Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 07:45 PM EDT

PDB ID	:	4EZM
Title	:	Crystal structure of the human IgE-Fc(epsilon)3-4 bound to its B cell receptor derCD23
Authors	:	Dhaliwal, B.; Yuan, D.; Sutton, B.J.
Deposited on	:	2012-05-03
Resolution	:	3.10 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:

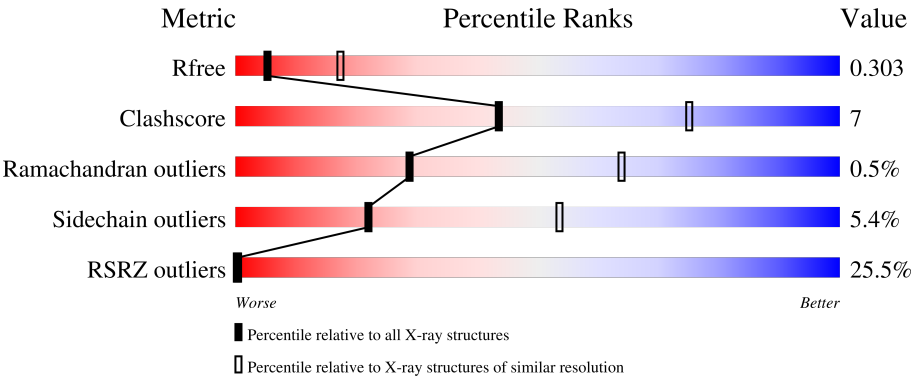
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	223	13% 82% 11% • 5%
1	B	223	17% 83% 10% 7%
1	C	223	19% 77% 9% • 12%
1	D	223	20% 83% 8% • 7%
1	E	223	33% 75% 9% • 14%

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Mol	Chain	Length	Quality of chain
1	F	223	36% 80% 11% 7%
2	G	143	16% 76% 14% 7%
2	H	143	19% 76% 15% 7%
2	I	143	44% 74% 18% 7%
2	J	143	12% 76% 17% 7%
2	K	143	29% 78% 15% 6%
2	L	143	27% 79% 12% 6%
3	M	5	60% 40%
3	N	5	80% 20%
3	O	5	40% 60%
3	P	5	80% 20%
3	Q	5	60% 40%
3	R	5	60% 40%

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
3	NAG	M	1	-	-	-	X
3	NAG	N	1	-	-	-	X
3	NAG	O	1	-	-	-	X
3	MAN	O	4	-	-	-	X
3	NAG	Q	1	-	-	-	X
4	MAN	C	606	-	-	-	X
4	MAN	C	607	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16496 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 Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1667	1044	307	310	6			
1	B	208	Total	C	N	O	S	0	0	0
			1650	1033	304	307	6			
1	C	197	Total	C	N	O	S	0	1	0
			1565	981	284	294	6			
1	D	207	Total	C	N	O	S	0	0	0
			1639	1027	302	304	6			
1	E	191	Total	C	N	O	S	0	0	0
			1509	945	276	283	5			
1	F	208	Total	C	N	O	S	0	0	0
			1645	1030	303	306	6			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ALA	-	expression tag	UNP P01854
A	326	ASP	-	expression tag	UNP P01854
A	327	PRO	-	expression tag	UNP P01854
A	371	GLN	ASN	engineered mutation	UNP P01854
A	383	GLN	ASN	engineered mutation	UNP P01854
B	325	ALA	-	expression tag	UNP P01854
B	326	ASP	-	expression tag	UNP P01854
B	327	PRO	-	expression tag	UNP P01854
B	371	GLN	ASN	engineered mutation	UNP P01854
B	383	GLN	ASN	engineered mutation	UNP P01854
C	325	ALA	-	expression tag	UNP P01854
C	326	ASP	-	expression tag	UNP P01854
C	327	PRO	-	expression tag	UNP P01854
C	371	GLN	ASN	engineered mutation	UNP P01854
C	383	GLN	ASN	engineered mutation	UNP P01854
D	325	ALA	-	expression tag	UNP P01854
D	326	ASP	-	expression tag	UNP P01854

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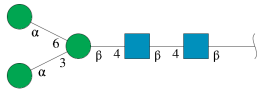
Chain	Residue	Modelled	Actual	Comment	Reference
D	327	PRO	-	expression tag	UNP P01854
D	371	GLN	ASN	engineered mutation	UNP P01854
D	383	GLN	ASN	engineered mutation	UNP P01854
E	325	ALA	-	expression tag	UNP P01854
E	326	ASP	-	expression tag	UNP P01854
E	327	PRO	-	expression tag	UNP P01854
E	371	GLN	ASN	engineered mutation	UNP P01854
E	383	GLN	ASN	engineered mutation	UNP P01854
F	325	ALA	-	expression tag	UNP P01854
F	326	ASP	-	expression tag	UNP P01854
F	327	PRO	-	expression tag	UNP P01854
F	371	GLN	ASN	engineered mutation	UNP P01854
F	383	GLN	ASN	engineered mutation	UNP P01854

- Molecule 2 is a protein called Low affinity immunoglobulin epsilon Fc receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	H	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	I	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	J	133	Total	C	N	O	S	0	0	0
			1070	673	191	195	11			
2	K	134	Total	C	N	O	S	0	0	0
			1074	675	192	196	11			
2	L	134	Total	C	N	O	S	0	0	0
			1078	677	192	198	11			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	M	5	Total	C	N	O	0	0	0
			61	34	2	25			

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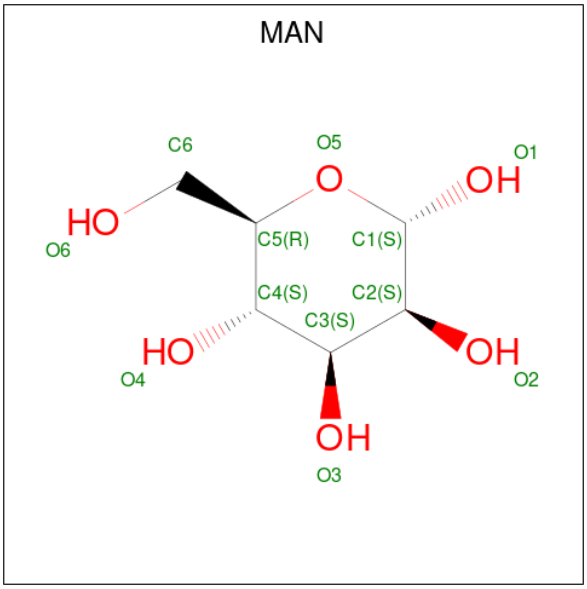
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	N	5	Total C N O 61 34 2 25	0	0	0
3	O	5	Total C N O 61 34 2 25	0	0	0
3	P	5	Total C N O 61 34 2 25	0	0	0
3	Q	5	Total C N O 61 34 2 25	0	0	0
3	R	5	Total C N O 61 34 2 25	0	0	0

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 11 6 5	0	0
4	C	1	Total C O 11 6 5	0	0

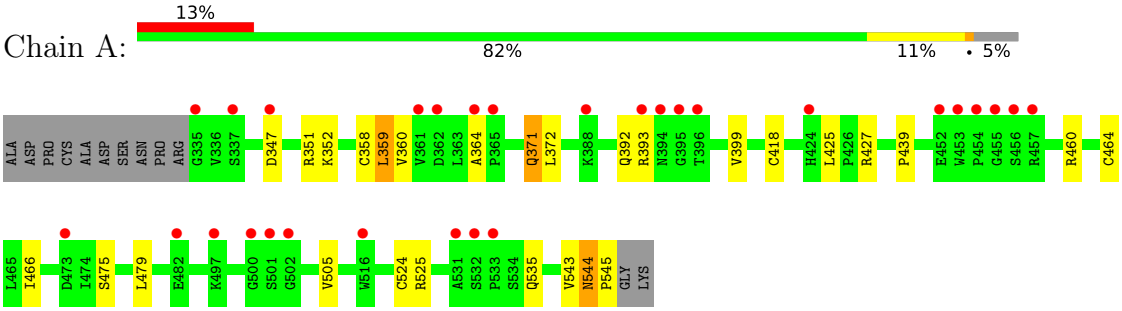
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total O 1 1	0	0

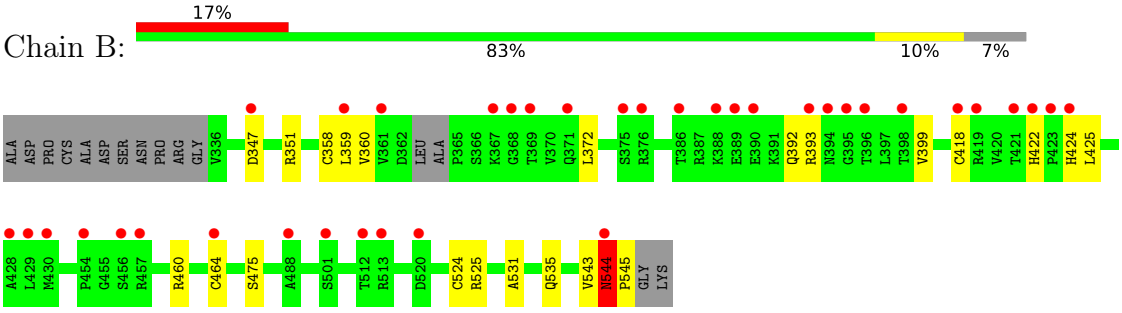
3 Residue-property plots

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.

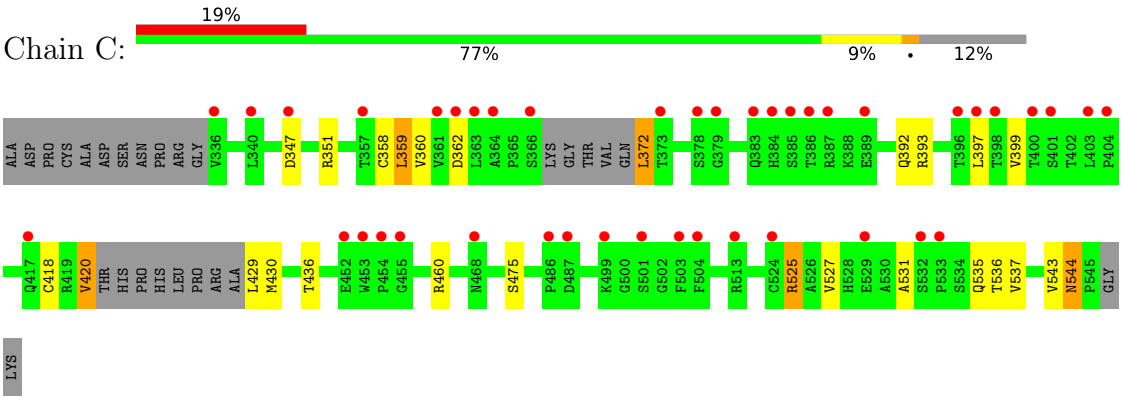
• Molecule 1: Ig epsilon chain C region



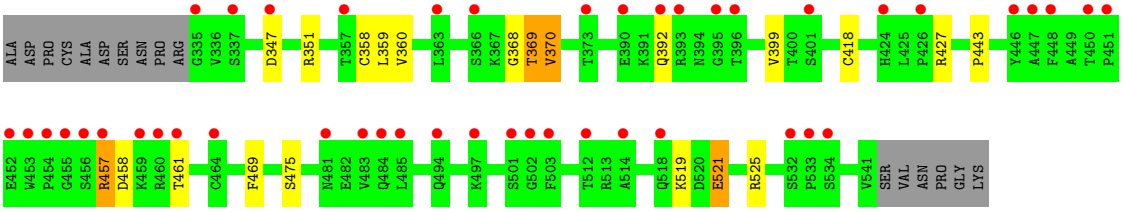
• Molecule 1: Ig epsilon chain C region



• Molecule 1: Ig epsilon chain C region

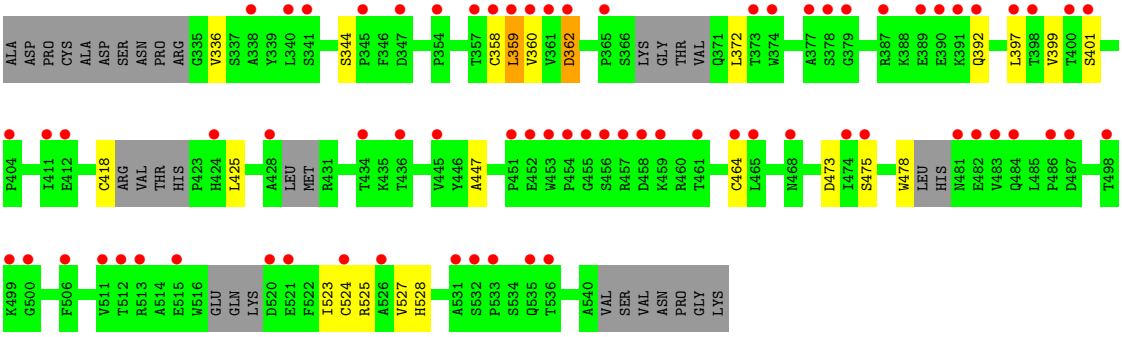


• Molecule 1: Ig epsilon chain C region



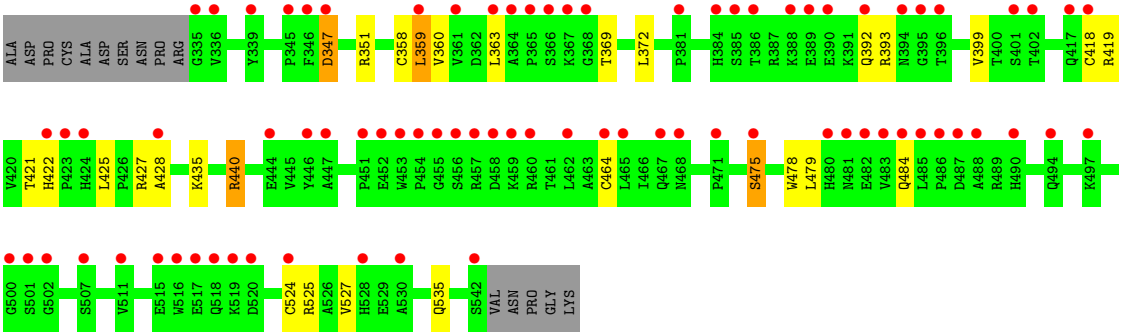
• Molecule 1: Ig epsilon chain C region

Chain E:



