



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:06 AM UTC

PDB ID : 5JPM / pdb_00005jpm
Title : Structure of the complex of human complement C4 with MASP-2 rebuilt using iMDFF
Authors : Croll, T.I.; Andersen, G.R.
Deposited on : 2016-05-03
Resolution : 3.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

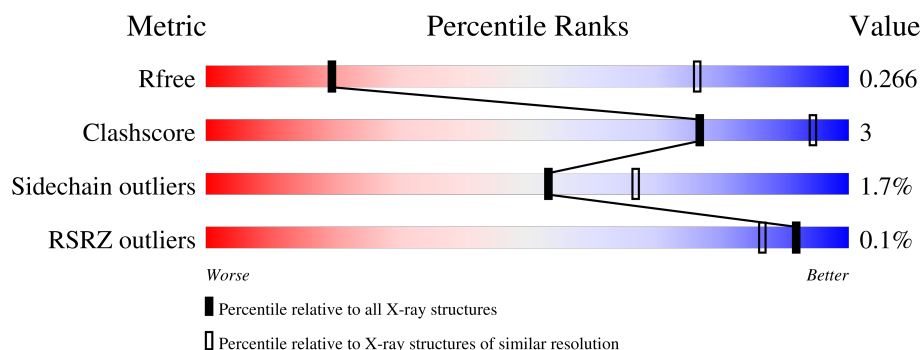
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



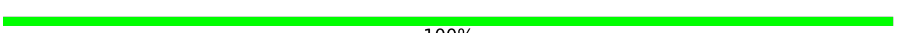
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	656	
1	D	656	
2	B	767	
2	E	767	
3	C	291	
3	F	291	

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Mol	Chain	Length	Quality of chain
4	G	154	 90% 5% 6%
4	I	154	 90% 5% 6%
5	H	242	 89% 11%
5	J	242	 95% 5%
6	K	3	 100%
6	L	3	 100%
6	M	3	 100%
6	N	3	 100%
6	O	3	 100%
6	P	3	 100%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 32214 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 Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			
1	D	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			

- Molecule 2 is a protein called Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	740	Total	C	N	O	S	0	0	0
			5718	3588	1002	1102	26			
2	E	740	Total	C	N	O	S	0	0	0
			5718	3588	1002	1102	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1201	SER	THR	variant	UNP P0C0L4
E	1201	SER	THR	variant	UNP P0C0L4

- Molecule 3 is a protein called Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	0	0	0
			2290	1437	407	429	17			
3	F	287	Total	C	N	O	S	0	0	0
			2290	1437	407	429	17			

- Molecule 4 is a protein called Mannan-binding lectin serine protease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	145	Total	C	N	O	S	0	0	0
			1103	701	177	213	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	145	Total	C	N	O	S	0	0	0
			1103	701	177	213	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	298	HIS	GLN	engineered mutation	UNP O00187
G	299	ALA	PRO	engineered mutation	UNP O00187
I	298	HIS	GLN	engineered mutation	UNP O00187
I	299	ALA	PRO	engineered mutation	UNP O00187

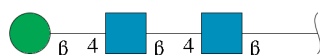
- Molecule 5 is a protein called Mannan-binding lectin serine protease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	242	Total	C	N	O	S	0	0	0
			1867	1190	317	350	10			
5	J	242	Total	C	N	O	S	0	0	0
			1867	1190	317	350	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	633	ALA	SER	engineered mutation	UNP O00187
J	633	ALA	SER	engineered mutation	UNP O00187

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	K	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	L	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	M	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

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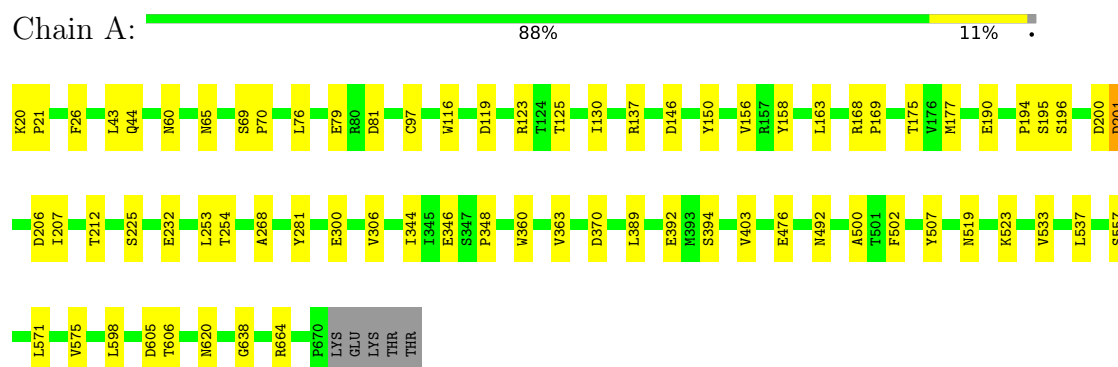
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	O	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	P	3	Total	C	N	O	0	0	0
			39	22	2	15			

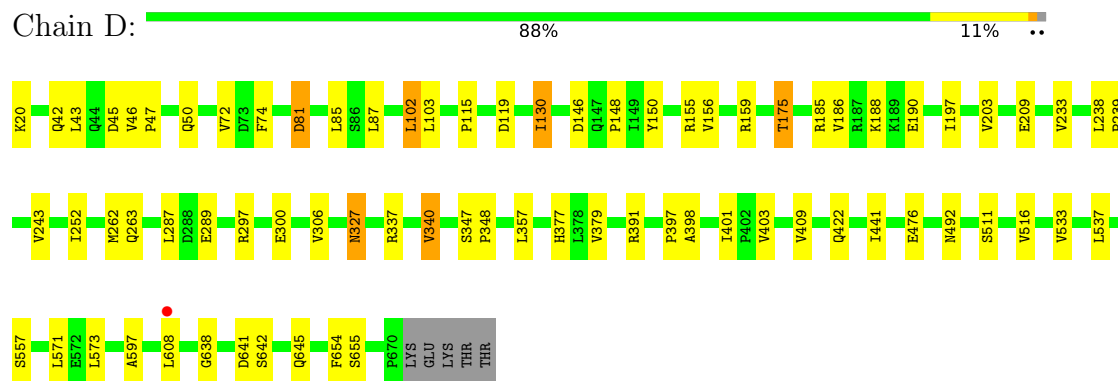
3 Residue-property plots

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.

