



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:31 AM BST

PDB ID : 4C83  
Title : Crystal Structure of the IgG2a LPT3 in complex with an 8-sugar inner core analogue of Neisseria meningitidis  
Authors : Parker, M.J.; Gomery, K.; Richard, G.; Mackenzie, C.R.; Cox, A.D.; Richards, J.C.; Evans, S.V.  
Deposited on : 2013-09-29  
Resolution : 2.69 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](mailto: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 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 : 2.13.1  
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) : 2.13.1

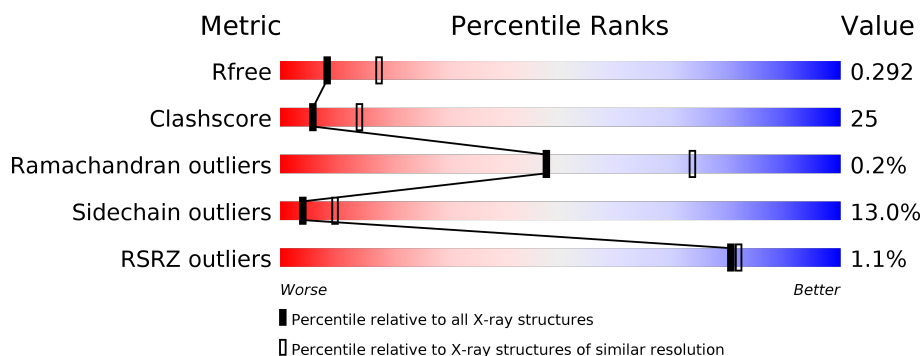
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	220	 62% 33% . .
1	C	220	 54% 40% 5% .
2	B	214	 53% 39% 8%
2	D	214	 59% 30% 10%
3	E	5	 20% 20% 60%
3	F	5	 40% 60%

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
4	SO4	A	1221	-	-	X	-
4	SO4	C	1221	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6691 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.

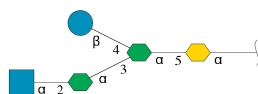
- Molecule 1 is a protein called LPT3 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1629	1034	274	313	8			
1	C	215	Total	C	N	O	S	0	0	0
			1629	1034	274	313	8			

- Molecule 2 is a protein called LPT3 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1647	1023	277	336	11			
2	D	213	Total	C	N	O	S	0	0	0
			1638	1018	275	334	11			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]L-glycero-alpha-D-manno-heptopyranose-(1-5)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	0	0	0
			67	36	1	30			
3	F	5	Total	C	N	O	0	0	0
			67	36	1	30			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

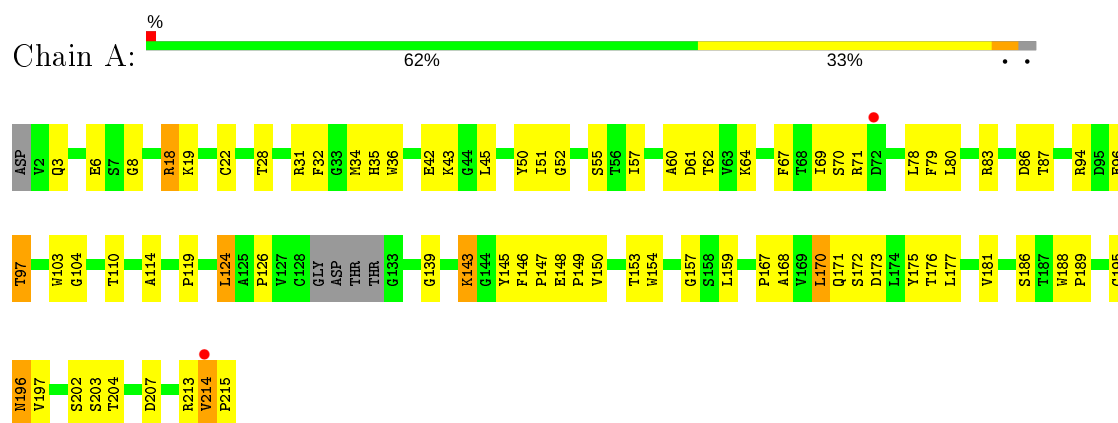
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	O	0	0
			2	2		
5	C	2	Total	O	0	0
			2	2		

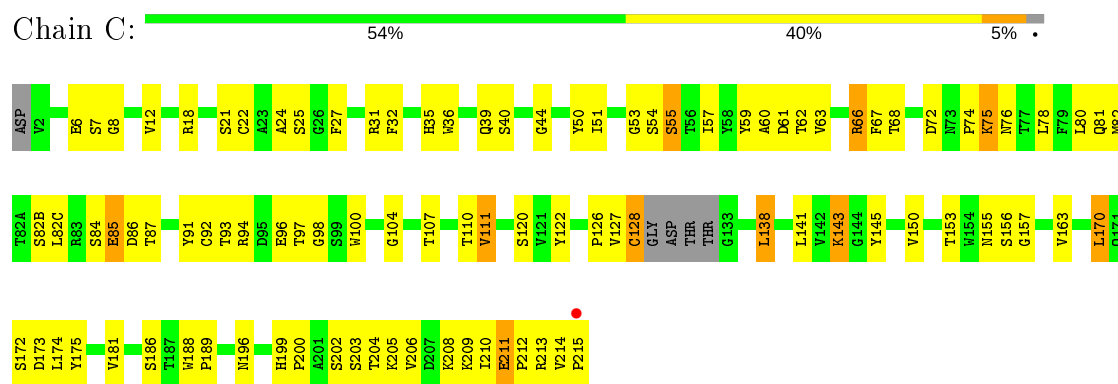
### 3 Residue-property plots [i](#)

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.

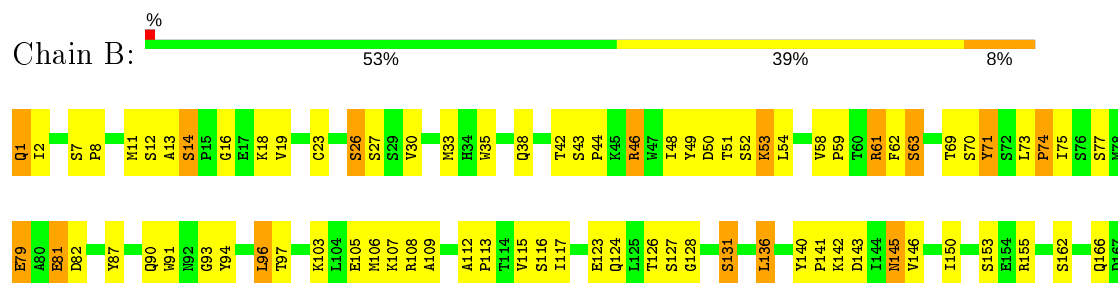
#### • Molecule 1: LPT3 HEAVY CHAIN



#### • Molecule 1: LPT3 HEAVY CHAIN

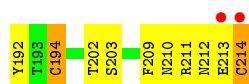


#### • Molecule 2: LPT3 LIGHT CHAIN





• Molecule 2: LPT3 LIGHT CHAIN



• Molecule 3: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]L-glycero-alpha-D-manno-heptopyranose-(1-5)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid



• Molecule 3: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-2)-L-glycero-alpha-D-manno-heptopyranose-(1-3)-[beta-D-glucopyranose-(1-4)]L-glycero-alpha-D-manno-heptopyranose-(1-5)-3-deoxy-alpha-D-manno-oct-2-ulopyranosonic acid



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.63Å 64.19Å 64.40Å 87.51° 89.82° 73.41°	Depositor
Resolution (Å)	37.90 – 2.69 37.87 – 2.69	Depositor EDS
% Data completeness (in resolution range)	97.4 (37.90-2.69) 97.5 (37.87-2.69)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.225 , 0.293 0.225 , 0.292	Depositor DCC
$R_{free}$ test set	1320 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l 0.000 for k,h,-l 0.000 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6691	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: KDO, GMH, BGC, SO4, NDG

