



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:28 AM UTC

PDB ID : 3V4P / pdb_00003v4p
Title : crystal structure of a4b7 headpiece complexed with Fab ACT-1
Authors : Yu, Y.; Zhu, J.; Springer, T.A.
Deposited on : 2011-12-15
Resolution : 3.15 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

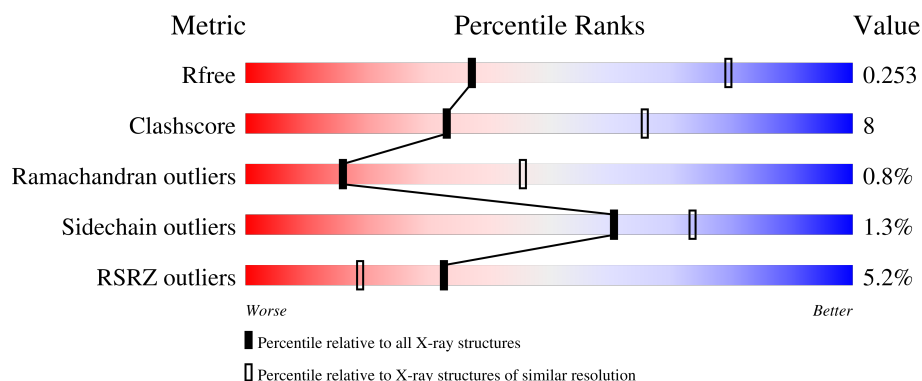
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	597	2% 74% 22% ..
1	C	597	% 73% 23% ..
2	B	503	3% 60% 14% 25%
2	D	503	5% 61% 13% 25%
3	H	219	10% 83% 13% ..

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Mol	Chain	Length	Quality of chain
3	M	219	13% 85% 10%
4	L	217	9% 85% 14%
4	N	217	9% 86% 13%
5	E	4	50% 25% 25%
5	F	4	25% 75%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21722 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 Integrin alpha-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	14	0	0
			4493	2834	773	864	22			
1	C	581	Total	C	N	O	S	19	0	0
			4496	2835	776	863	22			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	558	ALA	ARG	engineered mutation	UNP P13612
A	588	THR	-	expression tag	UNP P13612
A	589	GLY	-	expression tag	UNP P13612
A	590	GLY	-	expression tag	UNP P13612
A	591	LEU	-	expression tag	UNP P13612
A	592	GLU	-	expression tag	UNP P13612
A	593	ASN	-	expression tag	UNP P13612
A	594	LEU	-	expression tag	UNP P13612
A	595	TYR	-	expression tag	UNP P13612
A	596	PHE	-	expression tag	UNP P13612
A	597	GLN	-	expression tag	UNP P13612
C	558	ALA	ARG	engineered mutation	UNP P13612
C	588	THR	-	expression tag	UNP P13612
C	589	GLY	-	expression tag	UNP P13612
C	590	GLY	-	expression tag	UNP P13612
C	591	LEU	-	expression tag	UNP P13612
C	592	GLU	-	expression tag	UNP P13612
C	593	ASN	-	expression tag	UNP P13612
C	594	LEU	-	expression tag	UNP P13612
C	595	TYR	-	expression tag	UNP P13612
C	596	PHE	-	expression tag	UNP P13612
C	597	GLN	-	expression tag	UNP P13612

- Molecule 2 is a protein called Integrin beta-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	6	2	0
			2922	1828	519	563	12			
2	D	375	Total	C	N	O	S	0	1	0
			2916	1824	518	562	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	494	SER	-	expression tag	UNP P26010
B	495	ARG	-	expression tag	UNP P26010
B	496	GLY	-	expression tag	UNP P26010
B	497	LEU	-	expression tag	UNP P26010
B	498	GLU	-	expression tag	UNP P26010
B	499	ASN	-	expression tag	UNP P26010
B	500	LEU	-	expression tag	UNP P26010
B	501	TYR	-	expression tag	UNP P26010
B	502	PHE	-	expression tag	UNP P26010
B	503	GLN	-	expression tag	UNP P26010
D	494	SER	-	expression tag	UNP P26010
D	495	ARG	-	expression tag	UNP P26010
D	496	GLY	-	expression tag	UNP P26010
D	497	LEU	-	expression tag	UNP P26010
D	498	GLU	-	expression tag	UNP P26010
D	499	ASN	-	expression tag	UNP P26010
D	500	LEU	-	expression tag	UNP P26010
D	501	TYR	-	expression tag	UNP P26010
D	502	PHE	-	expression tag	UNP P26010
D	503	GLN	-	expression tag	UNP P26010

- Molecule 3 is a protein called MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	211	Total	C	N	O	S	0	0	0
			1607	1021	258	321	7			
3	M	211	Total	C	N	O	S	0	0	0
			1607	1021	258	321	7			

- Molecule 4 is a protein called MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN.

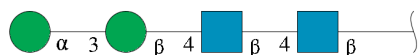
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	217	Total	C	N	O	S	0	0	0
			1681	1054	282	339	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	217	Total	C	N	O	S	0	0	0
			1681	1054	282	339	6			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

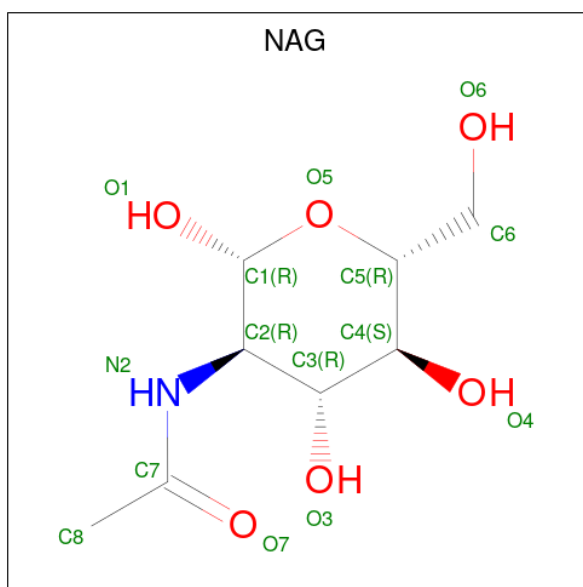


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

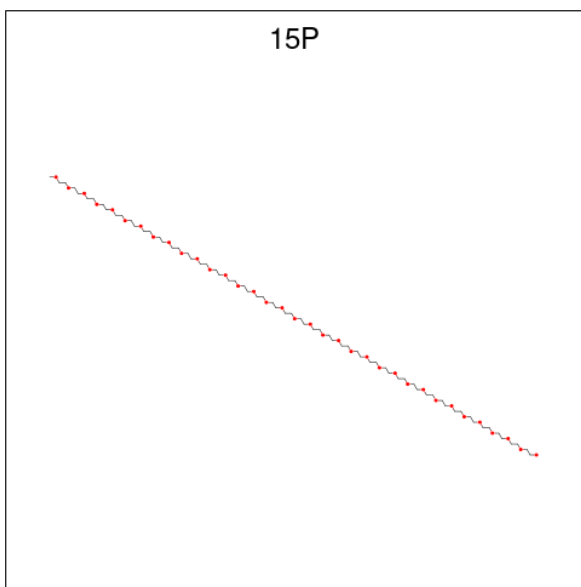
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Ca	0	0
			3	3		
6	B	2	Total	Ca	0	0
			2	2		
6	C	3	Total	Ca	0	0
			3	3		
6	D	2	Total	Ca	0	0
			2	2		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is POLYETHYLENE GLYCOL (N=34) (CCD ID: 15P) (formula: C₆₉H₁₄₀O₃₅).

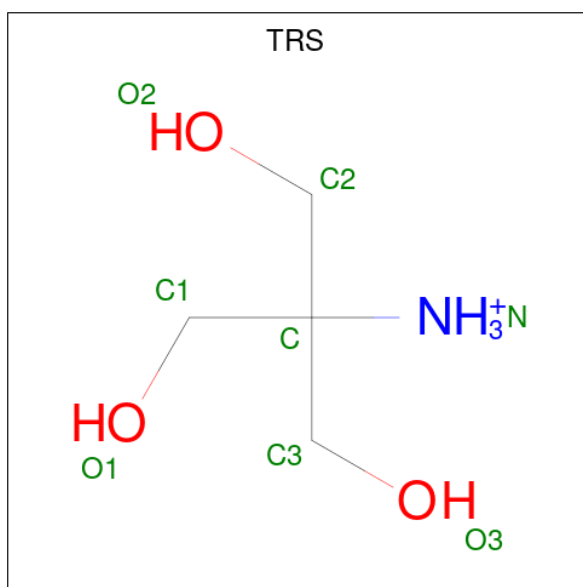


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			52	34	18		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

- Molecule 10 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	N	O	0	0
			8	4	1	3		

