WORLDWIDE
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 12:47 PM EST

PDB ID	:	4OZG
Title	:	D2 protein complex
Authors	:	Petersen, J.; Reid, H.H.; Rossjohn, J.
Deposited on	:	2014-02-16
Resolution	:	3.00 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		5.4%
RSRZ outliers		1.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
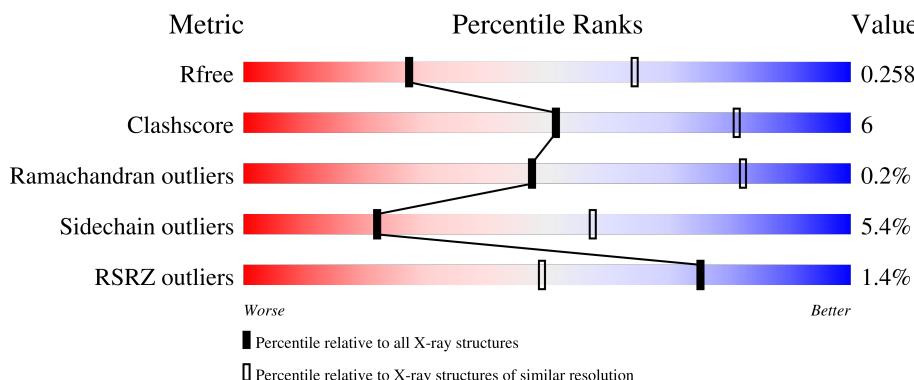
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	191	83%　　11%　・5%
1	C	191	8%　　80%　　13%　・6%
2	B	213	68%　　16%　・　15%
2	D	213	2%　　70%　　14%　　15%
3	E	202	80%　　14%　・・

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Mol	Chain	Length	Quality of chain
3	G	202	80% 15%
4	F	242	84% 13%
4	H	242	85% 13%
5	I	13	85% 15%
5	J	13	69% 23% 8%
6	K	2	50% 50%
6	L	2	50% 50%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 12715 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 HLA class II histocompatibility antigen, DQ alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1441	928	235	275	3			
1	C	180	Total	C	N	O	S	0	0	0
			1373	879	228	263	3			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DQ beta 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1480	935	264	274	7			
2	D	180	Total	C	N	O	S	0	0	0
			1437	907	257	266	7			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	GLY	-	expression tag	UNP Q5Y7D3
B	-11	GLY	-	expression tag	UNP Q5Y7D3
B	-10	SER	-	expression tag	UNP Q5Y7D3
B	-9	ILE	-	expression tag	UNP Q5Y7D3
B	-8	GLU	-	expression tag	UNP Q5Y7D3
B	-7	GLY	-	expression tag	UNP Q5Y7D3
B	-6	ARG	-	expression tag	UNP Q5Y7D3
B	-5	GLY	-	expression tag	UNP Q5Y7D3
B	-4	GLY	-	expression tag	UNP Q5Y7D3
B	-3	SER	-	expression tag	UNP Q5Y7D3
B	-2	GLY	-	expression tag	UNP Q5Y7D3
B	-1	ALA	-	expression tag	UNP Q5Y7D3
B	0	SER	-	expression tag	UNP Q5Y7D3
B	193	THR	-	expression tag	UNP Q5Y7D3
B	194	GLY	-	expression tag	UNP Q5Y7D3
B	195	GLY	-	expression tag	UNP Q5Y7D3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	196	ASP	-	expression tag	UNP Q5Y7D3
B	197	ASP	-	expression tag	UNP Q5Y7D3
B	198	ASP	-	expression tag	UNP Q5Y7D3
B	199	ASP	-	expression tag	UNP Q5Y7D3
B	200	LYS	-	expression tag	UNP Q5Y7D3
D	-12	GLY	-	expression tag	UNP Q5Y7D3
D	-11	GLY	-	expression tag	UNP Q5Y7D3
D	-10	SER	-	expression tag	UNP Q5Y7D3
D	-9	ILE	-	expression tag	UNP Q5Y7D3
D	-8	GLU	-	expression tag	UNP Q5Y7D3
D	-7	GLY	-	expression tag	UNP Q5Y7D3
D	-6	ARG	-	expression tag	UNP Q5Y7D3
D	-5	GLY	-	expression tag	UNP Q5Y7D3
D	-4	GLY	-	expression tag	UNP Q5Y7D3
D	-3	SER	-	expression tag	UNP Q5Y7D3
D	-2	GLY	-	expression tag	UNP Q5Y7D3
D	-1	ALA	-	expression tag	UNP Q5Y7D3
D	0	SER	-	expression tag	UNP Q5Y7D3
D	193	THR	-	expression tag	UNP Q5Y7D3
D	194	GLY	-	expression tag	UNP Q5Y7D3
D	195	GLY	-	expression tag	UNP Q5Y7D3
D	196	ASP	-	expression tag	UNP Q5Y7D3
D	197	ASP	-	expression tag	UNP Q5Y7D3
D	198	ASP	-	expression tag	UNP Q5Y7D3
D	199	ASP	-	expression tag	UNP Q5Y7D3
D	200	LYS	-	expression tag	UNP Q5Y7D3

- Molecule 3 is a protein called T-cell receptor, d2, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	194	Total 1479	C 930	N 249	O 290	S 10	0	0	0
3	G	194	Total 1489	C 935	N 250	O 294	S 10	0	0	0

- Molecule 4 is a protein called T-cell receptor, d2, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	240	Total 1872	C 1179	N 324	O 364	S 5	0	0	0
4	H	240	Total 1874	C 1182	N 326	O 361	S 5	0	0	0

- Molecule 5 is a protein called deamidated Gliadin-alpha2 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	13	Total 96	C 63	N 15	O 18	0	0	0
5	J	12	Total 91	C 60	N 14	O 17	0	0	0