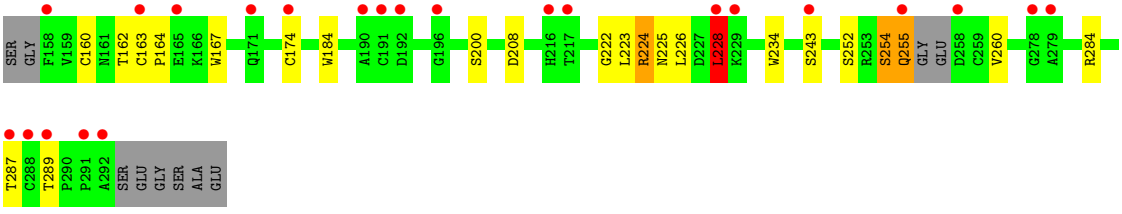
• Molecule 1: Ig epsilon chain C region

Chain F:



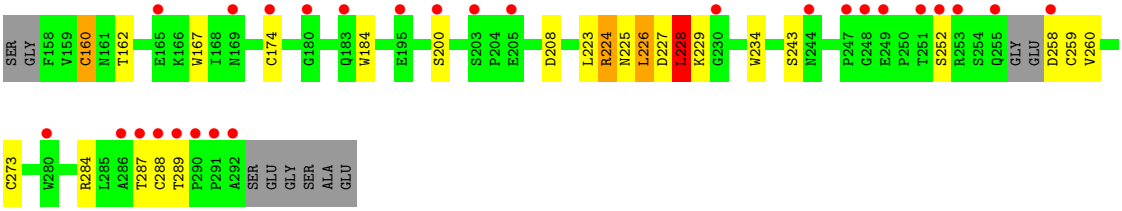
• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

Chain G:



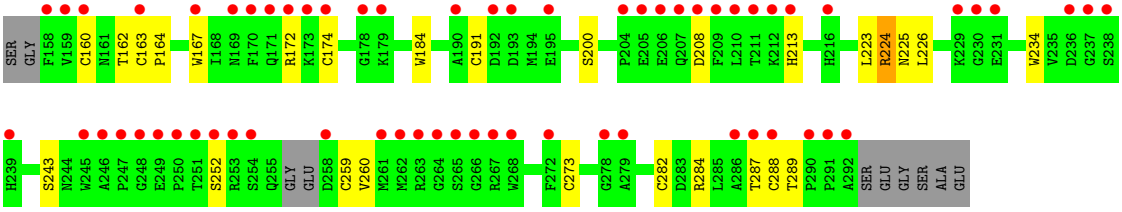
• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

Chain H:



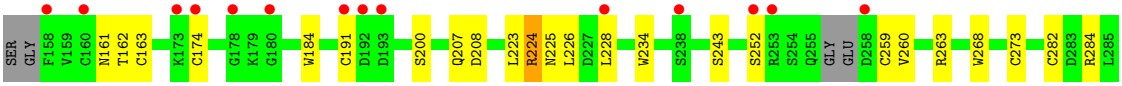
• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

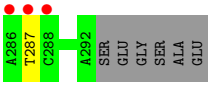
Chain I:



• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

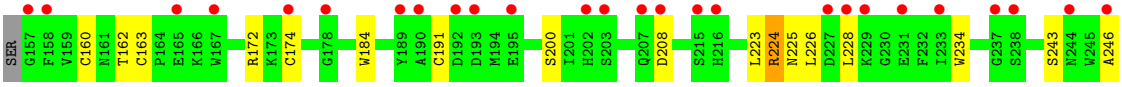
Chain J:

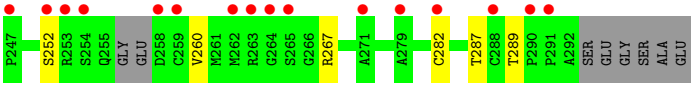




• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

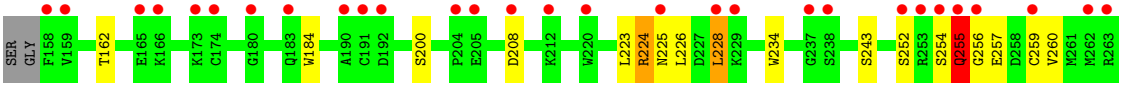
Chain K:

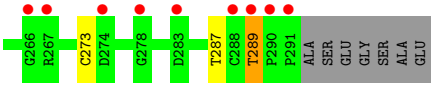




• Molecule 2: Low affinity immunoglobulin epsilon Fc receptor

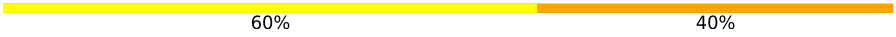
Chain L:





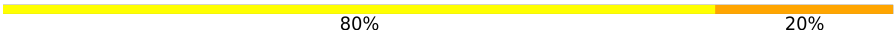
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

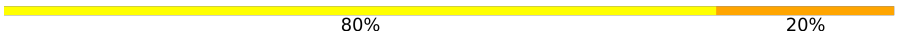


• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

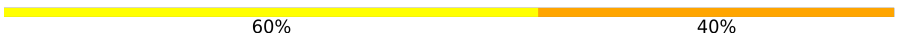
• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

NAG1
NAG2
BMA3
MAN4
MAN5

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.89Å 110.75Å 376.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 3.10 29.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.87-3.10) 98.7 (29.87-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 3.11Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.264 , 0.283 0.282 , 0.303	Depositor DCC
R_{free} test set	2437 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	98.7	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 72.4	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	0.80	EDS
Total number of atoms	16496	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.47	1/1710 (0.1%)	0.72	7/2328 (0.3%)
1	B	0.39	0/1692	0.65	1/2301 (0.0%)
1	C	0.37	0/1605	0.64	0/2182
1	D	0.40	0/1681	0.76	4/2287 (0.2%)
1	E	0.37	0/1544	0.61	0/2094
1	F	0.37	0/1687	0.62	0/2295
2	G	0.42	0/1103	0.69	1/1494 (0.1%)
2	H	0.43	0/1103	0.70	0/1494
2	I	0.40	0/1103	0.68	0/1494
2	J	0.41	0/1103	0.68	0/1494
2	K	0.39	0/1107	0.68	0/1499
2	L	0.39	0/1112	0.75	3/1507 (0.2%)
All	All	0.40	1/16550 (0.0%)	0.68	16/22469 (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
2	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	545	PRO	N-CD	10.62	1.62	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	369	THR	CB-CA-C	13.29	147.49	111.60
2	L	256	GLY	N-CA-C	10.56	139.50	113.10
1	D	369	THR	N-CA-C	-8.64	87.67	111.00
1	A	364	ALA	N-CA-C	-6.86	92.48	111.00
1	A	371	GLN	N-CA-C	6.16	127.64	111.00
1	B	544	ASN	N-CA-C	5.97	127.12	111.00
2	G	254	SER	N-CA-C	-5.96	94.91	111.00
1	A	544	ASN	N-CA-C	5.83	126.75	111.00
1	A	545	PRO	CA-N-CD	-5.61	103.65	111.50
2	L	289	THR	N-CA-CB	5.60	120.94	110.30
1	D	369	THR	C-N-CA	5.57	135.62	121.70
1	A	544	ASN	C-N-CD	-5.56	108.36	120.60
2	L	255	GLN	CB-CA-C	-5.38	99.63	110.40
1	A	545	PRO	N-CA-C	5.25	125.75	112.10
1	A	364	ALA	CB-CA-C	5.19	117.89	110.10
1	D	368	GLY	C-N-CA	5.18	134.64	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	255	GLN	Peptide

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	1667	0	1656	15	0
1	B	1650	0	1637	12	0
1	C	1565	0	1552	18	0
1	D	1639	0	1629	16	0
1	E	1509	0	1483	20	0
1	F	1645	0	1633	25	0
2	G	1070	0	994	20	0
2	H	1070	0	994	18	0
2	I	1070	0	994	17	0
2	J	1070	0	994	12	0
2	K	1074	0	996	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1078	0	999	14	0
3	M	61	0	52	5	0
3	N	61	0	52	4	0
3	O	61	0	52	9	0
3	P	61	0	52	4	0
3	Q	61	0	52	6	0
3	R	61	0	52	5	0
4	C	22	0	20	3	0
5	J	1	0	0	0	0
All	All	16496	0	15893	191	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 7.