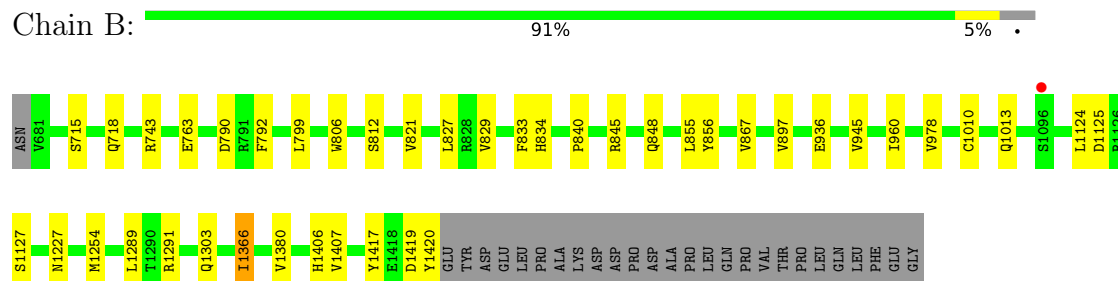
• Molecule 1: Complement C4-A



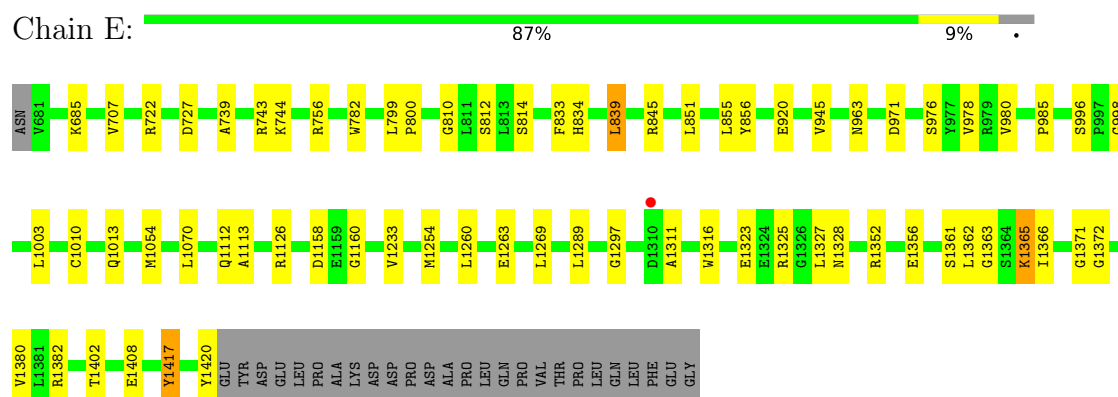
• Molecule 1: Complement C4-A



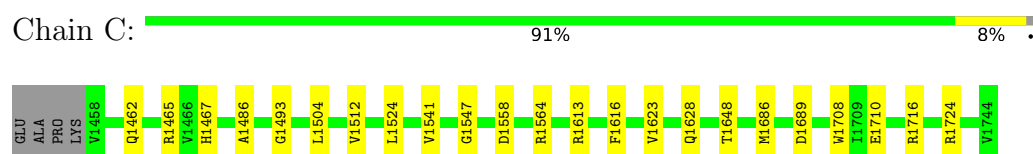
• Molecule 2: Complement C4-A



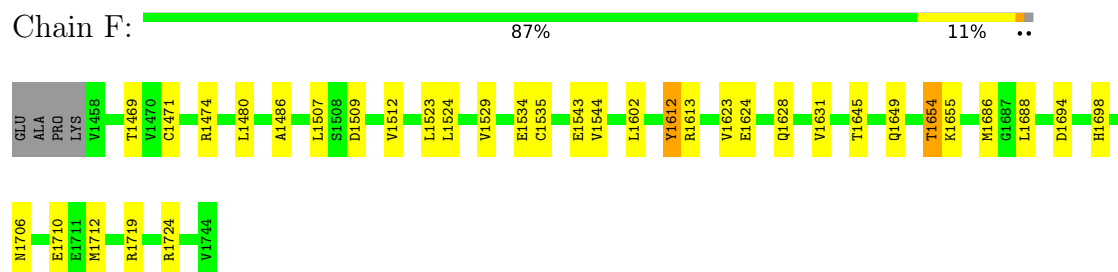
- Molecule 2: Complement C4-A



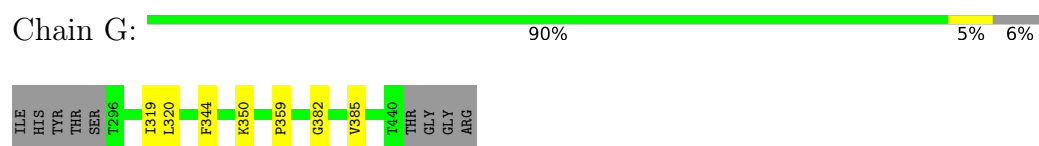
- Molecule 3: Complement C4-A



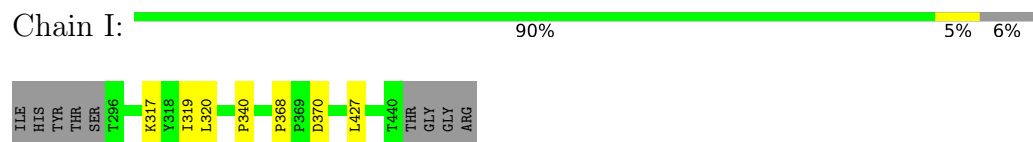
- Molecule 3: Complement C4-A



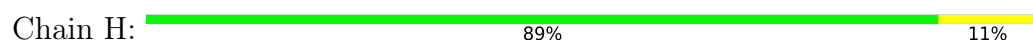
- Molecule 4: Mannan-binding lectin serine protease 2



- Molecule 4: Mannan-binding lectin serine protease 2



- Molecule 5: Mannan-binding lectin serine protease 2





- Molecule 5: Mannan-binding lectin serine protease 2

Chain J: 95% 5%



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

Chain K: 100%



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

Chain L: 100%



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

Chain M: 100%



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

Chain N: 100%



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

Chain O: 100%



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

Chain P:  100%

MAG1
MAG2
EMJ3

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.01Å 215.01Å 142.86Å 90.00° 110.11° 90.00°	Depositor
Resolution (Å)	48.97 – 3.75 48.97 – 3.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.97-3.75) 98.5 (48.97-3.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 3.77Å)	Xtriage
Refinement program	PHENIX (dev_2376)	Depositor
R, R_{free}	0.212 , 0.268 0.212 , 0.266	Depositor DCC
R_{free} test set	1727 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å ²)	118.2	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.083 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32214	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.09	0/5128	0.31	0/6961
1	D	0.09	0/5128	0.29	0/6961
2	B	0.08	0/5799	0.27	0/7875
2	E	0.08	0/5799	0.27	0/7875
3	C	0.09	0/2337	0.31	0/3158
3	F	0.09	0/2337	0.32	0/3158
4	G	0.09	0/1136	0.32	0/1549
4	I	0.08	0/1136	0.31	0/1549
5	H	0.09	0/1915	0.29	0/2604
5	J	0.09	0/1915	0.27	0/2604
All	All	0.09	0/32630	0.29	0/44294

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5012	0	5025	36	0
1	D	5012	0	5025	37	0
2	B	5718	0	5645	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	5718	0	5647	41	0
3	C	2290	0	2228	13	0
3	F	2290	0	2228	22	0
4	G	1103	0	1051	4	0
4	I	1103	0	1051	5	0
5	H	1867	0	1803	16	0
5	J	1867	0	1803	7	0
6	K	39	0	34	0	0
6	L	39	0	34	0	0
6	M	39	0	34	0	0
6	N	39	0	34	0	0
6	O	39	0	34	0	0
6	P	39	0	34	0	0
All	All	32214	0	31710	182	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 3.