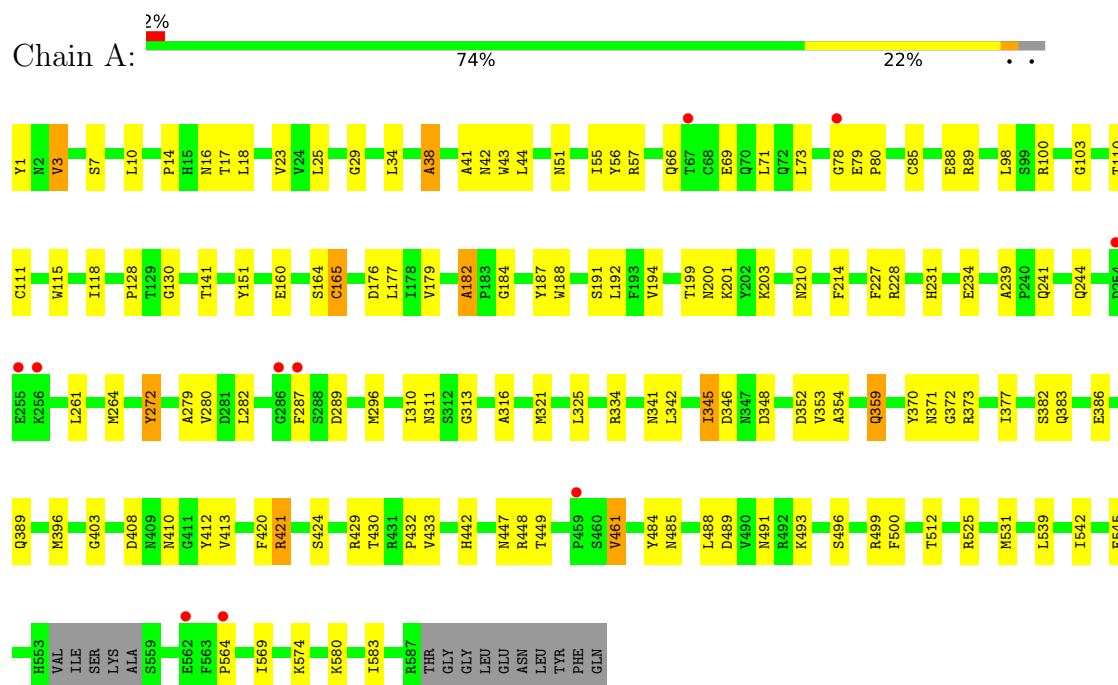
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	4	Total	O	0	0
			4	4		
11	B	7	Total	O	0	0
			7	7		
11	C	3	Total	O	0	0
			3	3		
11	D	7	Total	O	0	0
			7	7		

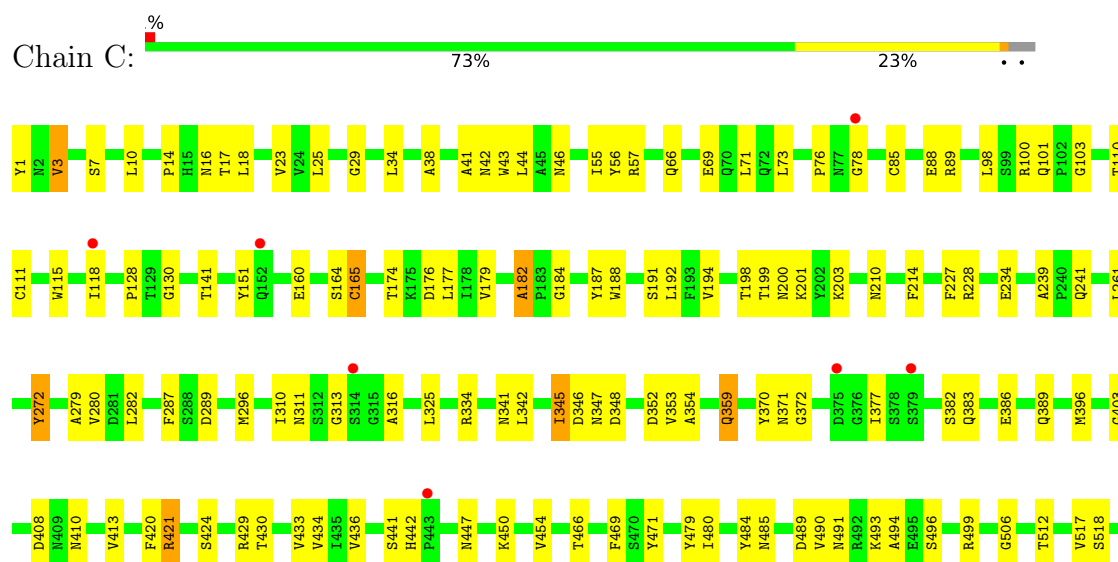
3 Residue-property plots

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: Integrin alpha-4

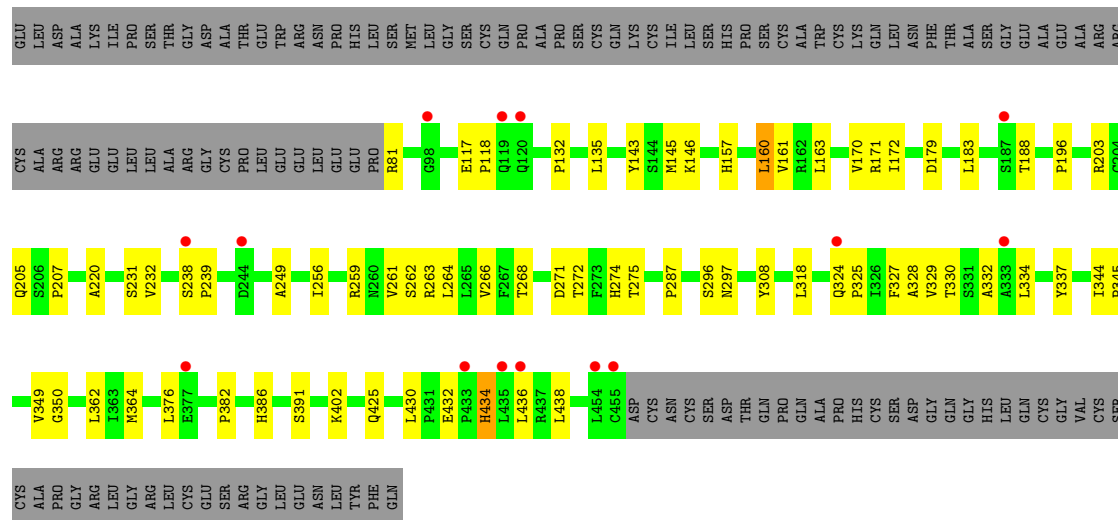


• Molecule 1: Integrin alpha-4

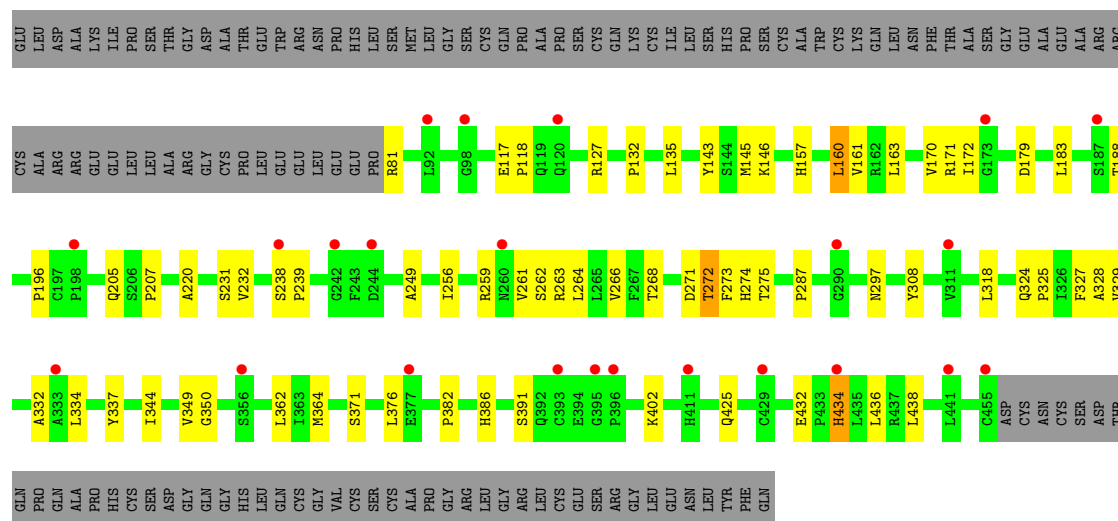




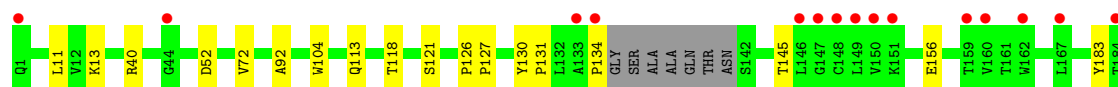
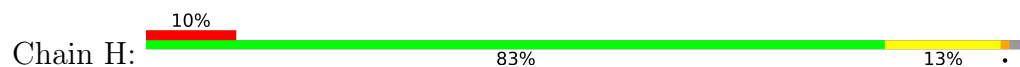
• Molecule 2: Integrin beta-7



• Molecule 2: Integrin beta-7

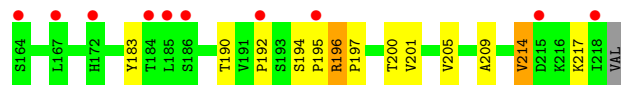
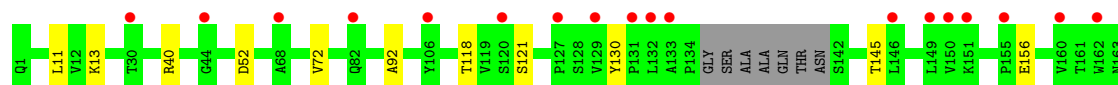
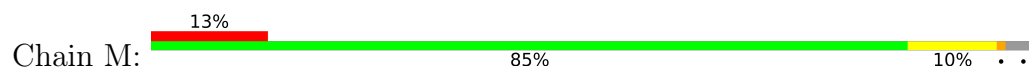


• Molecule 3: MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN

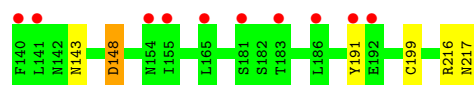
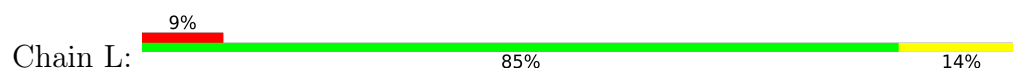




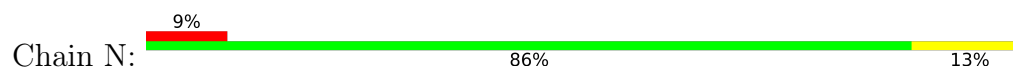
• Molecule 3: MONOCLONAL ANTIBODY Act-1 HEAVY CHAIN