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	0.53	0/1672	0.53	0/2280
1	C	0.59	1/1672 (0.1%)	0.63	3/2280 (0.1%)
2	B	0.52	0/1688	0.57	1/2290 (0.0%)
2	D	0.58	1/1679 (0.1%)	0.60	2/2278 (0.1%)
All	All	0.56	2/6711 (0.0%)	0.58	6/9128 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	120	PRO	N-CD	5.07	1.54	1.47
1	C	200	PRO	N-CD	5.02	1.54	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	CYS	CA-CB-SG	-9.13	97.56	114.00
2	B	73	LEU	C-N-CD	-6.78	105.67	120.60
1	C	211	GLU	C-N-CD	5.84	140.67	128.40
2	D	118	PHE	C-N-CD	5.77	140.52	128.40
1	C	199	HIS	C-N-CD	5.72	140.41	128.40
2	D	119	PRO	C-N-CD	5.63	140.22	128.40

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	1629	0	1592	69	0
1	C	1629	0	1592	83	0
2	B	1647	0	1567	90	1
2	D	1638	0	1556	94	1
3	E	67	0	55	4	0
3	F	67	0	55	4	0
4	A	5	0	0	2	0
4	C	5	0	0	4	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
All	All	6691	0	6417	330	1

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 25.

All (330) 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)
2:B:63:SER:O	2:B:74:PRO:HD2	1.49	1.10
2:D:21:MET:CE	2:D:102:THR:HB	1.81	1.09
2:D:21:MET:HE1	2:D:102:THR:HB	1.28	1.08
2:B:108:ARG:NH1	2:B:109:ALA:O	1.89	1.06
1:A:148:GLU:HG3	1:A:149:PRO:HA	1.33	1.06
1:C:55:SER:HB3	4:C:1221:SO4:O1	1.57	1.04
2:D:63:SER:O	2:D:74:PRO:CD	2.06	1.03
2:D:63:SER:O	2:D:74:PRO:HD2	1.61	1.01
2:B:12:SER:OG	2:B:107:LYS:HG2	1.61	1.00
2:D:161:ASN:HB3	2:D:175:MET:CE	1.93	0.99
1:C:85:GLU:N	1:C:85:GLU:OE1	1.96	0.98
1:C:87:THR:HG23	1:C:110:THR:HA	1.45	0.98
1:C:66:ARG:NH2	1:C:86:ASP:OD2	1.99	0.96
1:C:94:ARG:NH1	1:C:96:GLU:OE2	2.00	0.95
2:B:12:SER:OG	2:B:107:LYS:CG	2.18	0.91
1:C:66:ARG:NH1	1:C:82(B):SER:O	2.03	0.91
2:D:161:ASN:HB3	2:D:175:MET:HE3	1.49	0.91
2:D:188:ARG:HH11	2:D:188:ARG:HG3	1.36	0.90
2:B:61:ARG:HH11	2:B:61:ARG:HG3	1.37	0.90
2:D:8:PRO:HG3	2:D:11:MET:HE3	1.55	0.87
2:B:30:VAL:O	2:B:71:TYR:OH	1.93	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:CYS:O	2:B:70:SER:HA	1.75	0.86
2:D:21:MET:CE	2:D:102:THR:CB	2.54	0.86
1:C:173:ASP:O	1:C:174:LEU:HD23	1.76	0.85
2:B:136:LEU:HD21	2:B:146:VAL:HG22	1.59	0.84
1:A:148:GLU:HG3	1:A:149:PRO:CA	2.07	0.84
1:C:75:LYS:O	1:C:76:ASN:HB2	1.79	0.81
2:D:63:SER:O	2:D:74:PRO:HD3	1.78	0.81
1:C:59:TYR:OH	1:C:68:THR:HA	1.81	0.80
2:D:61:ARG:NH1	2:D:82:ASP:OD2	2.13	0.80
1:A:94:ARG:HD2	1:A:96:GLU:OE2	1.82	0.79
2:B:11:MET:CE	2:B:19:VAL:HG23	2.12	0.79
1:A:60:ALA:O	1:A:64:LYS:HG3	1.84	0.78
2:B:12:SER:OG	2:B:107:LYS:HE3	1.84	0.78
1:C:60:ALA:HB3	1:C:63:VAL:HG22	1.66	0.78
2:B:1:GLN:OE1	2:B:1:GLN:N	2.17	0.77
2:D:31:ARG:HB2	2:D:92:ASN:HA	1.67	0.77
2:D:21:MET:HE3	2:D:102:THR:CB	2.15	0.76
2:D:191:SER:OG	2:D:210:ASN:OD1	2.04	0.75
2:B:12:SER:OG	2:B:107:LYS:CE	2.34	0.75
2:B:11:MET:HE1	2:B:19:VAL:HG23	1.69	0.74
1:C:67:PHE:CE2	1:C:82:MET:HG2	2.21	0.74
2:D:61:ARG:HH12	2:D:82:ASP:CG	1.90	0.74
2:B:12:SER:HG	2:B:107:LYS:HG2	1.51	0.74
2:B:50:ASP:CB	2:B:53:LYS:HE3	2.17	0.74
2:B:103:LYS:HE2	2:B:105:GLU:OE2	1.87	0.74
1:A:94:ARG:NH1	1:A:96:GLU:OE2	2.14	0.73
1:A:61:ASP:HA	1:A:64:LYS:CD	2.18	0.73
1:A:32:PHE:CD1	1:A:94:ARG:HD3	2.23	0.73
1:C:31:ARG:HE	1:C:32:PHE:HE1	1.35	0.72
2:D:124:GLN:OE1	2:D:131:SER:HB2	1.88	0.72
1:C:57:ILE:O	1:C:57:ILE:HD12	1.90	0.71
2:B:191:SER:OG	2:B:210:ASN:OD1	2.07	0.70
2:B:63:SER:O	2:B:74:PRO:CD	2.36	0.70
1:A:188:TRP:CG	1:A:189:PRO:HA	2.26	0.70
1:C:12:VAL:HG11	1:C:82(C):LEU:HD12	1.74	0.70
2:B:103:LYS:HG2	2:B:105:GLU:OE2	1.92	0.69
2:B:50:ASP:HB3	2:B:53:LYS:HE3	1.76	0.68
1:A:153:THR:CG2	1:A:157:GLY:N	2.57	0.67
1:A:214:VAL:O	1:A:215:PRO:O	2.13	0.67
2:B:189:HIS:O	2:B:211:ARG:NH1	2.28	0.67
2:D:61:ARG:NH1	2:D:82:ASP:CG	2.48	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:MET:HE1	2:D:102:THR:CB	2.15	0.66
1:A:114:ALA:HB3	1:A:146:PHE:CE2	2.30	0.66
2:B:50:ASP:HB2	2:B:53:LYS:HG3	1.76	0.66
1:C:6:GLU:OE2	1:C:104:GLY:HA3	1.95	0.66
2:D:161:ASN:HB3	2:D:175:MET:HE2	1.76	0.66
1:A:6:GLU:OE2	1:A:104:GLY:HA3	1.96	0.66
1:C:31:ARG:NE	1:C:32:PHE:CE1	2.61	0.66
2:D:89:GLN:NE2	2:D:96:LEU:HD11	2.11	0.65
2:D:47:TRP:CZ2	2:D:58:VAL:HG13	2.32	0.65
2:D:5:SER:O	2:D:24:SER:N	2.30	0.64
2:B:61:ARG:NH1	2:B:61:ARG:HG3	2.11	0.64
2:B:90:GLN:HE21	2:B:97:THR:HB	1.63	0.64
2:B:49:TYR:CD2	2:B:50:ASP:OD2	2.51	0.64
1:A:171:GLN:HG3	2:D:69:THR:HG21	1.79	0.63
2:B:115:VAL:HG12	2:B:207:LYS:HG3	1.80	0.63
2:B:49:TYR:O	2:B:53:LYS:HG3	1.97	0.63
1:C:57:ILE:HD12	1:C:57:ILE:C	2.19	0.63
1:C:22:CYS:HB3	1:C:78:LEU:HB3	1.81	0.63
1:A:170:LEU:HB2	1:A:175:TYR:CE1	2.33	0.62
1:C:208:LYS:NZ	2:D:123:GLU:OE1	2.30	0.62
2:D:212:ASN:O	2:D:213:GLU:HG3	2.00	0.62
2:D:61:ARG:NH1	2:D:82:ASP:OD1	2.30	0.62
2:D:170:ASP:O	2:D:171:SER:HB2	2.00	0.62
2:D:188:ARG:NH1	2:D:188:ARG:HG3	2.09	0.62
1:C:35:HIS:HB2	1:C:93:THR:OG1	2.00	0.61
1:A:3:GLN:HA	1:A:3:GLN:OE1	2.00	0.61
1:C:172:SER:O	1:C:173:ASP:HB2	1.99	0.61
1:A:124:LEU:HB2	1:A:139:GLY:O	2.00	0.61
1:A:172:SER:O	1:A:173:ASP:HB2	1.99	0.61
2:B:123:GLU:O	2:B:126:THR:HG22	2.01	0.61
1:C:67:PHE:CD2	1:C:82:MET:HG2	2.36	0.61
2:B:59:PRO:HG2	2:B:62:PHE:HD1	1.66	0.61
2:D:117:ILE:HD12	2:D:194:CYS:HB2	1.83	0.61