All (191) 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:H:167:TRP:HB3	2:H:174:CYS:SG	1.43	1.57
1:E:478:TRP:CZ3	1:E:524:CYS:SG	2.15	1.37
2:I:163:CYS:SG	2:I:167:TRP:HB2	1.68	1.33
2:G:163:CYS:SG	2:G:167:TRP:HB2	1.72	1.27
2:H:167:TRP:CB	2:H:174:CYS:SG	2.25	1.22
1:E:478:TRP:CH2	1:E:524:CYS:SG	2.36	1.19
2:I:163:CYS:SG	2:I:167:TRP:CB	2.31	1.18
2:G:163:CYS:SG	2:G:167:TRP:CB	2.31	1.17
4:C:607:MAN:H2	3:O:5:MAN:O6	1.45	1.16
1:F:464:CYS:SG	1:F:478:TRP:CH2	2.53	1.00
2:H:259:CYS:HG	2:H:273:CYS:HG	1.07	0.97
1:E:478:TRP:CE3	1:E:524:CYS:SG	2.58	0.95
1:E:392:GLN:HG3	3:Q:1:NAG:O6	1.67	0.94
1:C:392:GLN:NE2	3:O:1:NAG:O6	2.02	0.93
1:F:358:CYS:HG	1:F:418:CYS:HG	1.10	0.93
1:A:358:CYS:HG	1:A:418:CYS:HG	1.06	0.91
1:D:358:CYS:HG	1:D:418:CYS:HG	1.14	0.91
2:G:163:CYS:SG	2:G:167:TRP:HB3	2.09	0.90
2:I:191:CYS:HG	2:I:282:CYS:HG	1.21	0.89
1:D:369:THR:O	1:D:370:VAL:HG23	1.72	0.88
1:A:464:CYS:HG	1:A:524:CYS:HG	1.11	0.86
1:C:392:GLN:HG3	3:O:1:NAG:O6	1.75	0.86
1:E:392:GLN:NE2	3:Q:1:NAG:O6	2.08	0.86
1:F:392:GLN:NE2	3:R:1:NAG:O6	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:GLN:CG	3:Q:1:NAG:O6	2.25	0.84
1:F:440:ARG:NH1	2:L:255:GLN:O	2.10	0.84
2:L:254:SER:O	2:L:255:GLN:HB2	1.79	0.83
2:I:259:CYS:HG	2:I:273:CYS:HG	1.06	0.83
1:E:358:CYS:HG	1:E:418:CYS:HG	1.22	0.82
2:I:163:CYS:SG	2:I:167:TRP:HB3	2.16	0.82
1:C:544:ASN:ND2	1:C:544:ASN:O	2.13	0.82
1:B:358:CYS:HG	1:B:418:CYS:HG	1.22	0.81
1:D:392:GLN:NE2	3:P:1:NAG:O6	2.13	0.81
1:C:392:GLN:CG	3:O:1:NAG:O6	2.30	0.79
1:A:392:GLN:HG3	3:M:1:NAG:O6	1.81	0.79
1:B:392:GLN:NE2	3:N:1:NAG:O6	2.14	0.79
4:C:607:MAN:C2	3:O:5:MAN:O6	2.30	0.78
2:J:259:CYS:HG	2:J:273:CYS:HG	1.28	0.78
1:F:392:GLN:HG3	3:R:1:NAG:O6	1.82	0.78
2:K:191:CYS:HG	2:K:282:CYS:HG	1.28	0.78
1:C:544:ASN:O	1:C:544:ASN:CG	2.23	0.75
1:A:392:GLN:CG	3:M:1:NAG:O6	2.36	0.73
4:C:607:MAN:H2	3:O:5:MAN:HO6	1.52	0.73
2:H:160:CYS:HG	2:H:288:CYS:HG	1.28	0.73
1:D:521:GLU:HG3	1:F:421:THR:HG21	1.72	0.71
2:J:191:CYS:HG	2:J:282:CYS:HG	1.27	0.71
1:B:392:GLN:HG3	3:N:1:NAG:O6	1.92	0.70
1:E:464:CYS:SG	1:E:478:TRP:CH2	2.84	0.70
1:F:392:GLN:CG	3:R:1:NAG:O6	2.38	0.70
2:G:163:CYS:SG	2:G:164:PRO:HD2	2.31	0.70
1:D:392:GLN:HG3	3:P:1:NAG:O6	1.94	0.67
2:L:259:CYS:HG	2:L:273:CYS:HG	1.40	0.66
2:H:167:TRP:CG	2:H:174:CYS:SG	2.89	0.65
1:C:392:GLN:HE21	3:O:1:NAG:C6	2.10	0.65
1:C:543:VAL:O	1:C:544:ASN:OD1	2.16	0.64
1:B:392:GLN:CG	3:N:1:NAG:O6	2.46	0.64
1:E:478:TRP:CZ2	1:E:524:CYS:SG	2.92	0.63
2:H:167:TRP:CE3	2:H:174:CYS:SG	2.90	0.63
1:D:392:GLN:CG	3:P:1:NAG:O6	2.48	0.62
2:I:160:CYS:HG	2:I:288:CYS:HG	1.22	0.62
2:H:167:TRP:HB3	2:H:174:CYS:HG	1.55	0.62
2:L:254:SER:O	2:L:255:GLN:CB	2.48	0.62
1:D:392:GLN:HE21	3:P:1:NAG:C6	2.15	0.60
1:F:392:GLN:HE21	3:R:1:NAG:C6	2.14	0.60
2:G:252:SER:HB2	2:G:255:GLN:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:GLN:HE21	3:Q:1:NAG:C6	2.15	0.59
1:F:440:ARG:NH1	2:L:257:GLU:H	2.01	0.59
2:G:163:CYS:SG	2:G:164:PRO:CD	2.93	0.57
1:C:531:ALA:O	1:C:535:GLN:HA	2.05	0.57
1:E:475:SER:HB2	1:E:527:VAL:HB	1.86	0.56
2:J:162:THR:HB	2:J:287:THR:HG23	1.88	0.56
1:B:392:GLN:HE21	3:N:1:NAG:C6	2.16	0.56
1:E:359:LEU:HD11	3:Q:2:NAG:O7	2.05	0.55
2:K:246:ALA:HA	2:K:267:ARG:HE	1.71	0.55
1:F:464:CYS:SG	1:F:478:TRP:HH2	2.18	0.55
2:I:162:THR:HB	2:I:287:THR:HG23	1.88	0.55
2:K:226:LEU:O	2:K:226:LEU:HG	2.07	0.55
1:A:360:VAL:HG13	1:A:399:VAL:HG13	1.89	0.55
1:B:464:CYS:HG	1:B:524:CYS:HG	0.59	0.55
2:H:162:THR:HB	2:H:287:THR:HG23	1.89	0.55
2:G:162:THR:HB	2:G:287:THR:HG23	1.88	0.54
2:J:174:CYS:HB2	2:J:284:ARG:HG2	1.90	0.54
1:F:464:CYS:SG	1:F:478:TRP:CZ2	2.92	0.54
1:B:360:VAL:HG13	1:B:399:VAL:HG13	1.90	0.54
2:I:163:CYS:SG	2:I:164:PRO:HD2	2.48	0.54
2:L:162:THR:HB	2:L:287:THR:HG23	1.90	0.54
1:E:336:VAL:HG12	1:E:362:ASP:HA	1.90	0.53
2:G:184:TRP:CH2	2:G:224:ARG:HG2	2.44	0.53
2:J:226:LEU:HG	2:J:226:LEU:O	2.08	0.53
2:L:226:LEU:HG	2:L:226:LEU:O	2.09	0.53
2:G:174:CYS:HB2	2:G:284:ARG:HG2	1.91	0.53
2:K:162:THR:HB	2:K:287:THR:HG23	1.89	0.53
1:C:360:VAL:HG13	1:C:399:VAL:HG13	1.91	0.52
1:D:360:VAL:HG13	1:D:399:VAL:HG13	1.91	0.52
1:F:360:VAL:HG13	1:F:399:VAL:HG13	1.91	0.52
1:E:360:VAL:HG13	1:E:399:VAL:HG13	1.91	0.52
2:J:184:TRP:CZ2	2:J:224:ARG:HG2	2.45	0.52
2:I:226:LEU:O	2:I:226:LEU:HG	2.09	0.52
1:F:347:ASP:HA	1:F:351:ARG:HB2	1.90	0.52
2:G:184:TRP:CZ2	2:G:224:ARG:HG2	2.45	0.51
1:D:443:PRO:HB3	1:D:469:PHE:HB3	1.91	0.51
1:C:359:LEU:HD11	3:O:2:NAG:O7	2.10	0.51
2:K:184:TRP:CH2	2:K:224:ARG:HG2	2.45	0.51
2:L:184:TRP:CH2	2:L:224:ARG:HG2	2.46	0.51
2:G:226:LEU:HG	2:G:226:LEU:O	2.09	0.51
2:H:226:LEU:HG	2:H:226:LEU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ARG:HG3	1:A:543:VAL:HG13	1.92	0.51
1:A:535:GLN:OE1	2:G:228:LEU:HG	2.10	0.51
1:C:475:SER:HB2	1:C:527:VAL:HB	1.92	0.51
2:K:184:TRP:CZ2	2:K:224:ARG:HG2	2.46	0.51
1:F:358:CYS:CB	1:F:418:CYS:HG	2.23	0.50
1:C:460:ARG:HG3	1:C:543:VAL:HG13	1.92	0.50
1:F:359:LEU:HD11	3:R:2:NAG:O7	2.11	0.50
2:H:223:LEU:HB3	2:H:260:VAL:HB	1.93	0.50
2:I:184:TRP:CZ2	2:I:224:ARG:HG2	2.47	0.50
1:D:358:CYS:CB	1:D:418:CYS:HG	2.25	0.50
1:F:479:LEU:HG	1:F:484:GLN:HA	1.93	0.50
2:G:163:CYS:HG	2:G:174:CYS:HB3	1.76	0.50
2:J:184:TRP:CH2	2:J:224:ARG:HG2	2.47	0.49
1:D:347:ASP:HA	1:D:351:ARG:HB2	1.94	0.49
1:B:460:ARG:HG3	1:B:543:VAL:HG13	1.94	0.49
2:L:184:TRP:CZ2	2:L:224:ARG:HG2	2.47	0.49
1:F:440:ARG:HH12	2:L:257:GLU:H	1.59	0.49
1:D:519:LYS:HD3	1:F:419:ARG:HH22	1.78	0.49
2:K:160:CYS:HB2	2:K:172:ARG:HG2	1.94	0.49
1:D:519:LYS:HA	1:F:419:ARG:HH22	1.77	0.48
1:B:347:ASP:HA	1:B:351:ARG:HB2	1.95	0.48
1:C:358:CYS:CB	1:C:418:CYS:HG	2.26	0.48
2:G:252:SER:C	2:G:254:SER:H	2.17	0.48
1:D:369:THR:O	1:D:370:VAL:CG2	2.54	0.48
1:F:478:TRP:CE2	1:F:524:CYS:SG	2.99	0.48
2:K:163:CYS:CB	2:K:174:CYS:HG	2.16	0.48
2:I:160:CYS:HB2	2:I:172:ARG:HG2	1.96	0.48
1:A:392:GLN:CD	3:M:1:NAG:HO6	2.14	0.48
2:I:184:TRP:CH2	2:I:224:ARG:HG2	2.48	0.48
2:K:163:CYS:HA	2:K:174:CYS:SG	2.54	0.48
1:C:392:GLN:CD	3:O:1:NAG:O6	2.52	0.47
2:H:167:TRP:HE3	2:H:174:CYS:SG	2.36	0.47
1:A:439:PRO:HA	2:G:254:SER:HA	1.96	0.47
1:D:519:LYS:HE3	1:F:428:ALA:H	1.79	0.47
1:E:447:ALA:CB	1:E:464:CYS:SG	3.02	0.47
1:F:535:GLN:OE1	2:L:228:LEU:HG	2.14	0.47
2:L:200:SER:HA	2:L:234:TRP:CE3	2.50	0.47
2:I:174:CYS:HB2	2:I:284:ARG:HG2	1.96	0.47
2:K:200:SER:HA	2:K:234:TRP:CE3	2.50	0.47
2:G:200:SER:HA	2:G:234:TRP:CE3	2.49	0.47
2:I:163:CYS:SG	2:I:174:CYS:SG	3.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:174:CYS:HB3	2:H:284:ARG:HG2	1.97	0.47
1:F:435:LYS:HE3	2:L:257:GLU:HG3	1.97	0.46
2:H:184:TRP:CH2	2:H:224:ARG:HG2	2.50	0.46
2:I:200:SER:HA	2:I:234:TRP:CE3	2.50	0.46
2:H:227:ASP:C	2:H:229:LYS:H	2.18	0.46
2:J:200:SER:HA	2:J:234:TRP:CE3	2.50	0.46
1:E:392:GLN:CD	3:Q:1:NAG:O6	2.54	0.46
2:H:226:LEU:H	2:H:229:LYS:HG3	1.81	0.46
2:G:163:CYS:SG	2:G:174:CYS:SG	3.14	0.45
2:J:207:GLN:OE1	2:J:268:TRP:NE1	2.48	0.45
2:H:167:TRP:HB2	2:H:174:CYS:SG	2.44	0.45
1:E:447:ALA:HB2	1:E:464:CYS:SG	2.56	0.45
1:D:457:ARG:HA	1:D:457:ARG:NE	2.32	0.44
1:A:358:CYS:CB	1:A:418:CYS:HG	2.31	0.44
1:B:544:ASN:HA	1:B:545:PRO:HD2	1.74	0.44
1:C:347:ASP:HA	1:C:351:ARG:HB2	1.99	0.44
1:A:392:GLN:OE1	3:M:1:NAG:O6	2.23	0.44
1:E:362:ASP:HB3	1:E:397:LEU:O	2.18	0.44
2:J:163:CYS:CB	2:J:174:CYS:SG	3.06	0.44
2:K:163:CYS:CB	2:K:174:CYS:SG	3.04	0.44
2:I:163:CYS:SG	2:I:164:PRO:CD	3.06	0.43
1:C:525:ARG:HD2	1:C:536:THR:HG21	2.01	0.43
1:B:422:HIS:HB3	1:B:425:LEU:HB3	2.01	0.42
2:G:222:GLY:O	2:G:234:TRP:HA	2.19	0.42
1:F:422:HIS:HB3	1:F:425:LEU:HD13	2.00	0.42
2:J:163:CYS:HG	2:J:174:CYS:HG	0.42	0.42
1:A:347:ASP:HA	1:A:351:ARG:HB2	2.01	0.42
2:L:223:LEU:HB3	2:L:260:VAL:HB	2.02	0.42
1:A:460:ARG:HG3	1:A:543:VAL:CG1	2.50	0.42
1:A:359:LEU:HD11	3:M:2:NAG:O7	2.20	0.41
1:B:531:ALA:O	1:B:535:GLN:HA	2.19	0.41
1:C:531:ALA:HB1	1:C:537:VAL:HG23	2.01	0.41
2:G:254:SER:O	2:G:255:GLN:OE1	2.39	0.41
2:G:223:LEU:HB3	2:G:260:VAL:HB	2.02	0.41
1:E:478:TRP:CD2	1:E:524:CYS:SG	3.09	0.41
2:K:223:LEU:HB3	2:K:260:VAL:HB	2.03	0.41
2:I:223:LEU:HB3	2:I:260:VAL:HB	2.02	0.41
2:H:226:LEU:O	2:H:228:LEU:N	2.54	0.41
1:C:372:LEU:HA	1:C:420:VAL:HG13	2.04	0.40
1:E:473:ASP:O	1:E:528:HIS:HD2	2.03	0.40
2:J:223:LEU:HB3	2:J:260:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:475:SER:HB2	1:F:527:VAL:HB	2.03	0.40
2:H:200:SER:HA	2:H:234:TRP:CE3	2.57	0.40
1:A:466:ILE:HD13	1:A:505:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	209/223 (94%)	198 (95%)	10 (5%)	1 (0%)	29	64
1	B	204/223 (92%)	190 (93%)	13 (6%)	1 (0%)	29	64
1	C	192/223 (86%)	183 (95%)	8 (4%)	1 (0%)	29	64
1	D	205/223 (92%)	193 (94%)	11 (5%)	1 (0%)	29	64
1	E	179/223 (80%)	171 (96%)	8 (4%)	0	100	100
1	F	206/223 (92%)	200 (97%)	5 (2%)	1 (0%)	29	64
2	G	129/143 (90%)	113 (88%)	15 (12%)	1 (1%)	19	54
2	H	129/143 (90%)	118 (92%)	9 (7%)	2 (2%)	9	37
2	I	129/143 (90%)	113 (88%)	16 (12%)	0	100	100
2	J	129/143 (90%)	116 (90%)	12 (9%)	1 (1%)	19	54
2	K	130/143 (91%)	118 (91%)	12 (9%)	0	100	100
2	L	132/143 (92%)	118 (89%)	14 (11%)	0	100	100
All	All	1973/2196 (90%)	1831 (93%)	133 (7%)	9 (0%)	29	64

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	370	VAL

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Mol	Chain	Res	Type
2	H	228	LEU
1	A	393	ARG
1	B	393	ARG
1	F	393	ARG
1	C	393	ARG
2	G	228	LEU
2	H	226	LEU
2	J	161	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	186/195 (95%)	176 (95%)	10 (5%)	22	53
1	B	185/195 (95%)	179 (97%)	6 (3%)	39	69
1	C	176/195 (90%)	166 (94%)	10 (6%)	20	52
1	D	182/195 (93%)	174 (96%)	8 (4%)	28	61
1	E	167/195 (86%)	159 (95%)	8 (5%)	25	58
1	F	183/195 (94%)	174 (95%)	9 (5%)	25	57
2	G	114/120 (95%)	106 (93%)	8 (7%)	15	45
2	H	114/120 (95%)	105 (92%)	9 (8%)	12	40
2	I	114/120 (95%)	107 (94%)	7 (6%)	18	49
2	J	114/120 (95%)	107 (94%)	7 (6%)	18	49
2	K	114/120 (95%)	107 (94%)	7 (6%)	18	49
2	L	115/120 (96%)	108 (94%)	7 (6%)	18	49
All	All	1764/1890 (93%)	1668 (95%)	96 (5%)	22	53

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

Mol	Chain	Res	Type
1	A	352	LYS
1	A	359	LEU

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Mol	Chain	Res	Type
1	A	371	GLN
1	A	372	LEU
1	A	425	LEU
1	A	427	ARG
1	A	475	SER
1	A	479	LEU
1	A	525	ARG
1	A	544	ASN
1	B	359	LEU
1	B	372	LEU
1	B	424	HIS
1	B	475	SER
1	B	525	ARG
1	B	544	ASN
1	C	359	LEU
1	C	362	ASP
1	C	372	LEU
1	C	397	LEU
1	C	420	VAL
1	C	429	LEU
1	C	430	MET
1	C	436	THR
1	C	525	ARG
1	C	544	ASN
1	D	359	LEU
1	D	427	ARG
1	D	457	ARG
1	D	458	ASP
1	D	461	THR
1	D	475	SER
1	D	521	GLU
1	D	525	ARG
1	E	344	SER
1	E	359	LEU
1	E	362	ASP
1	E	372	LEU
1	E	401	SER
1	E	425	LEU
1	E	523	ILE
1	E	525	ARG
1	F	347	ASP
1	F	359	LEU

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Mol	Chain	Res	Type
1	F	363	LEU
1	F	369	THR
1	F	372	LEU
1	F	427	ARG
1	F	440	ARG
1	F	475	SER
1	F	525	ARG
2	G	160	CYS
2	G	208	ASP
2	G	224	ARG
2	G	225	ASN
2	G	228	LEU
2	G	243	SER
2	G	255	GLN
2	G	289	THR
2	H	160	CYS
2	H	208	ASP
2	H	224	ARG
2	H	225	ASN
2	H	228	LEU
2	H	243	SER
2	H	252	SER
2	H	258	ASP
2	H	289	THR
2	I	208	ASP
2	I	213	HIS
2	I	224	ARG
2	I	225	ASN
2	I	243	SER
2	I	252	SER
2	I	289	THR
2	J	208	ASP
2	J	224	ARG
2	J	225	ASN
2	J	228	LEU
2	J	243	SER
2	J	252	SER
2	J	263	ARG
2	K	208	ASP
2	K	224	ARG
2	K	225	ASN
2	K	228	LEU