All (182) 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)
5:H:485:VAL:HG13	5:H:495:LEU:HD11	1.75	0.68
1:D:185:ARG:HD3	1:D:188:LYS:HB2	1.75	0.67
5:H:602:TYR:OH	5:H:666:TYR:O	2.14	0.65
1:A:346:GLU:HG2	1:A:348:PRO:HD2	1.79	0.65
5:H:491:ASP:HB3	5:H:494:ALA:HB2	1.79	0.63
2:E:845:ARG:NH2	2:E:971:ASP:O	2.28	0.61
1:A:571:LEU:HD22	2:B:812:SER:HB2	1.82	0.61
1:D:557:SER:OG	1:D:638:GLY:O	2.19	0.60
2:B:945:VAL:HG23	2:B:1254:MET:HB3	1.84	0.60
2:B:1227:ASN:OD1	2:B:1291:ARG:NH1	2.34	0.59
1:D:476:GLU:HB3	1:D:492:ASN:HB2	1.84	0.59
1:A:557:SER:OG	1:A:638:GLY:O	2.21	0.58
1:D:81:ASP:OD2	1:D:81:ASP:N	2.36	0.58
3:F:1543:GLU:HG3	3:F:1544:VAL:HG23	1.85	0.58
1:D:642:SER:HB3	1:D:645:GLN:HG2	1.85	0.58
2:E:978:VAL:HG22	2:E:1380:VAL:HG12	1.85	0.57
1:A:212:THR:HG22	1:A:232:GLU:HG2	1.84	0.57
2:E:1126:ARG:HD3	2:E:1260:LEU:HD13	1.86	0.57
1:A:146:ASP:OD1	1:A:150:TYR:OH	2.16	0.57
2:E:980:VAL:O	2:E:1352:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1361:SER:O	2:E:1363:GLY:N	2.34	0.57
2:B:1013:GLN:N	2:B:1013:GLN:OE1	2.39	0.56
2:E:1327:LEU:HA	2:E:1372:GLY:HA3	1.88	0.56
2:B:834:HIS:HB3	2:B:856:TYR:HB2	1.88	0.55
3:C:1462:GLN:HG2	5:J:488:GLN:HG2	1.89	0.54
2:E:722:ARG:NH2	3:F:1534:GLU:OE1	2.37	0.54
1:D:571:LEU:HD22	2:E:812:SER:HB2	1.88	0.54
1:D:391:ARG:HA	1:D:397:PRO:HA	1.89	0.54
3:F:1471:CYS:HA	3:F:1535:CYS:HA	1.88	0.54
1:D:209:GLU:HB2	2:E:1070:LEU:HD21	1.89	0.54
1:A:175:THR:HG22	1:A:190:GLU:HG2	1.90	0.54
1:D:409:VAL:HG13	1:D:441:ILE:HD13	1.88	0.54
5:H:671:LYS:HE2	5:H:673:ILE:HD11	1.89	0.53
3:F:1486:ALA:HB3	3:F:1524:LEU:HB2	1.90	0.53
2:E:744:LYS:NZ	2:E:1417:TYR:O3	2.39	0.53
1:A:500:ALA:HB3	1:A:502:PHE:HD1	1.74	0.53
2:E:1013:GLN:OE1	2:E:1013:GLN:N	2.38	0.53
2:E:945:VAL:HG23	2:E:1254:MET:HB3	1.90	0.52
3:F:1613:ARG:NH1	3:F:1710:GLU:OE2	2.38	0.52
3:F:1654:THR:HG23	3:F:1655:LYS:H	1.75	0.52
5:H:487:GLU:HG3	5:H:488:GLN:HG2	1.92	0.52
3:C:1613:ARG:NH1	3:C:1710:GLU:OE1	2.35	0.52
2:B:799:LEU:HD21	2:B:829:VAL:HB	1.91	0.52
2:B:1125:ASP:O	2:B:1127:SER:N	2.42	0.51
3:F:1631:VAL:HA	3:F:1645:THR:HG22	1.92	0.51
1:D:47:PRO:HG2	1:D:50:GLN:HB2	1.91	0.51
3:F:1688:LEU:HD13	3:F:1706:ASN:HB3	1.91	0.51
5:J:602:TYR:OH	5:J:666:TYR:O	2.21	0.51
1:D:42:GLN:NE2	1:D:43:LEU:O	2.45	0.50
4:I:319:ILE:HG22	4:I:320:LEU:H	1.76	0.50
2:B:960:ILE:HB	2:B:1366:ILE:HG23	1.94	0.50
1:A:123:ARG:HG3	1:A:125:THR:H	1.75	0.50
1:A:20:LYS:HB2	1:A:21:PRO:HD3	1.94	0.50
2:E:839:LEU:HA	3:F:1544:VAL:HG21	1.93	0.50
1:A:370:ASP:HB3	1:A:389:LEU:HB3	1.94	0.50
3:C:1716:ARG:HG2	4:I:368:PRO:HG3	1.94	0.49
5:H:471:ALA:HB2	5:H:636:ALA:HB2	1.94	0.49
5:J:463:LEU:HB2	5:J:496:ASP:HB3	1.94	0.49
1:D:597:ALA:HB2	2:E:814:SER:HB2	1.95	0.49
2:E:851:LEU:H	2:E:851:LEU:HD23	1.77	0.49
2:E:996:SER:OG	2:E:998:GLY:O	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:673:ILE:HA	5:H:676:ILE:HG12	1.95	0.49
2:B:833:PHE:HZ	2:B:855:LEU:HD22	1.79	0.48
3:C:1465:ARG:HG2	3:C:1541:VAL:HG22	1.94	0.48
2:E:1269:LEU:HD12	2:E:1311:ALA:HB1	1.95	0.48
1:D:340:VAL:HG23	1:D:357:LEU:HB3	1.95	0.48
3:F:1623:VAL:HG11	3:F:1686:MET:HB3	1.96	0.48
1:D:115:PRO:O	1:D:119:ASP:N	2.45	0.48
2:E:1408:GLU:CD	5:H:498:ARG:HH22	2.22	0.48
4:G:320:LEU:HD22	4:G:350:LYS:HA	1.96	0.48
4:G:319:ILE:HG22	4:G:320:LEU:H	1.77	0.48
3:C:1486:ALA:HB3	3:C:1524:LEU:HB2	1.96	0.47
1:D:533:VAL:HA	1:D:537:LEU:HD22	1.96	0.47
3:F:1612:TYR:HD2	3:F:1612:TYR:H	1.61	0.47
3:F:1712:MET:HA	3:F:1712:MET:HE2	1.97	0.47
1:D:148:PRO:HG2	1:D:608:LEU:HD13	1.97	0.47
1:A:281:TYR:OH	1:A:300:GLU:OE1	2.19	0.47
2:B:840:PRO:HB3	3:C:1493:GLY:HA2	1.95	0.47
3:F:1507:LEU:C	3:F:1509:ASP:H	2.21	0.47
2:B:978:VAL:HG22	2:B:1380:VAL:HG12	1.96	0.47
5:J:555:ARG:HG2	5:J:558:ALA:HB2	1.97	0.47
1:A:268:ALA:HB2	1:A:344:ILE:HD13	1.97	0.47
5:H:605:PRO:O	5:H:609:ARG:NH2	2.47	0.46
2:E:833:PHE:HZ	2:E:855:LEU:HD22	1.81	0.46
3:F:1624:GLU:HB3	3:F:1654:THR:HG21	1.98	0.46
5:J:557:GLU:OE1	5:J:557:GLU:N	2.45	0.46
1:D:377:HIS:CD2	1:D:641:ASP:HB2	2.51	0.46
5:H:447:GLY:HA2	5:H:577:GLN:HB3	1.98	0.46
2:B:848:GLN:O	3:C:1547:GLY:N	2.38	0.46
3:C:1558:ASP:OD1	3:C:1564:ARG:NH2	2.46	0.46
3:F:1507:LEU:O	3:F:1509:ASP:N	2.48	0.45
1:D:146:ASP:OD1	1:D:150:TYR:OH	2.19	0.45
5:H:445:ILE:HB	5:H:586:MET:HB2	1.98	0.45
1:A:60:ASN:O	1:A:65:ASN:HA	2.16	0.45
1:A:392:GLU:O	1:A:394:SER:N	2.43	0.45
2:E:1323:GLU:HG2	2:E:1325:ARG:HG3	1.97	0.45
2:E:727:ASP:OD1	2:E:727:ASP:N	2.50	0.45
1:A:620:ASN:HA	2:B:821:VAL:HG11	1.98	0.45
2:B:867:VAL:HG21	2:B:897:VAL:HG11	1.98	0.45
1:D:300:GLU:OE2	2:E:685:LYS:NZ	2.42	0.45
1:A:43:LEU:HD22	1:A:76:LEU:HD13	1.99	0.45
1:D:74:PHE:HB3	1:D:85:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ARG:HA	1:D:297:ARG:HE	1.81	0.44
1:D:327:ASN:N	1:D:327:ASN:OD1	2.51	0.44
4:I:370:ASP:HB2	4:I:427:LEU:HD21	1.98	0.44
1:A:194:PRO:C	1:A:196:SER:H	2.23	0.44
1:D:155:ARG:HA	1:D:203:VAL:HA	2.00	0.44
4:I:317:LYS:HE2	4:I:319:ILE:HD11	1.99	0.44
1:D:238:LEU:HD12	1:D:239:PRO:HD2	2.00	0.44
3:C:1686:MET:HG3	3:C:1708:TRP:HB3	2.00	0.44
2:E:1158:ASP:O	2:E:1160:GLY:N	2.43	0.43
5:H:563:ARG:H	5:H:563:ARG:HG2	1.59	0.43
2:B:1419:ASP:O	5:J:583:ARG:NH1	2.52	0.43
1:D:511:SER:HB3	1:D:516:VAL:HG21	2.00	0.43
1:A:116:TRP:HA	1:A:119:ASP:HB3	1.99	0.43
1:A:605:ASP:OD1	1:A:606:THR:N	2.51	0.43
2:B:845:ARG:HE	2:B:936:GLU:CD	2.26	0.43
1:D:289:GLU:HA	1:D:337:ARG:HH11	1.84	0.43
2:B:790:ASP:O	2:B:792:PHE:N	2.51	0.43
1:D:43:LEU:HD12	1:D:46:VAL:HG11	2.00	0.43
1:D:72:VAL:HG12	1:D:87:LEU:HD13	2.01	0.43
2:E:985:PRO:HB3	2:E:1316:TRP:CD2	2.53	0.43
3:F:1628:GLN:HB3	3:F:1649:GLN:HB2	2.01	0.43
4:G:382:GLY:O	4:G:385:VAL:HG12	2.18	0.43
1:D:20:LYS:HB3	1:D:45:ASP:OD2	2.19	0.43
1:D:186:VAL:HB	2:E:1054:MET:HG3	2.00	0.43
2:E:834:HIS:HB3	2:E:856:TYR:HB2	2.00	0.43
5:H:497:ILE:HD11	5:H:536:ILE:HG21	2.01	0.43
1:A:81:ASP:OD2	1:A:81:ASP:N	2.51	0.43
2:B:715:SER:HB2	2:B:718:GLN:HB3	2.01	0.43
1:D:573:LEU:HD11	2:E:810:GLY:HA3	2.00	0.43
2:E:963:ASN:HB2	2:E:1382:ARG:HD2	2.00	0.43
2:B:743:ARG:HD2	2:B:763:GLU:HB3	2.00	0.43
1:D:130:ILE:HG23	1:D:655:SER:HB3	2.01	0.43
1:A:476:GLU:HB2	1:A:492:ASN:HB2	2.01	0.42
1:A:69:SER:HB2	1:A:70:PRO:HD3	2.01	0.42
3:C:1616:PHE:CE1	3:C:1708:TRP:HB2	2.54	0.42
2:E:1112:GLN:HG3	2:E:1113:ALA:H	1.82	0.42
2:E:707:VAL:HG12	2:E:739:ALA:HB2	2.02	0.42
1:A:253:LEU:HD23	1:A:363:VAL:HG23	2.02	0.42
1:A:507:TYR:CZ	1:A:519:ASN:HB3	2.54	0.42
3:F:1623:VAL:HG21	3:F:1686:MET:HE3	2.01	0.42
1:A:201:ASP:OD2	1:A:201:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:ILE:HD13	1:D:262:MET:HG2	2.02	0.42
3:F:1612:TYR:N	3:F:1612:TYR:CD2	2.88	0.42
1:A:533:VAL:HA	1:A:537:LEU:HD22	2.02	0.42
1:A:195:SER:HB3	1:A:598:LEU:HD11	2.02	0.41
3:C:1628:GLN:O	3:C:1648:THR:OG1	2.33	0.41
2:E:1402:THR:HG23	3:F:1469:THR:HB	2.02	0.41
1:D:398:ALA:HB1	1:D:401:ILE:HD13	2.02	0.41
1:A:163:LEU:HD23	1:A:169:PRO:HA	2.02	0.41
2:E:1365:LYS:H	2:E:1365:LYS:HG3	1.65	0.41
2:E:799:LEU:HD12	2:E:800:PRO:HD2	2.01	0.41
5:J:485:VAL:HG13	5:J:495:LEU:HD11	2.01	0.41
1:A:137:ARG:HA	1:A:225:SER:HB2	2.02	0.41
2:E:1328:ASN:N	2:E:1371:GLY:O	2.39	0.41
2:E:1408:GLU:OE1	5:H:498:ARG:NH2	2.51	0.41
1:A:523:LYS:HE3	1:A:523:LYS:HB3	1.91	0.41
2:B:1406:HIS:HA	3:C:1467:HIS:CD2	2.56	0.41
1:D:175:THR:HB	1:D:190:GLU:HG2	2.03	0.41
1:D:347:SER:HB2	1:D:348:PRO:HD3	2.03	0.41
2:E:756:ARG:HG2	5:H:655:TRP:HA	2.02	0.41
2:E:782:TRP:CD1	2:E:800:PRO:HG2	2.56	0.41
2:E:1003:LEU:HB3	2:E:1297:GLY:HA3	2.03	0.41
4:G:344:PHE:CZ	4:G:359:PRO:HD3	2.56	0.41
5:H:465:GLY:HA3	5:H:487:GLU:HG2	2.03	0.41
1:A:158:TYR:CZ	1:A:200:ASP:HB3	2.56	0.41
1:A:206:ASP:OD2	1:A:206:ASP:N	2.48	0.41
3:F:1474:ARG:NH1	3:F:1529:VAL:O	2.54	0.41
1:A:168:ARG:HA	1:A:168:ARG:HD3	1.85	0.40
3:C:1724:ARG:HG2	4:I:340:PRO:HD3	2.04	0.40
2:E:1323:GLU:OE2	2:E:1325:ARG:NE	2.32	0.40
3:F:1719:ARG:O	3:F:1724:ARG:NH2	2.54	0.40
1:A:79:GLU:OE1	1:A:79:GLU:N	2.53	0.40
2:B:1124:LEU:HD21	2:B:1303:GLN:HG3	2.03	0.40
1:D:102:LEU:HD23	1:D:103:LEU:H	1.85	0.40
2:E:1126:ARG:HH12	2:E:1263:GLU:CD	2.29	0.40
3:F:1694:ASP:OD1	3:F:1698:HIS:N	2.54	0.40
2:B:1406:HIS:CD2	2:B:1407:VAL:HG13	2.57	0.40
1:A:575:VAL:HG21	2:B:827:LEU:HD11	2.03	0.40
1:A:500:ALA:HB3	1:A:502:PHE:CD1	2.56	0.40
2:E:976:SER:HB3	2:E:1362:LEU:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	557/562 (99%)	544 (98%)	13 (2%)	44	62
1	D	557/562 (99%)	539 (97%)	18 (3%)	34	55
2	B	615/639 (96%)	611 (99%)	4 (1%)	76	77
2	E	615/639 (96%)	606 (98%)	9 (2%)	57	68
3	C	246/249 (99%)	242 (98%)	4 (2%)	55	68
3	F	246/249 (99%)	240 (98%)	6 (2%)	43	61
4	G	124/131 (95%)	124 (100%)	0	100	100
4	I	124/131 (95%)	124 (100%)	0	100	100
5	H	193/193 (100%)	190 (98%)	3 (2%)	55	68
5	J	193/193 (100%)	191 (99%)	2 (1%)	68	73
All	All	3470/3548 (98%)	3411 (98%)	59 (2%)	53	67