1:C:126:PRO:HD3	1:C:138:LEU:HD23	1.83	0.60
2:D:212:ASN:C	2:D:213:GLU:HG3	2.21	0.60
1:C:12:VAL:HG11	1:C:82(C):LEU:CD1	2.31	0.60
1:A:148:GLU:CG	1:A:149:PRO:HA	2.21	0.59
1:C:54:SER:N	4:C:1221:SO4:O4	2.35	0.59
1:C:170:LEU:HB2	1:C:175:TYR:CE1	2.37	0.59
1:C:67:PHE:CE2	1:C:82:MET:SD	2.96	0.59
1:A:87:THR:HG23	1:A:110:THR:HA	1.85	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:ARG:HB2	2:D:92:ASN:OD1	2.03	0.59
2:D:8:PRO:HG3	2:D:11:MET:CE	2.28	0.59
1:C:7:SER:HA	1:C:107:THR:HG21	1.85	0.59
1:A:8:GLY:O	1:A:18:ARG:HD2	2.03	0.58
2:D:48:ILE:CD1	2:D:54:LEU:CD2	2.82	0.58
1:C:40:SER:O	1:C:44:GLY:N	2.36	0.58
2:D:118:PHE:CE1	2:D:135:PHE:HD2	2.22	0.58
2:D:161:ASN:CB	2:D:175:MET:CE	2.75	0.58
2:D:6:GLN:OE1	2:D:101:GLY:HA2	2.03	0.58
2:B:50:ASP:HB2	2:B:53:LYS:HE3	1.85	0.58
2:D:31:ARG:HD2	2:D:92:ASN:C	2.24	0.57
1:A:61:ASP:HA	1:A:64:LYS:HG3	1.85	0.57
2:B:71:TYR:HD1	2:B:71:TYR:H	1.49	0.57
2:D:48:ILE:CD1	2:D:54:LEU:HD23	2.34	0.57
1:C:214:VAL:HG23	1:C:215:PRO:HD2	1.86	0.57
2:B:49:TYR:HD2	2:B:50:ASP:OD2	1.87	0.56
2:B:61:ARG:CG	2:B:61:ARG:HH11	2.14	0.56
1:C:66:ARG:HH22	1:C:86:ASP:CG	2.02	0.56
2:D:48:ILE:HD13	2:D:54:LEU:HD23	1.86	0.56
2:D:10:ILE:HG23	2:D:103:LYS:HB3	1.88	0.56
2:B:124:GLN:HE22	2:B:131:SER:HB2	1.69	0.56
1:C:153:THR:CG2	1:C:157:GLY:N	2.69	0.56
2:B:59:PRO:HG2	2:B:62:PHE:CD1	2.41	0.56
1:A:45:LEU:HD12	2:B:87:TYR:CD2	2.40	0.56
2:B:2:ILE:O	2:B:97:THR:HG21	2.06	0.56
2:D:118:PHE:CE1	2:D:135:PHE:CD2	2.94	0.56
1:C:188:TRP:CH2	1:C:212:PRO:HG3	2.40	0.56
2:D:63:SER:OG	2:D:74:PRO:HG2	2.06	0.55
1:C:155:ASN:O	1:C:156:SER:HB2	2.07	0.55
2:D:118:PHE:HE1	2:D:135:PHE:HD2	1.55	0.55
1:A:124:LEU:HB2	1:A:139:GLY:C	2.27	0.55
1:A:42:GLU:O	1:A:43:LYS:HB2	2.07	0.55
2:B:136:LEU:CD2	2:B:146:VAL:HG22	2.33	0.55
1:A:50:TYR:CZ	3:E:4:NDG:H8C3	2.41	0.54
2:B:69:THR:HG22	2:B:70:SER:N	2.21	0.54
2:D:8:PRO:CG	2:D:11:MET:HE3	2.32	0.54
2:B:61:ARG:NH1	2:B:82:ASP:OD2	2.35	0.54
2:B:50:ASP:HB2	2:B:53:LYS:CG	2.38	0.54
2:B:16:GLY:HA2	2:B:77:SER:OG	2.07	0.54
1:C:72:ASP:OD1	1:C:74:PRO:HD2	2.06	0.54
2:D:63:SER:C	2:D:74:PRO:HD2	2.27	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:HA	1:A:64:LYS:CG	2.37	0.54
2:B:11:MET:HE2	2:B:19:VAL:HG23	1.87	0.54
2:B:14:SER:HA	2:B:107:LYS:HB2	1.89	0.54
4:C:1221:SO4:O3	3:F:5:BGC:O6	2.25	0.54
1:A:70:SER:OG	1:A:79:PHE:HB2	2.07	0.54
2:B:12:SER:CB	2:B:107:LYS:HE3	2.37	0.54
2:B:136:LEU:CD2	2:B:146:VAL:CG2	2.86	0.54
1:A:51:ILE:CD1	1:A:57:ILE:HG12	2.38	0.53
2:D:210:ASN:O	2:D:212:ASN:O	2.26	0.53
2:D:3:VAL:H	2:D:26:SER:HB2	1.74	0.53
1:C:214:VAL:HG22	1:C:215:PRO:O	2.09	0.53
1:A:159:LEU:HD13	1:A:181:VAL:HG21	1.91	0.53
1:C:66:ARG:C	1:C:67:PHE:HD1	2.11	0.53
2:D:6:GLN:HA	2:D:22:THR:O	2.09	0.53
1:C:67:PHE:CE2	1:C:82:MET:CG	2.91	0.53
2:D:21:MET:HE3	2:D:102:THR:HG21	1.90	0.53
2:B:71:TYR:CD1	2:B:71:TYR:N	2.75	0.53
2:B:124:GLN:O	2:B:127:SER:HB3	2.09	0.52
2:B:136:LEU:HD21	2:B:146:VAL:CG2	2.35	0.52
2:D:21:MET:HE3	2:D:102:THR:CG2	2.39	0.52
2:D:47:TRP:CE2	2:D:58:VAL:HG13	2.44	0.52
1:C:91:TYR:CE2	2:D:43:SER:HB3	2.44	0.52
1:A:28:THR:HG23	1:A:28:THR:O	2.09	0.52
1:C:31:ARG:NE	1:C:32:PHE:HE1	2.04	0.52
1:C:67:PHE:CZ	1:C:82:MET:SD	3.03	0.52
1:A:83:ARG:O	1:A:86:ASP:HB2	2.09	0.52
1:A:18:ARG:HG3	1:A:19:LYS:N	2.24	0.51
1:C:53:GLY:O	1:C:54:SER:CB	2.58	0.51
2:B:108:ARG:HG3	2:B:108:ARG:HH11	1.76	0.51
1:A:22:CYS:HB3	1:A:78:LEU:HB3	1.91	0.51
2:B:93:GLY:C	2:B:94:TYR:HD1	2.14	0.51
2:D:6:GLN:OE1	2:D:101:GLY:N	2.43	0.51
2:D:186:TYR:O	2:D:192:TYR:OH	2.29	0.51
2:D:116:SER:HB3	2:D:118:PHE:CE1	2.45	0.50
1:C:163:VAL:HG22	1:C:181:VAL:HG23	1.93	0.50
1:A:61:ASP:OD1	1:A:64:LYS:HD2	2.12	0.50
1:A:143:LYS:HG3	1:A:176:THR:HG23	1.93	0.50
1:A:94:ARG:HH11	1:A:96:GLU:CD	2.08	0.50
2:B:128:GLY:HA2	2:B:183:LYS:HD3	1.93	0.50
1:C:98:GLY:HA2	2:D:32:TYR:CZ	2.47	0.50
2:D:6:GLN:OE1	2:D:101:GLY:CA	2.60	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:ARG:CB	2:D:92:ASN:HA	2.40	0.50
3:E:3:GMH:H2	3:E:5:BGC:H6C2	1.94	0.50
1:C:188:TRP:CG	1:C:189:PRO:HA	2.47	0.50
1:C:66:ARG:NH2	1:C:86:ASP:CG	2.63	0.49
2:D:21:MET:CE	2:D:102:THR:CG2	2.90	0.49
2:B:140:TYR:CG	2:B:141:PRO:HA	2.47	0.49
2:B:61:ARG:NH1	2:B:61:ARG:CG	2.73	0.49
2:B:187:GLU:O	2:B:211:ARG:NH1	2.46	0.49
1:C:55:SER:N	4:C:1221:SO4:O4	2.45	0.49
1:C:39:GLN:HA	1:C:44:GLY:O	2.11	0.49
2:B:11:MET:HE2	2:B:19:VAL:CG2	2.43	0.49
1:C:100:TRP:HB3	2:D:34:HIS:CE1	2.48	0.49
2:D:150:ILE:O	2:D:153:SER:OG	2.29	0.49
2:D:63:SER:H	2:D:74:PRO:HD2	1.78	0.49
2:B:2:ILE:HG12	2:B:27:SER:HB2	1.95	0.48
2:D:2:ILE:O	2:D:97:THR:HG21	2.12	0.48
1:C:67:PHE:CZ	1:C:82:MET:HG2	2.48	0.48
2:B:69:THR:CG2	2:B:70:SER:N	2.76	0.48
1:A:213:ARG:HH11	1:A:213:ARG:HG2	1.78	0.48
1:A:34:MET:HB3	1:A:78:LEU:HD22	1.96	0.48
1:A:167:PRO:HG2	2:B:162:SER:OG	2.13	0.48
1:C:24:ALA:HB1	1:C:27:PHE:CZ	2.48	0.48
1:C:35:HIS:CE1	1:C:50:TYR:CD1	3.02	0.48
2:B:170:ASP:O	2:B:171:SER:HB2	2.12	0.48
1:A:154:TRP:CZ3	1:A:195:CYS:HB3	2.48	0.48
2:D:31:ARG:HB3	2:D:91:TRP:O	2.13	0.48
2:B:112:ALA:HA	2:B:200:THR:HG21	1.96	0.47
2:D:188:ARG:NH1	2:D:188:ARG:CG	2.76	0.47
1:C:122:TYR:HD2	1:C:141:LEU:HD23	1.78	0.47