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Mol	Chain	Res	Type
2	K	243	SER
2	K	252	SER
2	K	289	THR
2	L	208	ASP
2	L	224	ARG
2	L	225	ASN
2	L	228	LEU
2	L	243	SER
2	L	252	SER
2	L	289	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	392	GLN
1	B	481	ASN
1	C	392	GLN
1	C	544	ASN
1	D	392	GLN
1	E	392	GLN
1	F	392	GLN
2	G	213	HIS
2	G	225	ASN
2	G	255	GLN
2	G	269	ASN
2	H	213	HIS
2	H	269	ASN
2	I	225	ASN
2	I	269	ASN
2	J	213	HIS
2	J	225	ASN
2	J	269	ASN
2	K	213	HIS
2	K	225	ASN
2	K	269	ASN
2	L	213	HIS
2	L	225	ASN
2	L	269	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

30 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	M	1	3	14,14,15	0.52	0	17,19,21	1.47	2 (11%)
3	NAG	M	2	3	14,14,15	0.58	0	17,19,21	1.38	2 (11%)
3	BMA	M	3	3	11,11,12	0.71	0	15,15,17	2.17	3 (20%)
3	MAN	M	4	3	11,11,12	0.59	0	15,15,17	1.60	4 (26%)
3	MAN	M	5	3	11,11,12	0.65	0	15,15,17	1.56	3 (20%)
3	NAG	N	1	3	14,14,15	0.51	0	17,19,21	1.46	2 (11%)
3	NAG	N	2	3	14,14,15	0.57	0	17,19,21	1.37	1 (5%)
3	BMA	N	3	3	11,11,12	0.71	0	15,15,17	2.17	3 (20%)
3	MAN	N	4	3	11,11,12	0.61	0	15,15,17	1.60	4 (26%)
3	MAN	N	5	3	11,11,12	0.64	0	15,15,17	1.55	3 (20%)
3	NAG	O	1	3	14,14,15	0.52	0	17,19,21	1.47	2 (11%)
3	NAG	O	2	3	14,14,15	0.56	0	17,19,21	1.37	2 (11%)
3	BMA	O	3	3	11,11,12	0.71	0	15,15,17	2.17	3 (20%)
3	MAN	O	4	3	11,11,12	0.61	0	15,15,17	1.59	4 (26%)
3	MAN	O	5	3	11,11,12	0.64	0	15,15,17	1.55	3 (20%)
3	NAG	P	1	3	14,14,15	0.53	0	17,19,21	1.46	2 (11%)
3	NAG	P	2	3	14,14,15	0.57	0	17,19,21	1.37	1 (5%)
3	BMA	P	3	3	11,11,12	0.71	0	15,15,17	2.17	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MAN	P	4	3	11,11,12	0.61	0	15,15,17	1.59	4 (26%)
3	MAN	P	5	3	11,11,12	0.65	0	15,15,17	1.55	3 (20%)
3	NAG	Q	1	3	14,14,15	0.53	0	17,19,21	1.46	2 (11%)
3	NAG	Q	2	3	14,14,15	0.57	0	17,19,21	1.37	2 (11%)
3	BMA	Q	3	3	11,11,12	0.71	0	15,15,17	2.18	3 (20%)
3	MAN	Q	4	3	11,11,12	0.61	0	15,15,17	1.59	4 (26%)
3	MAN	Q	5	3	11,11,12	0.64	0	15,15,17	1.55	3 (20%)
3	NAG	R	1	3	14,14,15	0.52	0	17,19,21	1.46	2 (11%)
3	NAG	R	2	3	14,14,15	0.57	0	17,19,21	1.37	1 (5%)
3	BMA	R	3	3	11,11,12	0.71	0	15,15,17	2.17	3 (20%)
3	MAN	R	4	3	11,11,12	0.61	0	15,15,17	1.59	4 (26%)
3	MAN	R	5	3	11,11,12	0.64	0	15,15,17	1.57	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	M	1	3	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	BMA	M	3	3	-	2/2/19/22	0/1/1/1
3	MAN	M	4	3	-	1/2/19/22	0/1/1/1
3	MAN	M	5	3	-	2/2/19/22	0/1/1/1
3	NAG	N	1	3	-	1/6/23/26	0/1/1/1
3	NAG	N	2	3	-	1/6/23/26	0/1/1/1
3	BMA	N	3	3	-	2/2/19/22	0/1/1/1
3	MAN	N	4	3	-	1/2/19/22	0/1/1/1
3	MAN	N	5	3	-	2/2/19/22	0/1/1/1
3	NAG	O	1	3	-	1/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	BMA	O	3	3	-	2/2/19/22	0/1/1/1
3	MAN	O	4	3	-	1/2/19/22	0/1/1/1
3	MAN	O	5	3	-	2/2/19/22	0/1/1/1
3	NAG	P	1	3	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	1/6/23/26	0/1/1/1
3	BMA	P	3	3	-	2/2/19/22	0/1/1/1
3	MAN	P	4	3	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MAN	P	5	3	-	2/2/19/22	0/1/1/1
3	NAG	Q	1	3	-	1/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	2/2/19/22	0/1/1/1
3	MAN	Q	4	3	-	1/2/19/22	0/1/1/1
3	MAN	Q	5	3	-	2/2/19/22	0/1/1/1
3	NAG	R	1	3	-	1/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1
3	BMA	R	3	3	-	2/2/19/22	0/1/1/1
3	MAN	R	4	3	-	1/2/19/22	0/1/1/1
3	MAN	R	5	3	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	3	BMA	O5-C5-C6	6.47	117.35	107.20
3	P	3	BMA	O5-C5-C6	6.46	117.33	107.20
3	N	3	BMA	O5-C5-C6	6.45	117.32	107.20
3	M	3	BMA	O5-C5-C6	6.44	117.29	107.20
3	R	3	BMA	O5-C5-C6	6.43	117.29	107.20
3	O	3	BMA	O5-C5-C6	6.42	117.27	107.20
3	Q	1	NAG	O5-C5-C6	3.81	113.18	107.20
3	O	1	NAG	O5-C5-C6	3.81	113.17	107.20
3	M	1	NAG	O5-C5-C6	3.80	113.16	107.20
3	P	1	NAG	O5-C5-C6	3.79	113.14	107.20
3	R	1	NAG	O5-C5-C6	3.79	113.14	107.20
3	N	1	NAG	O5-C5-C6	3.78	113.14	107.20
3	M	4	MAN	O5-C1-C2	-3.31	105.67	110.77
3	M	5	MAN	O5-C1-C2	-3.29	105.70	110.77
3	R	4	MAN	O5-C1-C2	-3.28	105.70	110.77
3	R	5	MAN	O5-C1-C2	-3.28	105.70	110.77
3	P	4	MAN	O5-C1-C2	-3.27	105.72	110.77
3	N	4	MAN	O5-C1-C2	-3.27	105.72	110.77
3	O	5	MAN	O5-C1-C2	-3.26	105.74	110.77
3	P	5	MAN	O5-C1-C2	-3.26	105.74	110.77
3	Q	4	MAN	O5-C1-C2	-3.26	105.74	110.77
3	Q	5	MAN	O5-C1-C2	-3.25	105.75	110.77
3	N	5	MAN	O5-C1-C2	-3.24	105.77	110.77
3	O	4	MAN	O5-C1-C2	-3.23	105.78	110.77
3	Q	3	BMA	O3-C3-C4	-3.09	103.20	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	3	BMA	O3-C3-C4	-3.09	103.21	110.35
3	N	3	BMA	O3-C3-C4	-3.09	103.21	110.35
3	P	3	BMA	O3-C3-C4	-3.08	103.22	110.35
3	O	3	BMA	O3-C3-C4	-3.07	103.25	110.35
3	R	3	BMA	O3-C3-C4	-3.07	103.25	110.35
3	R	5	MAN	C3-C4-C5	3.06	115.69	110.24
3	N	5	MAN	C3-C4-C5	3.03	115.65	110.24
3	M	5	MAN	C3-C4-C5	3.02	115.64	110.24
3	O	5	MAN	C3-C4-C5	3.02	115.62	110.24
3	Q	5	MAN	C3-C4-C5	3.00	115.59	110.24
3	P	5	MAN	C3-C4-C5	3.00	115.58	110.24
3	O	3	BMA	C6-C5-C4	-3.00	105.99	113.00
3	R	3	BMA	C6-C5-C4	-2.99	105.99	113.00
3	N	3	BMA	C6-C5-C4	-2.99	106.01	113.00
3	Q	3	BMA	C6-C5-C4	-2.98	106.03	113.00
3	P	3	BMA	C6-C5-C4	-2.98	106.03	113.00
3	M	3	BMA	C6-C5-C4	-2.97	106.04	113.00
3	M	2	NAG	C1-O5-C5	2.86	116.07	112.19
3	N	2	NAG	C1-O5-C5	2.83	116.02	112.19
3	R	2	NAG	C1-O5-C5	2.82	116.01	112.19
3	O	2	NAG	C1-O5-C5	2.81	116.00	112.19
3	P	2	NAG	C1-O5-C5	2.81	116.00	112.19
3	Q	2	NAG	C1-O5-C5	2.80	115.99	112.19
3	N	4	MAN	C3-C4-C5	-2.77	105.30	110.24
3	M	4	MAN	C3-C4-C5	-2.76	105.31	110.24
3	P	4	MAN	C3-C4-C5	-2.75	105.33	110.24
3	R	4	MAN	C3-C4-C5	-2.74	105.34	110.24
3	O	4	MAN	C3-C4-C5	-2.74	105.35	110.24
3	Q	4	MAN	C3-C4-C5	-2.74	105.36	110.24
3	N	5	MAN	O4-C4-C3	-2.54	104.48	110.35
3	P	5	MAN	O4-C4-C3	-2.54	104.49	110.35
3	O	5	MAN	O4-C4-C3	-2.53	104.50	110.35
3	M	5	MAN	O4-C4-C3	-2.52	104.51	110.35
3	Q	5	MAN	O4-C4-C3	-2.52	104.52	110.35
3	R	5	MAN	O4-C4-C3	-2.52	104.52	110.35
3	O	1	NAG	O5-C1-C2	-2.37	107.54	111.29
3	Q	1	NAG	O5-C1-C2	-2.37	107.54	111.29
3	N	1	NAG	O5-C1-C2	-2.37	107.55	111.29
3	P	1	NAG	O5-C1-C2	-2.37	107.55	111.29
3	M	1	NAG	O5-C1-C2	-2.36	107.56	111.29
3	O	4	MAN	C2-C3-C4	-2.36	106.81	110.89
3	R	1	NAG	O5-C1-C2	-2.35	107.58	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	4	MAN	C2-C3-C4	-2.35	106.83	110.89
3	N	4	MAN	C2-C3-C4	-2.34	106.85	110.89
3	P	4	MAN	C2-C3-C4	-2.34	106.85	110.89
3	Q	4	MAN	C2-C3-C4	-2.34	106.85	110.89
3	R	4	MAN	C2-C3-C4	-2.32	106.88	110.89
3	N	4	MAN	C1-C2-C3	-2.07	107.12	109.67
3	O	4	MAN	C1-C2-C3	-2.06	107.14	109.67
3	R	4	MAN	C1-C2-C3	-2.06	107.14	109.67
3	Q	4	MAN	C1-C2-C3	-2.05	107.14	109.67
3	P	4	MAN	C1-C2-C3	-2.05	107.15	109.67
3	M	4	MAN	C1-C2-C3	-2.04	107.15	109.67
3	M	2	NAG	O5-C5-C6	2.02	110.38	107.20
3	O	2	NAG	O5-C5-C6	2.00	110.35	107.20
3	Q	2	NAG	O7-C7-C8	-2.00	118.34	122.06

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	M	5	MAN	O5-C5-C6-O6
3	N	5	MAN	O5-C5-C6-O6
3	O	5	MAN	O5-C5-C6-O6
3	P	5	MAN	O5-C5-C6-O6
3	Q	5	MAN	O5-C5-C6-O6
3	R	5	MAN	O5-C5-C6-O6
3	M	5	MAN	C4-C5-C6-O6
3	N	5	MAN	C4-C5-C6-O6
3	O	5	MAN	C4-C5-C6-O6
3	P	5	MAN	C4-C5-C6-O6
3	Q	5	MAN	C4-C5-C6-O6
3	R	5	MAN	C4-C5-C6-O6
3	M	3	BMA	O5-C5-C6-O6
3	N	3	BMA	O5-C5-C6-O6
3	O	3	BMA	O5-C5-C6-O6
3	P	3	BMA	O5-C5-C6-O6
3	Q	3	BMA	O5-C5-C6-O6
3	R	3	BMA	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	N	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	R	1	NAG	O5-C5-C6-O6
3	M	3	BMA	C4-C5-C6-O6
3	N	3	BMA	C4-C5-C6-O6
3	O	3	BMA	C4-C5-C6-O6
3	P	3	BMA	C4-C5-C6-O6
3	Q	3	BMA	C4-C5-C6-O6
3	R	3	BMA	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	N	4	MAN	C4-C5-C6-O6
3	O	4	MAN	C4-C5-C6-O6
3	P	4	MAN	C4-C5-C6-O6
3	R	4	MAN	C4-C5-C6-O6
3	M	4	MAN	C4-C5-C6-O6
3	Q	4	MAN	C4-C5-C6-O6

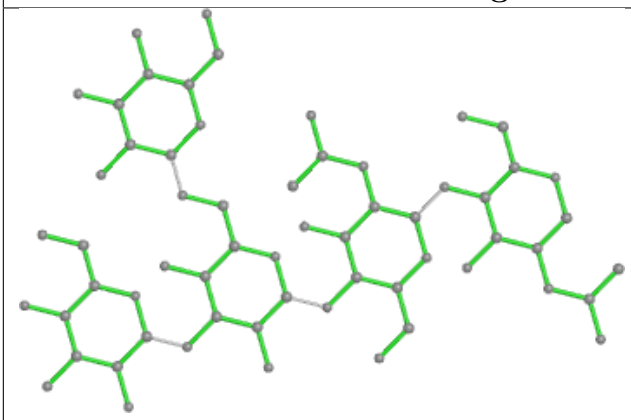
There are no ring outliers.