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

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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
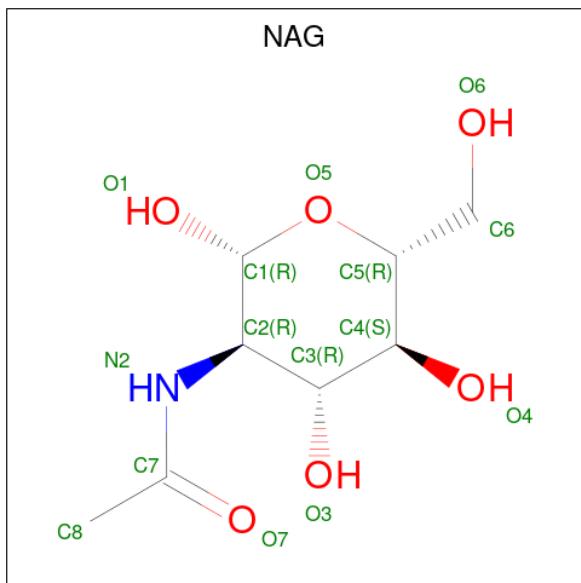
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total Ca 1 1	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	2	Total O 2 2	0	0
9	B	1	Total O 1 1	0	0
9	C	2	Total O 2 2	0	0
9	E	1	Total O 1 1	0	0
9	F	1	Total O 1 1	0	0
9	G	2	Total O 2 2	0	0
9	H	3	Total O 3 3	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: HLA class II histocompatibility antigen, DQ alpha 1 chain
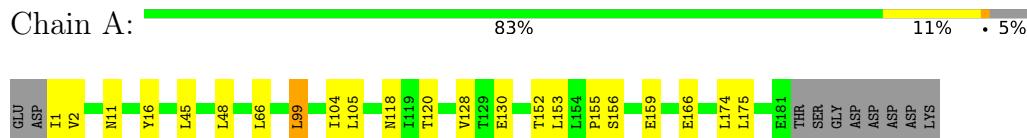
• Molecule 1: HLA class II histocompatibility antigen, DQ alpha 1 chain
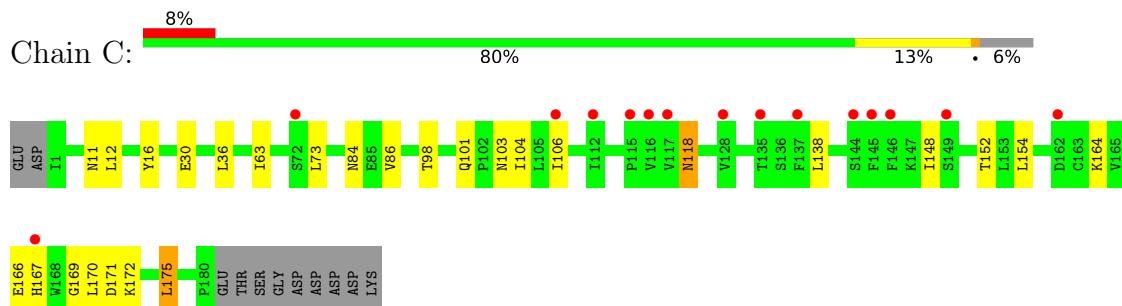

• Molecule 2: HLA class II histocompatibility antigen, DQ beta 1 chain
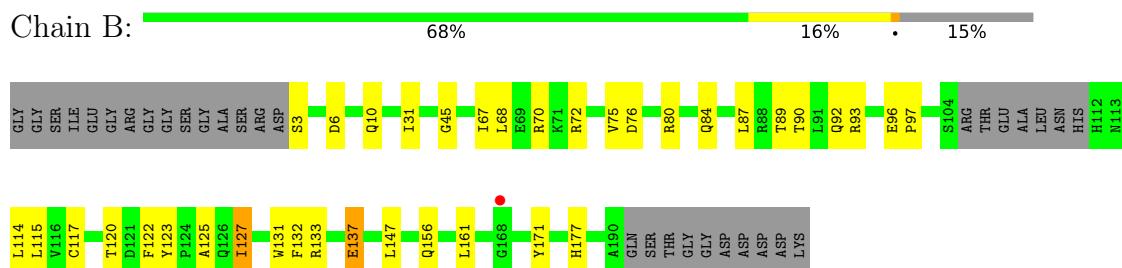
• Molecule 2: HLA class II histocompatibility antigen, DQ beta 1 chain

- Molecule 3: T-cell receptor, d2, alpha chain
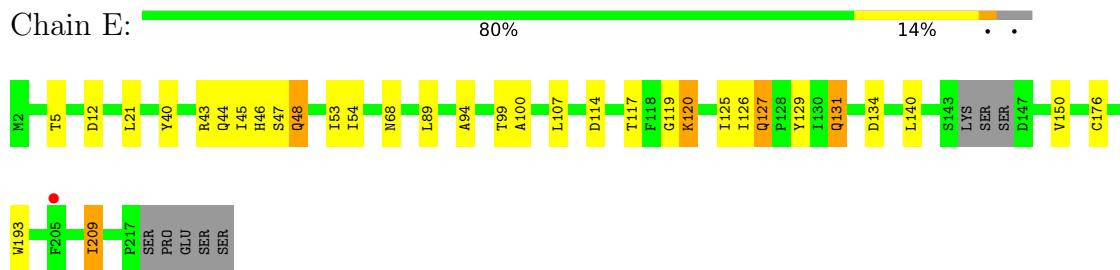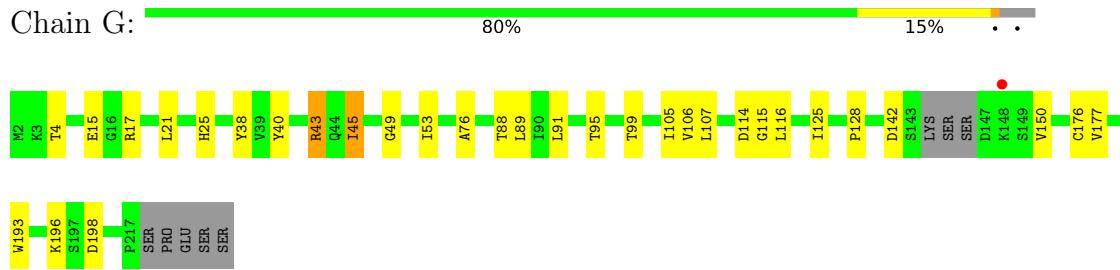
Chain E:

- Molecule 3: T-cell receptor, d2, alpha chain

Chain G:

- Molecule 4: T-cell receptor, d2, beta chain

Chain F:

- Molecule 4: T-cell receptor, d2, beta chain
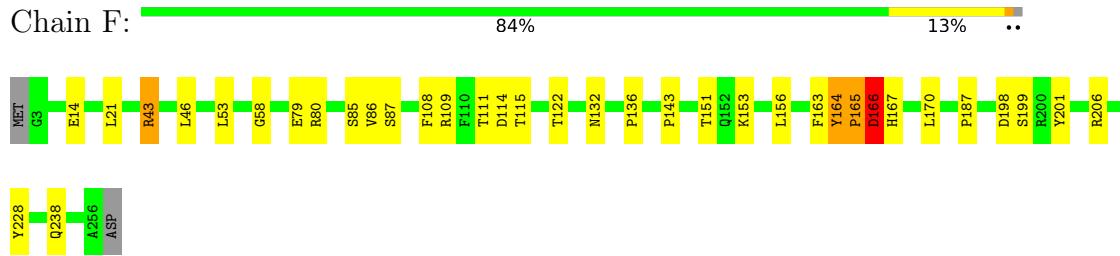
Chain H:

- Molecule 5: deamidated Gliadin-alpha2 peptide

Chain I:

- Molecule 5: deamidated Gliadin-alpha2 peptide

Chain J:

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

Chain K:

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

Chain L:
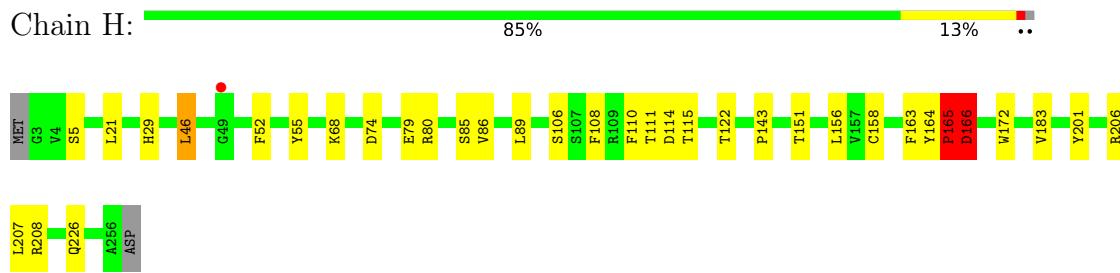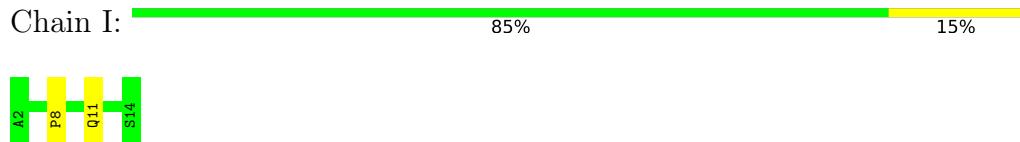
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	266.02Å 60.27Å 138.24Å 90.00° 114.04° 90.00°	Depositor
Resolution (Å)	43.48 – 3.00 113.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.5 (43.48-3.00) 96.5 (113.68-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.203 , 0.241 0.214 , 0.258	Depositor DCC
R_{free} test set	1958 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	66.5	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.9	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12715	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, CA

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	0.41	0/1483	0.60	0/2027
1	C	0.53	0/1411	0.66	3/1933 (0.2%)
2	B	0.59	0/1513	0.64	1/2056 (0.0%)
2	D	0.48	0/1469	0.59	1/2001 (0.0%)
3	E	0.55	0/1513	0.66	1/2063 (0.0%)
3	G	0.54	0/1523	0.66	1/2075 (0.0%)
4	F	0.54	2/1922 (0.1%)	0.62	3/2619 (0.1%)
4	H	0.60	1/1924 (0.1%)	0.63	1/2621 (0.0%)
5	I	0.38	0/101	0.51	0/141
5	J	0.43	0/96	0.63	0/134
All	All	0.53	3/12955 (0.0%)	0.63	11/17670 (0.1%)

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
3	G	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	165	PRO	N-CD	5.34	1.55	1.47
4	F	165	PRO	N-CD	5.08	1.54	1.47
4	F	164	TYR	CD2-CE2	-5.01	1.31	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	3	SER	C-N-CD	6.18	141.39	128.40
2	B	3	SER	C-N-CD	6.07	141.14	128.40
3	E	127	GLN	C-N-CD	6.04	141.09	128.40
1	C	86	VAL	C-N-CD	5.93	140.85	128.40
3	G	49	GLY	C-N-CD	5.92	140.82	128.40
1	C	172	LYS	C-N-CD	5.78	140.55	128.40
4	F	165	PRO	CA-N-CD	-5.53	103.76	111.50
4	F	164	TYR	C-N-CD	5.34	139.61	128.40
4	F	198	ASP	N-CA-C	-5.17	97.04	111.00
1	C	169	GLY	N-CA-C	5.12	125.91	113.10
4	H	165	PRO	CA-N-CD	-5.02	104.47	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	45	ILE	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	1441	0	1386	16	0
1	C	1373	0	1266	13	0
2	B	1480	0	1443	27	0
2	D	1437	0	1371	11	0
3	E	1479	0	1371	24	0
3	G	1489	0	1386	15	0
4	F	1872	0	1761	22	0
4	H	1874	0	1773	24	0
5	I	96	0	86	1	0
5	J	91	0	84	2	0
6	K	28	0	25	0	0
6	L	28	0	25	0	0
7	C	14	0	13	0	0
8	C	1	0	0	0	0
9	A	2	0	0	0	0
9	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	C	2	0	0	0	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	2	0	0	0	0
9	H	3	0	0	0	0
All	All	12715	0	11990	137	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 6.