1:C:7:SER:CA	1:C:107:THR:HG21	2.44	0.47
2:D:140:TYR:CG	2:D:141:PRO:HA	2.49	0.47
2:B:46:ARG:O	2:B:46:ARG:HG2	2.13	0.47
1:A:188:TRP:CD1	1:A:189:PRO:HA	2.50	0.47
2:B:166:GLN:HG2	2:B:171:SER:HA	1.97	0.47
2:D:66:GLY:HA3	2:D:71:TYR:HA	1.96	0.47
1:A:170:LEU:HB2	1:A:175:TYR:CD1	2.50	0.47
1:C:204:THR:HG22	1:C:206:VAL:HG23	1.97	0.47
1:C:211:GLU:HG3	1:C:212:PRO:O	2.14	0.47
1:A:55:SER:CB	4:A:1221:SO4:O3	2.62	0.47
2:B:108:ARG:HD2	2:B:171:SER:HB2	1.96	0.47
2:B:93:GLY:C	2:B:94:TYR:CD1	2.88	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:CE1	3:E:4:NDG:H8C3	2.50	0.47
2:B:117:ILE:HD12	2:B:194:CYS:HB2	1.97	0.47
1:C:145:TYR:CE2	1:C:150:VAL:HG23	2.49	0.47
1:C:68:THR:HG22	1:C:81:GLN:HB3	1.97	0.47
2:D:89:GLN:HE21	2:D:96:LEU:HD11	1.80	0.47
2:B:91:TRP:CE3	2:B:96:LEU:HD12	2.50	0.46
1:C:8:GLY:O	1:C:18:ARG:NH1	2.45	0.46
1:A:196:ASN:HD22	1:A:207:ASP:HB2	1.79	0.46
1:A:55:SER:HB3	4:A:1221:SO4:S	2.55	0.46
2:B:79:GLU:HG2	2:B:81:GLU:CD	2.36	0.46
1:C:138:LEU:HD22	1:C:210:ILE:HG21	1.98	0.46
2:D:170:ASP:HB3	2:D:172:THR:OG1	2.14	0.46
1:A:61:ASP:CA	1:A:64:LYS:HG3	2.46	0.46
1:A:70:SER:O	1:A:78:LEU:HD12	2.15	0.46
2:B:91:TRP:NE1	2:B:93:GLY:HA2	2.30	0.46
2:B:13:ALA:N	2:B:107:LYS:HG3	2.31	0.46
2:D:89:GLN:HB2	2:D:98:PHE:CD1	2.50	0.46
2:D:166:GLN:HG3	2:D:173:TYR:CZ	2.51	0.45
2:D:48:ILE:HD13	2:D:54:LEU:CD2	2.46	0.45
1:A:51:ILE:HD13	1:A:57:ILE:HD13	1.97	0.45
2:B:199:LYS:O	2:B:199:LYS:HG2	2.15	0.45
2:B:63:SER:C	2:B:74:PRO:HD2	2.27	0.45
2:D:11:MET:HE3	2:D:11:MET:HB3	1.77	0.45
1:A:196:ASN:HD22	1:A:207:ASP:CB	2.29	0.45
1:C:202:SER:CB	1:C:204:THR:OG1	2.65	0.45
1:C:31:ARG:HB3	1:C:32:PHE:CD1	2.52	0.45
2:D:35:TRP:HB2	2:D:48:ILE:HB	1.98	0.45
1:A:126:PRO:O	1:A:213:ARG:HD2	2.17	0.45
1:A:168:ALA:HB2	1:A:177:LEU:HD12	1.99	0.45
1:A:61:ASP:HA	1:A:64:LYS:HD2	1.98	0.45
2:B:54:LEU:HB3	2:B:58:VAL:CG2	2.47	0.45
2:D:14:SER:O	2:D:78:MET:HB3	2.17	0.45
1:A:51:ILE:HD13	1:A:57:ILE:CD1	2.46	0.45
3:F:2:GMH:H71	3:F:2:GMH:H4	1.79	0.45
1:A:52:GLY:O	1:A:71:ARG:NH1	2.50	0.44
1:C:6:GLU:CD	1:C:104:GLY:HA3	2.37	0.44
2:B:145:ASN:OD1	2:D:31:ARG:NH2	2.50	0.44
1:A:213:ARG:HG2	1:A:213:ARG:NH1	2.31	0.44
2:B:108:ARG:HG2	2:B:140:TYR:CD2	2.52	0.44
2:B:108:ARG:NH1	2:B:108:ARG:HG3	2.33	0.44
2:D:89:GLN:HB2	2:D:98:PHE:CE1	2.52	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:ASP:O	2:D:171:SER:CB	2.66	0.44
2:D:18:LYS:C	2:D:18:LYS:HE2	2.38	0.44
1:A:146:PHE:HA	1:A:147:PRO:HA	1.73	0.44
2:B:35:TRP:HB2	2:B:48:ILE:HB	2.00	0.44
2:B:59:PRO:HB2	2:B:61:ARG:HD3	1.98	0.44
1:C:67:PHE:CZ	1:C:82:MET:CG	3.00	0.43
2:D:213:GLU:O	2:D:214:CYS:CB	2.66	0.43
1:C:12:VAL:HB	1:C:111:VAL:HG13	1.99	0.43
2:D:106:MET:HE1	2:D:107:LYS:O	2.19	0.43
2:B:150:ILE:HD12	2:B:155:ARG:HD2	2.00	0.43
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.00	0.43
1:C:214:VAL:HG23	1:C:215:PRO:CD	2.48	0.43
1:C:98:GLY:HA2	2:D:32:TYR:CE1	2.54	0.43
1:C:50:TYR:OH	3:F:3:GMH:O3	2.28	0.43
1:C:35:HIS:CE1	1:C:50:TYR:HD1	2.35	0.43
1:C:68:THR:CG2	1:C:81:GLN:HB3	2.49	0.43
2:B:124:GLN:NE2	2:B:131:SER:HB2	2.34	0.43
2:D:47:TRP:CE3	2:D:58:VAL:HG22	2.53	0.43
1:C:53:GLY:O	1:C:54:SER:HB2	2.18	0.43
1:A:202:SER:HB3	1:A:204:THR:OG1	2.19	0.43
2:B:93:GLY:O	2:B:94:TYR:CD1	2.72	0.43
1:C:202:SER:HB3	1:C:204:THR:OG1	2.19	0.43
2:D:97:THR:HG22	2:D:98:PHE:N	2.33	0.42
2:D:120:PRO:HG3	2:D:131:SER:O	2.19	0.42
1:C:127:VAL:HG22	1:C:128:CYS:N	2.34	0.42
1:C:141:LEU:HD21	1:C:143:LYS:HD2	2.01	0.42
1:A:6:GLU:CD	1:A:104:GLY:HA3	2.39	0.42
2:B:14:SER:CA	2:B:107:LYS:HB2	2.49	0.42
2:D:8:PRO:CG	2:D:11:MET:CE	2.93	0.42
2:B:19:VAL:HG13	2:B:75:ILE:HG13	2.00	0.42
1:A:36:TRP:CE2	1:A:80:LEU:HB2	2.54	0.41
2:B:8:PRO:CG	2:B:11:MET:HB3	2.50	0.41
1:A:150:VAL:CG1	1:A:197:VAL:HG13	2.50	0.41
1:C:36:TRP:NE1	1:C:80:LEU:HB2	2.36	0.41
1:A:67:PHE:N	1:A:67:PHE:CD1	2.87	0.41
2:B:12:SER:OG	2:B:107:LYS:HG3	2.15	0.41
1:C:24:ALA:HB1	1:C:27:PHE:CE2	2.56	0.41
2:D:119:PRO:HB3	2:D:209:PHE:CE2	2.55	0.41
2:B:50:ASP:O	2:B:51:THR:HB	2.21	0.41
2:B:103:LYS:HE2	2:B:105:GLU:CD	2.39	0.41
1:C:8:GLY:O	1:C:18:ARG:HD3	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:30:VAL:CG2	2:D:71:TYR:CE1	3.04	0.41
2:D:48:ILE:HD11	2:D:54:LEU:CD2	2.50	0.41
1:C:51:ILE:HG23	1:C:51:ILE:O	2.19	0.41
1:A:57:ILE:CG2	1:A:69:ILE:CG2	2.98	0.41
1:C:143:LYS:HB2	1:C:143:LYS:HE2	1.78	0.41
2:D:15:PRO:HD3	2:D:106:MET:HE1	2.03	0.41
1:A:35:HIS:CE1	1:A:50:TYR:CD1	3.09	0.41
3:F:2:GMH:H72	3:F:5:BGC:C1	2.51	0.41
1:C:214:VAL:CG2	1:C:215:PRO:HD2	2.49	0.41
2:D:212:ASN:C	2:D:213:GLU:CG	2.87	0.41
1:A:51:ILE:HD12	1:A:57:ILE:HG12	2.03	0.41
1:C:210:ILE:HD13	1:C:210:ILE:N	2.36	0.41
2:D:161:ASN:CB	2:D:175:MET:HE2	2.47	0.41
2:B:113:PRO:HG2	2:B:205:ILE:HD12	2.03	0.40
2:B:38:GLN:HE21	2:B:38:GLN:HB3	1.69	0.40
1:A:28:THR:HG21	1:A:31:ARG:NE	2.35	0.40
1:A:97:THR:HG23	3:E:3:GMH:O7	2.21	0.40
2:D:212:ASN:O	2:D:213:GLU:CB	2.68	0.40
1:A:103:TRP:CE3	2:B:44:PRO:HD2	2.57	0.40
1:C:12:VAL:O	1:C:111:VAL:HA	2.20	0.40
1:C:82:MET:HB3	1:C:82(C):LEU:HD21	2.04	0.40
2:D:186:TYR:CE2	2:D:211:ARG:HD3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:SER:OG	2:D:157:ASN:OD1[1_556]	2.12	0.08