11 monomers are involved in 33 short contacts:

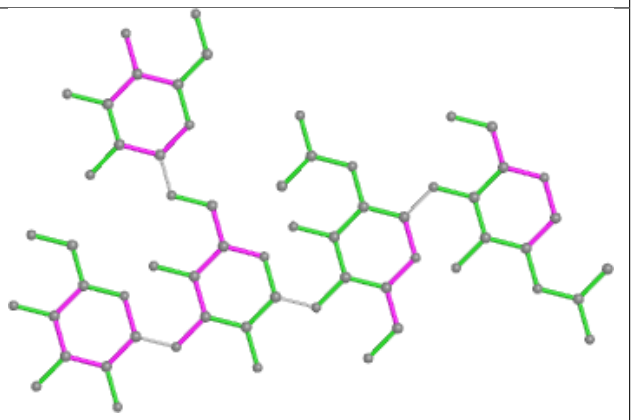
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	5	MAN	3	0
3	O	2	NAG	1	0
3	O	1	NAG	5	0
3	Q	1	NAG	5	0
3	M	1	NAG	4	0
3	R	1	NAG	4	0
3	N	1	NAG	4	0
3	P	1	NAG	4	0
3	Q	2	NAG	1	0
3	R	2	NAG	1	0
3	M	2	NAG	1	0