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	44	GLN
1	A	97	CYS
1	A	130	ILE
1	A	156	VAL
1	A	177	MET
1	A	201	ASP
1	A	207	ILE
1	A	254	THR
1	A	306	VAL

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Mol	Chain	Res	Type
1	A	360	TRP
1	A	403	VAL
1	A	664	ARG
2	B	806	TRP
2	B	1010	CYS
2	B	1289	LEU
2	B	1366	ILE
3	C	1504	LEU
3	C	1512	VAL
3	C	1623	VAL
3	C	1689	ASP
1	D	81	ASP
1	D	102	LEU
1	D	130	ILE
1	D	156	VAL
1	D	159	ARG
1	D	175	THR
1	D	197	ILE
1	D	233	VAL
1	D	243	VAL
1	D	263	GLN
1	D	287	LEU
1	D	306	VAL
1	D	327	ASN
1	D	340	VAL
1	D	379	VAL
1	D	403	VAL
1	D	422	GLN
1	D	654	PHE
2	E	743	ARG
2	E	839	LEU
2	E	920	GLU
2	E	1010	CYS
2	E	1233	VAL
2	E	1289	LEU
2	E	1356	GLU
2	E	1365	LYS
2	E	1366	ILE
3	F	1480	LEU
3	F	1512	VAL
3	F	1523	LEU
3	F	1602	LEU

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Mol	Chain	Res	Type
3	F	1612	TYR
3	F	1654	THR
5	H	463	LEU
5	H	563	ARG
5	H	583	ARG
5	J	543	VAL
5	J	555	ARG

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

Mol	Chain	Res	Type
1	A	263	GLN
1	A	320	GLN
1	A	648	GLN
2	B	826	GLN
2	B	834	HIS
2	B	967	ASN
2	B	1092	GLN
2	B	1345	GLN
2	B	1395	GLN
3	C	1521	HIS
1	D	101	GLN
1	D	199	GLN
1	D	536	HIS
1	D	616	HIS
2	E	1058	GLN
2	E	1296	GLN
2	E	1345	GLN
3	F	1514	HIS
3	F	1521	HIS
3	F	1731	ASN
4	G	310	HIS
4	G	338	HIS
5	H	490	HIS
4	I	315	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	TYS	E	1417	2	15,16,17	1.28	1 (6%)	15,22,24	0.90	1 (6%)
2	TYS	E	1420	2	15,16,17	1.25	1 (6%)	15,22,24	0.89	1 (6%)
2	TYS	B	1420	2	15,16,17	1.27	1 (6%)	15,22,24	1.04	1 (6%)
2	TYS	B	1417	2	15,16,17	1.26	1 (6%)	15,22,24	1.13	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	TYS	E	1417	2	-	5/10/11/13	0/1/1/1
2	TYS	E	1420	2	-	0/10/11/13	0/1/1/1
2	TYS	B	1420	2	-	4/10/11/13	0/1/1/1
2	TYS	B	1417	2	-	2/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1417	TYS	OH-S	3.84	1.65	1.58
2	B	1420	TYS	OH-S	3.78	1.65	1.58
2	E	1420	TYS	OH-S	3.71	1.65	1.58
2	B	1417	TYS	OH-S	3.70	1.65	1.58

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1417	TYS	O2-S-O1	-2.92	100.97	112.24
2	B	1420	TYS	O2-S-O1	-2.86	101.20	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1417	TYS	O3-S-O1	-2.15	101.04	108.56
2	E	1420	TYS	O3-S-O2	-2.12	101.13	108.56

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1420	TYS	N-CA-CB-CG
2	B	1420	TYS	C-CA-CB-CG
2	E	1417	TYS	N-CA-CB-CG
2	E	1417	TYS	C-CA-CB-CG
2	E	1417	TYS	O-C-CA-CB
2	B	1420	TYS	CA-CB-CG-CD1
2	B	1420	TYS	CA-CB-CG-CD2
2	B	1417	TYS	CA-CB-CG-CD1
2	B	1417	TYS	CA-CB-CG-CD2
2	E	1417	TYS	CA-CB-CG-CD1
2	E	1417	TYS	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1417	TYS	1	0

