Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 08:18 AM EDT

PDB ID	:	1MPN
Title	:	MALTOPORIN MALTOTRIOSE COMPLEX
Authors	:	Dutzler, R.; Schirmer, T.
Deposited on	:	1996-01-11
Resolution	:	3.20 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 (i) 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 (i)) were used in the production of this report:

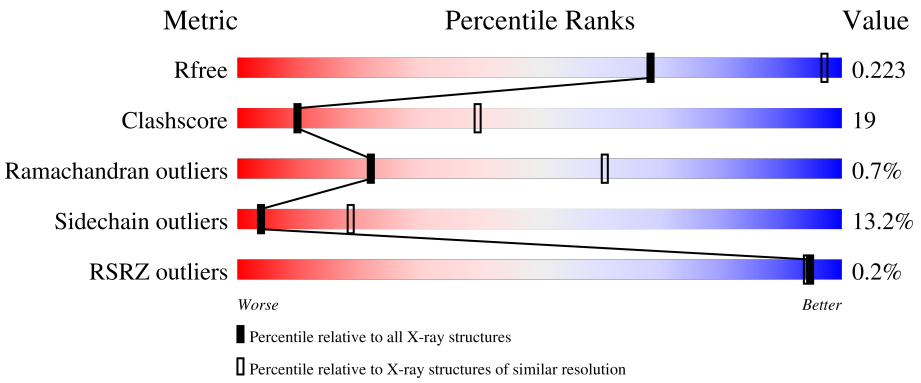
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	421	67% 27% 6%
1	B	421	67% 27% 6%
1	C	421	67% 27% 6%
2	D	3	33% 67%
2	E	3	33% 67%

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Mol	Chain	Length	Quality of chain
2	F	3	33% 67%

2 Entry composition (i)

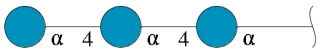
There are 3 unique types of molecules in this entry. The entry contains 10155 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MALTOPORIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	421	3350	2110	571	655	14	127	0	0
1	B	421	3350	2110	571	655	14	127	0	0
1	C	421	3350	2110	571	655	14	127	0	0

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	D	3	34	18	16	0	0	0
2	E	3	34	18	16	0	0	0
2	F	3	34	18	16	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

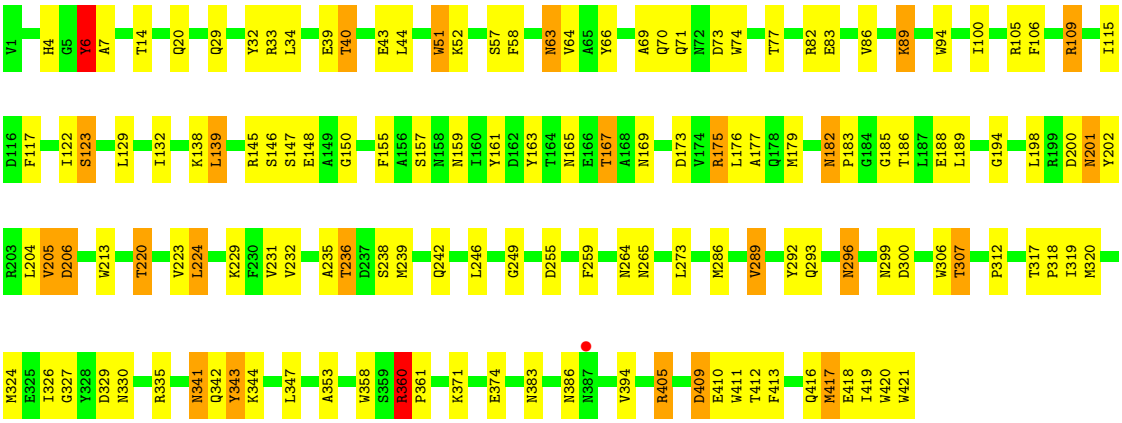
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0
3	C	1	1	1	0	0

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.

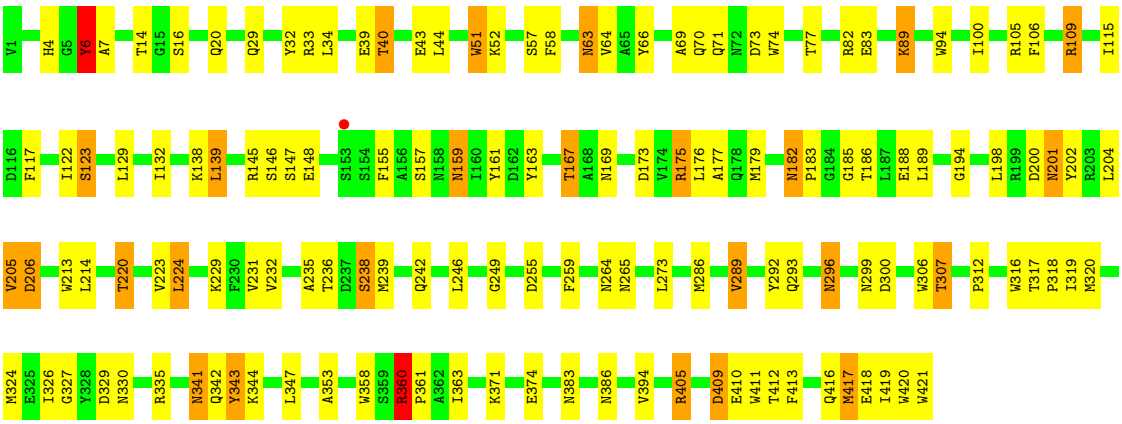
• Molecule 1: MALTOPORIN

Chain A: 67% 27% 6%



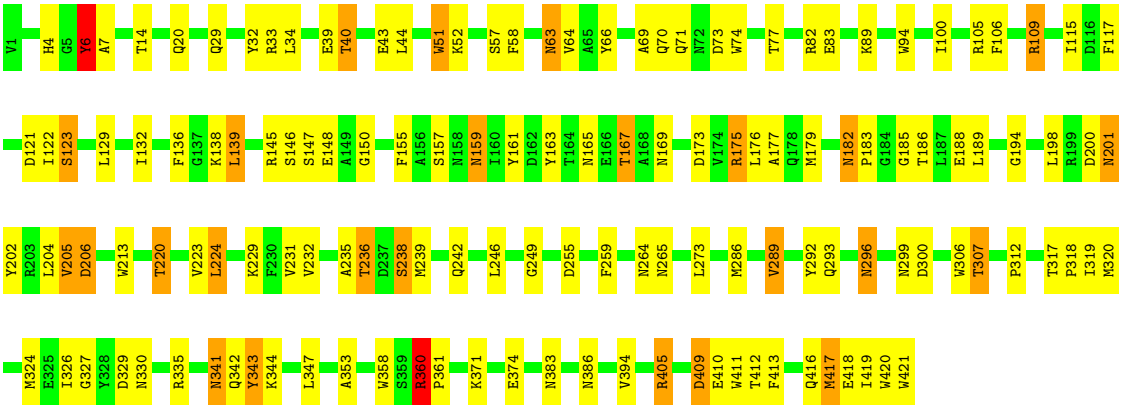
• Molecule 1: MALTOPORIN

Chain B: 67% 27% 6%



• Molecule 1: MALTOPORIN

Chain C: 67% 27% 6%



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:

• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	131.90Å 214.80Å 220.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20 38.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (8.00-3.20) 98.8 (38.95-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.98 (at 3.18Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.218 , 0.231 0.211 , 0.223	Depositor DCC
R_{free} test set	5111 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 102.1	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	0.90	EDS
Total number of atoms	10155	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GLC

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	0.77	1/3443 (0.0%)	0.95	2/4668 (0.0%)
1	B	0.77	2/3443 (0.1%)	0.95	2/4668 (0.0%)
1	C	0.77	1/3443 (0.0%)	0.95	2/4668 (0.0%)
All	All	0.77	4/10329 (0.0%)	0.95	6/14004 (0.0%)

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	2
1	B	0	2
1	C	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	TRP	CB-CG	-5.97	1.39	1.50
1	A	358	TRP	CB-CG	-5.96	1.39	1.50
1	C	358	TRP	CB-CG	-5.92	1.39	1.50
1	B	316	TRP	CB-CG	-5.00	1.41	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	289	VAL	CB-CA-C	-8.61	95.04	111.40
1	C	289	VAL	CB-CA-C	-8.61	95.05	111.40
1	B	289	VAL	CB-CA-C	-8.59	95.08	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	73	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	73	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	73	ASP	CB-CG-OD1	5.71	123.44	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	ARG	Peptide
1	A	6	TYR	Sidechain
1	B	360	ARG	Peptide
1	B	6	TYR	Sidechain
1	C	360	ARG	Peptide
1	C	6	TYR	Sidechain

5.2 Too-close contacts (i)

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	3350	0	3070	124	0
1	B	3350	0	3070	127	0
1	C	3350	0	3070	128	0
2	D	34	0	30	3	0
2	E	34	0	30	3	0
2	F	34	0	30	3	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
All	All	10155	0	9300	355	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 19.