All (137) 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:48:LEU:CD2	2:B:89:THR:HG21	1.93	0.99
1:A:48:LEU:HD23	2:B:89:THR:HG21	1.57	0.87
3:G:106:VAL:O	3:G:107:LEU:HD12	1.76	0.86
3:G:114:ASP:OD1	3:G:115:GLY:N	2.07	0.86
1:C:164:LYS:HA	1:C:175:LEU:HB3	1.59	0.82
4:F:80:ARG:NH1	4:F:85:SER:O	2.12	0.82
3:G:38:TYR:N	3:G:107:LEU:O	2.13	0.81
1:C:175:LEU:HD13	1:C:175:LEU:H	1.46	0.80
1:A:48:LEU:HD21	2:B:89:THR:HG21	1.63	0.80
1:C:175:LEU:HD22	1:C:175:LEU:O	1.81	0.80
3:E:45:ILE:O	3:E:48:GLN:HG2	1.83	0.79
3:E:120:LYS:H	3:E:120:LYS:CD	1.96	0.78
1:A:11:ASN:HB3	1:A:66:LEU:HD11	1.71	0.72
2:B:89:THR:HG22	2:B:90:THR:N	2.04	0.72
3:E:120:LYS:H	3:E:120:LYS:CE	2.02	0.72
4:H:85:SER:OG	4:H:86:VAL:N	2.23	0.72
1:A:48:LEU:HD21	2:B:89:THR:CG2	2.20	0.71
4:H:21:LEU:HD22	4:H:122:THR:HG21	1.73	0.71
4:H:110:PHE:O	4:H:111:THR:HB	1.91	0.71
1:A:48:LEU:CD2	2:B:89:THR:CG2	2.68	0.70
4:F:170:LEU:C	4:F:170:LEU:HD23	2.13	0.69
3:G:106:VAL:C	3:G:107:LEU:HD12	2.12	0.68
2:B:132:PHE:CE2	2:B:137:GLU:HG3	2.30	0.67
1:C:175:LEU:HD13	1:C:175:LEU:N	2.10	0.66
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.76	0.65
2:D:133:ARG:NH2	2:D:169:ASP:OD2	2.30	0.64
3:E:44:GLN:NE2	3:E:48:GLN:O	2.21	0.64
4:H:166:ASP:HB3	4:H:201:TYR:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:120:LYS:H	3:E:120:LYS:HE3	1.62	0.63
4:F:85:SER:OG	4:F:86:VAL:N	2.29	0.63
4:F:58:GLY:O	4:F:80:ARG:HD3	1.99	0.62
4:F:109:ARG:HH21	5:I:8:PRO:HD2	1.62	0.62
1:A:104:ILE:HG12	1:A:152:THR:HG22	1.83	0.61
2:B:123:TYR:O	2:B:177:HIS:HE1	1.84	0.60
4:F:111:THR:O	4:F:111:THR:HG22	2.01	0.59
4:F:21:LEU:HD22	4:F:122:THR:HG21	1.84	0.59
3:E:150:VAL:HG12	3:E:193:TRP:HB3	1.84	0.58
1:C:167:HIS:HB3	1:C:170:LEU:H	1.68	0.58
4:F:80:ARG:O	4:F:80:ARG:HG2	2.02	0.58
2:B:76:ASP:HA	2:B:80:ARG:HB2	1.85	0.58
1:A:48:LEU:HD23	2:B:89:THR:CG2	2.33	0.56
2:B:84:GLN:HA	2:B:87:LEU:HD12	1.85	0.56
1:A:16:TYR:HB2	2:B:6:ASP:OD1	2.05	0.56
3:E:21:LEU:HD12	3:E:89:LEU:HD23	1.89	0.55
4:F:86:VAL:HG12	4:F:87:SER:N	2.21	0.55
1:C:104:ILE:HG12	1:C:152:THR:HG22	1.87	0.55
2:D:41:ASP:HB3	2:D:44:VAL:HG22	1.89	0.54
2:D:76:ASP:HA	2:D:80:ARG:HB2	1.90	0.54
4:H:80:ARG:O	4:H:80:ARG:HG2	2.06	0.54
2:D:130:ARG:HB2	2:D:174:HIS:HB3	1.90	0.54
3:G:128:PRO:HG3	3:G:177:VAL:HG21	1.90	0.53
3:E:120:LYS:H	3:E:120:LYS:HD2	1.70	0.53
3:G:43:ARG:HB3	3:G:53:ILE:HD11	1.90	0.52
1:C:175:LEU:N	1:C:175:LEU:CD1	2.72	0.52
2:B:67:ILE:HD11	4:H:108:PHE:CE1	2.45	0.52
2:B:89:THR:HG22	2:B:90:THR:H	1.73	0.51
4:F:43:ARG:HB2	4:F:53:LEU:HD11	1.92	0.51
3:E:129:TYR:CE2	3:E:131:GLN:HG2	2.46	0.51
3:G:105:ILE:HG22	3:G:106:VAL:N	2.24	0.51
2:B:89:THR:HG22	2:B:90:THR:HG23	1.92	0.51
2:D:84:GLN:HA	2:D:87:LEU:HD12	1.92	0.50
3:E:54:ILE:HD12	3:E:68:ASN:HB2	1.94	0.50
3:E:12:ASP:HB3	3:E:127:GLN:HE21	1.77	0.50
3:E:120:LYS:HE3	3:E:120:LYS:N	2.26	0.50
3:G:150:VAL:HG12	3:G:193:TRP:HB3	1.94	0.49
3:G:43:ARG:O	3:G:43:ARG:HG3	2.13	0.48
1:A:16:TYR:N	2:B:6:ASP:OD1	2.46	0.48
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.96	0.47
3:E:40:TYR:OH	4:F:115:THR:OG1	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:158:CYS:HB2	4:H:172:TRP:CZ2	2.50	0.47
2:B:133:ARG:HG3	2:B:171:TYR:CE1	2.49	0.47
3:E:120:LYS:CE	3:E:120:LYS:N	2.73	0.47
4:H:183:VAL:HG22	4:H:207:LEU:HD12	1.97	0.47
2:D:82:ASN:HA	2:D:85:LEU:HD12	1.96	0.47
3:E:119:GLY:CA	3:E:120:LYS:HE3	2.45	0.47
4:F:167:HIS:HB2	4:F:228:TYR:HB2	1.95	0.47
4:H:151:THR:HG21	4:H:208:ARG:HH11	1.80	0.47
3:G:21:LEU:HD12	3:G:89:LEU:HD23	1.96	0.47
3:G:15:GLU:HG2	3:G:128:PRO:HA	1.96	0.46
4:F:166:ASP:HB3	4:F:201:TYR:CD1	2.49	0.46
2:D:129:VAL:HG11	2:D:159:VAL:HG21	1.97	0.46
1:C:30:GLU:HB2	1:C:138:LEU:HD21	1.97	0.46