5.5 Carbohydrates

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	K	1	6,1	14,14,15	0.27	0	17,19,21	0.46	0
6	NAG	K	2	6	14,14,15	0.25	0	17,19,21	0.45	0
6	BMA	K	3	6	11,11,12	0.59	0	15,15,17	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	L	1	6,2	14,14,15	0.21	0	17,19,21	0.43	0
6	NAG	L	2	6	14,14,15	0.27	0	17,19,21	0.50	0
6	BMA	L	3	6	11,11,12	0.60	0	15,15,17	0.65	0
6	NAG	M	1	6,2	14,14,15	0.31	0	17,19,21	0.45	0
6	NAG	M	2	6	14,14,15	0.27	0	17,19,21	0.58	0
6	BMA	M	3	6	11,11,12	0.54	0	15,15,17	0.80	0
6	NAG	N	1	6,1	14,14,15	0.26	0	17,19,21	0.44	0
6	NAG	N	2	6	14,14,15	0.26	0	17,19,21	0.42	0
6	BMA	N	3	6	11,11,12	0.57	0	15,15,17	0.65	0
6	NAG	O	1	6,2	14,14,15	0.28	0	17,19,21	0.46	0
6	NAG	O	2	6	14,14,15	0.25	0	17,19,21	0.42	0
6	BMA	O	3	6	11,11,12	0.56	0	15,15,17	0.70	0
6	NAG	P	1	6,2	14,14,15	0.28	0	17,19,21	0.49	0
6	NAG	P	2	6	14,14,15	0.20	0	17,19,21	0.48	0
6	BMA	P	3	6	11,11,12	0.64	0	15,15,17	0.76	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

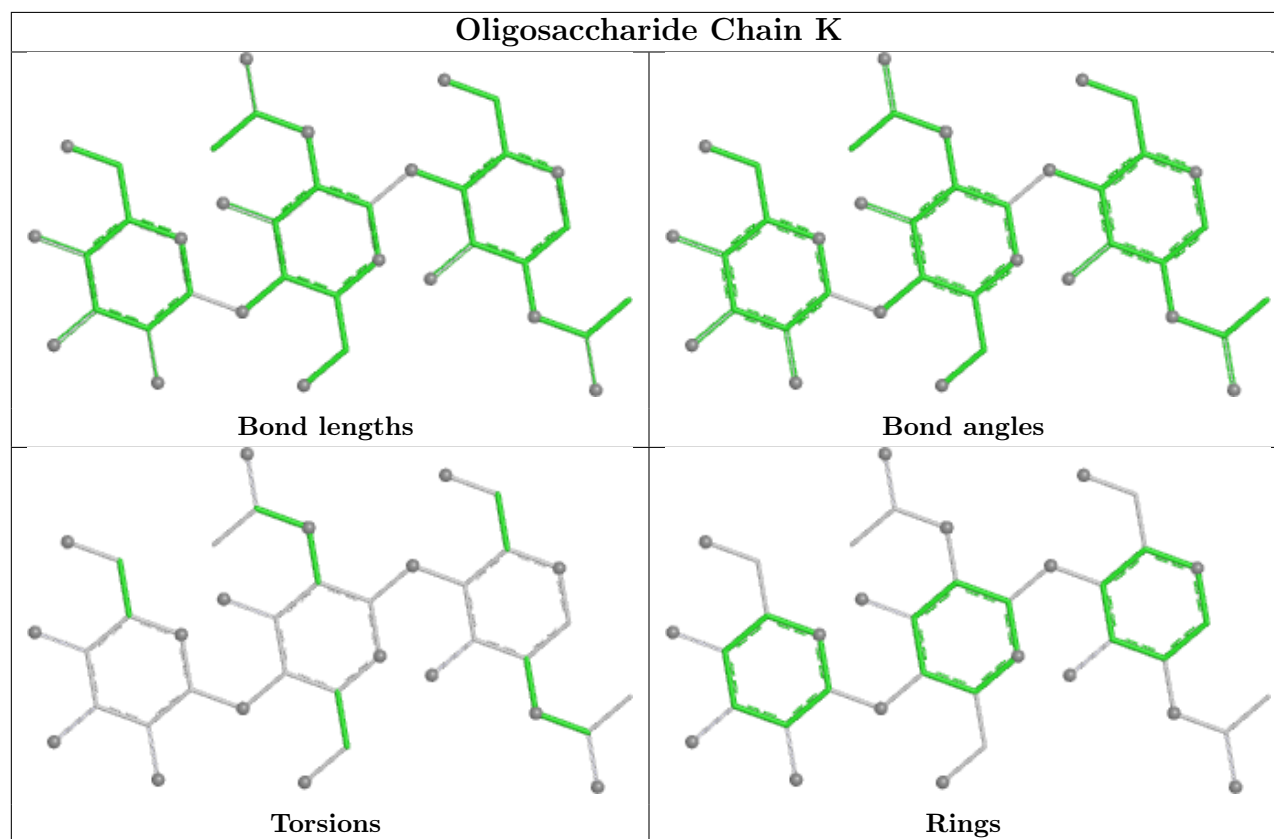
All (2) torsion outliers are listed below:

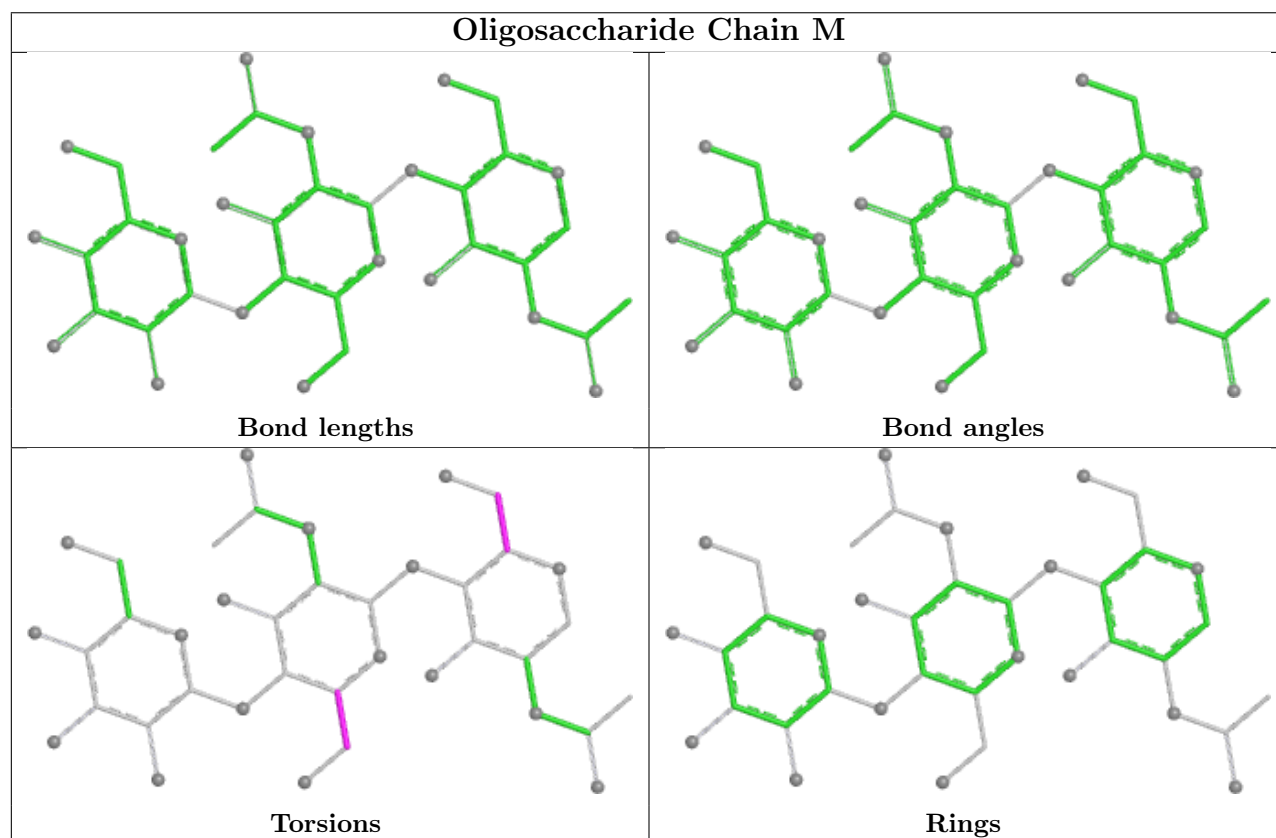
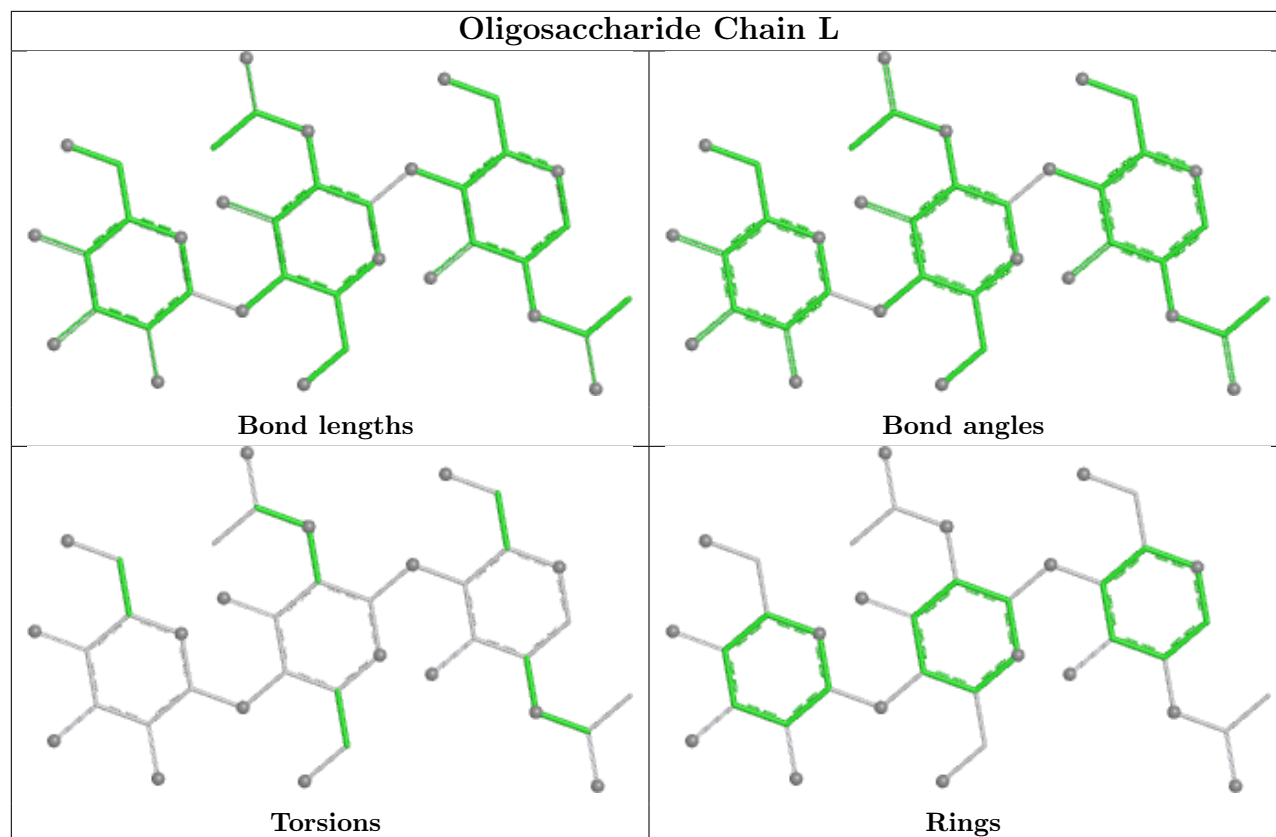
Mol	Chain	Res	Type	Atoms
6	M	1	NAG	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6