• Molecule 4: MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN



• Molecule 4: MONOCLONAL ANTIBODY Act-1 LIGHT CHAIN



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	137.78Å 122.74Å 158.14Å 90.00° 115.38° 90.00°	Depositor
Resolution (Å)	46.13 – 3.15 46.13 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.13-3.15) 99.4 (46.13-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.220 , 0.251 0.224 , 0.253	Depositor DCC
R_{free} test set	1067 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å ²)	54.1	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 119.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	21722	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, MAN, 15P, NAG, CA, TRS

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	0.31	0/4593	0.77	8/6221 (0.1%)
1	C	0.31	0/4596	0.78	8/6224 (0.1%)
2	B	0.29	0/2984	0.71	0/4053
2	D	0.29	0/2978	0.71	0/4044
3	H	0.29	0/1652	0.70	2/2259 (0.1%)
3	M	0.28	0/1652	0.70	2/2259 (0.1%)
4	L	0.27	0/1722	0.68	0/2340
4	N	0.27	0/1722	0.69	0/2340
All	All	0.29	0/21899	0.73	20/29740 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	ILE	N-CA-C	6.26	116.42	110.53
1	C	345	ILE	N-CA-C	6.20	116.36	110.53
3	H	52	ASP	CA-C-N	5.88	125.35	119.24
3	H	52	ASP	C-N-CA	5.88	125.35	119.24
3	M	52	ASP	CA-C-N	5.86	125.33	119.24
3	M	52	ASP	C-N-CA	5.86	125.33	119.24
1	C	239	ALA	CA-C-N	5.85	125.53	119.56
1	C	239	ALA	C-N-CA	5.85	125.53	119.56
1	A	239	ALA	CA-C-N	5.80	125.48	119.56
1	A	239	ALA	C-N-CA	5.80	125.48	119.56
1	C	182	ALA	CA-C-N	5.56	125.39	119.28
1	C	182	ALA	C-N-CA	5.56	125.39	119.28
1	A	182	ALA	CA-C-N	5.50	125.32	119.28
1	A	182	ALA	C-N-CA	5.50	125.32	119.28
1	A	111	CYS	N-CA-C	5.17	116.84	109.14
1	C	38	ALA	CA-C-N	5.12	124.84	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	ALA	C-N-CA	5.12	124.84	119.82
1	C	111	CYS	N-CA-C	5.09	116.73	109.14
1	A	38	ALA	CA-C-N	5.07	124.79	119.82
1	A	38	ALA	C-N-CA	5.07	124.79	119.82

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	4493	0	4351	96	0
1	C	4496	0	4361	95	0
2	B	2922	0	2848	45	0
2	D	2916	0	2842	42	0
3	H	1607	0	1552	18	0
3	M	1607	0	1552	12	0
4	L	1681	0	1616	20	0
4	N	1681	0	1616	17	0
5	E	50	0	43	1	0
5	F	50	0	43	1	0
6	A	3	0	0	0	0
6	B	2	0	0	0	0
6	C	3	0	0	0	0
6	D	2	0	0	0	0
7	A	56	0	52	0	0
7	B	14	0	13	0	0
7	C	56	0	52	1	0
8	A	52	0	69	17	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	C	8	0	12	0	0
11	A	4	0	0	4	0
11	B	7	0	0	1	0
11	C	3	0	0	4	0
11	D	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21722	0	21022	332	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 8.