All (355) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ARG:CD	1:C:71:GLN:HE22	1.70	1.04
1:A:353:ALA:HB2	1:C:58:PHE:CD2	1.98	0.99
1:A:71:GLN:HE22	1:C:145:ARG:CD	1.74	0.98
1:B:58:PHE:CD2	1:C:353:ALA:HB2	2.03	0.93
1:B:145:ARG:HD3	1:C:71:GLN:NE2	1.84	0.91
1:A:71:GLN:NE2	1:C:145:ARG:HD3	1.86	0.91
1:A:63:ASN:HB3	1:A:83:GLU:HG2	1.53	0.91
1:C:155:PHE:CE1	1:C:157:SER:HB3	2.06	0.91
1:B:155:PHE:CE1	1:B:157:SER:HB3	2.06	0.90
1:A:71:GLN:HE22	1:C:145:ARG:HD2	1.36	0.90
1:B:145:ARG:CD	1:C:71:GLN:NE2	2.34	0.90
1:A:155:PHE:CE1	1:A:157:SER:HB3	2.06	0.90
1:A:71:GLN:NE2	1:C:145:ARG:CD	2.36	0.89
1:B:63:ASN:HB3	1:B:83:GLU:HG2	1.53	0.89
1:A:145:ARG:CD	1:B:71:GLN:HE22	1.86	0.89
1:C:63:ASN:HB3	1:C:83:GLU:HG2	1.53	0.89
1:B:145:ARG:HD2	1:C:71:GLN:HE22	1.34	0.88
1:B:317:THR:HG22	1:B:319:ILE:H	1.38	0.88
1:C:317:THR:HG22	1:C:319:ILE:H	1.38	0.86
1:A:317:THR:HG22	1:A:319:ILE:H	1.38	0.85
1:B:145:ARG:HD3	1:C:71:GLN:HE22	1.41	0.85
1:A:58:PHE:CD2	1:B:353:ALA:HB2	2.12	0.83
1:A:353:ALA:HB2	1:C:58:PHE:CE2	2.13	0.82
1:C:198:LEU:HD11	1:C:204:LEU:HG	1.65	0.79
1:A:198:LEU:HD11	1:A:204:LEU:HG	1.65	0.78
1:C:155:PHE:HE1	1:C:157:SER:HB3	1.49	0.77
1:C:317:THR:HG23	1:C:318:PRO:HD2	1.65	0.77
1:B:155:PHE:HE1	1:B:157:SER:HB3	1.49	0.77
1:B:317:THR:HG23	1:B:318:PRO:HD2	1.65	0.77
1:B:198:LEU:HD11	1:B:204:LEU:HG	1.65	0.77
1:A:317:THR:HG23	1:A:318:PRO:HD2	1.66	0.77
1:A:155:PHE:HE1	1:A:157:SER:HB3	1.49	0.76
1:A:145:ARG:HD3	1:B:71:GLN:NE2	2.00	0.76
1:A:145:ARG:HD2	1:B:71:GLN:HE22	1.49	0.75
1:A:63:ASN:HD22	1:A:64:VAL:N	1.86	0.74
1:B:63:ASN:HD22	1:B:64:VAL:N	1.86	0.74
1:C:63:ASN:HD22	1:C:64:VAL:N	1.86	0.74
1:A:145:ARG:CD	1:B:71:GLN:NE2	2.51	0.74
1:A:71:GLN:HE22	1:C:145:ARG:HD3	1.45	0.73
1:A:145:ARG:HD3	1:B:71:GLN:HE22	1.53	0.73
1:B:148:GLU:HG3	1:B:167:THR:HG23	1.71	0.71
1:A:148:GLU:HG3	1:A:167:THR:HG23	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:PHE:HA	1:A:123:SER:HB3	1.73	0.71
1:B:58:PHE:CE2	1:C:353:ALA:HB2	2.27	0.70
1:C:148:GLU:HG3	1:C:167:THR:HG23	1.71	0.70
1:C:106:PHE:HA	1:C:123:SER:HB3	1.73	0.70
1:B:106:PHE:HA	1:B:123:SER:HB3	1.73	0.69
1:A:58:PHE:CE2	1:B:353:ALA:HB2	2.31	0.66
1:A:63:ASN:CB	1:A:83:GLU:HG2	2.24	0.66
1:B:223:VAL:HG12	1:B:224:LEU:N	2.11	0.65
1:C:109:ARG:HG3	1:C:109:ARG:HH11	1.62	0.65
1:A:6:TYR:CD1	1:A:7:ALA:N	2.66	0.64
1:A:223:VAL:HG12	1:A:224:LEU:N	2.11	0.64
1:B:109:ARG:HG3	1:B:109:ARG:HH11	1.62	0.64
1:C:223:VAL:HG12	1:C:224:LEU:N	2.11	0.64
1:A:33:ARG:NH2	2:D:2:GLC:O3	2.30	0.64
1:B:176:LEU:HG	1:B:179:MET:CE	2.28	0.64
1:C:63:ASN:CB	1:C:83:GLU:HG2	2.24	0.64
1:C:6:TYR:CD1	1:C:7:ALA:N	2.66	0.64
1:B:6:TYR:CD1	1:B:7:ALA:N	2.66	0.63
1:B:63:ASN:CB	1:B:83:GLU:HG2	2.24	0.63
1:C:312:PRO:HD2	1:C:324:MET:O	1.99	0.63
1:C:169:ASN:HD21	1:C:249:GLY:H	1.47	0.63
1:A:109:ARG:HG3	1:A:109:ARG:HH11	1.62	0.63
1:A:176:LEU:HG	1:A:179:MET:HE2	1.80	0.63
1:A:312:PRO:HD2	1:A:324:MET:O	1.99	0.63
1:C:176:LEU:HG	1:C:179:MET:CE	2.28	0.63
1:C:71:GLN:NE2	1:C:71:GLN:HA	2.15	0.62
1:A:176:LEU:HG	1:A:179:MET:CE	2.28	0.62
1:B:71:GLN:NE2	1:B:71:GLN:HA	2.15	0.62
1:A:71:GLN:NE2	1:A:71:GLN:HA	2.15	0.62
1:B:169:ASN:HD21	1:B:249:GLY:H	1.47	0.62
1:B:312:PRO:HD2	1:B:324:MET:O	1.99	0.62
1:B:33:ARG:NH2	2:E:2:GLC:O3	2.30	0.61
1:A:173:ASP:OD1	1:A:175:ARG:HD2	2.01	0.61
1:A:169:ASN:HD21	1:A:249:GLY:H	1.47	0.60
1:C:173:ASP:OD1	1:C:175:ARG:HD2	2.01	0.60
1:B:14:THR:HA	1:B:412:THR:HG22	1.83	0.60
1:A:163:TYR:CD2	1:A:205:VAL:HG23	2.37	0.60
1:C:100:ILE:HG22	1:C:129:LEU:HD13	1.84	0.60
1:A:100:ILE:HG22	1:A:129:LEU:HD13	1.84	0.60
1:C:163:TYR:CD2	1:C:205:VAL:HG23	2.37	0.60
1:B:163:TYR:CD2	1:B:205:VAL:HG23	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:THR:HA	1:C:412:THR:HG22	1.83	0.60
1:C:32:TYR:CB	1:C:344:LYS:HE2	2.31	0.59
1:B:32:TYR:CB	1:B:344:LYS:HE2	2.31	0.59
1:B:100:ILE:HG22	1:B:129:LEU:HD13	1.84	0.59
1:B:173:ASP:OD1	1:B:175:ARG:HD2	2.01	0.59
1:A:32:TYR:CB	1:A:344:LYS:HE2	2.31	0.59
1:A:14:THR:HA	1:A:412:THR:HG22	1.83	0.59
1:C:145:ARG:HG3	1:C:146:SER:N	2.18	0.59
1:C:33:ARG:NH2	2:F:2:GLC:O3	2.30	0.59
1:A:145:ARG:HG3	1:A:146:SER:N	2.18	0.58
1:B:43:GLU:HB3	1:B:63:ASN:HD21	1.69	0.58
1:B:182:ASN:HB2	1:B:183:PRO:HD2	1.85	0.58
1:A:182:ASN:HB2	1:A:183:PRO:HD2	1.84	0.58
1:B:145:ARG:HG3	1:B:146:SER:N	2.18	0.58
1:C:182:ASN:HB2	1:C:183:PRO:HD2	1.85	0.58
1:B:176:LEU:HG	1:B:179:MET:HE3	1.85	0.57
1:C:32:TYR:HB2	1:C:344:LYS:HE2	1.87	0.57
1:C:176:LEU:HG	1:C:179:MET:HE2	1.85	0.57
1:B:32:TYR:HB2	1:B:344:LYS:HE2	1.87	0.57
1:C:43:GLU:HB3	1:C:63:ASN:HD21	1.69	0.57
1:A:43:GLU:HB3	1:A:63:ASN:HD21	1.69	0.57
1:A:202:TYR:N	1:A:202:TYR:CD1	2.72	0.57
1:C:202:TYR:CD1	1:C:202:TYR:N	2.72	0.56
1:B:202:TYR:N	1:B:202:TYR:CD1	2.72	0.56
1:B:202:TYR:N	1:B:202:TYR:HD1	2.04	0.56
1:C:202:TYR:N	1:C:202:TYR:HD1	2.04	0.56
1:B:6:TYR:CD1	1:B:6:TYR:C	2.80	0.56
1:B:82:ARG:HH12	2:E:1:GLC:H61	1.71	0.55
1:C:163:TYR:N	1:C:163:TYR:CD1	2.74	0.55
1:B:163:TYR:N	1:B:163:TYR:CD1	2.74	0.55
1:C:6:TYR:CD1	1:C:6:TYR:C	2.80	0.55
1:C:82:ARG:HH12	2:F:1:GLC:H61	1.71	0.55
1:A:32:TYR:HB2	1:A:344:LYS:HE2	1.87	0.55
1:A:43:GLU:C	1:A:44:LEU:HD23	2.27	0.55
1:A:6:TYR:CD1	1:A:6:TYR:C	2.80	0.55
1:A:163:TYR:N	1:A:163:TYR:CD1	2.74	0.55
1:C:200:ASP:O	1:C:201:ASN:HB2	2.05	0.55
1:A:202:TYR:N	1:A:202:TYR:HD1	2.04	0.55