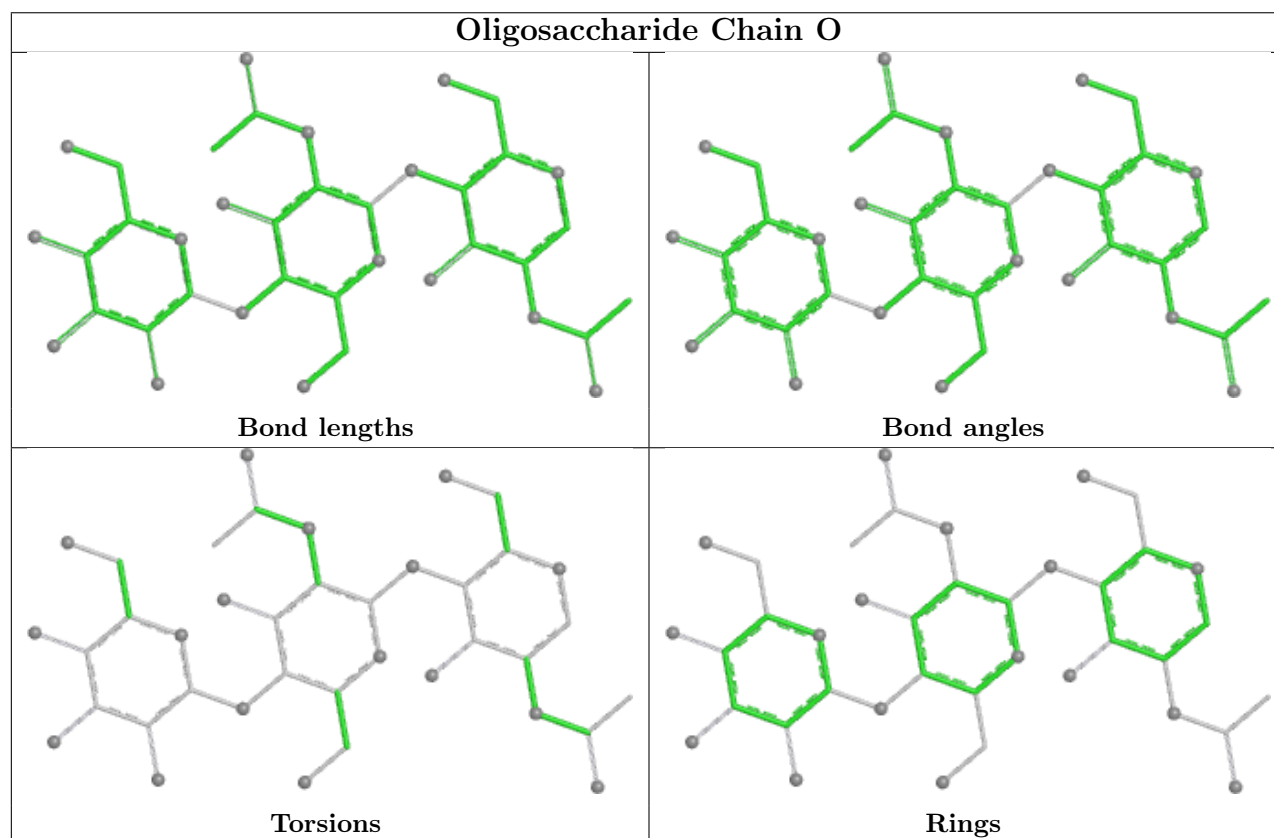
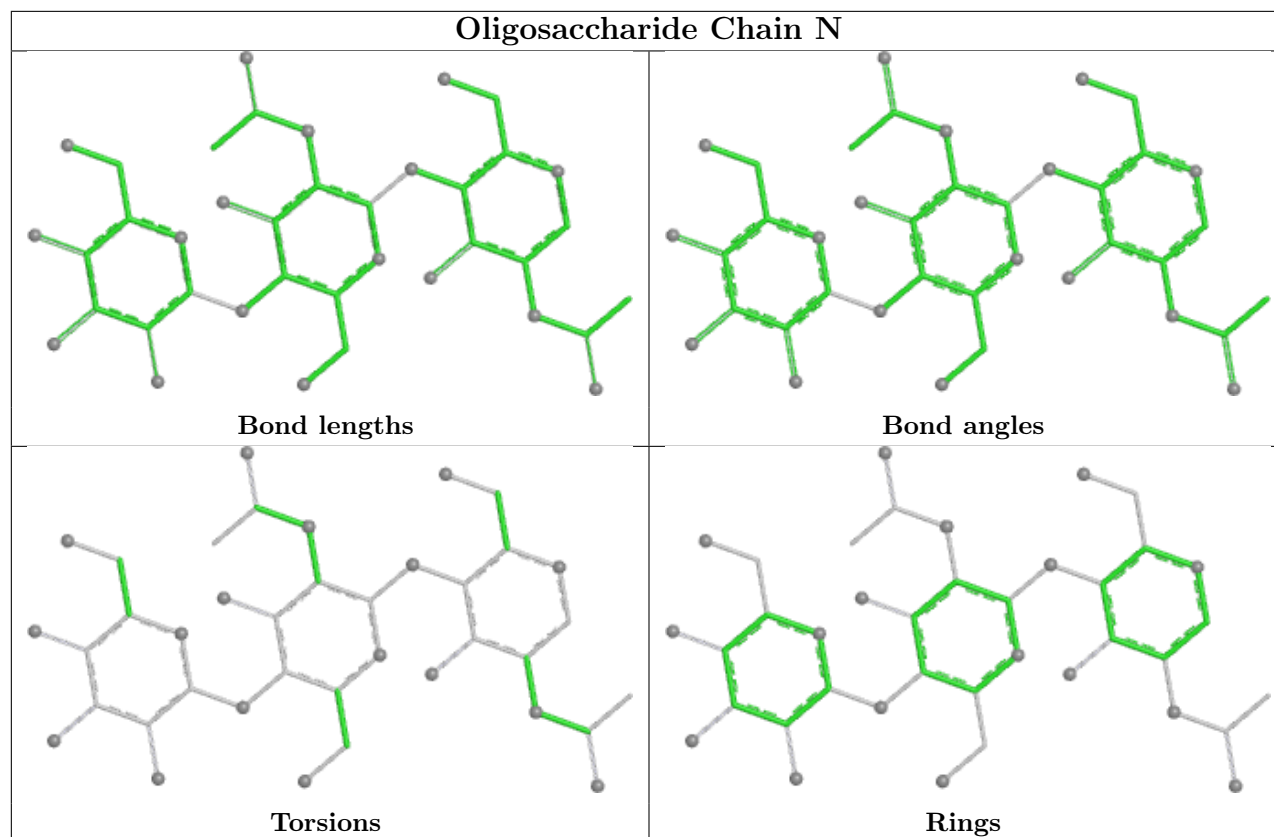
There are no ring outliers.