All (332) 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)
3:M:196:ARG:HD2	3:M:197:PRO:HA	1.59	0.83
3:H:196:ARG:HD2	3:H:197:PRO:HA	1.59	0.82
1:A:372:GLY:O	11:A:702:HOH:O	1.99	0.79
1:A:372:GLY:HA2	1:A:377:ILE:HG22	1.65	0.77
1:C:372:GLY:HA2	1:C:377:ILE:HG22	1.65	0.76
2:B:160:LEU:HD22	2:B:220:ALA:HB2	1.67	0.76
2:D:160:LEU:HD22	2:D:220:ALA:HB2	1.67	0.75
1:C:442:HIS:HE1	1:C:583:ILE:HB	1.53	0.74
1:A:442:HIS:HE1	1:A:583:ILE:HB	1.51	0.73
2:B:350:GLY:HA3	2:B:362:LEU:HD11	1.72	0.72
2:D:327:PHE:HB2	2:D:349:VAL:HG22	1.71	0.72
2:D:350:GLY:HA3	2:D:362:LEU:HD11	1.72	0.72
1:A:311:ASN:O	11:A:701:HOH:O	2.07	0.71
1:C:241:GLN:HE22	2:D:275:THR:HB	1.55	0.71
2:B:327:PHE:HB2	2:B:349:VAL:HG22	1.71	0.71
1:A:71:LEU:HB3	1:A:141:THR:HG21	1.73	0.71
1:C:71:LEU:HB3	1:C:141:THR:HG21	1.73	0.70
8:A:612:15P:H101	1:C:42:ASN:HD22	1.56	0.70
1:A:442:HIS:CE1	1:A:583:ILE:HB	2.26	0.69
1:A:16:ASN:HD22	8:A:612:15P:H252	1.57	0.68
2:D:146:LYS:HA	2:D:232:VAL:HG11	1.73	0.68
1:A:88:GLU:HB2	1:A:118:ILE:HG13	1.76	0.68
2:B:146:LYS:HA	2:B:232:VAL:HG11	1.74	0.68
1:C:88:GLU:HB2	1:C:118:ILE:HG13	1.76	0.67
1:C:372:GLY:O	11:C:702:HOH:O	2.13	0.67
1:C:430:THR:N	11:C:703:HOH:O	2.27	0.67
8:A:612:15P:H132	1:C:44:LEU:HD21	1.77	0.66
4:L:88:LEU:HD11	4:L:111:ILE:HD11	1.78	0.66
4:N:88:LEU:HD11	4:N:111:ILE:HD11	1.78	0.66
8:A:612:15P:H111	1:C:42:ASN:H	1.61	0.65
2:B:118:PRO:HB3	2:B:425:GLN:HB3	1.78	0.65
1:A:1:TYR:HA	1:A:383:GLN:HB2	1.79	0.64
1:C:1:TYR:HA	1:C:383:GLN:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:PRO:HB3	2:D:425:GLN:HB3	1.78	0.64
1:A:199:THR:O	1:A:201:LYS:N	2.31	0.63
2:D:382:PRO:HD3	2:D:436:LEU:HD21	1.80	0.63
1:C:199:THR:O	1:C:201:LYS:N	2.32	0.62
2:D:163:LEU:HB3	2:D:170:VAL:HG11	1.81	0.62
2:B:382:PRO:HD3	2:B:436:LEU:HD21	1.80	0.62
4:L:17:ASP:H	4:L:83:ILE:HG22	1.65	0.62
3:M:13:LYS:HG2	3:M:121:SER:HA	1.83	0.61
4:N:17:ASP:H	4:N:83:ILE:HG22	1.65	0.60
2:B:163:LEU:HB3	2:B:170:VAL:HG11	1.81	0.60
3:H:40:ARG:HG2	3:H:92:ALA:HB2	1.83	0.60
1:C:128:PRO:HD2	1:C:164:SER:HB3	1.85	0.59
3:M:40:ARG:HG2	3:M:92:ALA:HB2	1.82	0.59
1:A:128:PRO:HD2	1:A:164:SER:HB3	1.85	0.59
1:C:543:GLN:HG2	1:C:582:THR:HB	1.86	0.58
1:A:56:TYR:HE2	8:A:612:15P:H191	1.68	0.57
3:H:130:TYR:CG	4:L:129:GLN:HG2	2.40	0.57
1:C:311:ASN:O	11:C:701:HOH:O	2.18	0.57
1:A:17:THR:HB	1:A:41:ALA:HB2	1.86	0.57
4:L:216:ARG:HG2	4:L:217:ASN:H	1.71	0.56
1:A:545:GLU:HG2	1:A:580:LYS:HG2	1.86	0.56
3:M:200:THR:HG23	3:M:217:LYS:HD3	1.87	0.56
4:N:148:ASP:N	4:N:148:ASP:OD1	2.39	0.56
1:C:17:THR:HB	1:C:41:ALA:HB2	1.87	0.56
1:C:14:PRO:HB2	1:C:17:THR:HG21	1.88	0.56
3:H:200:THR:HG23	3:H:217:LYS:HD3	1.87	0.55
1:A:287:PHE:HB3	1:A:311:ASN:ND2	2.20	0.55
1:C:491:ASN:C	1:C:493:LYS:H	2.14	0.55
1:A:14:PRO:HB2	1:A:17:THR:HG21	1.89	0.55
1:A:100:ARG:NH2	1:A:103:GLY:O	2.40	0.55
2:B:132:PRO:HB2	2:B:261:VAL:HG11	1.87	0.55
1:C:228:ARG:HD3	1:C:261:LEU:HD11	1.87	0.55
1:C:493:LYS:HB2	1:C:496:SER:HB2	1.89	0.55
4:L:148:ASP:OD1	4:L:148:ASP:N	2.39	0.55
2:B:376:LEU:HD11	2:B:438:LEU:HB3	1.90	0.54
1:C:287:PHE:HB3	1:C:311:ASN:ND2	2.22	0.54
1:A:342:LEU:HB3	1:A:352:ASP:O	2.08	0.54
1:C:100:ARG:NH2	1:C:103:GLY:O	2.40	0.54
1:C:371:ASN:HB3	11:C:702:HOH:O	2.07	0.54
4:L:122:ILE:HD12	4:L:199:CYS:HB2	1.90	0.54
1:A:56:TYR:CE2	8:A:612:15P:H191	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:ASN:HB3	1:C:450:LYS:HG2	1.89	0.54
1:A:228:ARG:HD3	1:A:261:LEU:HD11	1.88	0.54
1:A:346:ASP:HB2	1:A:433:VAL:HG11	1.90	0.54
1:C:359:GLN:HE21	2:D:287:PRO:HG3	1.71	0.54
2:B:135:LEU:HD11	2:B:266:VAL:HG23	1.89	0.54
1:C:442:HIS:CE1	1:C:583:ILE:HB	2.39	0.54
2:D:264:LEU:HD23	2:D:324:GLN:HB2	1.90	0.54
2:D:376:LEU:HD11	2:D:438:LEU:HB3	1.90	0.54
2:D:135:LEU:HD11	2:D:266:VAL:HG23	1.89	0.53
1:A:228:ARG:HH11	1:A:261:LEU:HD11	1.74	0.53
2:B:264:LEU:HD23	2:B:324:GLN:HB2	1.90	0.53
4:N:122:ILE:HD12	4:N:199:CYS:HB2	1.90	0.53
2:B:205:GLN:HE21	2:B:231:SER:H	1.57	0.53
2:D:135:LEU:HB3	2:D:172:ILE:HG22	1.91	0.53
1:C:469:PHE:HB2	1:C:517:VAL:HG21	1.90	0.53
3:H:130:TYR:CD1	4:L:129:GLN:HG2	2.44	0.53
3:H:205:VAL:HB	3:H:214:VAL:HG13	1.91	0.53
1:C:342:LEU:HB3	1:C:352:ASP:O	2.08	0.52
3:M:205:VAL:HB	3:M:214:VAL:HG13	1.92	0.52
1:A:461:VAL:HG13	1:A:531:MET:HB3	1.91	0.52
1:A:491:ASN:HD21	1:A:542:ILE:HA	1.75	0.52
2:B:183:LEU:HG	2:B:188:THR:HG23	1.92	0.52
1:C:228:ARG:HH11	1:C:261:LEU:HD11	1.74	0.52
1:A:493:LYS:HB2	1:A:496:SER:HB2	1.92	0.52
2:D:183:LEU:HG	2:D:188:THR:HG23	1.92	0.52
2:D:205:GLN:HE21	2:D:231:SER:H	1.57	0.52
1:A:57:ARG:HD3	1:A:71:LEU:HD21	1.92	0.52
1:A:408:ASP:OD2	1:A:429:ARG:HD2	2.10	0.52
2:D:238:SER:N	2:D:239:PRO:HD2	2.25	0.52
2:B:238:SER:N	2:B:239:PRO:HD2	2.24	0.51
2:B:261:VAL:O	2:B:263:ARG:HG3	2.10	0.51
1:A:184:GLY:HA2	1:A:188:TRP:CD1	2.45	0.51
2:B:135:LEU:HB3	2:B:172:ILE:HG22	1.92	0.51
1:C:57:ARG:HD3	1:C:71:LEU:HD21	1.92	0.51
1:C:184:GLY:HA2	1:C:188:TRP:CD1	2.46	0.51
4:N:216:ARG:HG2	4:N:217:ASN:H	1.75	0.51
8:A:612:15P:H14	1:C:16:ASN:HD21	1.75	0.51
2:D:261:VAL:O	2:D:263:ARG:HG3	2.10	0.51
2:D:179:ASP:OD1	2:D:308:TYR:OH	2.26	0.51
1:C:18:LEU:HD22	1:C:420:PHE:HD2	1.76	0.51
1:C:408:ASP:OD2	1:C:429:ARG:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:330:THR:HG21	11:B:2106:HOH:O	2.11	0.50
1:C:485:ASN:HB3	1:C:512:THR:HG22	1.93	0.50
1:A:41:ALA:HA	8:A:612:15P:H231	1.92	0.50
1:C:272:TYR:HB2	1:C:296:MET:HB2	1.94	0.50
1:A:396:MET:HG3	1:A:421:ARG:HG3	1.92	0.50
2:D:127:ARG:NH2	2:D:371:SER:OG	2.44	0.50
1:A:241:GLN:HE22	2:B:275:THR:HB	1.77	0.50
2:B:261:VAL:HG12	2:B:262:SER:N	2.27	0.50
1:A:210:ASN:O	1:A:210:ASN:ND2	2.45	0.50
1:A:447:ASN:C	1:A:449:THR:H	2.20	0.50
1:C:179:VAL:HG22	1:C:194:VAL:HG12	1.93	0.50
1:A:359:GLN:HE21	2:B:287:PRO:HG3	1.77	0.50
1:A:489:ASP:OD2	1:A:499:ARG:HD3	2.12	0.50
1:C:342:LEU:HD22	1:C:354:ALA:HB2	1.94	0.49
1:A:231:HIS:CD2	5:E:4:MAN:H62	2.47	0.49
1:C:346:ASP:HB2	1:C:433:VAL:HG11	1.94	0.49
1:A:429:ARG:HH12	1:A:564:PRO:HD2	1.78	0.49
1:A:18:LEU:HD22	1:A:420:PHE:HD2	1.76	0.49
1:A:179:VAL:HG22	1:A:194:VAL:HG12	1.93	0.49
1:A:272:TYR:HB2	1:A:296:MET:HB2	1.94	0.49
1:C:10:LEU:HD11	1:C:424:SER:HB2	1.95	0.49
4:N:42:LEU:HB2	4:N:52:LEU:HD11	1.95	0.49
1:A:342:LEU:HD22	1:A:354:ALA:HB2	1.94	0.49
4:L:42:LEU:HB2	4:L:52:LEU:HD11	1.95	0.49
1:C:396:MET:HG3	1:C:421:ARG:HG3	1.94	0.48
2:D:261:VAL:HG12	2:D:262:SER:N	2.28	0.48
1:C:280:VAL:O	1:C:289:ASP:HB2	2.13	0.48
1:C:25:LEU:HD12	1:C:403:GLY:HA2	1.95	0.48
4:L:42:LEU:HD13	4:L:91:TYR:CZ	2.48	0.48
2:B:268:THR:HA	2:B:328:ALA:O	2.14	0.48
1:C:489:ASP:O	1:C:493:LYS:HE3	2.13	0.48
4:L:125:PRO:HD3	4:L:137:VAL:HG22	1.95	0.48
1:A:10:LEU:HD11	1:A:424:SER:HB2	1.96	0.48
1:C:489:ASP:OD2	1:C:499:ARG:HD3	2.13	0.48
2:D:272:THR:OG1	2:D:273:PHE:N	2.45	0.48
1:A:16:ASN:ND2	8:A:612:15P:H252	2.27	0.48
1:A:484:TYR:OH	1:A:525:ARG:HD3	2.13	0.48
1:A:280:VAL:O	1:A:289:ASP:HB2	2.13	0.48
2:B:179:ASP:OD1	2:B:308:TYR:OH	2.26	0.48
1:C:261:LEU:HD13	1:C:316:ALA:HB2	1.96	0.47
4:N:125:PRO:HD3	4:N:137:VAL:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:156:GLU:HG2	3:H:183:TYR:CE2	2.48	0.47
1:C:334:ARG:HG3	1:C:359:GLN:OE1	2.15	0.47
4:N:71:GLY:HA3	4:N:76:PHE:HA	1.96	0.47
1:C:210:ASN:O	1:C:210:ASN:ND2	2.47	0.47
1:A:1:TYR:HD1	1:A:569:ILE:HD13	1.79	0.47
1:C:436:VAL:HA	1:C:471:TYR:HA	1.96	0.47
2:D:268:THR:HA	2:D:328:ALA:O	2.14	0.47
3:H:13:LYS:HG2	3:H:121:SER:HA	1.96	0.47
4:N:42:LEU:HD13	4:N:91:TYR:CZ	2.49	0.47
1:A:7:SER:HB3	1:A:429:ARG:HH11	1.79	0.47
2:B:196:PRO:HG3	2:B:207:PRO:HD3	1.97	0.47
1:C:194:VAL:HG23	1:C:203:LYS:HB2	1.97	0.47
3:M:156:GLU:HG2	3:M:183:TYR:CE2	2.49	0.47
3:M:145:THR:HG22	3:M:190:THR:HG23	1.97	0.47