1:B:200:ASP:O	1:B:201:ASN:HB2	2.05	0.55
1:A:82:ARG:HH12	2:D:1:GLC:H61	1.71	0.54
1:C:43:GLU:C	1:C:44:LEU:HD23	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ILE:O	1:B:100:ILE:HG13	2.07	0.54
1:A:200:ASP:O	1:A:201:ASN:HB2	2.05	0.54
1:C:100:ILE:O	1:C:100:ILE:HG13	2.07	0.54
1:C:242:GLN:CD	1:C:246:LEU:HB2	2.28	0.54
1:B:43:GLU:C	1:B:44:LEU:HD23	2.27	0.54
1:A:100:ILE:HG13	1:A:100:ILE:O	2.07	0.53
1:A:242:GLN:CD	1:A:246:LEU:HB2	2.28	0.53
1:B:242:GLN:CD	1:B:246:LEU:HB2	2.28	0.53
1:A:194:GLY:HA3	1:A:239:MET:CE	2.39	0.53
1:C:194:GLY:HA3	1:C:239:MET:CE	2.39	0.52
1:B:194:GLY:HA3	1:B:239:MET:CE	2.39	0.52
1:A:307:THR:HG23	1:A:329:ASP:OD1	2.10	0.52
1:C:307:THR:HG23	1:C:329:ASP:OD1	2.10	0.52
1:A:353:ALA:CB	1:C:58:PHE:CE2	2.90	0.52
1:B:307:THR:HG23	1:B:329:ASP:OD1	2.10	0.51
1:A:40:THR:OG1	1:A:70:GLN:NE2	2.43	0.51
1:B:342:GLN:HG2	1:B:343:TYR:N	2.26	0.51
1:C:342:GLN:HG2	1:C:343:TYR:N	2.26	0.51
1:A:185:GLY:HA2	1:A:220:THR:O	2.10	0.51
1:C:185:GLY:HA2	1:C:220:THR:O	2.10	0.51
1:B:40:THR:OG1	1:B:70:GLN:NE2	2.43	0.51
1:B:185:GLY:HA2	1:B:220:THR:O	2.10	0.51
1:C:40:THR:OG1	1:C:70:GLN:NE2	2.43	0.51
1:B:161:TYR:HE2	1:B:259:PHE:CD1	2.29	0.51
1:C:317:THR:CG2	1:C:318:PRO:HD2	2.39	0.51
1:C:360:ARG:HA	1:C:361:PRO:O	2.11	0.51
1:C:43:GLU:O	1:C:44:LEU:HD23	2.11	0.50
1:A:342:GLN:HG2	1:A:343:TYR:N	2.26	0.50
1:B:43:GLU:O	1:B:44:LEU:HD23	2.11	0.50
1:C:115:ILE:HG13	1:C:117:PHE:HB2	1.94	0.50
1:A:43:GLU:O	1:A:44:LEU:HD23	2.11	0.50
1:A:115:ILE:HG13	1:A:117:PHE:HB2	1.94	0.50
1:C:161:TYR:HE2	1:C:259:PHE:CD1	2.29	0.50
1:A:161:TYR:HE2	1:A:259:PHE:CD1	2.29	0.50
1:B:145:ARG:HD2	1:C:71:GLN:NE2	2.11	0.50
1:A:409:ASP:O	1:A:410:GLU:HB2	2.12	0.50
1:A:360:ARG:HA	1:A:361:PRO:O	2.12	0.50
1:C:161:TYR:CE2	1:C:259:PHE:CD1	3.00	0.50
1:A:71:GLN:NE2	1:C:145:ARG:HD2	2.10	0.50
1:B:106:PHE:HA	1:B:123:SER:CB	2.41	0.49
1:B:360:ARG:HA	1:B:361:PRO:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:VAL:CG1	1:C:224:LEU:N	2.75	0.49
1:B:115:ILE:HG13	1:B:117:PHE:HB2	1.94	0.49
1:C:63:ASN:HD22	1:C:63:ASN:C	2.14	0.49
1:A:161:TYR:CE2	1:A:259:PHE:CD1	3.00	0.49
1:A:383:ASN:HB3	1:A:386:ASN:H	1.78	0.49
1:B:63:ASN:HD22	1:B:63:ASN:C	2.14	0.49
1:B:409:ASP:O	1:B:410:GLU:HB2	2.12	0.49
1:B:383:ASN:HB3	1:B:386:ASN:H	1.78	0.49
1:C:63:ASN:CB	1:C:83:GLU:CG	2.91	0.49
1:B:145:ARG:CG	1:B:146:SER:N	2.76	0.49
1:C:409:ASP:O	1:C:410:GLU:HB2	2.12	0.49
1:A:145:ARG:CG	1:A:146:SER:N	2.76	0.49
1:B:161:TYR:CE2	1:B:259:PHE:CD1	3.00	0.49
1:C:383:ASN:HB3	1:C:386:ASN:H	1.78	0.49
1:A:63:ASN:CB	1:A:83:GLU:CG	2.91	0.49
1:A:223:VAL:CG1	1:A:224:LEU:N	2.75	0.48
1:B:317:THR:CG2	1:B:318:PRO:HD2	2.39	0.48
1:C:176:LEU:HG	1:C:179:MET:HE3	1.95	0.48
1:B:109:ARG:HG3	1:B:109:ARG:NH1	2.28	0.48
1:C:145:ARG:CG	1:C:146:SER:N	2.76	0.48
1:A:317:THR:CG2	1:A:318:PRO:HD2	2.39	0.48
1:B:223:VAL:CG1	1:B:224:LEU:N	2.75	0.48
1:C:106:PHE:HA	1:C:123:SER:CB	2.41	0.48
1:B:335:ARG:HH11	1:B:335:ARG:HG2	1.78	0.48
1:A:292:TYR:HD1	1:A:306:TRP:CE2	2.32	0.48
1:A:374:GLU:CD	1:A:405:ARG:HB2	2.34	0.48
1:C:374:GLU:CD	1:C:405:ARG:HB2	2.34	0.48
1:C:335:ARG:HG2	1:C:335:ARG:HH11	1.78	0.47
1:A:163:TYR:N	1:A:163:TYR:HD1	2.12	0.47
1:B:374:GLU:CD	1:B:405:ARG:HB2	2.34	0.47
1:C:163:TYR:N	1:C:163:TYR:HD1	2.12	0.47
1:C:292:TYR:HD1	1:C:306:TRP:CE2	2.32	0.47
1:A:220:THR:HG23	1:A:229:LYS:HD3	1.95	0.47
1:B:89:LYS:H	1:B:89:LYS:HG2	1.49	0.47
2:E:1:GLC:H62	2:E:2:GLC:C1	2.44	0.47
2:F:1:GLC:H62	2:F:2:GLC:C1	2.44	0.47
1:A:335:ARG:HG2	1:A:335:ARG:HH11	1.78	0.47
1:A:106:PHE:HA	1:A:123:SER:CB	2.41	0.47
1:B:292:TYR:HD1	1:B:306:TRP:CE2	2.32	0.47
1:B:330:ASN:HD22	1:B:341:ASN:HB3	1.79	0.47
1:C:220:THR:HG23	1:C:229:LYS:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:GLN:OE1	1:A:246:LEU:HB2	2.15	0.47
1:C:4:HIS:HA	1:C:421:TRP:CD1	2.50	0.47
2:D:1:GLC:H62	2:D:2:GLC:C1	2.44	0.47
1:A:330:ASN:HD22	1:A:341:ASN:HB3	1.79	0.47
1:B:417:MET:SD	1:B:417:MET:C	2.93	0.47
1:B:220:THR:HG23	1:B:229:LYS:HD3	1.95	0.46
1:B:242:GLN:OE1	1:B:246:LEU:HB2	2.15	0.46
1:B:163:TYR:N	1:B:163:TYR:HD1	2.12	0.46
1:C:64:VAL:HG12	1:C:66:TYR:CE1	2.51	0.46
1:C:106:PHE:HB3	1:C:109:ARG:HD3	1.98	0.46
1:C:242:GLN:OE1	1:C:246:LEU:HB2	2.15	0.46
1:A:198:LEU:HD21	1:A:204:LEU:CD2	2.45	0.46
1:A:417:MET:SD	1:A:417:MET:C	2.93	0.46
1:B:4:HIS:HA	1:B:421:TRP:CD1	2.50	0.46
1:B:198:LEU:HD21	1:B:204:LEU:CD2	2.45	0.46
1:C:330:ASN:HD22	1:C:341:ASN:HB3	1.79	0.46
1:A:4:HIS:HA	1:A:421:TRP:CD1	2.50	0.46
1:C:109:ARG:HG3	1:C:109:ARG:NH1	2.28	0.46
1:A:64:VAL:HG12	1:A:66:TYR:CE1	2.50	0.46
1:C:198:LEU:HD21	1:C:204:LEU:CD2	2.45	0.46
1:C:417:MET:C	1:C:417:MET:SD	2.94	0.46
1:A:115:ILE:HG13	1:A:117:PHE:CB	2.46	0.46
1:B:176:LEU:HG	1:B:179:MET:HE2	1.96	0.46
1:B:64:VAL:HG12	1:B:66:TYR:CE1	2.50	0.46
1:B:115:ILE:HG13	1:B:117:PHE:CB	2.46	0.46
1:B:63:ASN:CB	1:B:83:GLU:CG	2.91	0.46
1:C:136:PHE:CD1	1:C:136:PHE:N	2.82	0.46
1:A:177:ALA:HB2	1:A:188:GLU:HG3	1.99	0.45
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.72	0.45
1:C:115:ILE:HG13	1:C:117:PHE:CB	2.46	0.45
1:C:161:TYR:CE2	1:C:259:PHE:HD1	2.34	0.45
1:B:177:ALA:HB2	1:B:188:GLU:HG3	1.98	0.45
1:B:106:PHE:HB3	1:B:109:ARG:HD3	1.98	0.45
1:A:106:PHE:HB3	1:A:109:ARG:HD3	1.98	0.45
1:A:32:TYR:CD2	1:A:327:GLY:HA3	2.52	0.45
1:A:231:VAL:HG12	1:A:232:VAL:N	2.32	0.45
1:B:52:LYS:HG3	1:B:57:SER:HB3	1.99	0.45