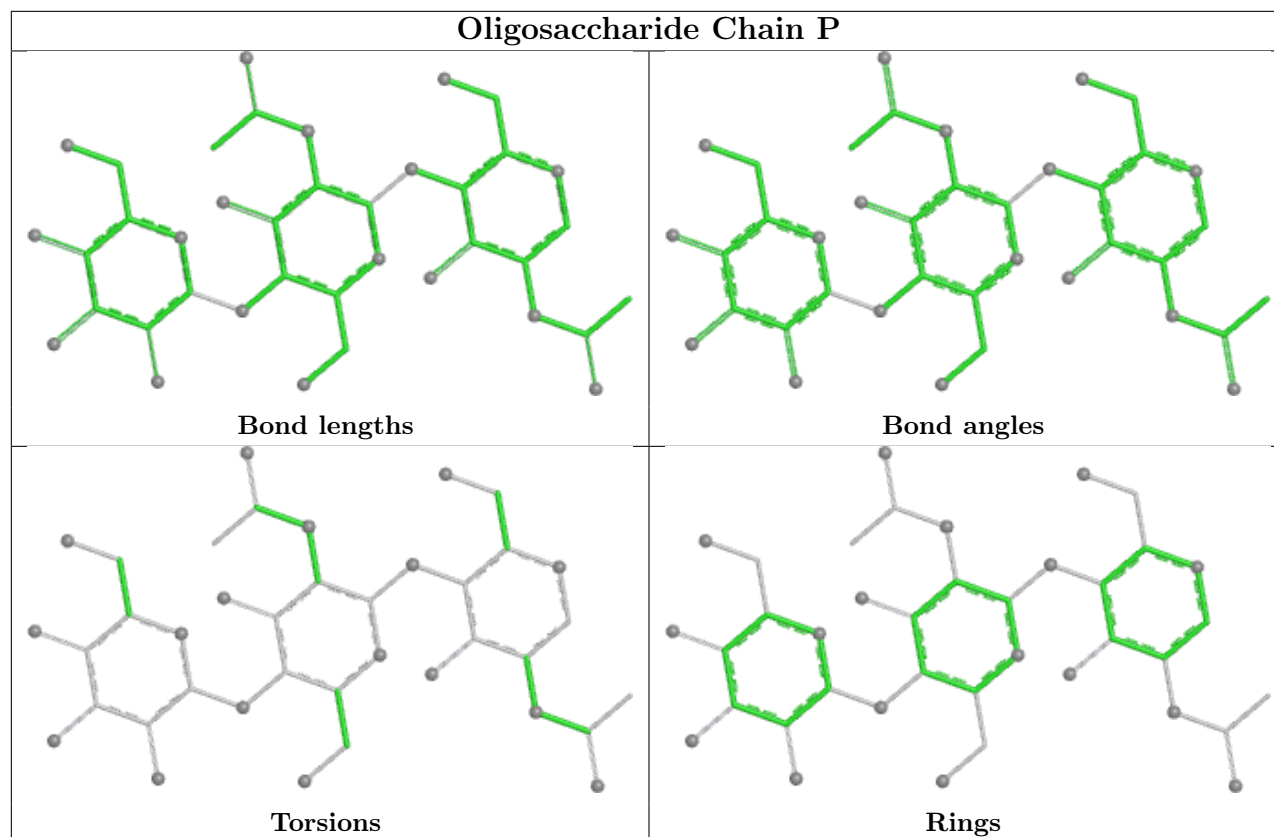
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	651/656 (99%)	-0.46	0 100 100	86, 135, 179, 201	0
1	D	651/656 (99%)	-0.47	1 (0%) 91 81	82, 122, 170, 205	0
2	B	738/767 (96%)	-0.39	1 (0%) 92 86	85, 131, 178, 239	0
2	E	738/767 (96%)	-0.46	1 (0%) 92 86	91, 135, 199, 257	0
3	C	287/291 (98%)	-0.37	0 100 100	74, 111, 154, 186	0
3	F	287/291 (98%)	-0.44	0 100 100	74, 115, 161, 218	0
4	G	145/154 (94%)	-0.53	0 100 100	117, 143, 178, 213	0
4	I	145/154 (94%)	-0.57	0 100 100	121, 146, 199, 232	0
5	H	242/242 (100%)	-0.26	0 100 100	160, 205, 245, 258	0
5	J	242/242 (100%)	-0.31	0 100 100	104, 154, 202, 234	0
All	All	4126/4220 (97%)	-0.43	3 (0%) 92 86	74, 133, 202, 258	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1096	SER	2.4
1	D	608	LEU	2.2
2	E	1310	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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	TYS	B	1420	16/17	0.21	0.16	236,247,264,264	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TYS	E	1417	16/17	0.57	0.10	218,242,263,264	0
2	TYS	E	1420	16/17	0.57	0.10	241,269,310,311	0
2	TYS	B	1417	16/17	0.75	0.12	197,209,219,226	0

6.3 Carbohydrates

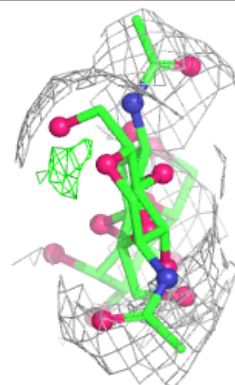
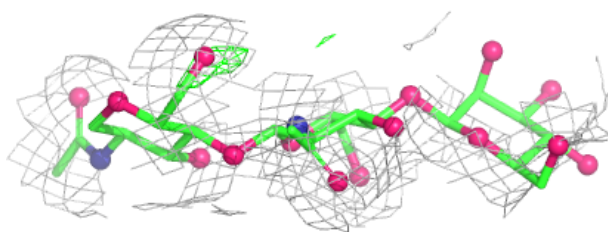
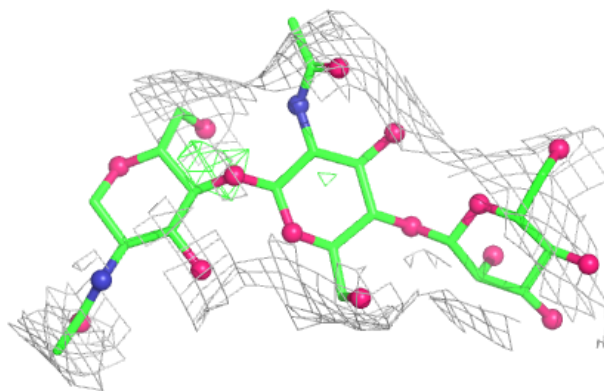
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	M	3	11/12	0.03	0.09	232,237,241,242	0
6	BMA	L	3	11/12	0.44	0.08	302,309,311,313	0
6	BMA	N	3	11/12	0.44	0.11	197,212,219,225	0
6	NAG	M	2	14/15	0.48	0.09	224,232,239,240	0
6	BMA	O	3	11/12	0.48	0.07	239,249,265,267	0
6	BMA	P	3	11/12	0.53	0.09	202,204,206,206	0
6	NAG	O	2	14/15	0.56	0.07	201,211,226,232	0
6	NAG	M	1	14/15	0.61	0.07	220,227,232,233	0
6	NAG	L	1	14/15	0.63	0.10	309,315,319,319	0
6	NAG	O	1	14/15	0.65	0.08	189,195,200,203	0
6	NAG	P	1	14/15	0.73	0.07	210,217,220,221	0
6	NAG	L	2	14/15	0.73	0.08	300,306,310,312	0
6	NAG	P	2	14/15	0.77	0.07	202,205,207,208	0
6	BMA	K	3	11/12	0.77	0.06	187,197,203,210	0
6	NAG	K	2	14/15	0.81	0.06	162,171,180,181	0
6	NAG	K	1	14/15	0.87	0.07	143,148,158,160	0
6	NAG	N	2	14/15	0.90	0.08	169,179,189,193	0
6	NAG	N	1	14/15	0.90	0.08	143,151,162,165	0