3:E:209:ILE:H	3:E:209:ILE:HG13	1.61	0.45
4:H:163:PHE:CE1	4:H:166:ASP:HA	2.51	0.45
1:A:156:SER:HB3	1:A:159:GLU:HB2	1.99	0.45
3:G:4:THR:HG22	3:G:25:HIS:HB3	1.97	0.45
1:A:99:LEU:HA	1:A:155:PRO:HB2	1.97	0.45
4:F:136:PRO:HB3	4:F:163:PHE:CD2	2.52	0.45
3:G:76:ALA:HB2	3:G:91:LEU:HD23	1.97	0.45
4:H:108:PHE:HE1	5:J:10:PRO:HD2	1.82	0.45
4:H:21:LEU:HD12	4:H:89:LEU:HD23	1.99	0.45
4:H:29:HIS:HA	4:H:108:PHE:HA	1.97	0.45
1:C:118:ASN:HB3	1:C:166:GLU:HG3	1.99	0.44
4:H:46:LEU:HD12	4:H:46:LEU:HA	1.90	0.44
3:E:99:THR:HG23	3:E:125:ILE:HA	1.99	0.44
4:H:164:TYR:HA	4:H:165:PRO:HA	1.80	0.44
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.53	0.44
1:C:98:THR:HB	1:C:101:GLN:HB2	1.99	0.44
3:G:99:THR:HG23	3:G:125:ILE:HA	1.99	0.44
1:C:170:LEU:O	1:C:171:ASP:HB3	2.16	0.44
3:E:46:HIS:CE1	4:F:187:PRO:HB2	2.53	0.44
3:E:94:ALA:HB1	3:E:126:ILE:HD12	1.99	0.44
4:F:164:TYR:CG	4:F:165:PRO:HA	2.53	0.43
2:B:70:ARG:HD3	2:B:70:ARG:HA	1.89	0.43
1:A:45:LEU:HD21	2:B:93:ARG:HD2	1.98	0.43
2:D:67:ILE:HD11	4:F:108:PHE:CE1	2.54	0.43
3:G:40:TYR:HH	4:H:115:THR:HG1	1.59	0.43
2:D:10:GLN:HB2	2:D:31:ILE:HB	2.00	0.42
3:E:120:LYS:CD	3:E:120:LYS:N	2.73	0.42
1:A:105:LEU:HD12	1:A:153:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:THR:HG22	2:B:156:GLN:HB2	2.00	0.42
3:E:140:LEU:HD22	4:F:143:PRO:HA	2.01	0.42
4:H:164:TYR:CG	4:H:165:PRO:HA	2.55	0.42
1:A:1:ILE:HG23	1:A:2:VAL:HG23	2.02	0.42
3:E:129:TYR:HE2	3:E:131:GLN:HG2	1.84	0.42
2:B:67:ILE:HD11	4:H:108:PHE:CZ	2.55	0.42
2:B:125:ALA:HB1	2:B:147:LEU:HD21	2.02	0.41
2:B:45:GLY:O	2:B:72:ARG:NH1	2.54	0.41
4:F:163:PHE:CE1	4:F:201:TYR:HB2	2.55	0.41
4:H:52:PHE:HZ	4:H:55:TYR:HB3	1.86	0.41
2:B:10:GLN:HB2	2:B:31:ILE:HB	2.02	0.41
4:H:143:PRO:HD3	4:H:156:LEU:HG	2.02	0.41
3:E:43:ARG:HB3	3:E:53:ILE:HD11	2.02	0.41
4:F:151:THR:HG23	4:F:153:LYS:HB2	2.03	0.41
4:H:151:THR:HG21	4:H:208:ARG:NH1	2.35	0.41
1:C:106:ILE:HG23	1:C:148:ILE:HG23	2.03	0.41
4:F:109:ARG:O	4:F:114:ASP:HB2	2.21	0.41
5:J:12:PRO:HA	5:J:13:GLY:HA2	1.77	0.41
1:C:36:LEU:HD21	1:C:63:ILE:HG13	2.03	0.40
2:D:150:ASN:HB2	2:D:154:THR:HB	2.03	0.40
4:H:111:THR:O	4:H:111:THR:CG2	2.69	0.40
2:B:127:ILE:HD12	2:B:177:HIS:HD2	1.86	0.40
2:D:64:GLN:HB2	2:D:67:ILE:HD12	2.03	0.40
4:H:80:ARG:NE	4:H:85:SER:O	2.36	0.40
4:F:164:TYR:CD1	4:F:199:SER:O	2.74	0.40
3:E:45:ILE:HG12	3:E:100:ALA:HB2	2.04	0.40
4:H:165:PRO:O	4:H:166:ASP:CB	2.69	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	179/191 (94%)	171 (96%)	8 (4%)	0	100	100
1	C	178/191 (93%)	168 (94%)	10 (6%)	0	100	100
2	B	177/213 (83%)	170 (96%)	7 (4%)	0	100	100
2	D	176/213 (83%)	167 (95%)	8 (4%)	1 (1%)	25	64
3	E	190/202 (94%)	182 (96%)	8 (4%)	0	100	100
3	G	190/202 (94%)	183 (96%)	7 (4%)	0	100	100
4	F	238/242 (98%)	228 (96%)	9 (4%)	1 (0%)	34	72
4	H	238/242 (98%)	226 (95%)	11 (5%)	1 (0%)	34	72
5	I	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
5	J	10/13 (77%)	10 (100%)	0	0	100	100
All	All	1587/1722 (92%)	1515 (96%)	69 (4%)	3 (0%)	47	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	166	ASP
4	F	166	ASP
2	D	4	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	164/174 (94%)	158 (96%)	6 (4%)	34	70
1	C	146/174 (84%)	137 (94%)	9 (6%)	18	52
2	B	164/188 (87%)	155 (94%)	9 (6%)	21	57
2	D	154/188 (82%)	146 (95%)	8 (5%)	23	59
3	E	159/180 (88%)	148 (93%)	11 (7%)	15	48
3	G	162/180 (90%)	152 (94%)	10 (6%)	18	52
4	F	202/210 (96%)	193 (96%)	9 (4%)	27	64
4	H	202/210 (96%)	191 (95%)	11 (5%)	22	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	I	10/11 (91%)	9 (90%)	1 (10%)	7	29
5	J	10/11 (91%)	10 (100%)	0	100	100
All	All	1373/1526 (90%)	1299 (95%)	74 (5%)	22	57