1:C:360:ARG:NH1	1:C:420:TRP:CH2	2.82	0.45
1:B:231:VAL:HG12	1:B:232:VAL:N	2.32	0.45
1:C:32:TYR:CD2	1:C:327:GLY:HA3	2.52	0.45
1:B:360:ARG:NH1	1:B:420:TRP:CH2	2.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LYS:HG3	1:C:57:SER:HB3	1.98	0.45
1:A:109:ARG:HG3	1:A:109:ARG:NH1	2.28	0.44
1:B:109:ARG:H	1:B:109:ARG:HG2	1.51	0.44
1:C:182:ASN:ND2	1:C:183:PRO:O	2.51	0.44
1:A:360:ARG:NH1	1:A:420:TRP:CH2	2.82	0.44
1:B:182:ASN:ND2	1:B:183:PRO:O	2.51	0.44
1:C:231:VAL:HG12	1:C:232:VAL:N	2.32	0.44
1:B:32:TYR:CD2	1:B:327:GLY:HA3	2.52	0.44
1:B:74:TRP:CD1	1:B:74:TRP:C	2.91	0.44
1:C:177:ALA:HB2	1:C:188:GLU:HG3	1.99	0.44
1:C:324:MET:CE	1:C:326:ILE:HD11	2.48	0.44
1:A:52:LYS:HG3	1:A:57:SER:HB3	1.99	0.44
1:A:182:ASN:ND2	1:A:183:PRO:O	2.51	0.44
1:C:292:TYR:CD1	1:C:306:TRP:CE2	3.06	0.44
1:A:29:GLN:NE2	1:A:293:GLN:HE22	2.16	0.44
1:C:74:TRP:CD1	1:C:74:TRP:C	2.91	0.44
1:A:74:TRP:CD1	1:A:74:TRP:C	2.91	0.44
1:A:161:TYR:CE2	1:A:259:PHE:HD1	2.34	0.44
1:B:161:TYR:CE2	1:B:259:PHE:HD1	2.34	0.44
1:B:246:LEU:HA	1:B:246:LEU:HD23	1.72	0.44
1:C:29:GLN:NE2	1:C:293:GLN:HE22	2.16	0.44
1:A:63:ASN:HD22	1:A:63:ASN:C	2.14	0.43
1:B:292:TYR:CD1	1:B:306:TRP:CE2	3.06	0.43
1:A:324:MET:CE	1:A:326:ILE:HD11	2.48	0.43
1:A:292:TYR:CD1	1:A:306:TRP:CE2	3.06	0.43
1:B:324:MET:CE	1:B:326:ILE:HD11	2.48	0.43
1:A:418:GLU:HG2	1:A:419:ILE:N	2.33	0.43
1:A:200:ASP:HB2	1:B:16:SER:OG	2.19	0.43
1:B:132:ILE:HB	1:B:139:LEU:O	2.19	0.43
1:A:205:VAL:HG13	1:A:206:ASP:N	2.34	0.43
1:C:159:ASN:HD22	1:C:159:ASN:HA	1.64	0.43
1:B:58:PHE:CE2	1:C:353:ALA:CB	3.00	0.43
1:B:205:VAL:HG13	1:B:206:ASP:N	2.34	0.43
1:C:132:ILE:HB	1:C:139:LEU:O	2.19	0.43
1:A:132:ILE:HB	1:A:139:LEU:O	2.19	0.42
1:A:213:TRP:O	1:A:235:ALA:HA	2.19	0.42
1:A:176:LEU:HG	1:A:179:MET:HE3	2.01	0.42
1:B:159:ASN:HD22	1:B:159:ASN:HA	1.64	0.42
1:C:213:TRP:O	1:C:235:ALA:HA	2.19	0.42
1:C:418:GLU:HG2	1:C:419:ILE:N	2.34	0.42
1:B:296:ASN:C	1:B:296:ASN:ND2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ASP:CG	1:C:259:PHE:HB2	2.40	0.42
1:A:109:ARG:H	1:A:109:ARG:HG2	1.51	0.42
1:A:353:ALA:CA	1:C:58:PHE:CE2	3.02	0.42
1:C:51:TRP:O	1:C:57:SER:HA	2.20	0.42
1:A:255:ASP:CG	1:A:259:PHE:HB2	2.40	0.42
1:A:296:ASN:C	1:A:296:ASN:ND2	2.72	0.42
1:B:29:GLN:NE2	1:B:293:GLN:HE22	2.16	0.42
1:B:418:GLU:HG2	1:B:419:ILE:N	2.34	0.42
1:C:296:ASN:HD22	1:C:296:ASN:C	2.23	0.42
1:B:296:ASN:C	1:B:296:ASN:HD22	2.23	0.42
1:C:205:VAL:HG13	1:C:206:ASP:N	2.34	0.42
1:C:296:ASN:C	1:C:296:ASN:ND2	2.72	0.42
1:B:51:TRP:O	1:B:57:SER:HA	2.20	0.42
1:C:238:SER:HB2	1:C:249:GLY:HA2	2.02	0.42
1:C:246:LEU:HD23	1:C:246:LEU:HA	1.72	0.42
1:C:416:GLN:CG	1:C:417:MET:N	2.82	0.42
1:A:86:VAL:HG12	1:B:363:ILE:HD11	2.02	0.41
1:A:122:ILE:O	1:A:122:ILE:HG13	2.20	0.41
1:A:51:TRP:O	1:A:57:SER:HA	2.20	0.41
1:B:419:ILE:O	1:B:419:ILE:HG23	2.20	0.41
1:C:122:ILE:O	1:C:122:ILE:HG13	2.20	0.41
1:A:416:GLN:CG	1:A:417:MET:N	2.82	0.41
1:B:44:LEU:HD23	1:B:44:LEU:N	2.35	0.41
1:B:416:GLN:CG	1:B:417:MET:N	2.82	0.41
1:C:109:ARG:H	1:C:109:ARG:HG2	1.51	0.41
1:A:44:LEU:HD23	1:A:44:LEU:N	2.35	0.41
1:A:205:VAL:CG1	1:A:206:ASP:N	2.83	0.41
1:B:122:ILE:O	1:B:122:ILE:HG13	2.20	0.41
1:C:44:LEU:HD23	1:C:44:LEU:N	2.35	0.41
1:C:69:ALA:O	1:C:70:GLN:HG2	2.21	0.41
1:B:213:TRP:O	1:B:235:ALA:HA	2.20	0.41
1:B:238:SER:HB2	1:B:249:GLY:HA2	2.02	0.41
1:B:317:THR:CG2	1:B:318:PRO:CD	2.99	0.41
1:B:343:TYR:CD1	1:B:343:TYR:C	2.93	0.41
1:C:63:ASN:HD22	1:C:64:VAL:H	1.67	0.41
1:C:419:ILE:HG23	1:C:419:ILE:O	2.21	0.41
1:A:343:TYR:CD1	1:A:343:TYR:C	2.93	0.41
1:B:255:ASP:CG	1:B:259:PHE:HB2	2.40	0.41
3:B:422:MG:MG	3:C:422:MG:MG	0.59	0.41
1:C:205:VAL:CG1	1:C:206:ASP:N	2.83	0.41
1:B:202:TYR:HD1	1:B:202:TYR:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:VAL:CG1	1:B:206:ASP:N	2.83	0.41
1:B:69:ALA:O	1:B:70:GLN:HG2	2.21	0.41
1:B:194:GLY:HA3	1:B:239:MET:HE1	2.03	0.41
1:B:411:TRP:CZ3	1:B:413:PHE:CD2	3.09	0.41
1:C:343:TYR:CD1	1:C:343:TYR:C	2.93	0.41
1:A:89:LYS:H	1:A:89:LYS:HG2	1.49	0.40
1:A:236:THR:O	1:A:236:THR:HG22	2.20	0.40
1:A:317:THR:HG23	1:A:318:PRO:CD	2.46	0.40
1:A:419:ILE:HG23	1:A:419:ILE:O	2.21	0.40
1:B:214:LEU:HD13	1:B:235:ALA:HB2	2.03	0.40
1:C:236:THR:O	1:C:236:THR:HG22	2.20	0.40
1:C:317:THR:CG2	1:C:318:PRO:CD	2.99	0.40
1:C:411:TRP:CZ3	1:C:413:PHE:CD2	3.09	0.40
1:A:69:ALA:O	1:A:70:GLN:HG2	2.21	0.40
1:A:296:ASN:C	1:A:296:ASN:HD22	2.23	0.40
1:B:324:MET:HE2	1:B:326:ILE:HD11	2.04	0.40
1:A:150:GLY:HA2	1:A:165:ASN:O	2.22	0.40
1:B:360:ARG:HD2	1:B:420:TRP:CH2	2.57	0.40
1:C:121:ASP:OD1	1:C:123:SER:OG	2.39	0.40
1:C:150:GLY:HA2	1:C:165:ASN:O	2.22	0.40
1:C:182:ASN:HD22	1:C:183:PRO:CD	2.35	0.40
1:A:317:THR:CG2	1:A:318:PRO:CD	2.99	0.40
1:A:360:ARG:HD2	1:A:420:TRP:CH2	2.57	0.40
1:A:411:TRP:CZ3	1:A:413:PHE:CD2	3.09	0.40
1:B:182:ASN:HD22	1:B:183:PRO:CD	2.35	0.40
1:C:194:GLY:HA3	1:C:239:MET:HE1	2.03	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	419/421 (100%)	380 (91%)	36 (9%)	3 (1%)	22	61
1	B	419/421 (100%)	380 (91%)	36 (9%)	3 (1%)	22	61
1	C	419/421 (100%)	380 (91%)	36 (9%)	3 (1%)	22	61
All	All	1257/1263 (100%)	1140 (91%)	108 (9%)	9 (1%)	22	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	224	LEU
1	A	264	ASN
1	B	224	LEU
1	B	264	ASN
1	C	224	LEU
1	C	264	ASN
1	A	201	ASN
1	B	201	ASN
1	C	201	ASN