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

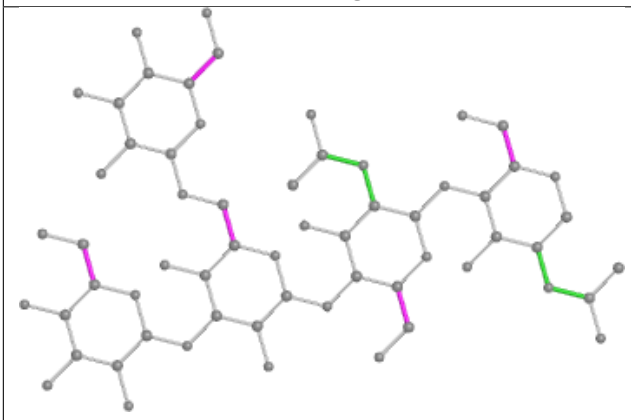
Oligosaccharide Chain M



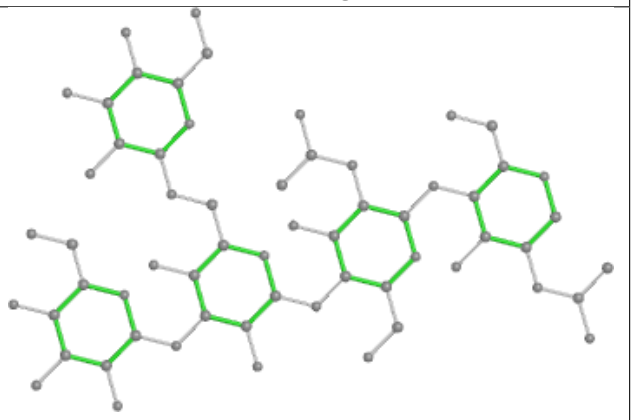
Bond lengths



Bond angles

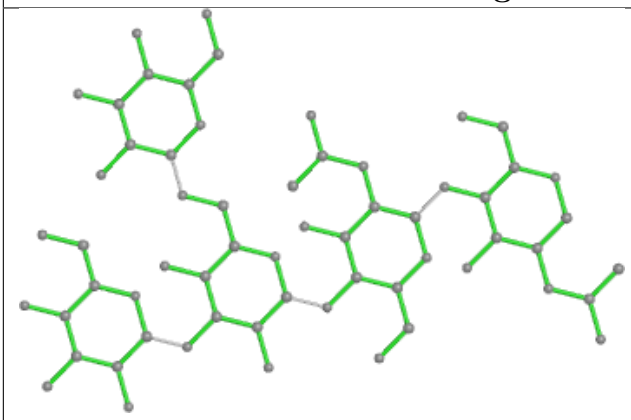


Torsions

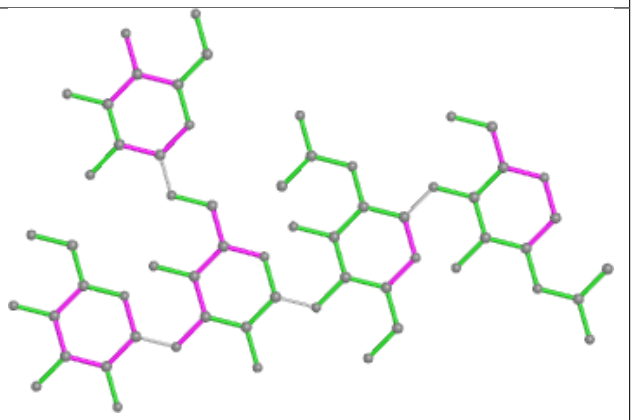


Rings

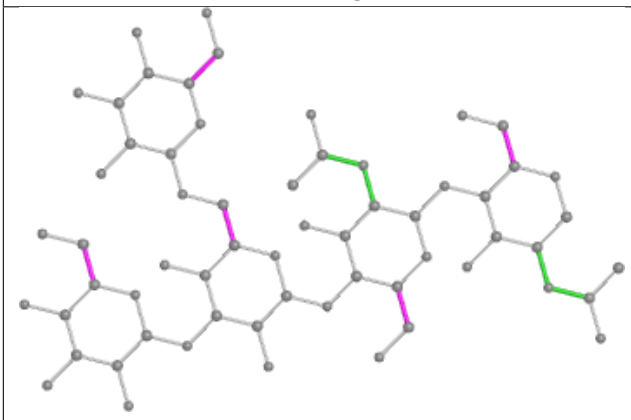
Oligosaccharide Chain N



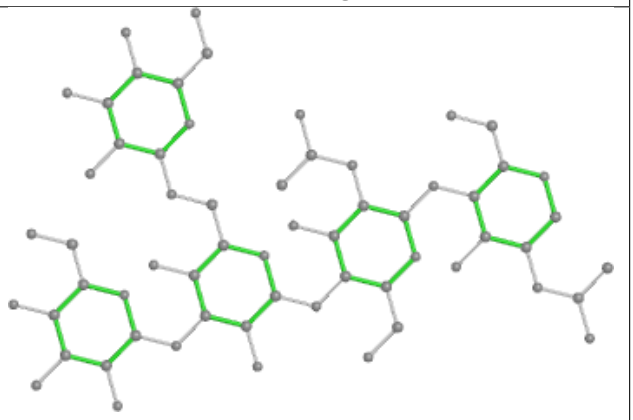
Bond lengths



Bond angles

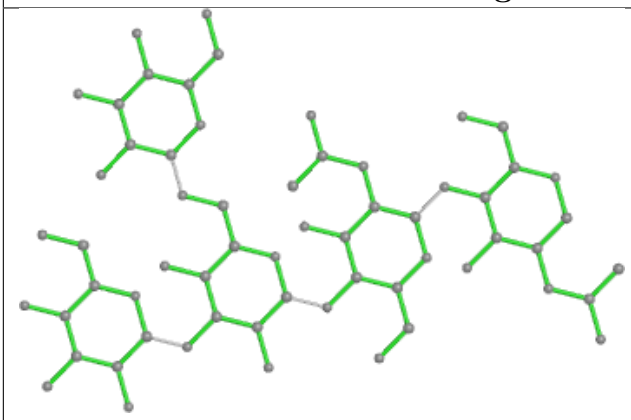


Torsions

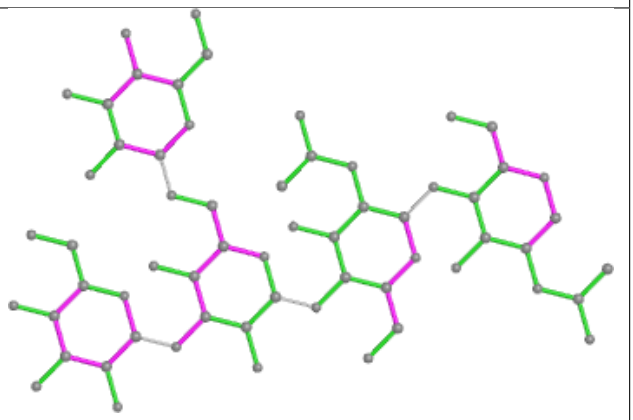


Rings

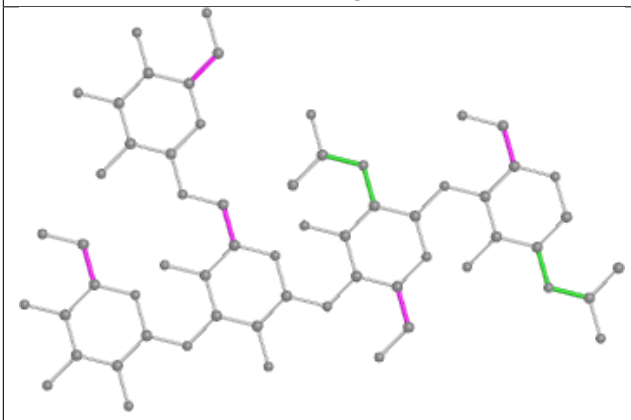
Oligosaccharide Chain O



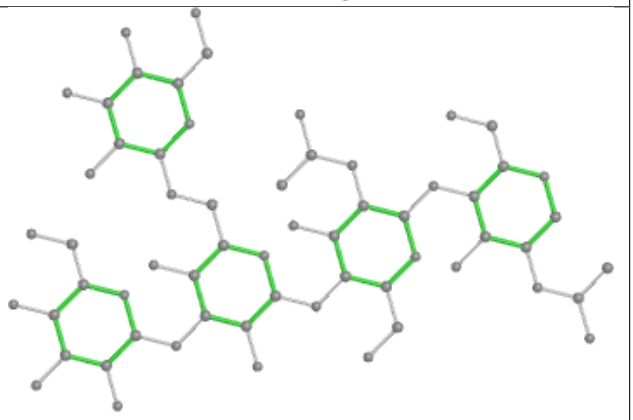
Bond lengths



Bond angles

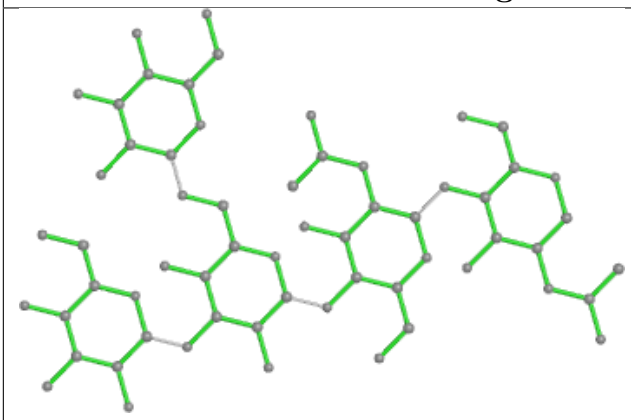


Torsions

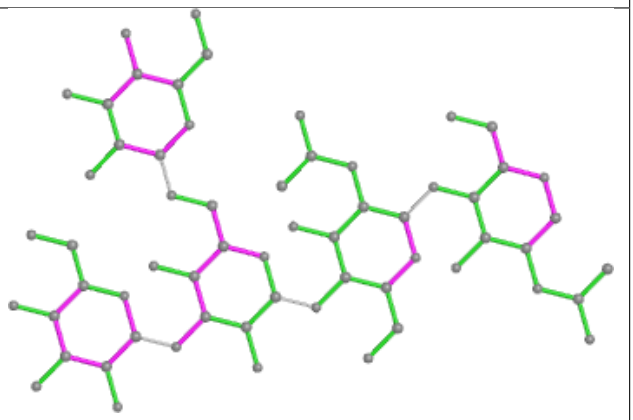


Rings

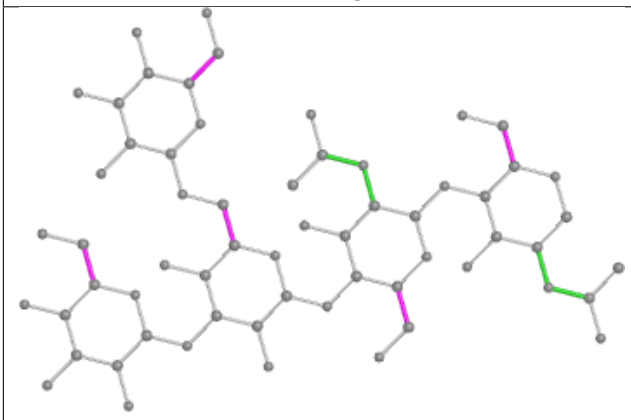
Oligosaccharide Chain P



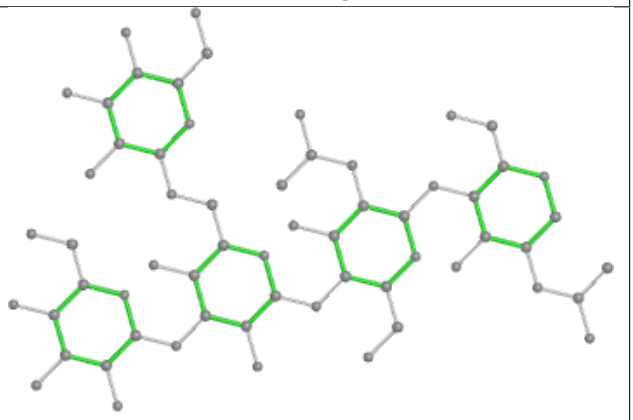
Bond lengths



Bond angles

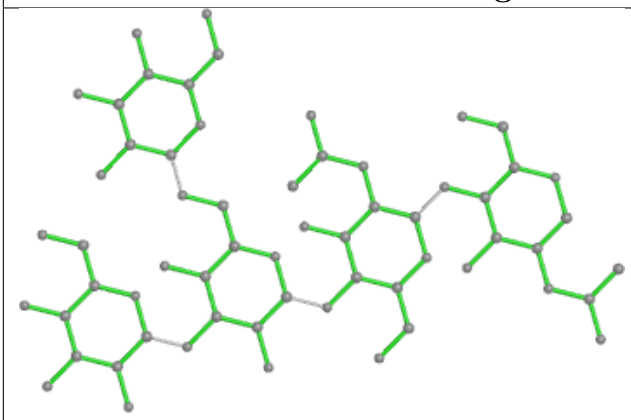


Torsions

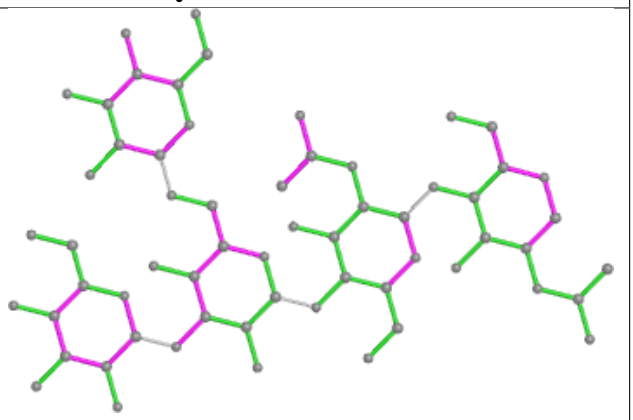


Rings

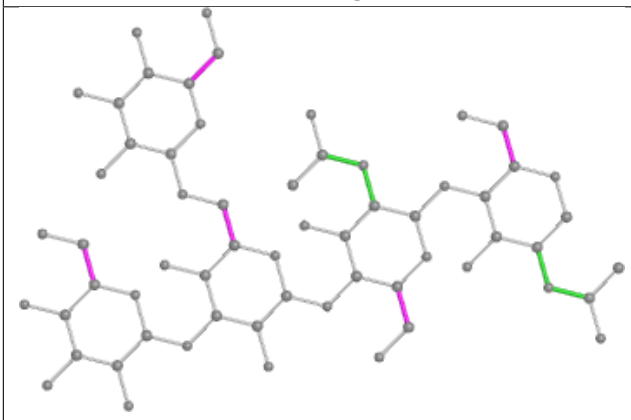
Oligosaccharide Chain Q



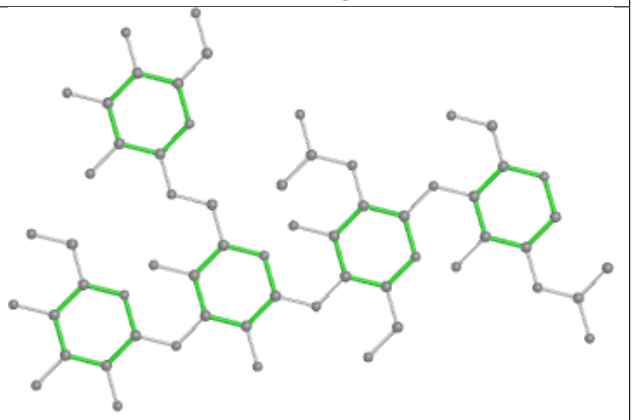
Bond lengths



Bond angles

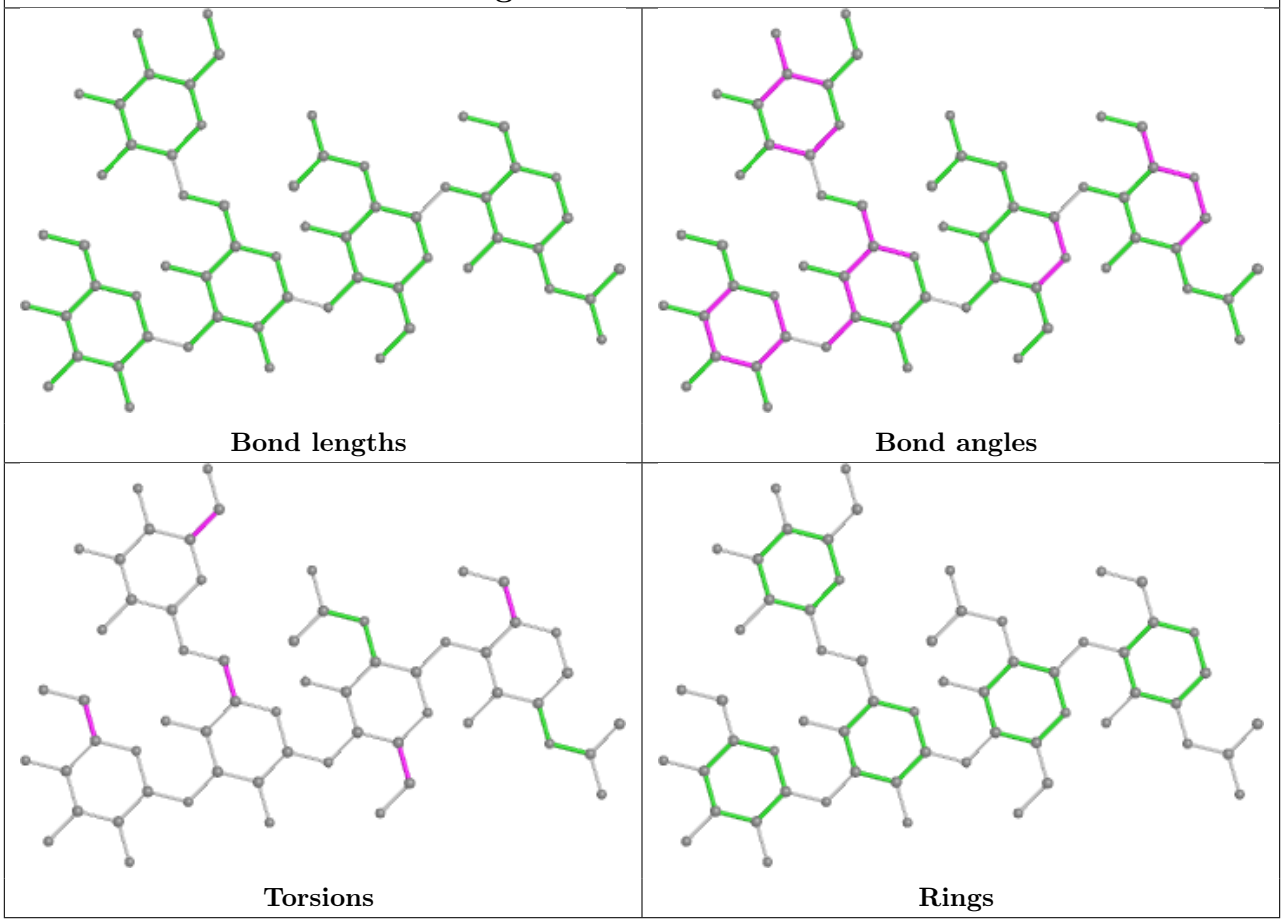


Torsions



Rings

Oligosaccharide Chain R



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	MAN	C	607	-	11,11,12	1.62	3 (27%)	15,15,17	1.32	2 (13%)
4	MAN	C	606	-	11,11,12	1.43	2 (18%)	15,15,17	1.93	8 (53%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	C	607	-	-	0/2/19/22	0/1/1/1
4	MAN	C	606	-	-	1/2/19/22	1/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	606	MAN	C4-C5	2.53	1.58	1.53
4	C	607	MAN	C4-C5	2.45	1.58	1.53
4	C	607	MAN	O5-C5	2.31	1.48	1.43
4	C	607	MAN	C4-C3	2.16	1.57	1.52
4	C	606	MAN	C1-C2	2.11	1.57	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	606	MAN	C1-O5-C5	3.42	116.83	112.19
4	C	606	MAN	O5-C1-C2	2.73	114.99	110.77
4	C	607	MAN	O3-C3-C4	2.69	116.57	110.35
4	C	606	MAN	C3-C4-C5	-2.48	105.81	110.24
4	C	606	MAN	O3-C3-C4	2.31	115.68	110.35
4	C	606	MAN	C6-C5-C4	2.20	118.15	113.00
4	C	606	MAN	O5-C5-C4	2.15	116.05	110.83
4	C	607	MAN	O5-C1-C2	2.14	114.07	110.77
4	C	606	MAN	O4-C4-C5	2.10	114.52	109.30
4	C	606	MAN	C1-C2-C3	2.07	112.21	109.67

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	606	MAN	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	606	MAN	C1-C2-C3-C4-C5-O5

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	607	MAN	3	0

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, 95^{th} 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	211/223 (94%)	1.04	29 (13%)	3	1	58, 83, 128, 143	0
1	B	208/223 (93%)	1.07	37 (17%)	1	0	55, 84, 162, 190	0
1	C	197/223 (88%)	1.23	42 (21%)	0	0	70, 100, 137, 178	0
1	D	207/223 (92%)	1.28	45 (21%)	0	0	65, 93, 144, 186	0
1	E	191/223 (85%)	2.16	73 (38%)	0	0	103, 134, 192, 213	0
1	F	208/223 (93%)	1.93	80 (38%)	0	0	97, 125, 172, 194	0
2	G	133/143 (93%)	1.04	23 (17%)	1	0	68, 91, 140, 176	0
2	H	133/143 (93%)	1.13	27 (20%)	1	0	66, 98, 129, 153	0
2	I	133/143 (93%)	2.48	63 (47%)	0	0	109, 140, 171, 197	0
2	J	133/143 (93%)	0.89	17 (12%)	3	1	62, 85, 120, 158	0
2	K	134/143 (93%)	1.65	42 (31%)	0	0	92, 122, 148, 168	0
2	L	134/143 (93%)	1.60	38 (28%)	0	0	91, 122, 155, 183	0
All	All	2022/2196 (92%)	1.45	516 (25%)	0	0	55, 109, 161, 213	0

All (516) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	292	ALA	23.2
2	I	264	GLY	12.8
1	E	456	SER	10.5
2	I	173	LYS	9.8
1	E	515	GLU	9.8
1	A	395	GLY	9.7
1	F	500	GLY	9.6
1	E	532	SER	9.4
2	I	291	PRO	9.3
1	D	454	PRO	9.2
2	H	292	ALA	8.8

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Mol	Chain	Res	Type	RSRZ
2	I	205	GLU	8.4
1	E	424	HIS	8.2
1	D	452	GLU	8.2
2	I	193	ASP	8.1
1	A	501	SER	8.0
1	F	480	HIS	7.8
1	D	335	GLY	7.8
2	K	264	GLY	7.8
2	I	265	SER	7.8
1	C	533	PRO	7.6
1	B	369	THR	7.5
1	D	533	PRO	7.5
1	F	542	SER	7.5
2	K	259	CYS	7.5
1	E	359	LEU	7.2
1	D	459	LYS	7.1
1	E	452	GLU	7.1
1	D	483	VAL	7.1
1	F	396	THR	7.1
1	F	464	CYS	7.1
2	K	247	PRO	7.0
1	E	531	ALA	7.0
2	G	288	CYS	6.9
2	I	158	PHE	6.9
2	I	178	GLY	6.8
1	F	424	HIS	6.7
1	F	487	ASP	6.7
2	I	216	HIS	6.7
2	L	253	ARG	6.6
1	E	358	CYS	6.6
2	K	178	GLY	6.5
2	L	205	GLU	6.5
1	F	486	PRO	6.5
1	E	484	GLN	6.5
1	B	395	GLY	6.4
1	D	366	SER	6.4
2	L	252	SER	6.3
2	I	231	GLU	6.2
1	E	434	THR	6.1
1	F	481	ASN	6.0
1	C	373	THR	6.0
1	E	457	ARG	6.0