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	120	THR
1	A	128	VAL
1	A	130	GLU
1	A	174	LEU
1	A	175	LEU
2	B	68	LEU
2	B	75	VAL
2	B	92	GLN
2	B	96	GLU
2	B	114	LEU
2	B	115	LEU
2	B	127	ILE
2	B	137	GLU
2	B	161	LEU
1	C	11	ASN
1	C	12	LEU
1	C	16	TYR
1	C	73	LEU
1	C	84	ASN
1	C	103	ASN
1	C	118	ASN
1	C	154	LEU
1	C	175	LEU
2	D	22	GLU
2	D	34	ARG
2	D	68	LEU
2	D	92	GLN
2	D	135	ASP
2	D	137	GLU
2	D	172	THR
2	D	180	LEU
3	E	5	THR
3	E	47	SER

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Mol	Chain	Res	Type
3	E	48	GLN
3	E	107	LEU
3	E	114	ASP
3	E	117	THR
3	E	120	LYS
3	E	131	GLN
3	E	134	ASP
3	E	176	CYS
3	E	209	ILE
4	F	14	GLU
4	F	43	ARG
4	F	46	LEU
4	F	79	GLU
4	F	132	ASN
4	F	156	LEU
4	F	166	ASP
4	F	206	ARG
4	F	238	GLN
3	G	17	ARG
3	G	43	ARG
3	G	45	ILE
3	G	88	THR
3	G	95	THR
3	G	116	LEU
3	G	142	ASP
3	G	176	CYS
3	G	196	LYS
3	G	198	ASP
4	H	5	SER
4	H	46	LEU
4	H	68	LYS
4	H	74	ASP
4	H	79	GLU
4	H	106	SER
4	H	114	ASP
4	H	165	PRO
4	H	166	ASP
4	H	206	ARG
4	H	226	GLN
5	I	11	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	123	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
6	NAG	K	1	6,1	14,14,15	0.28	0	17,19,21	1.40	2 (11%)
6	NAG	K	2	6	14,14,15	0.27	0	17,19,21	0.50	0
6	NAG	L	1	6,1	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
6	NAG	L	2	6	14,14,15	0.27	0	17,19,21	0.56	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