5.3.2 Protein sidechains (i)

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	340/340 (100%)	295 (87%)	45 (13%)	4	19
1	B	340/340 (100%)	295 (87%)	45 (13%)	4	19
1	C	340/340 (100%)	295 (87%)	45 (13%)	4	19
All	All	1020/1020 (100%)	885 (87%)	135 (13%)	4	19

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	20	GLN
1	A	34	LEU
1	A	39	GLU

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Mol	Chain	Res	Type
1	A	40	THR
1	A	51	TRP
1	A	63	ASN
1	A	77	THR
1	A	89	LYS
1	A	94	TRP
1	A	105	ARG
1	A	109	ARG
1	A	123	SER
1	A	138	LYS
1	A	139	LEU
1	A	147	SER
1	A	159	ASN
1	A	167	THR
1	A	175	ARG
1	A	182	ASN
1	A	186	THR
1	A	189	LEU
1	A	205	VAL
1	A	206	ASP
1	A	220	THR
1	A	236	THR
1	A	238	SER
1	A	265	ASN
1	A	273	LEU
1	A	286	MET
1	A	289	VAL
1	A	296	ASN
1	A	299	ASN
1	A	300	ASP
1	A	307	THR
1	A	320	MET
1	A	341	ASN
1	A	343	TYR
1	A	347	LEU
1	A	360	ARG
1	A	371	LYS
1	A	394	VAL
1	A	405	ARG
1	A	409	ASP
1	A	417	MET
1	B	6	TYR

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Mol	Chain	Res	Type
1	B	20	GLN
1	B	34	LEU
1	B	39	GLU
1	B	40	THR
1	B	51	TRP
1	B	63	ASN
1	B	77	THR
1	B	89	LYS
1	B	94	TRP
1	B	105	ARG
1	B	109	ARG
1	B	123	SER
1	B	138	LYS
1	B	139	LEU
1	B	147	SER
1	B	159	ASN
1	B	167	THR
1	B	175	ARG
1	B	182	ASN
1	B	186	THR
1	B	189	LEU
1	B	205	VAL
1	B	206	ASP
1	B	220	THR
1	B	236	THR
1	B	238	SER
1	B	265	ASN
1	B	273	LEU
1	B	286	MET
1	B	289	VAL
1	B	296	ASN
1	B	299	ASN
1	B	300	ASP
1	B	307	THR
1	B	320	MET
1	B	341	ASN
1	B	343	TYR
1	B	347	LEU
1	B	360	ARG
1	B	371	LYS
1	B	394	VAL
1	B	405	ARG

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Mol	Chain	Res	Type
1	B	409	ASP
1	B	417	MET
1	C	6	TYR
1	C	20	GLN
1	C	34	LEU
1	C	39	GLU
1	C	40	THR
1	C	51	TRP
1	C	63	ASN
1	C	77	THR
1	C	89	LYS
1	C	94	TRP
1	C	105	ARG
1	C	109	ARG
1	C	123	SER
1	C	138	LYS
1	C	139	LEU
1	C	147	SER
1	C	159	ASN
1	C	167	THR
1	C	175	ARG
1	C	182	ASN
1	C	186	THR
1	C	189	LEU
1	C	205	VAL
1	C	206	ASP
1	C	220	THR
1	C	236	THR
1	C	238	SER
1	C	265	ASN
1	C	273	LEU
1	C	286	MET
1	C	289	VAL
1	C	296	ASN
1	C	299	ASN
1	C	300	ASP
1	C	307	THR
1	C	320	MET
1	C	341	ASN
1	C	343	TYR
1	C	347	LEU
1	C	360	ARG