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Mol	Chain	Res	Type	RSRZ
1	F	454	PRO	5.9
2	H	252	SER	5.8
1	D	456	SER	5.8
1	F	455	GLY	5.8
1	F	483	VAL	5.8
1	E	390	GLU	5.7
1	B	424	HIS	5.7
1	A	394	ASN	5.6
1	C	417	GLN	5.6
2	J	193	ASP	5.6
2	H	289	THR	5.6
2	L	291	PRO	5.6
1	C	378	SER	5.6
1	E	487	ASP	5.5
1	F	501	SER	5.5
2	I	250	PRO	5.5
1	B	418	CYS	5.5
1	A	393	ARG	5.5
2	I	174	CYS	5.5
1	B	419	ARG	5.5
2	I	172	ARG	5.4
2	K	253	ARG	5.4
1	F	335	GLY	5.4
2	L	256	GLY	5.4
1	C	347	ASP	5.3
1	E	458	ASP	5.3
2	G	289	THR	5.3
1	E	454	PRO	5.3
2	K	174	CYS	5.3
2	I	279	ALA	5.3
1	A	533	PRO	5.3
1	F	402	THR	5.3
1	A	454	PRO	5.2
2	L	266	GLY	5.2
1	C	363	LEU	5.2
1	F	368	GLY	5.2
2	K	165	GLU	5.2
1	C	501	SER	5.2
1	C	336	VAL	5.1
1	B	454	PRO	5.1
1	E	378	SER	5.1
2	K	229	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	377	ALA	5.1
2	G	228	LEU	5.0
1	E	428	ALA	5.0
1	E	392	GLN	5.0
1	F	451	PRO	5.0
1	A	482	GLU	5.0
1	B	393	ARG	4.9
2	J	174	CYS	4.9
2	L	191	CYS	4.9
2	K	238	SER	4.9
2	L	254	SER	4.9
1	D	393	ARG	4.9
1	F	456	SER	4.8
1	C	389	GLU	4.8
2	L	255	GLN	4.8
2	L	190	ALA	4.8
2	G	216	HIS	4.7
1	F	347	ASP	4.7
1	F	390	GLU	4.7
2	I	249	GLU	4.7
2	K	216	HIS	4.7
2	G	192	ASP	4.6
2	K	193	ASP	4.6
1	E	499	LYS	4.6
2	I	272	PHE	4.6
1	F	365	PRO	4.6
1	E	533	PRO	4.6
1	B	347	ASP	4.6
1	D	424	HIS	4.6
1	B	394	ASN	4.5
1	E	373	THR	4.5
2	G	278	GLY	4.5
1	C	379	GLY	4.5
1	F	519	LYS	4.5
1	D	460	ARG	4.5
1	A	531	ALA	4.5
2	H	253	ARG	4.5
1	E	361	VAL	4.5
1	E	482	GLU	4.5
2	L	278	GLY	4.5
1	C	453	TRP	4.5
1	E	451	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	459	LYS	4.5
2	L	263	ARG	4.4
1	F	361	VAL	4.4
2	I	167	TRP	4.4
2	I	263	ARG	4.4
2	L	159	VAL	4.4
1	F	418	CYS	4.4
1	E	512	THR	4.4
1	D	457	ARG	4.3
2	I	248	GLY	4.3
1	B	386	THR	4.3
2	J	287	THR	4.3
1	E	464	CYS	4.3
2	K	263	ARG	4.3
1	C	397	LEU	4.3
2	I	229	LYS	4.3
1	B	501	SER	4.2
1	F	363	LEU	4.2
2	L	289	THR	4.2
1	E	341	SER	4.2
1	B	512	THR	4.2
1	C	383	GLN	4.2
1	F	389	GLU	4.2
2	K	190	ALA	4.2
1	E	340	LEU	4.2
1	F	345	PRO	4.2
1	F	516	TRP	4.2
1	D	512	THR	4.2
1	D	392	GLN	4.1
1	E	486	PRO	4.1
1	F	417	GLN	4.1
1	A	456	SER	4.1
1	F	524	CYS	4.1
1	A	532	SER	4.1
1	E	459	LYS	4.1
1	D	455	GLY	4.1
2	I	266	GLY	4.1
2	I	251	THR	4.1
1	E	468	ASN	4.0
2	L	212	LYS	4.0
1	C	487	ASP	4.0
2	I	236	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
2	I	207	GLN	4.0
1	F	460	ARG	4.0
1	A	335	GLY	4.0
2	I	290	PRO	4.0
2	L	288	CYS	4.0
1	E	453	TRP	3.9
1	C	364	ALA	3.9
2	H	291	PRO	3.9
1	F	485	LEU	3.9
1	A	453	TRP	3.9
2	K	192	ASP	3.9
2	G	165	GLU	3.9
2	K	228	LEU	3.9
1	B	396	THR	3.9
1	E	481	ASN	3.9
1	C	454	PRO	3.9
2	K	262	MET	3.9
1	E	511	VAL	3.8
1	D	373	THR	3.8
2	K	271	ALA	3.8
1	E	389	GLU	3.8
2	I	163	CYS	3.8
1	E	400	THR	3.8
1	D	518	GLN	3.8
1	E	357	THR	3.8
1	D	401	SER	3.8
1	D	481	ASN	3.8
1	E	401	SER	3.8
1	A	424	HIS	3.7
2	G	229	LYS	3.7
2	L	229	LYS	3.7
2	H	203	SER	3.7
2	I	160	CYS	3.7
2	G	279	ALA	3.6
1	A	455	GLY	3.6
1	E	520	ASP	3.6
2	H	174	CYS	3.6
1	F	458	ASP	3.6
1	B	457	ARG	3.6
2	K	157	GLY	3.6
1	E	338	ALA	3.6
2	K	258	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	532[A]	SER	3.6
1	C	503	PHE	3.6
1	C	452	GLU	3.6
1	F	490	HIS	3.6
2	J	238	SER	3.6
1	E	498	THR	3.5
1	E	354	PRO	3.5
2	K	246	ALA	3.5
1	F	511	VAL	3.5
2	L	225	ASN	3.5
1	E	536	THR	3.5
1	E	535	GLN	3.5
2	L	165	GLU	3.5
1	E	465	LEU	3.5
2	L	173	LYS	3.5
1	F	446	TYR	3.5
1	F	482	GLU	3.5
2	I	238	SER	3.5
2	I	171	GLN	3.4
2	J	288	CYS	3.4
2	L	238	SER	3.4
2	K	282	CYS	3.4
1	F	385	SER	3.4
1	C	384	HIS	3.4
1	F	517	GLU	3.4
1	D	532	SER	3.4
2	I	288	CYS	3.4
1	F	392	GLN	3.3
1	E	404	PRO	3.3
2	I	246	ALA	3.3
1	C	386	THR	3.3
2	L	180	GLY	3.3
2	L	237	GLY	3.3
2	H	183	GLN	3.3
2	I	212	LYS	3.3
2	G	191	CYS	3.3
1	E	391	LYS	3.3
1	A	364	ALA	3.3
1	B	423	PRO	3.3
1	B	371	GLN	3.3
1	B	389	GLU	3.2
1	F	364	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	365	PRO	3.2
2	H	169	ASN	3.2
1	A	452	GLU	3.2
1	F	346	PHE	3.2
1	F	465	LEU	3.2
2	G	292	ALA	3.2
1	A	361	VAL	3.2
2	L	158	PHE	3.2
1	C	385	SER	3.2
2	G	287	THR	3.2
1	A	388	LYS	3.2
1	F	452	GLU	3.2
1	C	499	LYS	3.2
2	L	204	PRO	3.2
1	A	347	ASP	3.2
1	A	396	THR	3.2
2	K	231	GLU	3.2
2	K	252	SER	3.1
1	E	362	ASP	3.1
1	E	500	GLY	3.1
2	H	286	ALA	3.1
1	E	374	TRP	3.1
1	F	444	GLU	3.1
2	K	233	ILE	3.1
1	B	421	THR	3.1
2	L	259	CYS	3.1
2	H	205	GLU	3.1
2	J	286	ALA	3.1
2	K	189	TYR	3.1
2	L	192	ASP	3.1
1	F	367	LYS	3.1
1	F	497	LYS	3.1
1	C	401	SER	3.1
1	B	428	ALA	3.1
1	D	503	PHE	3.0
1	E	506	PHE	3.0
1	F	395	GLY	3.0
1	D	464	CYS	3.0
1	A	516	TRP	3.0
1	F	494	GLN	3.0
2	I	258	ASP	3.0
2	K	207	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	I	210	LEU	3.0
1	B	398	THR	3.0
1	A	502	GLY	3.0
2	I	159	VAL	3.0
1	D	451	PRO	3.0
1	E	513	ARG	3.0
2	L	228	LEU	3.0
1	D	497	LYS	3.0
2	H	251	THR	3.0
2	H	230	GLY	3.0
2	H	288	CYS	3.0
1	D	461	THR	2.9
1	E	455	GLY	2.9
1	B	422	HIS	2.9
1	F	471	PRO	2.9
1	F	339	TYR	2.9
1	E	347	ASP	2.9
2	L	267	ARG	2.9
2	H	247	PRO	2.9
2	K	288	CYS	2.9
2	K	208	ASP	2.9
2	I	190	ALA	2.9
2	K	203	SER	2.9
1	A	337	SER	2.8
1	B	456	SER	2.8
2	H	255	GLN	2.8
2	J	180	GLY	2.8
1	D	484	GLN	2.8
2	H	248	GLY	2.8
1	D	447	ALA	2.8
2	H	165	GLU	2.8
2	I	206	GLU	2.8
1	F	359	LEU	2.8
1	C	361	VAL	2.8
2	J	191	CYS	2.8
1	C	400	THR	2.8
1	C	362	ASP	2.8
1	F	388	LYS	2.8
2	H	287	THR	2.8
2	I	209	PHE	2.8
1	E	461	THR	2.8
1	F	518	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	J	252	SER	2.7
2	J	253	ARG	2.7
1	F	507	SER	2.7
2	J	158	PHE	2.7
1	F	515	GLU	2.7
1	F	528	HIS	2.7
1	A	362	ASP	2.7
2	I	179	LYS	2.7
1	C	387	ARG	2.7
2	G	291	PRO	2.7
2	I	230	GLY	2.7
1	A	457	ARG	2.7
2	I	278	GLY	2.7
2	I	254	SER	2.7
2	K	215	SER	2.7
2	K	279	ALA	2.7
1	F	386	THR	2.7
1	B	390	GLU	2.7
1	D	347	ASP	2.6
2	K	237	GLY	2.6
1	B	359	LEU	2.6
1	F	366	SER	2.6
2	I	211	THR	2.6
1	B	367	LYS	2.6
1	F	468	ASN	2.6
1	F	520	ASP	2.6
2	H	180	GLY	2.6
1	F	488	ALA	2.6
1	C	455	GLY	2.6
2	H	290	PRO	2.6
2	I	245	TRP	2.6
1	B	488	ALA	2.6
1	B	361	VAL	2.6
2	H	195	GLU	2.6
2	L	174	CYS	2.6
2	L	262	MET	2.6
1	F	428	ALA	2.6
1	E	436	THR	2.6
1	A	473	ASP	2.6
1	E	387	ARG	2.6
2	I	286	ALA	2.6
1	F	394	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	237	GLY	2.6
1	D	534	SER	2.6
2	J	178	GLY	2.6
2	I	252	SER	2.6
1	B	388	LYS	2.6
1	E	365	PRO	2.6
1	E	524	CYS	2.6
1	D	395	GLY	2.5
1	D	446	TYR	2.5
1	D	485	LEU	2.5
1	B	430	MET	2.5
1	F	381	PRO	2.5
2	J	192	ASP	2.5
1	D	357	THR	2.5
2	G	217	THR	2.5
1	E	397	LEU	2.5
2	L	283	ASP	2.5
2	J	173	LYS	2.5
1	C	403	LEU	2.5
1	F	467	GLN	2.5
2	I	213	HIS	2.5
1	F	484	GLN	2.5
2	G	243	SER	2.5
2	I	169	ASN	2.5
2	H	249	GLU	2.5
2	G	190	ALA	2.5
1	E	360	VAL	2.4
2	I	208	ASP	2.4
2	I	262	MET	2.4
2	K	291	PRO	2.4
1	E	398	THR	2.4
1	F	475	SER	2.4
2	K	167	TRP	2.4
2	K	202	HIS	2.4
1	F	401	SER	2.4
2	K	254	SER	2.4
1	D	426	PRO	2.4
1	D	514	ALA	2.4
1	B	464	CYS	2.4
1	D	501	SER	2.4
2	K	265	SER	2.4
1	E	445	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	G	258	ASP	2.4
1	C	524	CYS	2.4
2	I	192	ASP	2.3
2	I	268	TRP	2.3
1	E	483	VAL	2.3
1	F	336	VAL	2.3
1	E	379	GLY	2.3
2	I	267	ARG	2.3
1	F	423	PRO	2.3
1	D	502	GLY	2.3
2	G	196	GLY	2.3
2	H	258	ASP	2.3
2	J	160	CYS	2.3
2	J	228	LEU	2.3
2	H	244	ASN	2.3
1	B	520	ASP	2.3
2	K	227	ASP	2.3
1	F	453	TRP	2.3
2	H	280	TRP	2.3
1	D	337	SER	2.3
1	B	513	ARG	2.3
1	E	475	SER	2.3
1	E	521	GLU	2.2
1	C	504	PHE	2.2
1	D	448	PHE	2.2
2	L	290	PRO	2.2
1	D	396	THR	2.2
1	C	513	ARG	2.2
1	C	404	PRO	2.2
2	G	171	GLN	2.2
2	L	208	ASP	2.2
2	I	170	PHE	2.2
2	K	158	PHE	2.2
1	E	474	ILE	2.2
2	L	166	LYS	2.2
1	B	375	SER	2.2
1	F	530	ALA	2.2
2	I	253	ARG	2.2
2	I	239	HIS	2.2
2	L	220	TRP	2.2
1	F	447	ALA	2.2
2	G	163	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	247	PRO	2.2
1	A	500	GLY	2.2
1	F	422	HIS	2.1
1	E	526	ALA	2.1
1	B	376	ARG	2.1
2	L	274	ASP	2.1
1	D	450	THR	2.1
1	D	453	TRP	2.1
1	D	390	GLU	2.1
1	D	494	GLN	2.1
2	I	195	GLU	2.1
2	K	195	GLU	2.1
1	C	366	SER	2.1
1	C	357	THR	2.1
1	B	368	GLY	2.1
1	E	345	PRO	2.1
2	L	183	GLN	2.1
2	J	258	ASP	2.1
2	K	244	ASN	2.1
1	E	412	GLU	2.1
1	C	340	LEU	2.1
2	H	200	SER	2.1
1	F	457	ARG	2.1
2	G	174	CYS	2.1
1	C	468	ASN	2.1
2	I	204	PRO	2.1
2	G	158	PHE	2.0
1	B	429	LEU	2.0
1	A	497	LYS	2.0
2	G	255	GLN	2.0
2	I	261	MET	2.0
1	D	363	LEU	2.0
1	C	529	GLU	2.0
1	F	384	HIS	2.0
1	C	396	THR	2.0
1	C	486	PRO	2.0
2	I	287	THR	2.0
1	E	411	ILE	2.0
1	F	462	LEU	2.0
1	C	398	THR	2.0
1	F	502	GLY	2.0
2	K	290	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	544	ASN	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	O	1	14/15	0.41	0.60	148,155,161,164	0
3	NAG	N	1	14/15	0.52	0.50	185,189,195,198	0
3	MAN	R	5	11/12	0.65	0.36	154,155,156,157	0
3	NAG	Q	1	14/15	0.67	0.80	158,160,162,164	0
3	MAN	O	4	11/12	0.68	0.41	164,166,168,169	0
3	MAN	M	5	11/12	0.72	0.34	153,154,155,156	0
3	NAG	M	1	14/15	0.72	0.44	142,147,153,157	0
3	MAN	O	5	11/12	0.73	0.31	142,142,144,144	0
3	MAN	P	5	11/12	0.74	0.34	146,148,149,150	0
3	MAN	Q	5	11/12	0.75	0.38	138,139,140,141	0
3	NAG	Q	2	14/15	0.76	0.21	132,134,136,136	0
3	MAN	Q	4	11/12	0.78	0.24	153,155,156,157	0
3	NAG	P	1	14/15	0.79	0.31	139,144,146,147	0
3	MAN	N	4	11/12	0.79	0.32	155,157,160,161	0
3	BMA	Q	3	11/12	0.79	0.21	150,152,153,153	0
3	MAN	N	5	11/12	0.81	0.28	155,156,157,157	0
3	MAN	M	4	11/12	0.82	0.38	163,165,168,169	0
3	NAG	R	2	14/15	0.83	0.40	147,150,151,151	0
3	NAG	R	1	14/15	0.84	0.28	142,147,151,153	0
3	BMA	O	3	11/12	0.84	0.17	139,143,145,146	0
3	NAG	N	2	14/15	0.84	0.31	120,124,127,128	0
3	MAN	R	4	11/12	0.85	0.16	147,149,151,151	0
3	NAG	O	2	14/15	0.87	0.30	135,137,142,143	0
3	BMA	R	3	11/12	0.87	0.25	137,139,139,139	0
3	MAN	P	4	11/12	0.88	0.21	156,157,159,159	0
3	NAG	M	2	14/15	0.88	0.51	146,148,151,152	0
3	BMA	N	3	11/12	0.89	0.19	123,126,128,128	0