6	NAG	K	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	0/6/23/26	0/1/1/1
6	NAG	L	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	L	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	K	1	NAG	C1-C2-N2	4.31	117.86	110.49
6	K	1	NAG	O5-C1-C2	-2.50	107.34	111.29
6	L	1	NAG	C1-O5-C5	2.17	115.14	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	K	1	NAG	C1-C2-N2-C7
6	K	1	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings
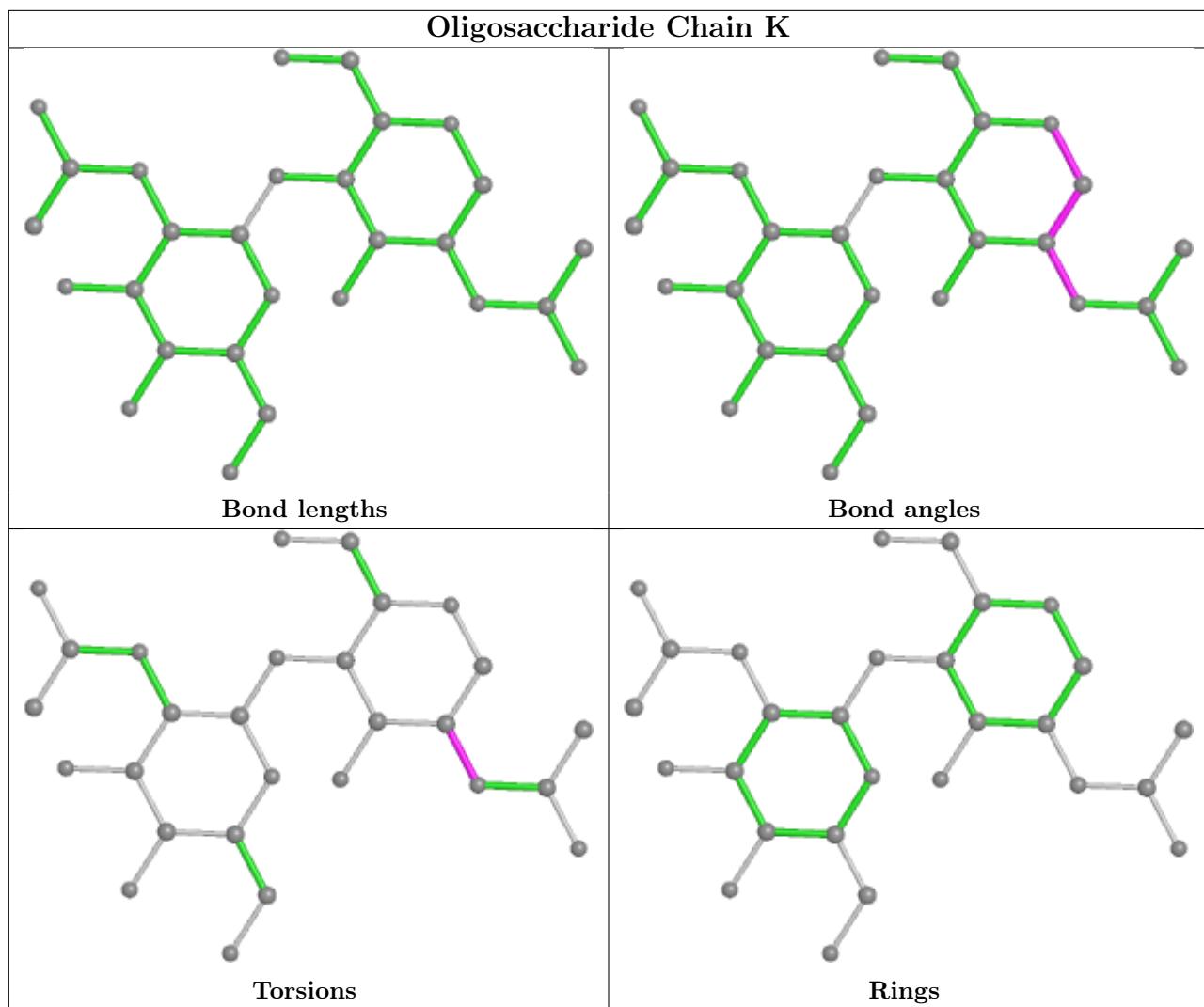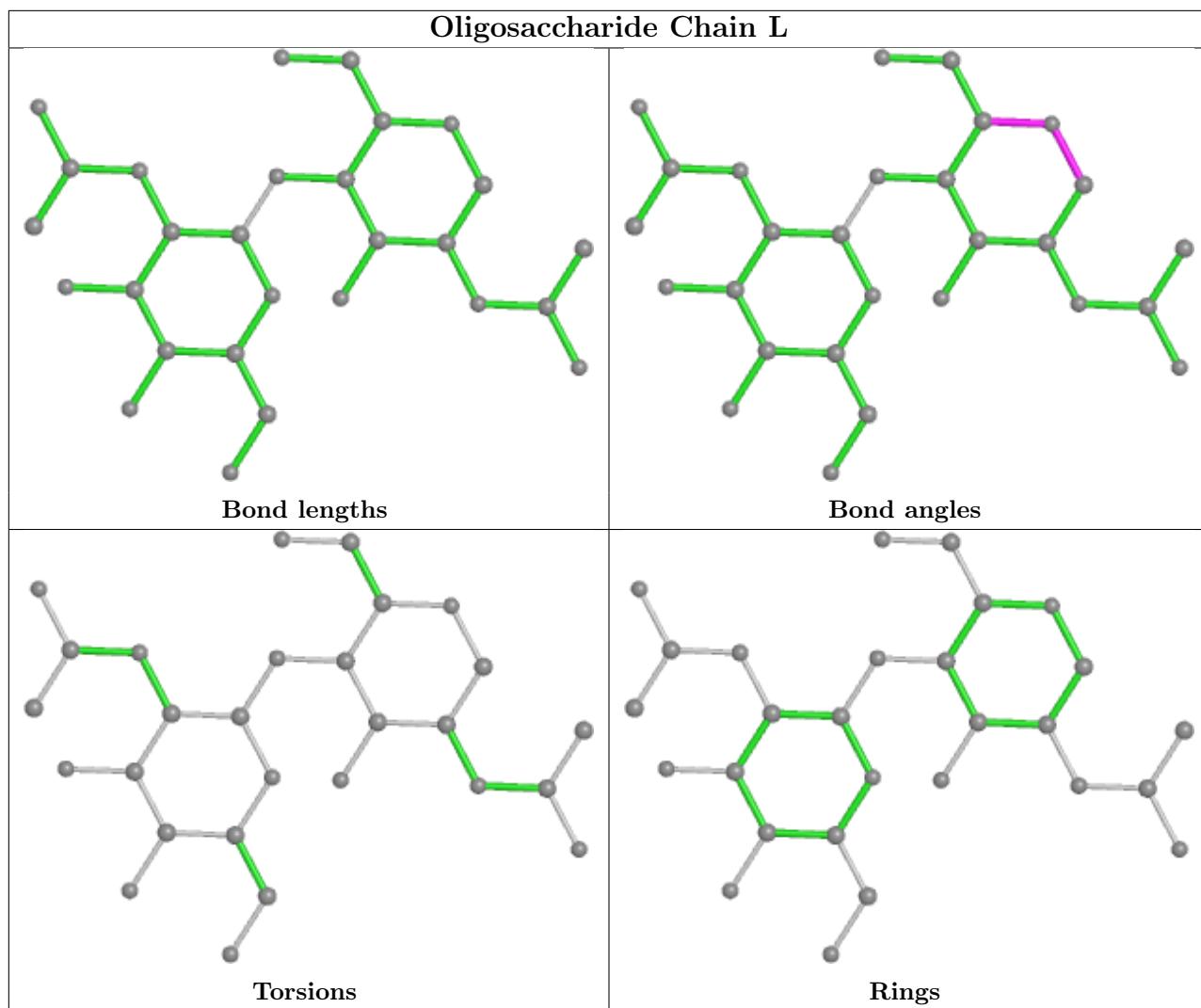
5.6　Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	#$|Z| > 2$
7	NAG	C	301	1	14,14,15	0.28	0	17,19,21	0.47	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
7	NAG	C	301	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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	181/191 (94%)	-0.19	0	100 100	36, 69, 108, 145	0
1	C	180/191 (94%)	0.43	15 (8%)	11 3	69, 118, 170, 180	0
2	B	181/213 (84%)	-0.27	1 (0%)	89 72	39, 65, 102, 135	0
2	D	180/213 (84%)	0.23	4 (2%)	62 33	55, 109, 158, 166	0
3	E	194/202 (96%)	-0.17	1 (0%)	91 75	44, 72, 102, 118	0
3	G	194/202 (96%)	-0.13	1 (0%)	91 75	41, 69, 104, 120	0
4	F	240/242 (99%)	-0.21	0	100 100	46, 71, 102, 118	0
4	H	240/242 (99%)	-0.29	1 (0%)	92 79	38, 61, 96, 111	0
5	I	13/13 (100%)	0.47	0	100 100	65, 76, 84, 117	0
5	J	12/13 (92%)	0.16	0	100 100	48, 52, 67, 74	0