1:A:23:VAL:HG13	1:A:34:LEU:HD11	1.97	0.47
1:A:42:ASN:H	8:A:612:15P:C23	2.28	0.47
1:A:334:ARG:HG3	1:A:359:GLN:OE1	2.14	0.47
2:B:132:PRO:HB2	2:B:261:VAL:CG1	2.46	0.47
4:L:125:PRO:HG2	4:L:191:TYR:CE1	2.50	0.47
1:A:194:VAL:HG23	1:A:203:LYS:HB2	1.97	0.46
2:D:196:PRO:HG3	2:D:207:PRO:HD3	1.95	0.46
2:D:386:HIS:HB2	2:D:425:GLN:HG3	1.96	0.46
1:C:7:SER:HB3	1:C:429:ARG:HH11	1.80	0.46
2:D:324:GLN:HA	2:D:325:PRO:HD3	1.71	0.46
4:N:125:PRO:HG2	4:N:191:TYR:CE1	2.50	0.46
1:A:227:PHE:HD1	1:A:234:GLU:HB2	1.80	0.46
1:A:261:LEU:HD13	1:A:316:ALA:HB2	1.97	0.46
2:B:329:VAL:HG11	2:B:337:TYR:CD2	2.51	0.46
1:C:434:VAL:HG23	1:C:570:LEU:HA	1.97	0.46
4:L:71:GLY:HA3	4:L:76:PHE:HA	1.96	0.46
1:A:25:LEU:HD12	1:A:403:GLY:HA2	1.96	0.46
1:A:165:CYS:HB2	1:A:182:ALA:HB1	1.98	0.46
2:B:203:ARG:HB3	3:H:104:TRP:CD1	2.51	0.46
2:D:325:PRO:HG2	2:D:344:ILE:HG21	1.98	0.46
1:A:371:ASN:HB3	11:A:702:HOH:O	2.16	0.46
1:C:227:PHE:HD1	1:C:234:GLU:HB2	1.80	0.46
1:C:434:VAL:HG23	1:C:570:LEU:HD23	1.98	0.46
1:A:289:ASP:OD1	1:A:310:ILE:HA	2.16	0.46
1:C:479:TYR:HA	1:C:518:SER:HA	1.97	0.46
1:A:429:ARG:HB3	11:A:704:HOH:O	2.15	0.46
1:C:23:VAL:HG13	1:C:34:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:CYS:HB2	1:C:182:ALA:HB1	1.98	0.46
1:A:227:PHE:CD1	1:A:234:GLU:HB2	2.51	0.46
1:C:289:ASP:OD1	1:C:310:ILE:HA	2.15	0.46
2:B:325:PRO:HG2	2:B:344:ILE:HG21	1.98	0.45
2:B:386:HIS:HB2	2:B:425:GLN:HG3	1.96	0.45
2:B:432:GLU:HB2	2:B:434:HIS:NE2	2.31	0.45
1:C:85:CYS:HB2	1:C:151:TYR:CE1	2.51	0.45
3:H:145:THR:HG22	3:H:190:THR:HG23	1.97	0.45
1:A:44:LEU:HD22	8:A:612:15P:H131	1.97	0.45
1:C:73:LEU:HD23	1:C:141:THR:HB	1.98	0.45
1:C:89:ARG:NH2	7:C:604:NAG:O6	2.42	0.45
2:D:329:VAL:HG11	2:D:337:TYR:CD2	2.51	0.45
1:A:73:LEU:HD23	1:A:141:THR:HB	1.99	0.45
1:A:85:CYS:HB2	1:A:151:TYR:CE1	2.51	0.45
8:A:612:15P:H161	1:C:69:GLU:HA	1.99	0.45
1:C:227:PHE:CD1	1:C:234:GLU:HB2	2.51	0.45
1:C:287:PHE:CE2	1:C:313:GLY:HA2	2.51	0.45
2:D:332:ALA:C	2:D:334:LEU:H	2.25	0.45
1:A:115:TRP:HB3	1:A:130:GLY:HA2	1.97	0.45
1:A:287:PHE:CE2	1:A:313:GLY:HA2	2.52	0.45
1:C:115:TRP:HB3	1:C:130:GLY:HA2	1.97	0.45
1:C:198:THR:HG21	5:F:2:NAG:H82	1.98	0.45
2:D:432:GLU:HB2	2:D:434:HIS:NE2	2.31	0.44
1:C:176:ASP:HB3	1:C:177:LEU:HD12	2.00	0.44
1:C:282:LEU:HD13	1:C:377:ILE:HG23	2.00	0.44
1:A:373:ARG:NH1	1:A:574:LYS:HA	2.32	0.44
2:D:391:SER:H	2:D:402:LYS:HE3	1.83	0.44
1:A:346:ASP:O	1:A:433:VAL:HG21	2.17	0.44
1:C:441:SER:HB2	1:C:466:THR:HB	2.00	0.44
3:H:126:PRO:HA	3:H:127:PRO:HD3	1.85	0.44
3:H:134:PRO:HD3	4:L:123:PHE:CE1	2.52	0.44
1:A:282:LEU:HD13	1:A:377:ILE:HG23	2.00	0.44
2:B:296:SER:HB3	4:N:65:ASP:CG	2.43	0.44
2:B:332:ALA:C	2:B:334:LEU:H	2.25	0.44
1:C:279:ALA:O	1:C:341:ASN:ND2	2.49	0.44
1:A:493:LYS:HD2	1:A:496:SER:HB2	1.99	0.44
1:A:191:SER:O	1:A:192:LEU:HD23	2.18	0.44
1:A:485:ASN:HB3	1:A:512:THR:HG22	2.00	0.44
4:N:8:PRO:O	4:N:107:THR:OG1	2.30	0.44
2:B:171:ARG:HD3	2:B:259:ARG:HD3	2.00	0.44
1:A:491:ASN:C	1:A:493:LYS:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:201:VAL:O	3:M:217:LYS:HG3	2.18	0.43
2:B:249:ALA:HA	2:B:256:ILE:HD11	1.99	0.43
1:C:480:ILE:HD12	1:C:480:ILE:HA	1.89	0.43
1:A:386:GLU:HG2	1:A:389:GLN:HG3	2.00	0.43
2:B:324:GLN:HA	2:B:325:PRO:HD3	1.71	0.43
1:C:386:GLU:HG2	1:C:389:GLN:HG3	2.00	0.43
1:A:279:ALA:O	1:A:341:ASN:ND2	2.51	0.43
3:H:201:VAL:O	3:H:217:LYS:HG3	2.18	0.43
8:A:612:15P:H152	1:C:56:TYR:HE2	1.84	0.43
2:B:81:ARG:HA	2:B:117:GLU:OE1	2.18	0.43
2:B:391:SER:H	2:B:402:LYS:HE3	1.83	0.43
1:C:3:VAL:HA	1:C:430:THR:HA	2.01	0.43
1:C:442:HIS:HE1	1:C:583:ILE:CB	2.28	0.43
4:N:31:LYS:HE2	4:N:97:THR:HA	1.99	0.43
4:L:8:PRO:O	4:L:107:THR:OG1	2.30	0.43
2:B:163:LEU:HD23	2:B:364:MET:HE1	2.01	0.42
1:C:98:LEU:HD23	1:C:110:THR:HB	2.00	0.42
1:A:160:GLU:HB3	1:A:187:TYR:CE2	2.54	0.42
1:C:57:ARG:HE	1:C:69:GLU:CD	2.27	0.42
1:C:191:SER:O	1:C:192:LEU:HD23	2.18	0.42
1:A:244:GLN:HE21	1:A:244:GLN:HB3	1.71	0.42
1:C:160:GLU:HB3	1:C:187:TYR:CE2	2.54	0.42
2:D:81:ARG:HA	2:D:117:GLU:OE1	2.18	0.42
1:A:98:LEU:HD23	1:A:110:THR:HB	2.01	0.42
1:A:321:MET:HE2	1:A:321:MET:HB3	1.96	0.42
3:H:130:TYR:HA	3:H:131:PRO:HD3	1.88	0.42
1:A:176:ASP:HB3	1:A:177:LEU:HD12	2.00	0.42
1:A:412:TYR:CZ	1:A:432:PRO:HA	2.54	0.42
1:C:43:TRP:CH2	1:C:89:ARG:HD2	2.55	0.42
1:C:348:ASP:OD1	1:C:348:ASP:C	2.63	0.42
2:D:171:ARG:HD3	2:D:259:ARG:HD3	2.00	0.42
2:D:239:PRO:O	2:D:274:HIS:CD2	2.73	0.42
2:D:132:PRO:HB2	2:D:261:VAL:CG1	2.49	0.42
2:D:249:ALA:HA	2:D:256:ILE:HD11	2.00	0.42
2:D:259:ARG:O	2:D:261:VAL:N	2.53	0.42
4:L:31:LYS:HE2	4:L:97:THR:HA	2.00	0.42
3:M:11:LEU:HB3	3:M:118:THR:HB	2.01	0.42
1:A:57:ARG:HE	1:A:69:GLU:CD	2.28	0.42
8:A:612:15P:H142	1:C:56:TYR:CE2	2.55	0.42
1:C:410:ASN:OD1	1:C:410:ASN:C	2.63	0.42
3:H:11:LEU:HB3	3:H:118:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:130:TYR:HD1	4:N:128:GLU:HB2	1.84	0.42
3:M:194:SER:HB2	3:M:195:PRO:HD3	2.01	0.42
2:B:259:ARG:O	2:B:261:VAL:N	2.52	0.42
3:M:192:PRO:O	3:M:195:PRO:HD2	2.20	0.42
4:N:31:LYS:HE3	4:N:37:TYR:CE2	2.54	0.42
1:A:43:TRP:CH2	1:A:89:ARG:HD2	2.55	0.41
2:B:318:LEU:HD13	2:B:325:PRO:HG3	2.01	0.41
4:L:117:ALA:HA	4:L:118:PRO:HD3	1.89	0.41
1:A:42:ASN:H	8:A:612:15P:H231	1.85	0.41
3:H:194:SER:HB2	3:H:195:PRO:HD3	2.01	0.41
1:A:10:LEU:O	1:A:66:GLN:HG3	2.20	0.41
2:D:318:LEU:HD13	2:D:325:PRO:HG3	2.02	0.41
4:L:31:LYS:HE3	4:L:37:TYR:CE2	2.55	0.41
1:C:241:GLN:NE2	2:D:275:THR:HB	2.27	0.41
2:D:163:LEU:HD23	2:D:364:MET:HE1	2.01	0.41
1:C:10:LEU:O	1:C:66:GLN:HG3	2.21	0.41
1:C:325:LEU:HD22	1:C:370:TYR:CE2	2.55	0.41
1:C:46:ASN:ND2	1:C:76:PRO:O	2.50	0.41
1:A:1:TYR:HB3	1:A:382:SER:HB3	2.03	0.41
1:A:51:ASN:HD21	8:A:612:15P:H261	1.86	0.41
1:C:187:TYR:HB2	1:C:214:PHE:CD1	2.56	0.41
1:C:494:ALA:C	1:C:496:SER:H	2.29	0.41
1:A:17:THR:HB	1:A:38:ALA:HB1	2.03	0.41
1:A:187:TYR:HB2	1:A:214:PHE:CD1	2.56	0.41
1:A:410:ASN:OD1	1:A:410:ASN:C	2.63	0.41
2:B:430:LEU:HD13	2:B:434:HIS:CD2	2.56	0.41
1:C:345:ILE:HG22	1:C:352:ASP:OD2	2.21	0.41
3:H:192:PRO:O	3:H:195:PRO:HD2	2.20	0.41
1:A:325:LEU:HD22	1:A:370:TYR:CE2	2.56	0.41
1:C:540:THR:HA	1:C:541:PRO:HD3	1.88	0.41
2:D:143:TYR:C	2:D:145:MET:H	2.29	0.41
3:H:113:GLN:HA	4:L:48:SER:HB3	2.02	0.41
1:A:3:VAL:HA	1:A:430:THR:HA	2.03	0.40
1:A:345:ILE:HG22	1:A:352:ASP:OD2	2.22	0.40
2:B:239:PRO:O	2:B:274:HIS:CD2	2.74	0.40
2:B:344:ILE:HA	2:B:345:PRO:HD3	1.94	0.40
1:C:101:GLN:HG3	1:C:174:THR:O	2.21	0.40
1:C:484:TYR:OH	1:C:525:ARG:HD3	2.21	0.40
4:N:154:ASN:HB2	4:N:198:THR:HB	2.03	0.40
1:A:348:ASP:OD1	1:A:348:ASP:C	2.63	0.40
1:A:488:LEU:HD13	1:A:500:PHE:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:TYR:C	2:B:145:MET:H	2.30	0.40
2:B:203:ARG:HD3	4:L:33:TYR:CZ	2.56	0.40
1:C:347:ASN:O	1:C:347:ASN:ND2	2.55	0.40
1:A:16:ASN:HD21	8:A:612:15P:H302	1.85	0.40
1:A:79:GLU:HA	1:A:80:PRO:HD3	1.99	0.40
1:A:264:MET:HE3	1:A:264:MET:HB2	2.02	0.40
2:D:157:HIS:O	2:D:161:VAL:HG23	2.21	0.40
2:D:239:PRO:HB3	2:D:272:THR:HG23	2.03	0.40
4:L:23:CYS:HB2	4:L:40:TRP:CH2	2.57	0.40
1:C:1:TYR:HB3	1:C:382:SER:HB3	2.03	0.40
4:N:23:CYS:HB2	4:N:40:TRP:CH2	2.57	0.40
2:B:157:HIS:O	2:B:161:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	578/597 (97%)	520 (90%)	53 (9%)	5 (1%)	14	43
1	C	577/597 (97%)	523 (91%)	48 (8%)	6 (1%)	12	41
2	B	375/503 (75%)	328 (88%)	44 (12%)	3 (1%)	16	46
2	D	374/503 (74%)	330 (88%)	42 (11%)	2 (0%)	24	55
3	H	207/219 (94%)	186 (90%)	20 (10%)	1 (0%)	24	55
3	M	207/219 (94%)	186 (90%)	20 (10%)	1 (0%)	24	55
4	L	215/217 (99%)	201 (94%)	12 (6%)	2 (1%)	14	43
4	N	215/217 (99%)	201 (94%)	12 (6%)	2 (1%)	14	43
All	All	2748/3072 (90%)	2475 (90%)	251 (9%)	22 (1%)	16	46