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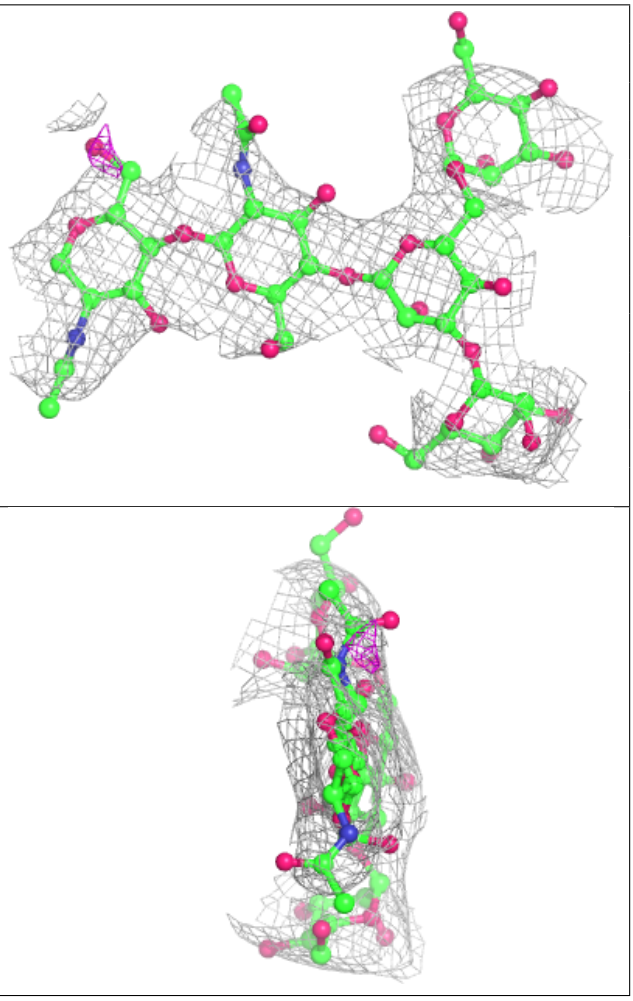
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	P	3	11/12	0.89	0.21	105,106,107,108	0
3	NAG	P	2	14/15	0.90	0.28	103,105,106,107	0
3	BMA	M	3	11/12	0.90	0.21	141,143,145,146	0

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.

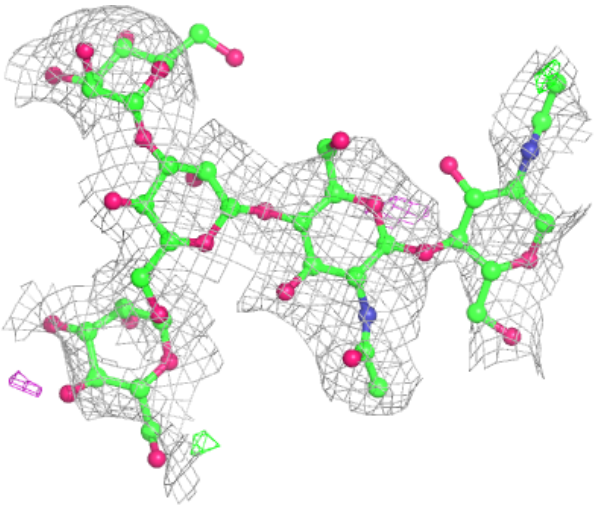
Electron density around Chain M:

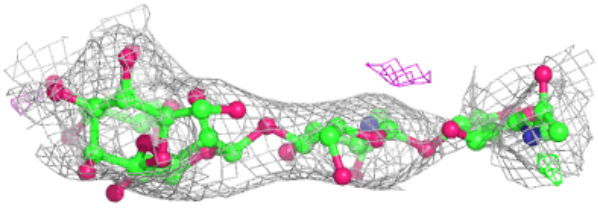
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

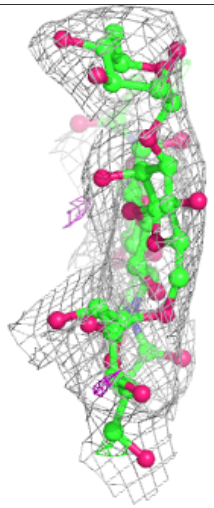


Electron density around Chain N:

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

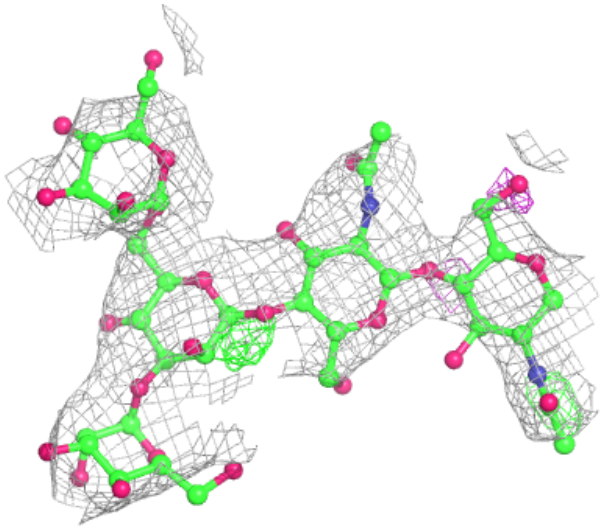


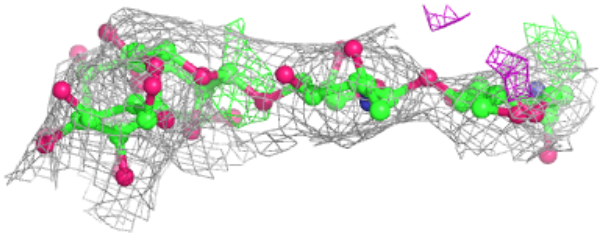


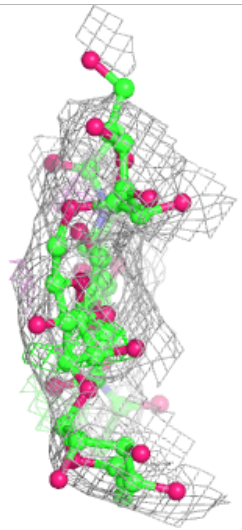


Electron density around Chain O:

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

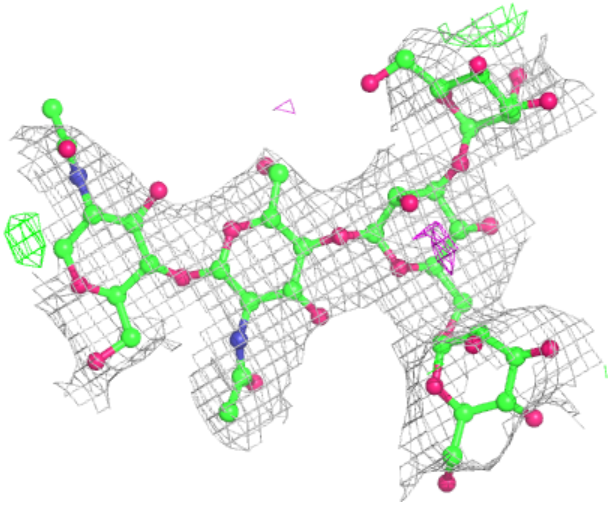


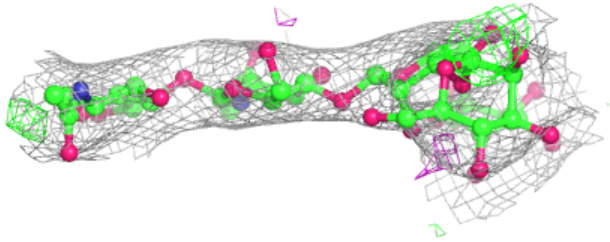


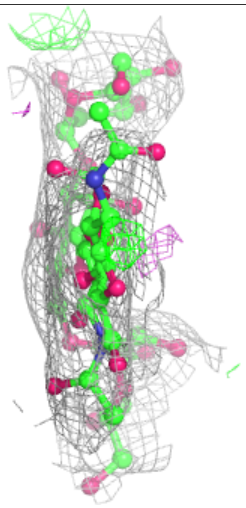


Electron density around Chain P:

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

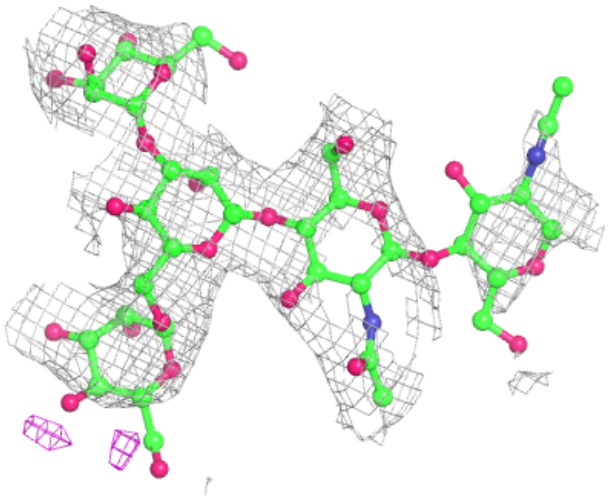


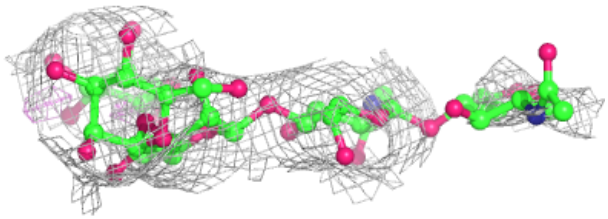


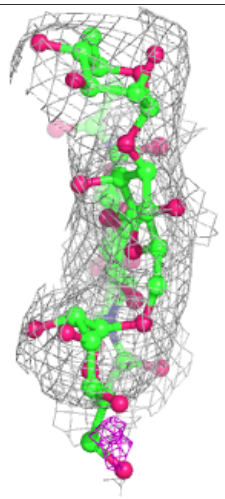


Electron density around Chain Q:

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

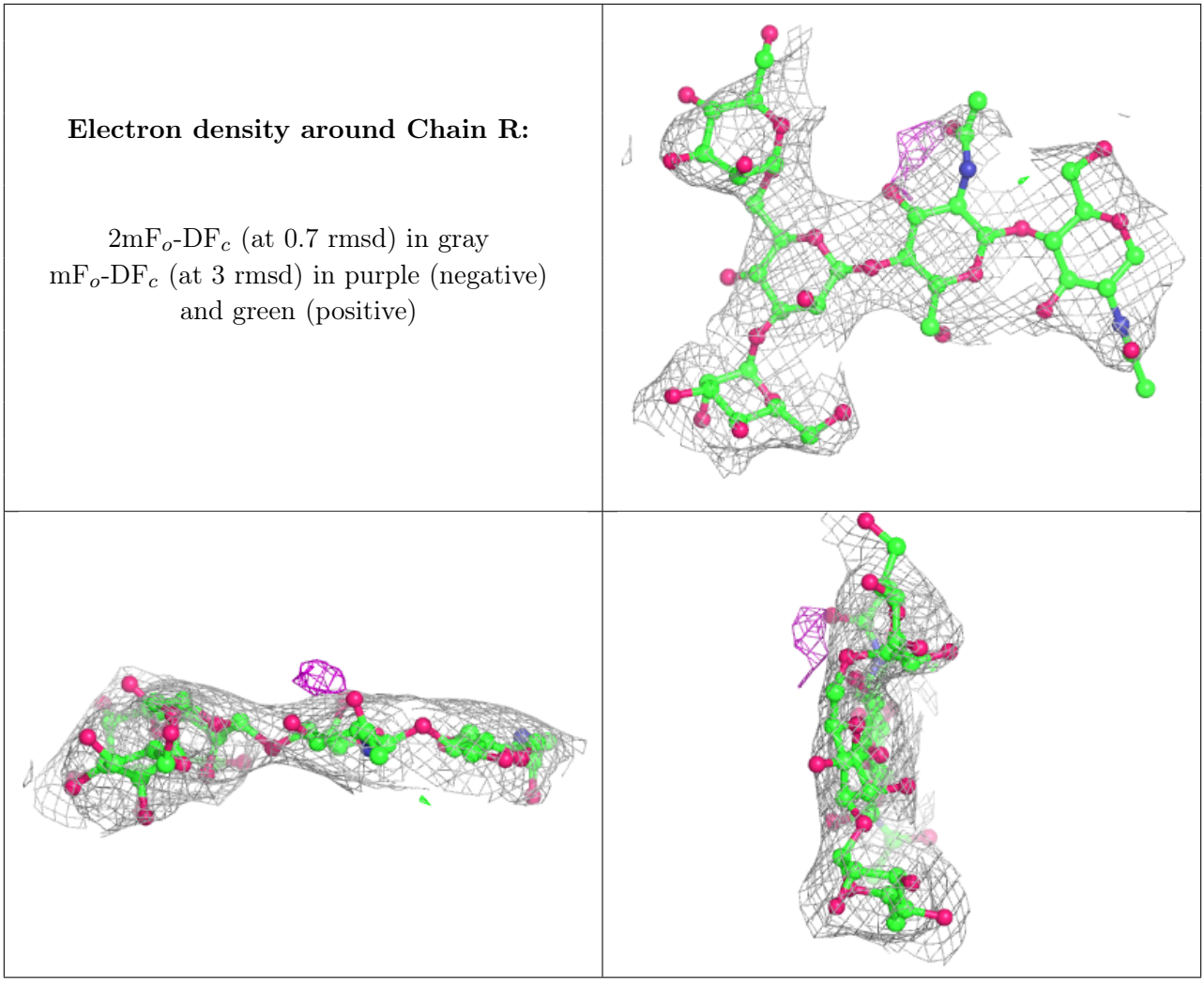






Electron density around Chain R:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
4	MAN	C	607	11/12	0.44	0.84	122,122,126,128	0
4	MAN	C	606	11/12	0.57	0.53	127,128,130,131	0

6.5 Other polymers

There are no such residues in this entry.