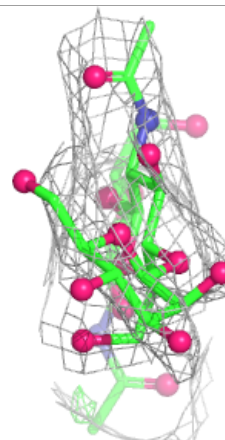
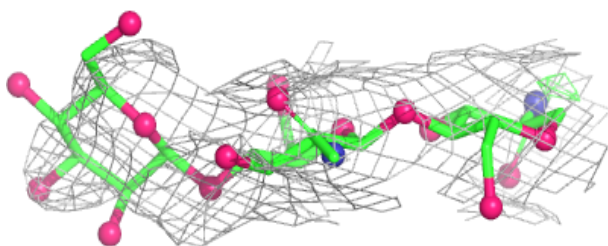
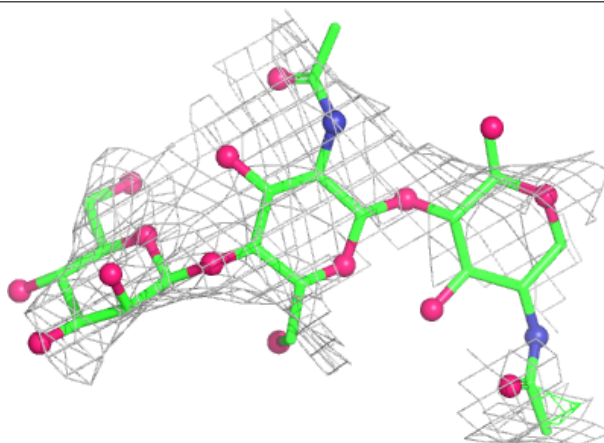
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain K:

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

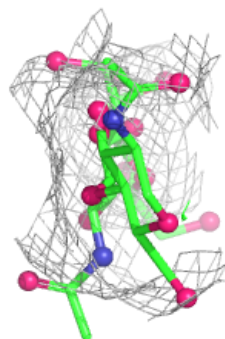
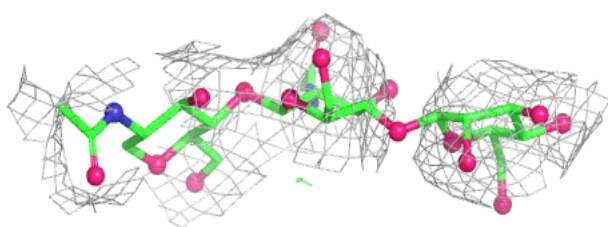
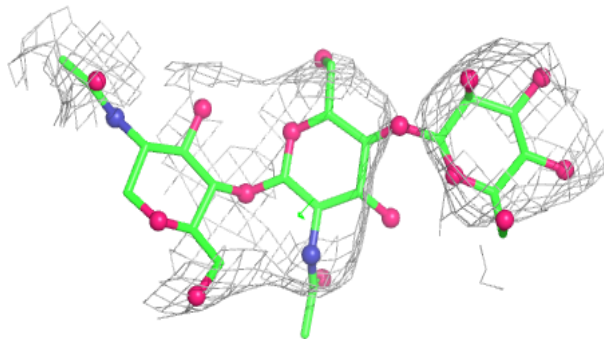
**Electron density around Chain L:**

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

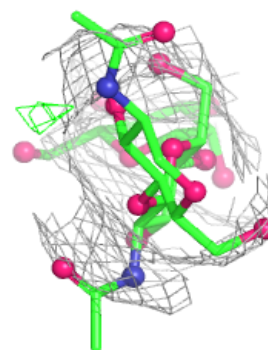
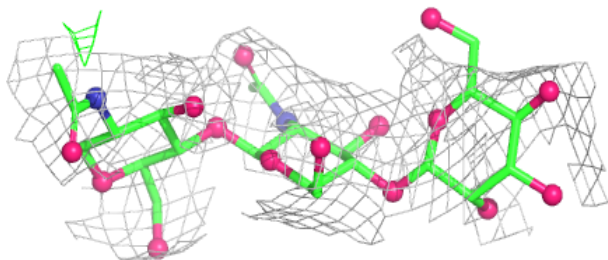
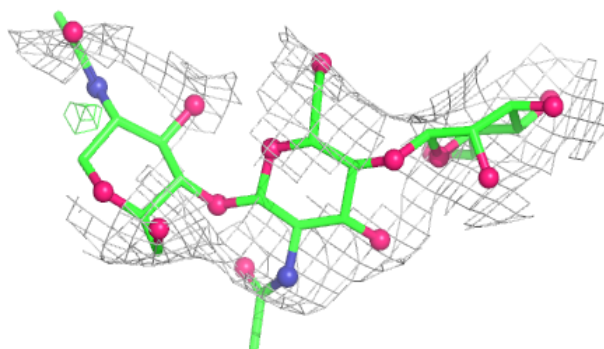


Electron density around Chain M:

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

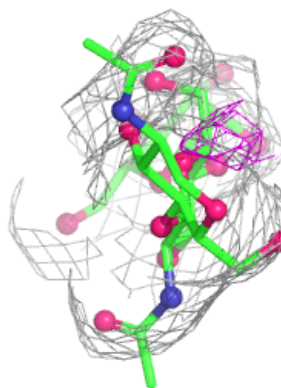
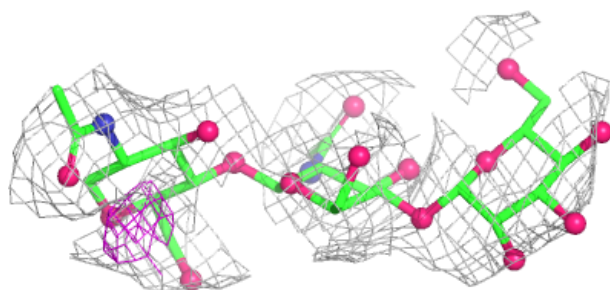
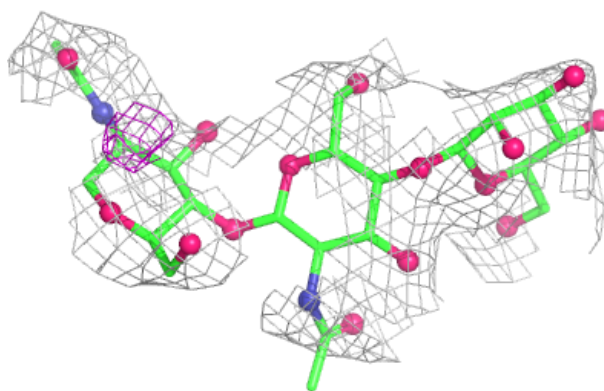
**Electron density around Chain N:**

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

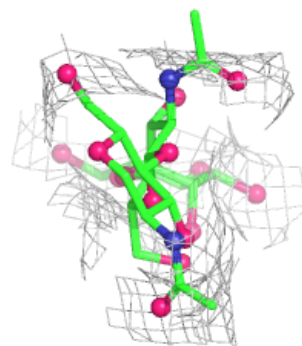
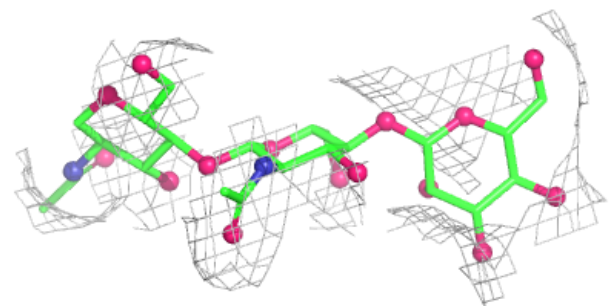
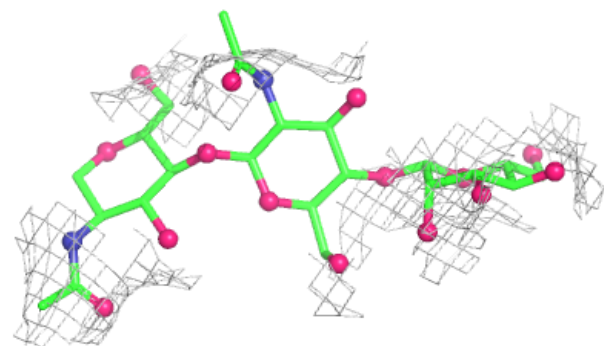


Electron density around Chain O:

$2mF_o-DF_c$ (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)



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.