All	All	1615/1722 (93%)	-0.08	23 (1%)	75 49	36, 74, 151, 180	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	PRO	5.2
1	C	117	VAL	5.0
1	C	167	HIS	3.7
1	C	145	PHE	3.6
2	D	119	VAL	3.4
1	C	106	ILE	3.3
1	C	162	ASP	3.3
1	C	112	ILE	3.3
2	D	124	PRO	3.2
2	D	97	PRO	3.2
4	H	49	GLY	3.1
1	C	149	SER	3.0
1	C	146	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	116	VAL	2.9
3	G	148	LYS	2.9
1	C	128	VAL	2.7
1	C	72	SER	2.6
2	B	168	GLY	2.6
3	E	205	PHE	2.5
1	C	137	PHE	2.5
1	C	135	THR	2.4
1	C	144	SER	2.2
2	D	6	ASP	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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
6	NAG	L	2	14/15	0.66	0.27	212,216,219,221	0
6	NAG	L	1	14/15	0.79	0.21	201,204,208,211	0
6	NAG	K	2	14/15	0.81	0.24	132,144,153,156	0
6	NAG	K	1	14/15	0.91	0.24	121,127,135,135	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.
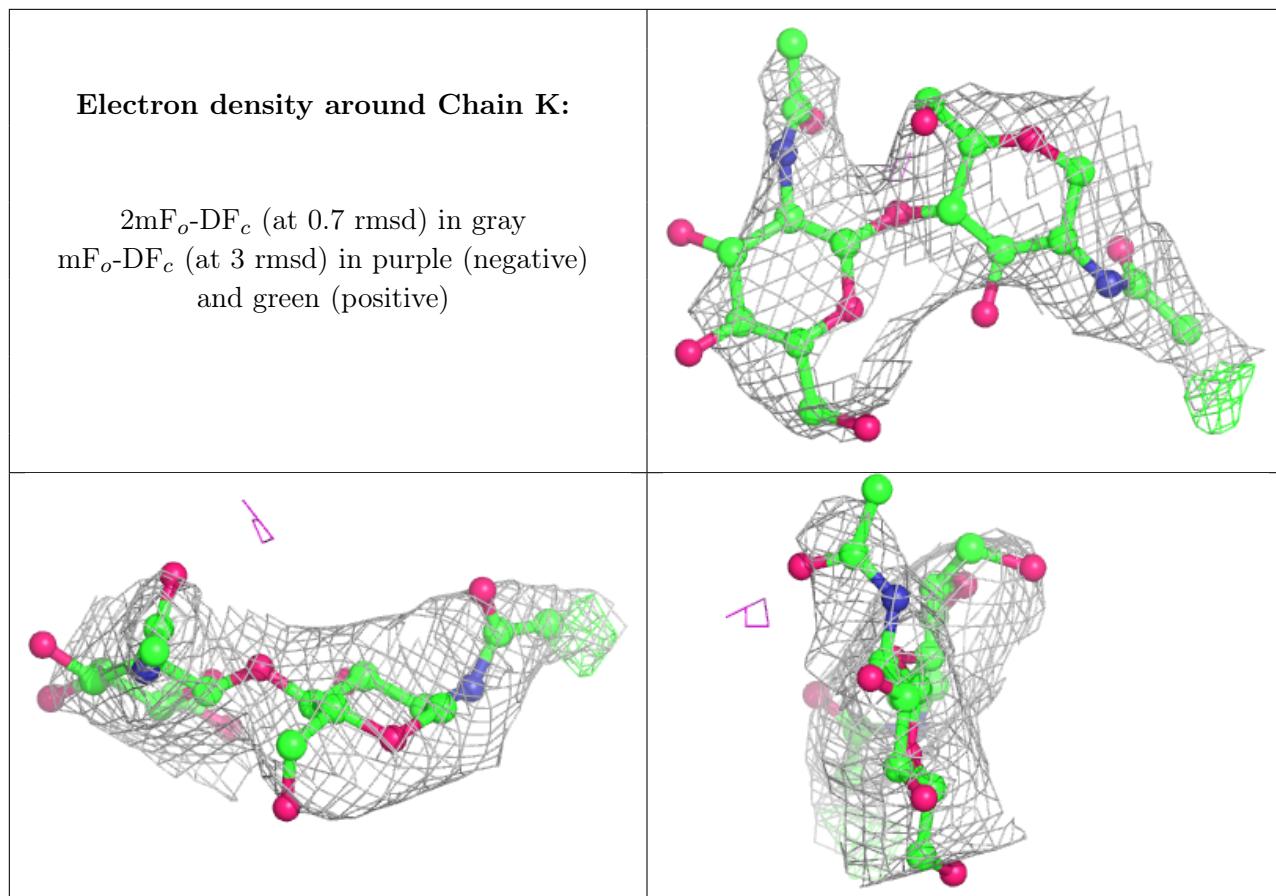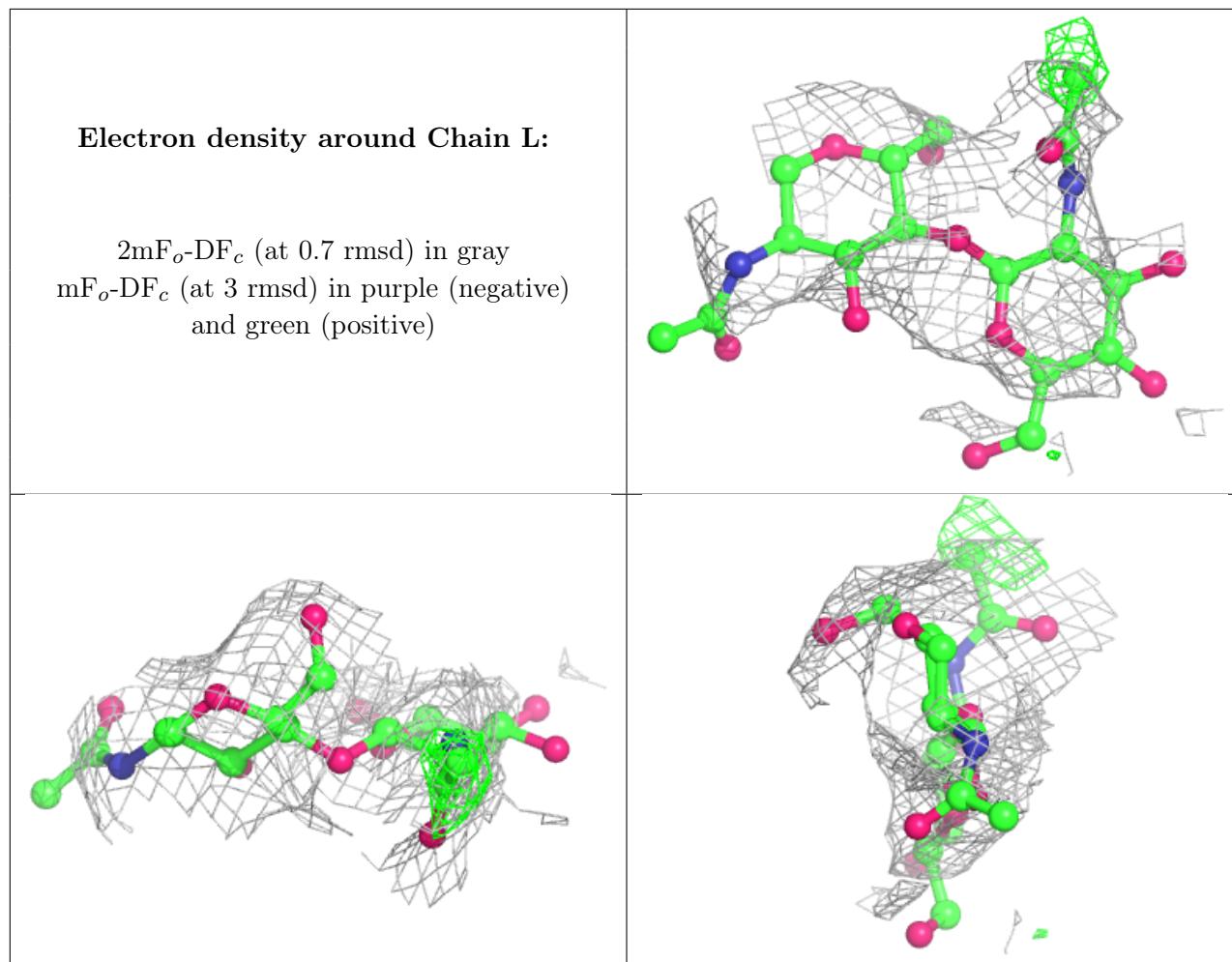
Electron density around Chain K:

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

Electron density around Chain L:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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($\mathring{A}^2$)	Q<0.9
7	NAG	C	301	14/15	0.78	0.18	144,148,155,155	0
8	CA	C	304	1/1	0.84	0.10	104,104,104,104	0

6.5 Other polymers ⓘ

There are no such residues in this entry.