## 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	211/220 (96%)	206 (98%)	5 (2%)	0	100	100
1	C	211/220 (96%)	207 (98%)	4 (2%)	0	100	100
2	B	212/214 (99%)	207 (98%)	4 (2%)	1 (0%)	29	54
2	D	211/214 (99%)	206 (98%)	4 (2%)	1 (0%)	29	54
All	All	845/868 (97%)	826 (98%)	17 (2%)	2 (0%)	47	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	74	PRO
2	D	74	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	182/186 (98%)	172 (94%)	10 (6%)	21	46
1	C	182/186 (98%)	160 (88%)	22 (12%)	5	11
2	B	188/188 (100%)	154 (82%)	34 (18%)	1	4
2	D	187/188 (100%)	157 (84%)	30 (16%)	2	6
All	All	739/748 (99%)	643 (87%)	96 (13%)	4	10

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	62	THR
1	A	97	THR
1	A	124	LEU
1	A	143	LYS
1	A	170	LEU
1	A	186	SER
1	A	196	ASN
1	A	203	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	214	VAL
2	B	1	GLN
2	B	7	SER
2	B	14	SER
2	B	18	LYS
2	B	26	SER
2	B	33	MET
2	B	42	THR
2	B	43	SER
2	B	46	ARG
2	B	52	SER
2	B	53	LYS
2	B	61	ARG
2	B	63	SER
2	B	71	TYR
2	B	79	GLU
2	B	81	GLU
2	B	96	LEU
2	B	106	MET
2	B	116	SER
2	B	131	SER
2	B	136	LEU
2	B	142	LYS
2	B	143	ASP
2	B	145	ASN
2	B	153	SER
2	B	168	SER
2	B	175	MET
2	B	177	SER
2	B	180	THR
2	B	187	GLU
2	B	194	CYS
2	B	202	THR
2	B	208	SER
2	B	214	CYS
1	C	21	SER
1	C	25	SER
1	C	55	SER
1	C	61	ASP
1	C	62	THR
1	C	66	ARG
1	C	75	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	84	SER
1	C	85	GLU
1	C	92	CYS
1	C	97	THR
1	C	111	VAL
1	C	120	SER
1	C	138	LEU
1	C	143	LYS
1	C	170	LEU
1	C	186	SER
1	C	196	ASN
1	C	203	SER
1	C	205	LYS
1	C	209	LYS
1	C	213	ARG
2	D	7	SER
2	D	10	ILE
2	D	14	SER
2	D	18	LYS
2	D	26	SER
2	D	29	SER
2	D	31	ARG
2	D	43	SER
2	D	46	ARG
2	D	47	TRP
2	D	52	SER
2	D	63	SER
2	D	70	SER
2	D	79	GLU
2	D	90	GLN
2	D	106	MET
2	D	107	LYS
2	D	131	SER
2	D	134	CYS
2	D	153	SER
2	D	157	ASN
2	D	162	SER
2	D	168	SER
2	D	170	ASP
2	D	175	MET
2	D	188	ARG
2	D	194	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	202	THR
2	D	203	SER
2	D	214	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
2	B	90	GLN