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Mol	Chain	Res	Type
1	C	371	LYS
1	C	394	VAL
1	C	405	ARG
1	C	409	ASP
1	C	417	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	63	ASN
1	A	70	GLN
1	A	71	GLN
1	A	110	HIS
1	A	159	ASN
1	A	169	ASN
1	A	182	ASN
1	A	221	GLN
1	A	248	GLN
1	A	265	ASN
1	A	266	ASN
1	A	268	HIS
1	A	296	ASN
1	A	330	ASN
1	A	341	ASN
1	A	349	GLN
1	B	29	GLN
1	B	63	ASN
1	B	70	GLN
1	B	71	GLN
1	B	110	HIS
1	B	159	ASN
1	B	169	ASN
1	B	182	ASN
1	B	221	GLN
1	B	248	GLN
1	B	265	ASN
1	B	266	ASN
1	B	296	ASN
1	B	330	ASN
1	B	341	ASN
1	B	349	GLN

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Mol	Chain	Res	Type
1	C	29	GLN
1	C	63	ASN
1	C	70	GLN
1	C	71	GLN
1	C	110	HIS
1	C	159	ASN
1	C	169	ASN
1	C	182	ASN
1	C	221	GLN
1	C	248	GLN
1	C	265	ASN
1	C	266	ASN
1	C	268	HIS
1	C	296	ASN
1	C	330	ASN
1	C	341	ASN
1	C	349	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

9 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	D	1	2	12,12,12	0.83	0	17,17,17	0.95	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLC	D	2	2	11,11,12	0.49	0	15,15,17	0.88	1 (6%)
2	GLC	D	3	2	11,11,12	0.51	0	15,15,17	1.07	1 (6%)
2	GLC	E	1	2	12,12,12	0.83	0	17,17,17	0.95	2 (11%)
2	GLC	E	2	2	11,11,12	0.49	0	15,15,17	0.88	1 (6%)
2	GLC	E	3	2	11,11,12	0.52	0	15,15,17	1.07	1 (6%)
2	GLC	F	1	2	12,12,12	0.83	0	17,17,17	0.95	2 (11%)
2	GLC	F	2	2	11,11,12	0.49	0	15,15,17	0.89	1 (6%)
2	GLC	F	3	2	11,11,12	0.50	0	15,15,17	1.07	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
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1
2	GLC	D	2	2	-	2/2/19/22	0/1/1/1
2	GLC	D	3	2	-	1/2/19/22	0/1/1/1
2	GLC	E	1	2	-	2/2/22/22	0/1/1/1
2	GLC	E	2	2	-	2/2/19/22	0/1/1/1
2	GLC	E	3	2	-	1/2/19/22	0/1/1/1
2	GLC	F	1	2	-	2/2/22/22	0/1/1/1
2	GLC	F	2	2	-	2/2/19/22	0/1/1/1
2	GLC	F	3	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	3	GLC	C2-C3-C4	2.59	115.37	110.89
2	D	3	GLC	C2-C3-C4	2.57	115.35	110.89
2	E	3	GLC	C2-C3-C4	2.57	115.33	110.89
2	F	2	GLC	C1-O5-C5	2.31	115.32	112.19
2	D	1	GLC	C4-C3-C2	2.30	114.84	110.82
2	D	2	GLC	C1-O5-C5	2.30	115.31	112.19
2	E	1	GLC	C4-C3-C2	2.30	114.84	110.82
2	F	1	GLC	C4-C3-C2	2.29	114.82	110.82
2	E	2	GLC	C1-O5-C5	2.28	115.28	112.19
2	F	1	GLC	C1-C2-C3	2.03	114.52	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	GLC	C1-C2-C3	2.02	114.51	110.31
2	E	1	GLC	C1-C2-C3	2.01	114.48	110.31

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	GLC	O5-C5-C6-O6
2	E	2	GLC	O5-C5-C6-O6
2	F	2	GLC	O5-C5-C6-O6
2	D	1	GLC	C4-C5-C6-O6
2	D	2	GLC	C4-C5-C6-O6
2	E	1	GLC	C4-C5-C6-O6
2	E	2	GLC	C4-C5-C6-O6
2	F	1	GLC	C4-C5-C6-O6
2	F	2	GLC	C4-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	E	1	GLC	O5-C5-C6-O6
2	F	1	GLC	O5-C5-C6-O6
2	F	3	GLC	O5-C5-C6-O6
2	D	3	GLC	O5-C5-C6-O6
2	E	3	GLC	O5-C5-C6-O6

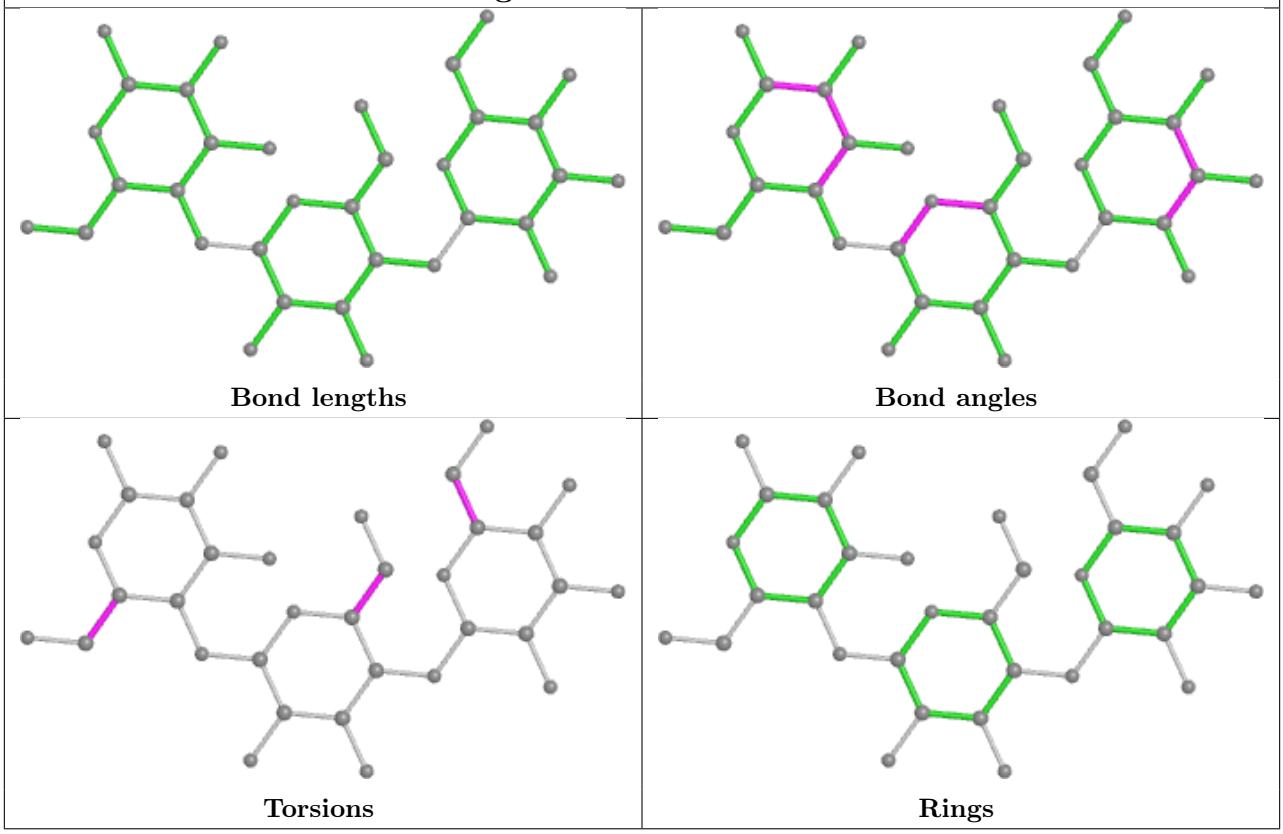
There are no ring outliers.