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	ASN
1	C	200	ASN
4	L	73	GLY
4	N	73	GLY
1	A	29	GLY
1	A	448	ARG
1	C	29	GLY
2	D	272	THR
1	A	539	LEU
2	B	434	HIS
2	D	434	HIS
3	H	209	ALA
4	L	143	ASN
3	M	209	ALA
4	N	143	ASN
2	B	272[A]	THR
2	B	272[B]	THR
1	C	454	VAL
1	C	490	VAL
1	C	506	GLY
1	A	78	GLY
1	C	78	GLY

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	486/500 (97%)	477 (98%)	9 (2%)	50	69
1	C	487/500 (97%)	478 (98%)	9 (2%)	51	70
2	B	325/431 (75%)	321 (99%)	4 (1%)	63	74
2	D	324/431 (75%)	320 (99%)	4 (1%)	63	74
3	H	183/188 (97%)	180 (98%)	3 (2%)	55	71
3	M	183/188 (97%)	180 (98%)	3 (2%)	55	71
4	L	194/194 (100%)	193 (100%)	1 (0%)	81	82
4	N	194/194 (100%)	193 (100%)	1 (0%)	81	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2376/2626 (90%)	2342 (99%)	34 (1%)	61	73

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	55	ILE
1	A	165	CYS
1	A	272	TYR
1	A	353	VAL
1	A	359	GLN
1	A	413	VAL
1	A	421	ARG
1	A	461	VAL
2	B	160	LEU
2	B	271[A]	ASP
2	B	271[B]	ASP
2	B	297	ASN
1	C	3	VAL
1	C	55	ILE
1	C	165	CYS
1	C	272	TYR
1	C	353	VAL
1	C	359	GLN
1	C	413	VAL
1	C	421	ARG
1	C	550	LEU
2	D	160	LEU
2	D	271[A]	ASP
2	D	271[B]	ASP
2	D	297	ASN
3	H	72	VAL
3	H	196	ARG
3	H	214	VAL
4	L	148	ASP
3	M	72	VAL
3	M	196	ARG
3	M	214	VAL
4	N	148	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	28	HIS
1	A	51	ASN
1	A	161	ASN
1	A	211	GLN
1	A	242	HIS
1	A	347	ASN
1	A	359	GLN
1	A	399	GLN
1	A	404	GLN
2	B	120	GLN
2	B	154	GLN
2	B	157	HIS
2	B	313	GLN
2	B	368	ASN
1	C	16	ASN
1	C	28	HIS
1	C	42	ASN
1	C	125	ASN
1	C	161	ASN
1	C	211	GLN
1	C	241	GLN
1	C	242	HIS
1	C	347	ASN
1	C	359	GLN
1	C	399	GLN
1	C	404	GLN
1	C	442	HIS
2	D	154	GLN
2	D	157	HIS
2	D	205	GLN
2	D	230	GLN
2	D	322	ASN
2	D	368	ASN
2	D	452	HIS
3	H	59	ASN
4	L	47	GLN
4	L	50	GLN
3	M	59	ASN
3	M	172	HIS
4	N	43	HIS
4	N	47	GLN
4	N	50	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 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	$\# Z > 2$
5	NAG	E	1	1,5	14,14,15	0.62	0	17,19,21	0.73	0
5	NAG	E	2	5	14,14,15	0.54	0	17,19,21	0.66	0
5	BMA	E	3	5	11,11,12	0.80	0	15,15,17	1.44	2 (13%)
5	MAN	E	4	5	11,11,12	0.44	0	15,15,17	1.49	1 (6%)
5	NAG	F	1	1,5	14,14,15	0.57	0	17,19,21	1.30	3 (17%)
5	NAG	F	2	5	14,14,15	0.61	0	17,19,21	0.78	0
5	BMA	F	3	5	11,11,12	0.58	0	15,15,17	0.82	1 (6%)
5	MAN	F	4	5	11,11,12	0.58	0	15,15,17	0.61	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
5	NAG	E	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	NAG	F	1	1,5	-	1/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	4	MAN	C1-O5-C5	5.34	119.34	112.19
5	E	3	BMA	C1-C2-C3	4.01	115.48	109.64
5	E	3	BMA	C2-C3-C4	2.99	116.11	110.86
5	F	1	NAG	C2-N2-C7	2.60	126.38	122.90
5	F	1	NAG	C3-C4-C5	2.47	114.72	110.23
5	F	3	BMA	C1-C2-C3	2.14	112.76	109.64
5	F	1	NAG	O5-C1-C2	-2.04	108.14	111.29

There are no chirality outliers.

All (10) torsion outliers are listed below:

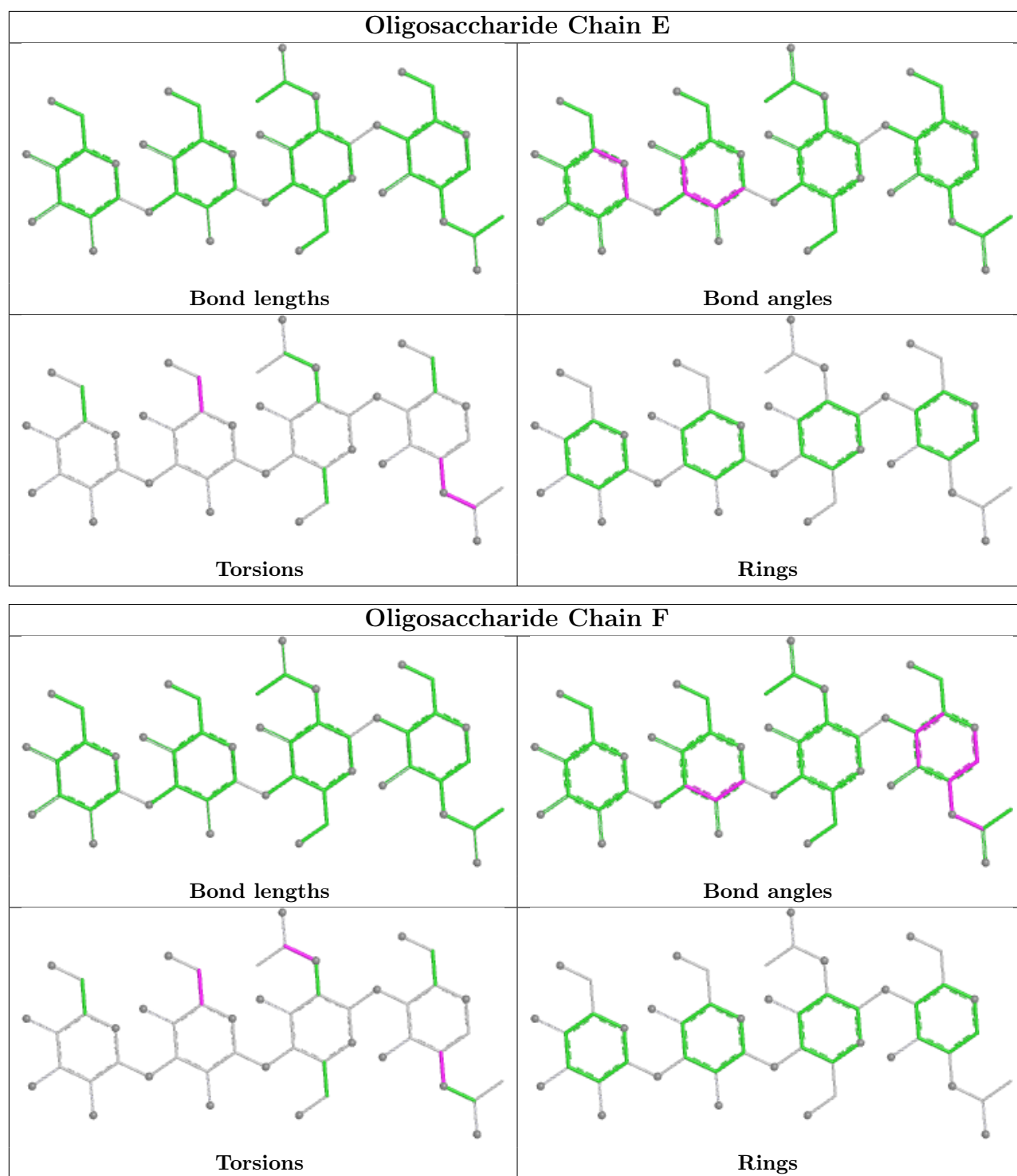
Mol	Chain	Res	Type	Atoms
5	E	1	NAG	C3-C2-N2-C7
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	F	1	NAG	C3-C2-N2-C7
5	F	3	BMA	C4-C5-C6-O6
5	E	3	BMA	O5-C5-C6-O6
5	F	2	NAG	C8-C7-N2-C2
5	F	3	BMA	O5-C5-C6-O6
5	F	2	NAG	O7-C7-N2-C2
5	E	3	BMA	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	2	NAG	1	0
5	E	4	MAN	1	0