### 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 ⓘ

10 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	KDO	E	1	3	13,16,16	1.54	2 (15%)	14,24,24	0.69	0
3	GMH	E	2	3	13,13,14	0.95	0	17,18,20	0.83	0
3	GMH	E	3	3	13,13,14	0.84	0	17,18,20	1.95	3 (17%)
3	NDG	E	4	3	14,14,15	0.63	0	17,19,21	1.02	3 (17%)
3	BGC	E	5	3	11,11,12	0.65	0	15,15,17	1.41	3 (20%)
3	KDO	F	1	3	13,16,16	1.78	3 (23%)	14,24,24	1.24	2 (14%)
3	GMH	F	2	3	13,13,14	0.94	0	17,18,20	1.44	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GMH	F	3	3	13,13,14	1.01	1 (7%)	17,18,20	1.69	4 (23%)
3	NDG	F	4	3	14,14,15	0.71	1 (7%)	17,19,21	1.10	1 (5%)
3	BGC	F	5	3	11,11,12	0.33	0	15,15,17	0.96	1 (6%)

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	KDO	E	1	3	-	2/6/30/30	0/1/1/1
3	GMH	E	2	3	-	6/6/23/26	0/1/1/1
3	GMH	E	3	3	-	1/6/23/26	0/1/1/1
3	NDG	E	4	3	-	0/6/23/26	0/1/1/1
3	BGC	E	5	3	-	1/2/19/22	0/1/1/1
3	KDO	F	1	3	-	0/6/30/30	0/1/1/1
3	GMH	F	2	3	-	4/6/23/26	0/1/1/1
3	GMH	F	3	3	-	4/6/23/26	0/1/1/1
3	NDG	F	4	3	-	1/6/23/26	0/1/1/1
3	BGC	F	5	3	-	2/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	KDO	O6-C2	4.53	1.47	1.43
3	E	1	KDO	C3-C2	3.28	1.55	1.51
3	E	1	KDO	O2-C2	3.08	1.44	1.39
3	F	1	KDO	O2-C2	3.06	1.44	1.39
3	F	1	KDO	C3-C2	2.98	1.55	1.51
3	F	3	GMH	O5-C1	-2.28	1.40	1.43
3	F	4	NDG	O5-C1	-2.08	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	GMH	C1-C2-C3	-5.93	102.37	109.67
3	F	3	GMH	C1-C2-C3	-4.66	103.94	109.67
3	F	2	GMH	C1-O5-C5	4.23	118.41	111.48
3	E	3	GMH	O2-C2-C1	3.50	116.32	109.15
3	E	5	BGC	C1-O5-C5	3.00	116.26	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	NDG	O5-C1-C2	-2.50	107.35	111.29
3	E	5	BGC	C2-C3-C4	-2.46	106.63	110.89
3	E	4	NDG	O5-C1-C2	-2.46	107.41	111.29
3	E	5	BGC	C1-C2-C3	-2.40	106.71	109.67
3	E	3	GMH	O5-C1-C2	2.32	114.36	110.77
3	F	3	GMH	O5-C1-C2	2.31	114.34	110.77
3	F	1	KDO	C4-C5-C6	-2.29	105.80	110.41
3	F	3	GMH	O6-C6-C5	2.28	114.61	109.14
3	F	1	KDO	C7-C6-C5	-2.26	110.29	114.03
3	F	5	BGC	O5-C5-C6	2.24	110.72	107.20
3	F	2	GMH	O5-C5-C4	2.17	114.55	110.73
3	E	4	NDG	C1-C2-N2	2.04	113.98	110.49
3	F	2	GMH	C3-C4-C5	2.04	114.33	109.68
3	F	3	GMH	O2-C2-C1	2.02	113.28	109.15
3	E	4	NDG	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	GMH	C4-C5-C6-C7
3	F	2	GMH	C4-C5-C6-O6
3	F	2	GMH	O5-C5-C6-C7
3	F	2	GMH	O5-C5-C6-O6
3	E	2	GMH	C4-C5-C6-C7
3	E	2	GMH	C4-C5-C6-O6
3	E	2	GMH	O5-C5-C6-C7
3	E	2	GMH	O5-C5-C6-O6
3	F	3	GMH	C4-C5-C6-C7
3	F	3	GMH	C4-C5-C6-O6
3	F	3	GMH	O5-C5-C6-C7
3	F	3	GMH	O5-C5-C6-O6
3	F	5	BGC	C4-C5-C6-O6
3	F	5	BGC	O5-C5-C6-O6
3	E	1	KDO	O7-C7-C8-O8
3	E	5	BGC	O5-C5-C6-O6
3	E	1	KDO	C6-C7-C8-O8
3	E	2	GMH	C5-C6-C7-O7
3	E	3	GMH	C4-C5-C6-C7
3	F	4	NDG	C4-C5-C6-O6
3	E	2	GMH	O6-C6-C7-O7