6 monomers are involved in 9 short contacts:

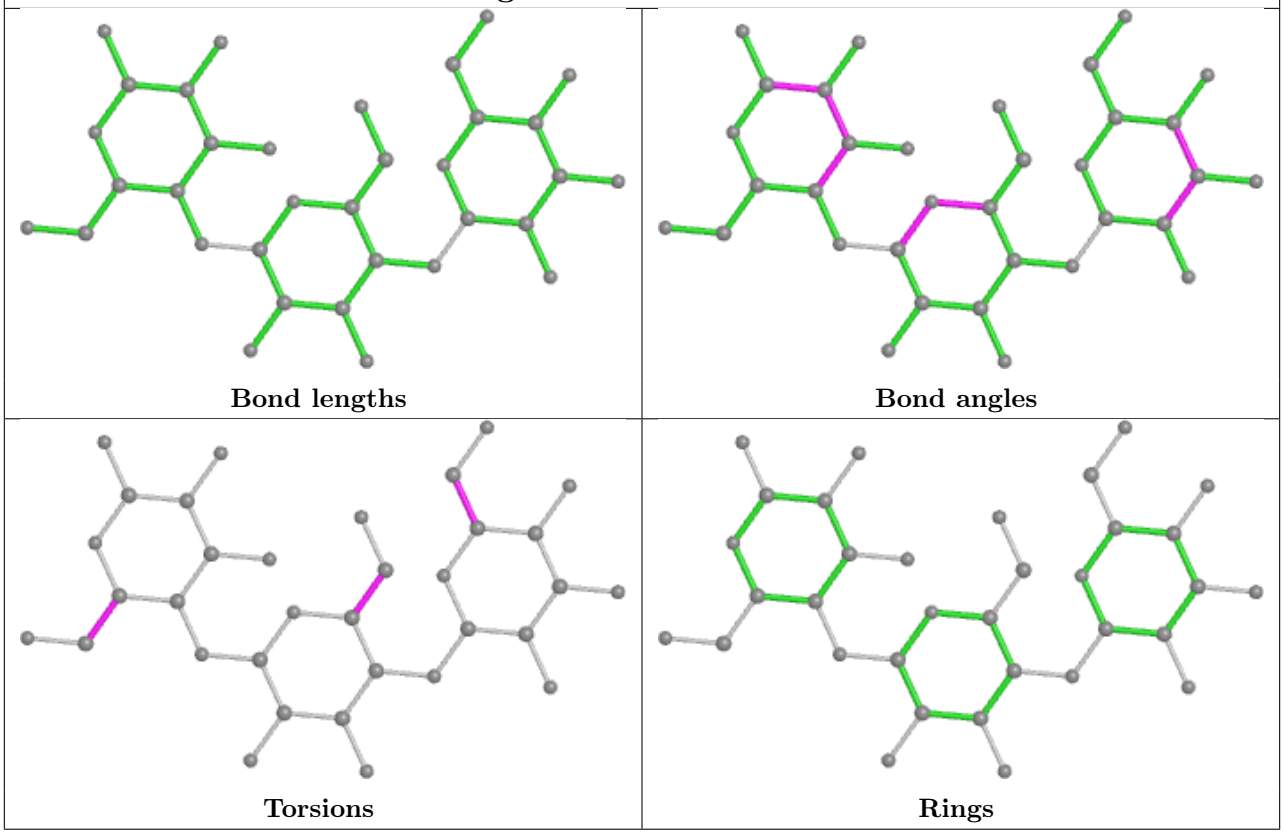
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	GLC	2	0
2	D	1	GLC	2	0
2	F	2	GLC	2	0
2	E	2	GLC	2	0
2	F	1	GLC	2	0
2	E	1	GLC	2	0

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

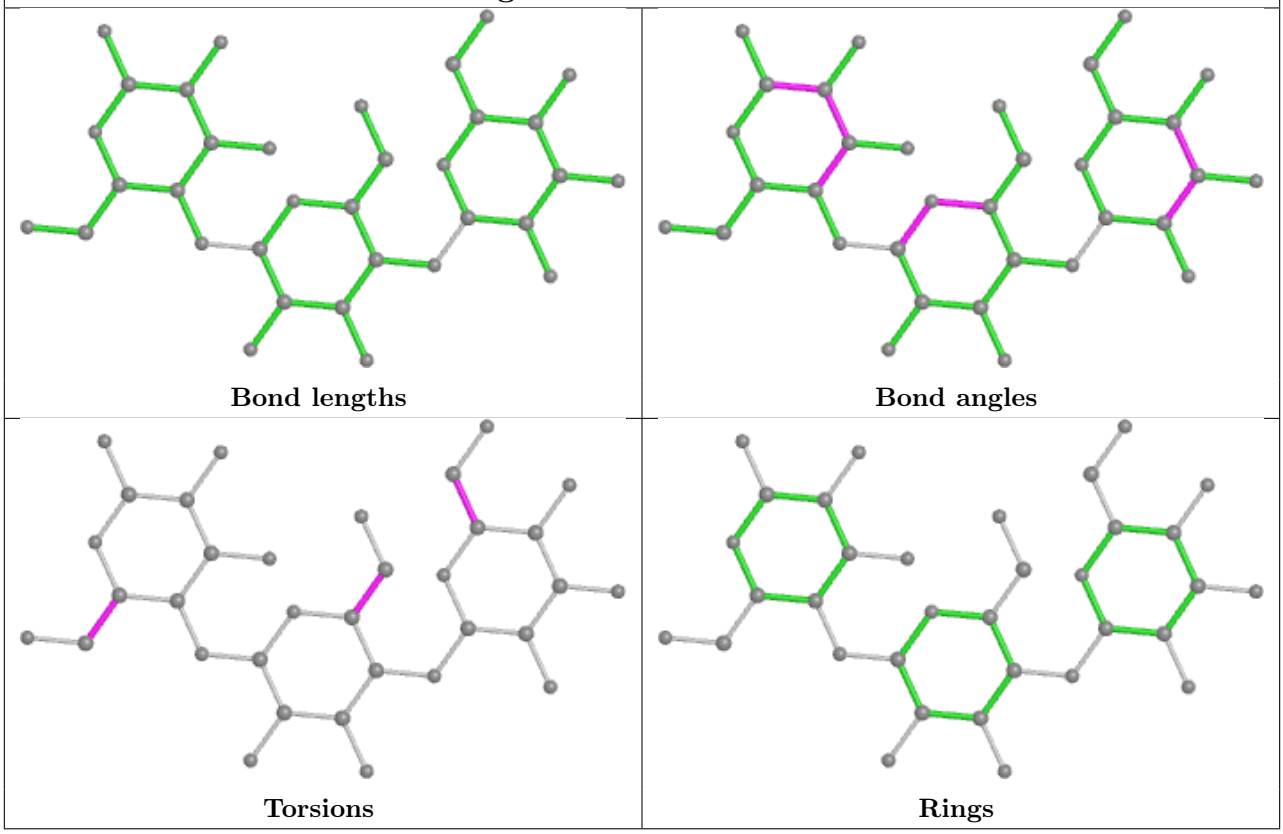
Oligosaccharide Chain D



Oligosaccharide Chain E



Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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 (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	421/421 (100%)	-0.45	1 (0%) 95 94	9, 26, 47, 58	45 (10%)
1	B	421/421 (100%)	-0.42	1 (0%) 95 94	9, 26, 47, 58	45 (10%)
1	C	421/421 (100%)	-0.47	0 100 100	9, 26, 47, 58	45 (10%)
All	All	1263/1263 (100%)	-0.44	2 (0%) 95 94	9, 27, 47, 58	135 (10%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	SER	2.4
1	A	387	ASN	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
2	GLC	D	1	12/12	0.81	0.36	81,81,81,81	0
2	GLC	F	3	11/12	0.85	0.25	54,54,54,54	0
2	GLC	E	1	12/12	0.86	0.28	81,81,81,81	0
2	GLC	E	3	11/12	0.88	0.28	54,54,54,54	0
2	GLC	F	1	12/12	0.88	0.28	81,81,81,81	0
2	GLC	D	3	11/12	0.88	0.25	54,54,54,54	0

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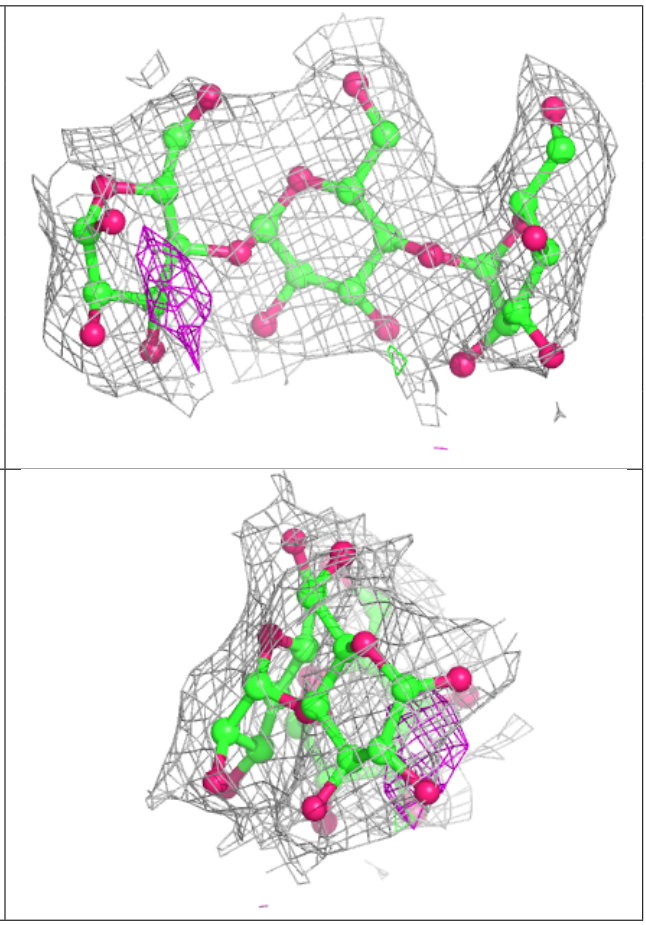
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	E	2	11/12	0.93	0.18	46,46,46,46	0
2	GLC	D	2	11/12	0.94	0.18	46,46,46,46	0
2	GLC	F	2	11/12	0.95	0.16	46,46,46,46	0