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



5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	605	1	14,14,15	0.53	0	17,19,21	0.66	0
7	NAG	B	2004	2	14,14,15	1.02	1 (7%)	17,19,21	1.53	2 (11%)
7	NAG	C	611	1	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
7	NAG	A	611	1	14,14,15	0.53	0	17,19,21	0.65	0
7	NAG	A	604	1	14,14,15	0.54	0	17,19,21	0.65	0
7	NAG	A	610	1	14,14,15	0.53	0	17,19,21	0.75	1 (5%)
7	NAG	C	604	1	14,14,15	0.58	0	17,19,21	0.77	0
7	NAG	C	605	1	14,14,15	0.55	0	17,19,21	0.58	0
8	15P	A	612	-	51,51,103	0.54	0	50,50,102	1.51	2 (4%)
7	NAG	C	610	1	14,14,15	0.51	0	17,19,21	0.74	0
10	TRS	C	612	-	7,7,7	1.30	0	9,9,9	1.42	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	605	1	-	1/6/23/26	0/1/1/1
7	NAG	B	2004	2	-	2/6/23/26	0/1/1/1
7	NAG	C	611	1	-	2/6/23/26	0/1/1/1
7	NAG	A	611	1	-	0/6/23/26	0/1/1/1
7	NAG	A	604	1	-	2/6/23/26	0/1/1/1
7	NAG	A	610	1	-	0/6/23/26	0/1/1/1
7	NAG	C	604	1	-	2/6/23/26	0/1/1/1
7	NAG	C	605	1	-	0/6/23/26	0/1/1/1
8	15P	A	612	-	-	19/49/49/101	-
7	NAG	C	610	1	-	1/6/23/26	0/1/1/1
10	TRS	C	612	-	-	0/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2004	NAG	C1-C2	2.92	1.56	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2004	NAG	C1-O5-C5	5.18	119.13	112.19
10	C	612	TRS	O1-C1-C	2.60	118.13	110.88
10	C	612	TRS	O3-C3-C	2.25	117.16	110.88
10	C	612	TRS	O2-C2-C	2.24	117.11	110.88
7	A	610	NAG	C1-O5-C5	2.11	115.01	112.19
7	B	2004	NAG	O5-C1-C2	2.06	114.48	111.29
8	A	612	15P	O11-C23-C24	2.05	119.69	110.35
7	C	611	NAG	C1-O5-C5	2.04	114.91	112.19
8	A	612	15P	O15-C30-C29	2.03	119.62	110.35

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	611	NAG	C8-C7-N2-C2
7	C	611	NAG	O7-C7-N2-C2
7	A	604	NAG	O5-C5-C6-O6
8	A	612	15P	O10-C21-C22-O11
8	A	612	15P	O12-C25-C26-O13
7	A	604	NAG	C4-C5-C6-O6
7	C	604	NAG	O5-C5-C6-O6
8	A	612	15P	O11-C23-C24-O12
7	C	604	NAG	C4-C5-C6-O6
8	A	612	15P	O5-C10-C9-O4
8	A	612	15P	O8-C17-C18-O9
8	A	612	15P	O13-C27-C28-O14
8	A	612	15P	C32-C31-O15-C30
8	A	612	15P	O15-C31-C32-O16
8	A	612	15P	O2-C5-C6-O3
8	A	612	15P	O6-C13-C14-O7
7	A	605	NAG	O5-C5-C6-O6
8	A	612	15P	C27-C28-O14-C29
8	A	612	15P	C15-C16-O8-C17
7	B	2004	NAG	O5-C5-C6-O6
8	A	612	15P	C6-C5-O2-C4
8	A	612	15P	C10-C9-O4-C8
8	A	612	15P	OXT-C1-C2-O1
8	A	612	15P	C18-C17-O8-C16
7	B	2004	NAG	C4-C5-C6-O6
8	A	612	15P	O5-C11-C12-O6
8	A	612	15P	C28-C27-O13-C26

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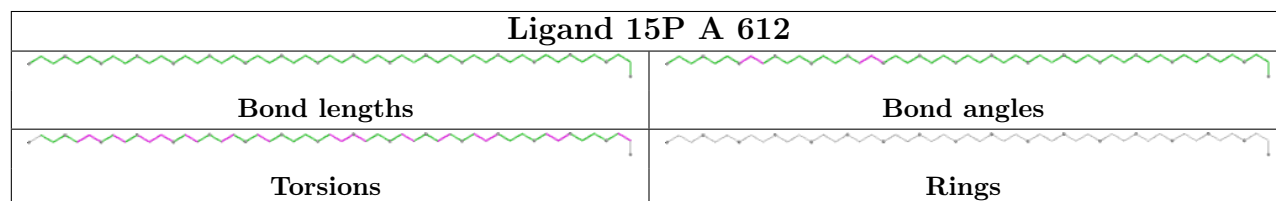
Mol	Chain	Res	Type	Atoms
8	A	612	15P	O14-C29-C30-O15
7	C	610	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	604	NAG	1	0
8	A	612	15P	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	582/597 (97%)	0.10	10 (1%) 69 48	33, 89, 161, 227	3 (0%)
1	C	581/597 (97%)	0.20	8 (1%) 73 53	35, 96, 166, 213	4 (0%)
2	B	375/503 (74%)	0.43	14 (3%) 45 26	36, 126, 203, 263	2 (0%)
2	D	375/503 (74%)	0.60	23 (6%) 27 15	57, 131, 198, 240	1 (0%)
3	H	211/219 (96%)	0.86	21 (9%) 12 7	83, 168, 230, 247	0
3	M	211/219 (96%)	1.07	28 (13%) 7 5	101, 176, 231, 246	0
4	L	217/217 (100%)	0.90	19 (8%) 15 9	93, 167, 249, 274	0
4	N	217/217 (100%)	0.83	20 (9%) 14 8	102, 168, 251, 276	0
All	All	2769/3072 (90%)	0.48	143 (5%) 33 19	33, 125, 224, 276	10 (0%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	L	183	THR	8.2
4	N	183	THR	5.9
3	H	206	ALA	4.7
4	N	136	SER	4.7
4	N	197	TYR	4.6
3	H	149	LEU	4.4
3	H	185	LEU	4.3
3	H	150	VAL	4.0
3	H	218	ILE	4.0
1	A	564	PRO	4.0
4	L	186	LEU	3.9
4	N	186	LEU	3.9
3	H	184	THR	3.8
4	L	136	SER	3.8
4	L	135	ALA	3.8
3	M	186	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	455	CYS	3.6
4	L	124	PRO	3.6
4	L	141	LEU	3.5
3	H	191	VAL	3.5
1	C	152	GLN	3.4
2	D	395	GLY	3.3
4	N	185	THR	3.2
3	M	184	THR	3.2
2	B	435	LEU	3.1
4	N	126	SER	3.1
3	M	146	LEU	3.1
1	A	255	GLU	3.1
2	D	311	VAL	3.1
4	N	138	VAL	3.0
1	C	379	SER	3.0
2	D	455	CYS	3.0
4	L	165	LEU	2.9
3	H	134	PRO	2.9
3	M	127	PRO	2.9
3	H	160	VAL	2.9
3	M	129	VAL	2.9
2	B	98	GLY	2.9
4	L	155	ILE	2.9
2	B	238	SER	2.8
3	M	164	SER	2.8
1	C	375	ASP	2.8
2	D	244	ASP	2.8
1	A	459	PRO	2.8
4	N	118	PRO	2.8
3	M	149	LEU	2.8
2	D	187	SER	2.8
2	B	333	ALA	2.8
2	D	393	CYS	2.8
1	A	254	ASP	2.8
4	N	210	ILE	2.8
3	M	44	GLY	2.8
3	M	185	LEU	2.8
3	M	132	LEU	2.7
4	L	125	PRO	2.7
4	L	127	SER	2.7
2	B	454	LEU	2.7
4	L	191	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	314	SER	2.7
3	M	120	SER	2.7
3	M	192	PRO	2.6
1	A	562	GLU	2.6
3	H	162	TRP	2.6
3	M	133	ALA	2.6
1	C	586	ALA	2.6
3	H	159	THR	2.6
1	A	286	GLY	2.5
2	D	92	LEU	2.5
3	H	151	LYS	2.5
3	M	30	THR	2.5
3	H	44	GLY	2.5
3	M	131	PRO	2.5
3	H	167	LEU	2.5
4	L	105	GLY	2.5
1	A	78	GLY	2.5
2	D	242	GLY	2.5
3	M	195	PRO	2.5
4	N	124	PRO	2.4
2	D	429	CYS	2.4
2	B	187	SER	2.4
4	L	116	ALA	2.3
2	B	244	ASP	2.3
2	D	333	ALA	2.3
3	H	148	CYS	2.3
3	M	160	VAL	2.3
2	D	98	GLY	2.3
2	B	120	GLN	2.3
3	M	218	ILE	2.3
3	M	167	LEU	2.3
3	M	68	ALA	2.3
3	H	146	LEU	2.3
2	D	377	GLU	2.2
2	D	290	GLY	2.2
4	L	130	LEU	2.2
3	M	151	LYS	2.2
4	L	181	SER	2.2
4	N	208	SER	2.2
2	D	260	ASN	2.2
3	M	215	ASP	2.2
4	N	165	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	M	162	TRP	2.2
1	C	78	GLY	2.2
2	D	173	GLY	2.2
3	H	147	GLY	2.2
2	D	238	SER	2.2
3	M	82	GLN	2.2
3	H	214	VAL	2.2
2	B	119	GLN	2.2
2	D	441	LEU	2.2
2	B	433	PRO	2.1
2	D	198	PRO	2.1
4	N	153	TRP	2.1
2	D	411	HIS	2.1
2	D	434	HIS	2.1
4	N	191	TYR	2.1
3	M	150	VAL	2.1
4	N	168	TRP	2.1
3	M	106	TYR	2.1
2	D	120	GLN	2.1
3	H	133	ALA	2.1
4	N	117	ALA	2.1
2	B	377	GLU	2.1
4	L	192	GLU	2.1
4	L	137	VAL	2.1
4	N	137	VAL	2.1
3	M	172	HIS	2.1
1	C	443	PRO	2.1
2	D	356	SER	2.1
2	B	324	GLN	2.1
4	N	129	GLN	2.1
4	N	125	PRO	2.1
2	B	436	LEU	2.0
4	L	154	ASN	2.0
3	H	195	PRO	2.0
3	M	155	PRO	2.0
4	L	140	PHE	2.0
1	A	67	THR	2.0
1	A	287	PHE	2.0
1	A	256	LYS	2.0
2	D	396	PRO	2.0
3	H	1	GLN	2.0
4	N	130	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	118	ILE	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](#)