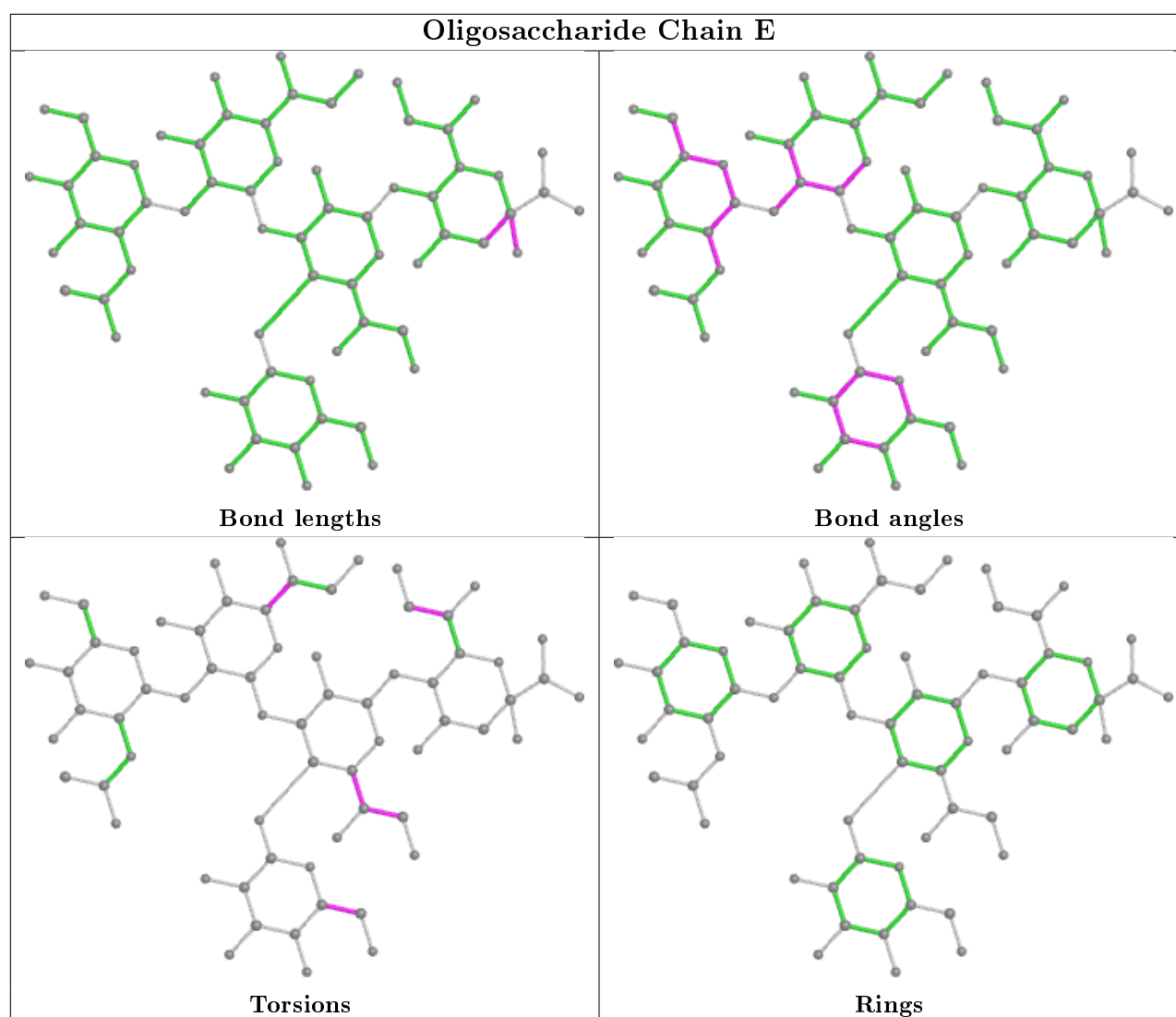


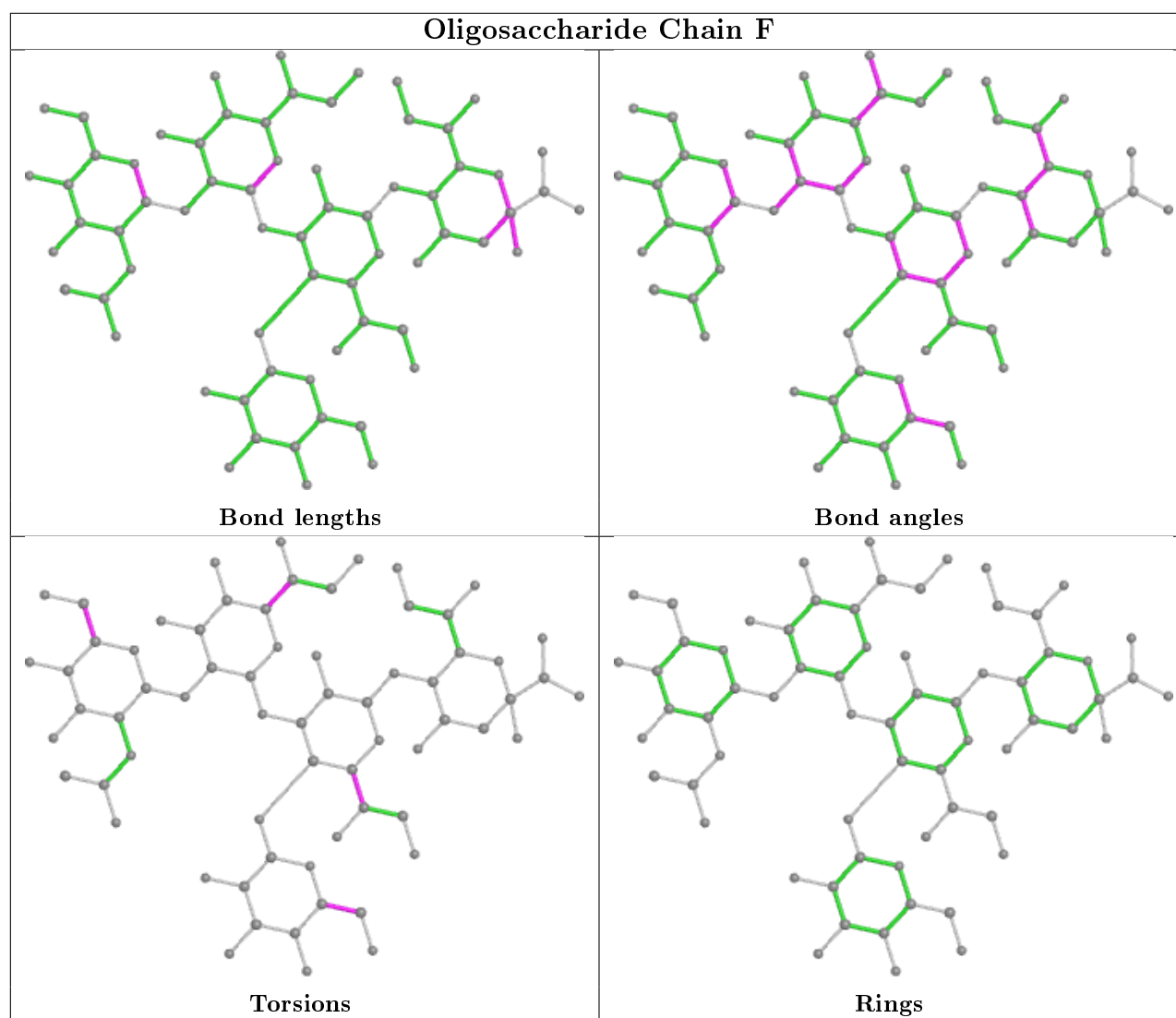
There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3	GMH	2	0
3	F	2	GMH	2	0
3	F	5	BGC	2	0
3	E	5	BGC	1	0
3	E	4	NDG	2	0
3	F	3	GMH	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](#)

2 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	SO4	C	1221	-	4,4,4	0.43	0	6,6,6	0.20	0
4	SO4	A	1221	-	4,4,4	0.35	0	6,6,6	0.30	0

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.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1221	SO4	4	0
4	A	1221	SO4	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	215/220 (97%)	-0.15	2 (0%) 84 85	32, 49, 68, 92	0
1	C	215/220 (97%)	-0.13	1 (0%) 91 92	32, 47, 68, 86	0
2	B	214/214 (100%)	0.05	2 (0%) 84 85	30, 52, 80, 94	0
2	D	213/214 (99%)	0.02	4 (1%) 66 69	31, 52, 76, 91	0
All	All	857/868 (98%)	-0.05	9 (1%) 80 82	30, 49, 74, 94	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	215	PRO	3.6
2	B	214	CYS	3.5
2	D	214	CYS	3.4
2	B	212	ASN	3.3
2	D	58	VAL	2.6
2	D	213	GLU	2.6
2	D	81	GLU	2.5
1	A	72	ASP	2.3
1	A	214	VAL	2.2