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

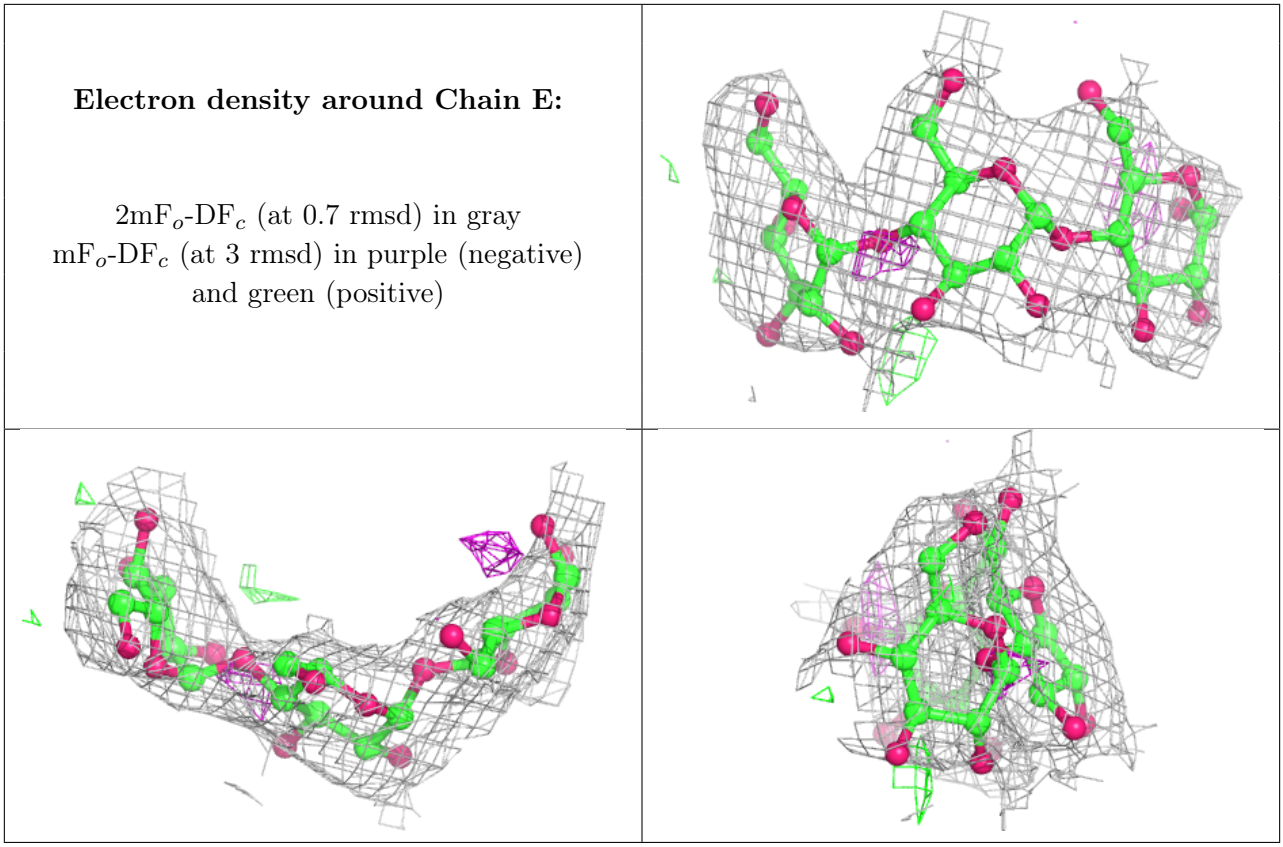
Electron density around Chain D:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



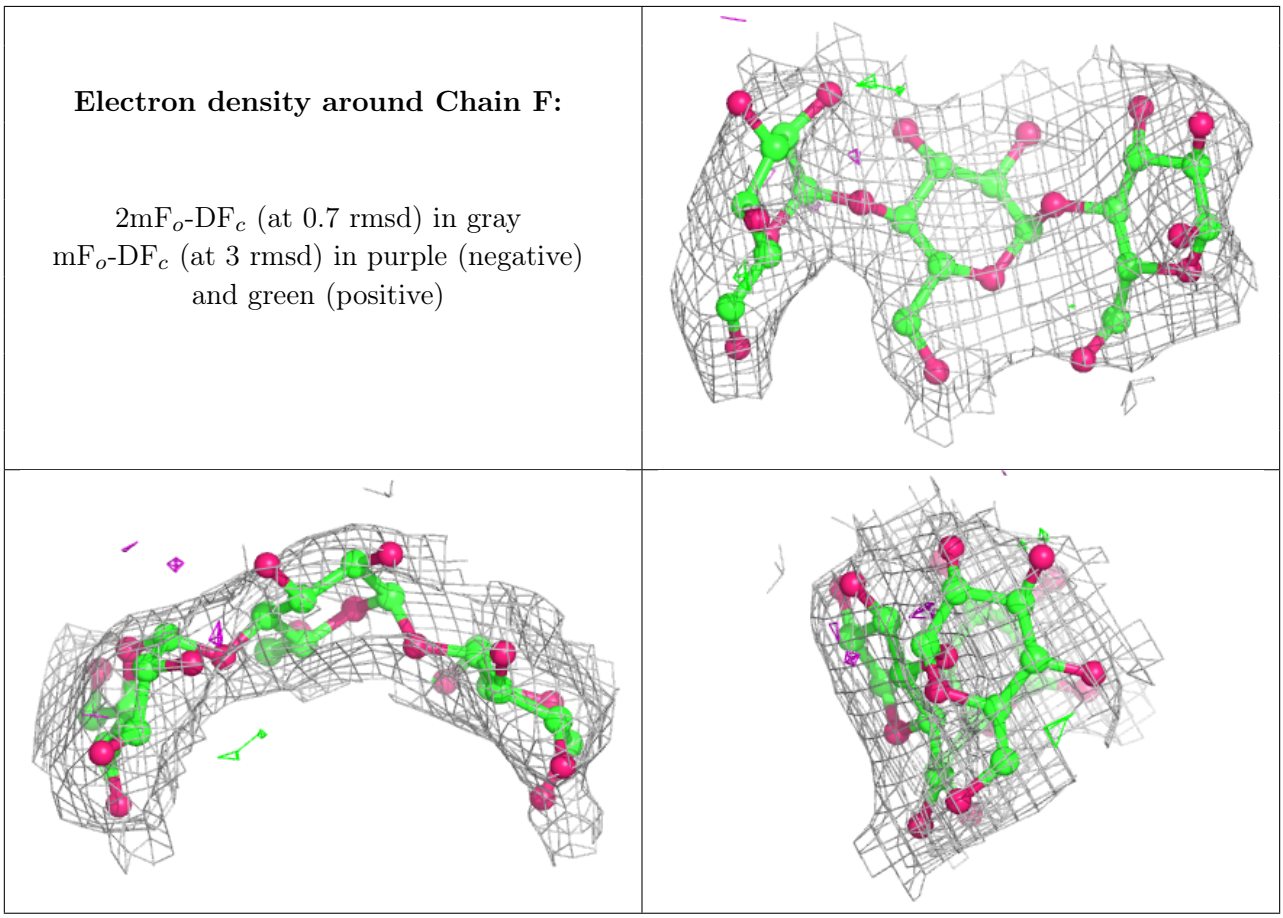
Electron density around Chain E:

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



Electron density around Chain F:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	422	1/1	0.95	0.12	11,11,11,11	1
3	MG	A	422	1/1	0.97	0.13	11,11,11,11	1
3	MG	C	422	1/1	0.97	0.13	11,11,11,11	1

6.5 Other polymers (i)

There are no such residues in this entry.