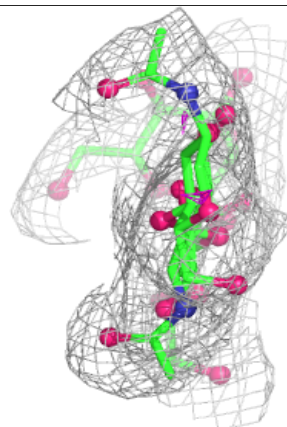
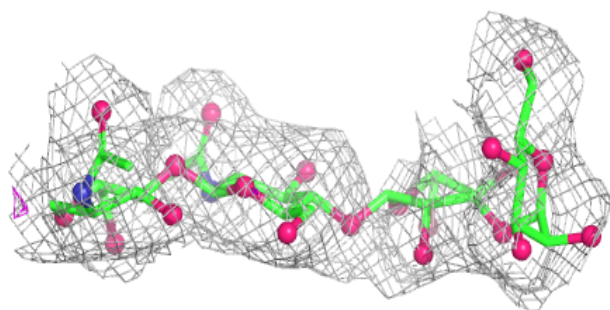
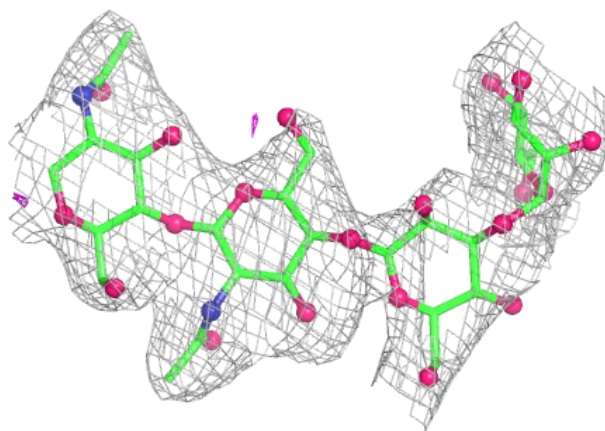
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	E	1	14/15	-	-	45,111,145,158	0
5	NAG	E	2	14/15	-	-	58,121,166,179	0
5	BMA	E	3	11/12	-	-	112,197,215,224	0
5	MAN	E	4	11/12	-	-	115,192,228,245	0
5	NAG	F	1	14/15	-	-	60,152,181,188	0
5	NAG	F	2	14/15	-	-	130,154,204,205	0
5	BMA	F	3	11/12	-	-	182,203,226,244	0
5	MAN	F	4	11/12	-	-	180,237,249,252	0

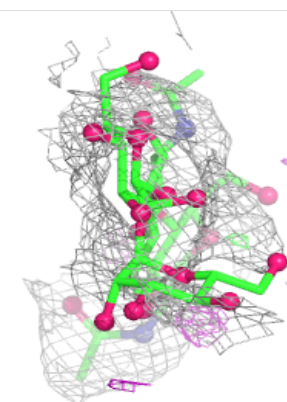
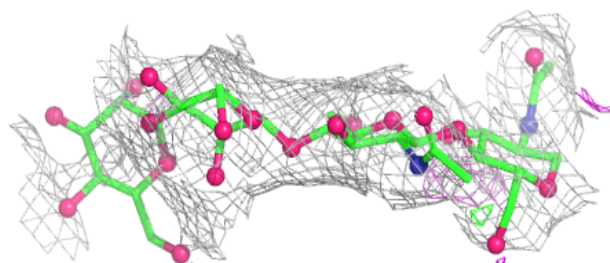
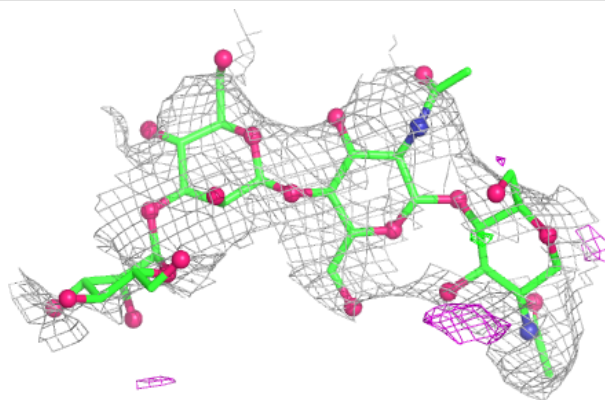
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

**Electron density around Chain F:**

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



6.4 Ligands ⓘ

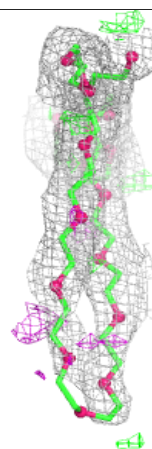
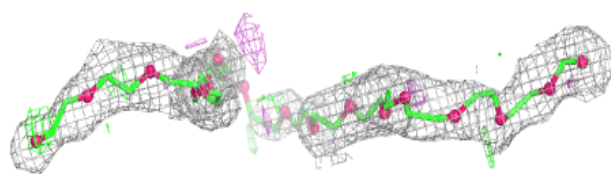
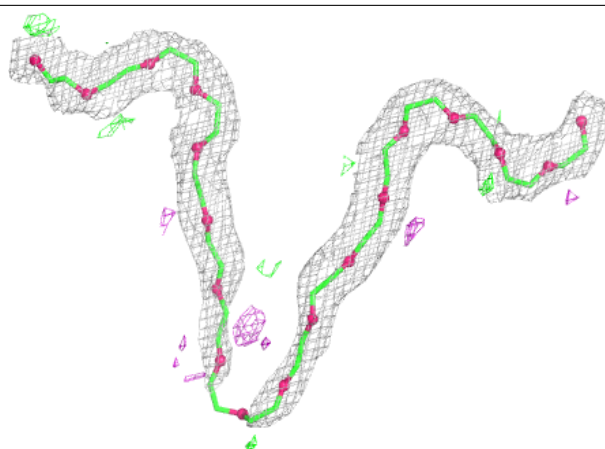
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NAG	C	610	14/15	0.60	0.14	119,164,193,202	0
7	NAG	A	610	14/15	0.66	0.15	133,157,188,195	0
7	NAG	B	2004	14/15	0.72	0.17	143,177,230,235	0
7	NAG	C	611	14/15	0.73	0.19	135,147,173,176	0
7	NAG	C	605	14/15	0.74	0.13	69,157,189,199	0
10	TRS	C	612	8/8	0.76	0.16	114,148,166,167	0
7	NAG	A	611	14/15	0.77	0.17	110,149,210,214	0
7	NAG	A	605	14/15	0.78	0.13	67,160,177,193	0
9	MG	B	2001	1/1	0.80	0.26	100,100,100,100	0
6	CA	B	2002	1/1	0.87	0.11	125,125,125,125	0
6	CA	C	601	1/1	0.90	0.13	86,86,86,86	0
6	CA	A	601	1/1	0.90	0.15	81,81,81,81	0
6	CA	D	2002	1/1	0.92	0.12	132,132,132,132	0
7	NAG	C	604	14/15	0.93	0.11	52,87,127,156	0
6	CA	A	602	1/1	0.93	0.12	78,78,78,78	0
9	MG	D	2001	1/1	0.93	0.12	104,104,104,104	0
6	CA	D	2003	1/1	0.93	0.09	115,115,115,115	0
8	15P	A	612	52/104	0.94	0.14	3,88,137,176	0
6	CA	B	2003	1/1	0.94	0.10	87,87,87,87	0
6	CA	A	603	1/1	0.95	0.12	69,69,69,69	0
7	NAG	A	604	14/15	0.95	0.09	47,75,103,114	0
6	CA	C	602	1/1	0.97	0.12	86,86,86,86	0
6	CA	C	603	1/1	0.98	0.14	68,68,68,68	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 15P A 612:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.