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

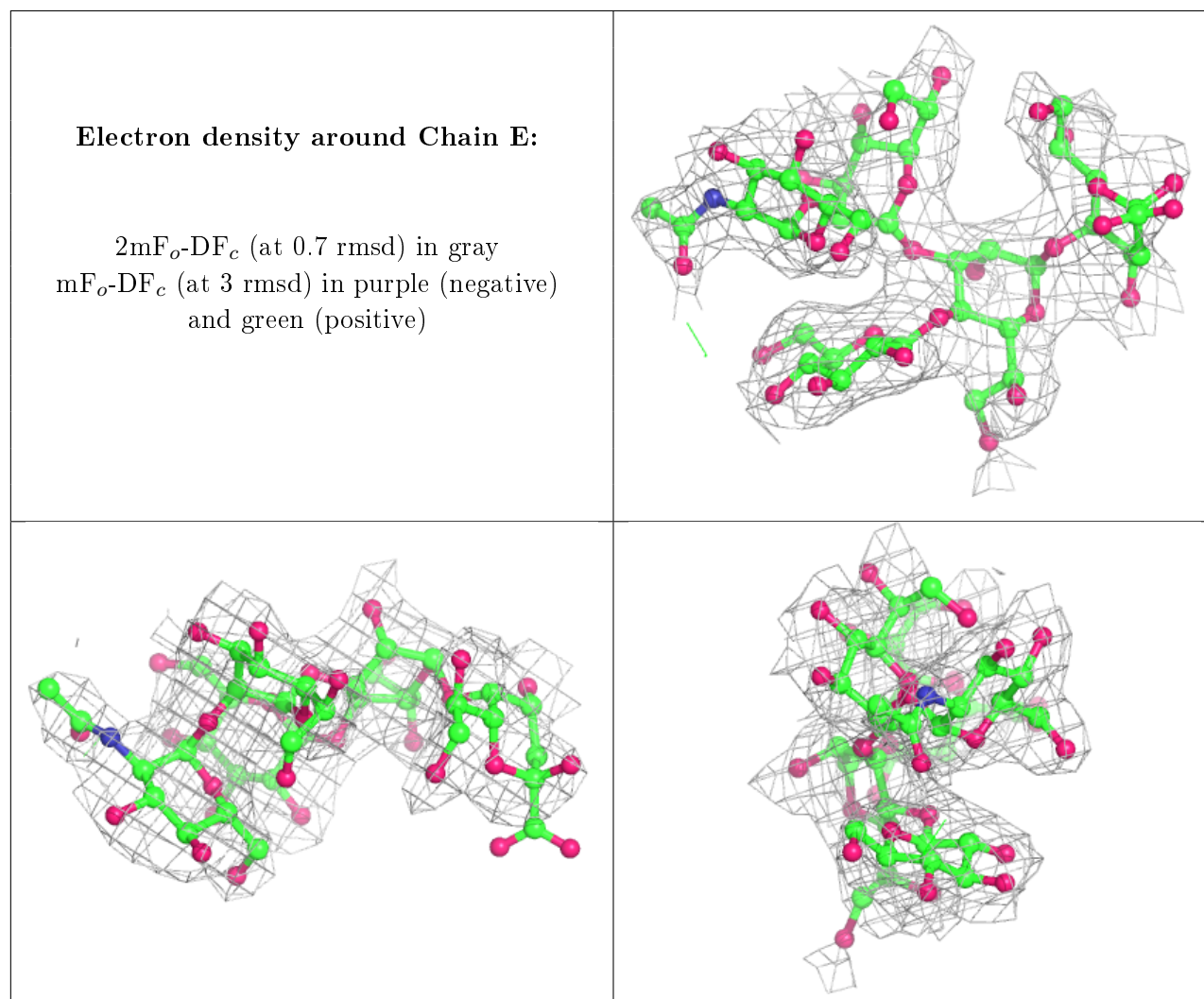
There are no non-standard protein/DNA/RNA residues in this entry.

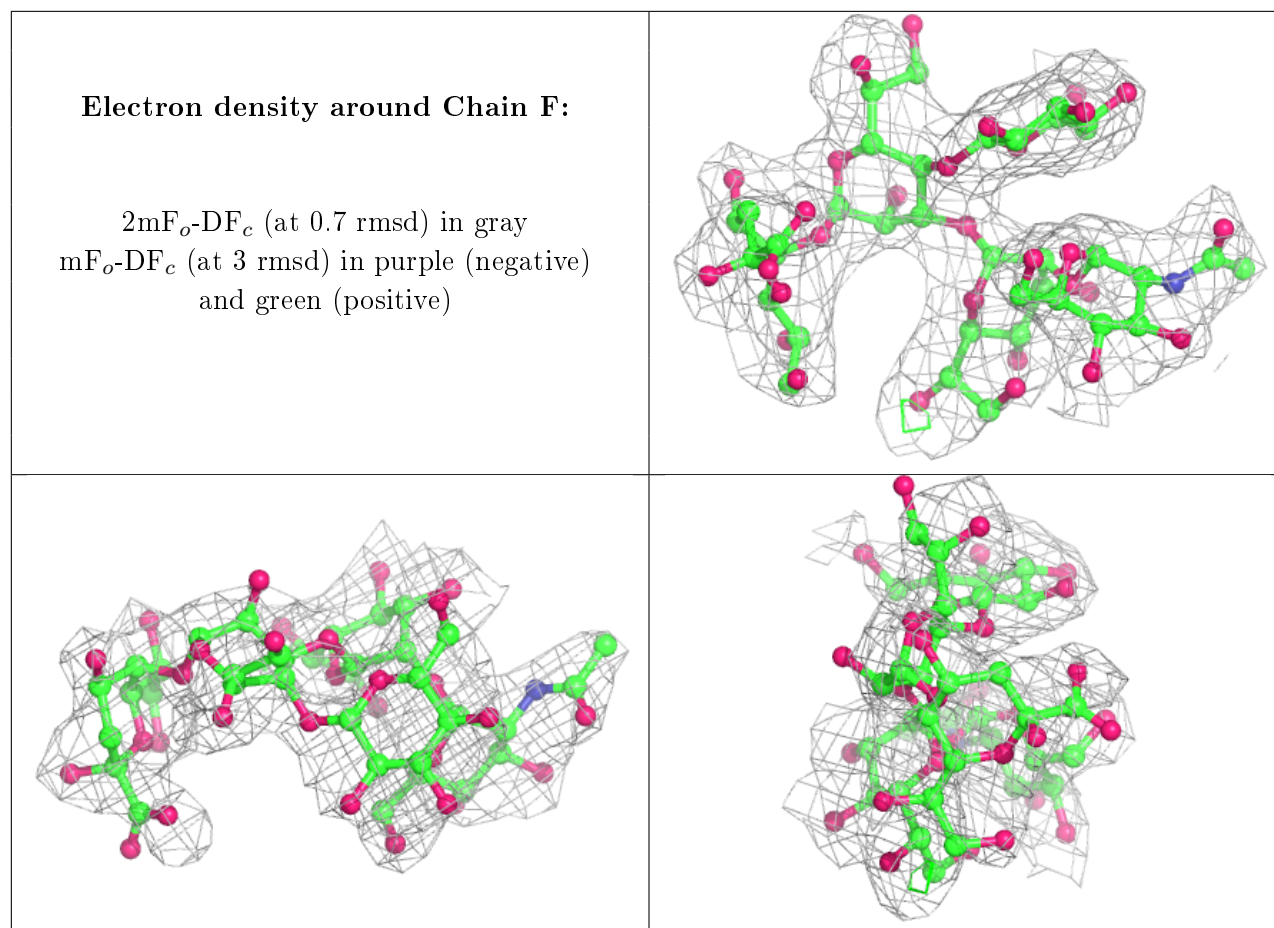
### 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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
3	KDO	E	1	16/16	0.76	0.26	74,94,112,120	0
3	KDO	F	1	16/16	0.87	0.23	75,85,98,111	0
3	GMH	F	2	13/14	0.92	0.17	54,63,70,71	0
3	GMH	E	2	13/14	0.93	0.16	58,67,79,86	0
3	NDG	E	4	14/15	0.93	0.15	45,61,67,72	0
3	GMH	F	3	13/14	0.93	0.17	34,48,62,85	0
3	BGC	F	5	11/12	0.94	0.14	61,65,72,76	0
3	NDG	F	4	14/15	0.94	0.15	42,48,52,52	0
3	BGC	E	5	11/12	0.95	0.16	56,57,63,72	0
3	GMH	E	3	13/14	0.95	0.22	49,57,78,97	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, 95<sup>th</sup> 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	SO4	C	1221	5/5	0.95	0.08	45,53,58,60	0
4	SO4	A	1221	5/5	0.98	0.13	53,54,60,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.