



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:18 PM UTC

PDB ID : 7T2D / pdb_00007t2d
Title : Crystal structure of the B1 TCR in complex with HLA-DP4-Ply
Authors : Ciacchi, L.; Farenc, C.; Petersen, J.; Reid, H.H.; Rossjohn, J.
Deposited on : 2021-12-03
Resolution : 3.40 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

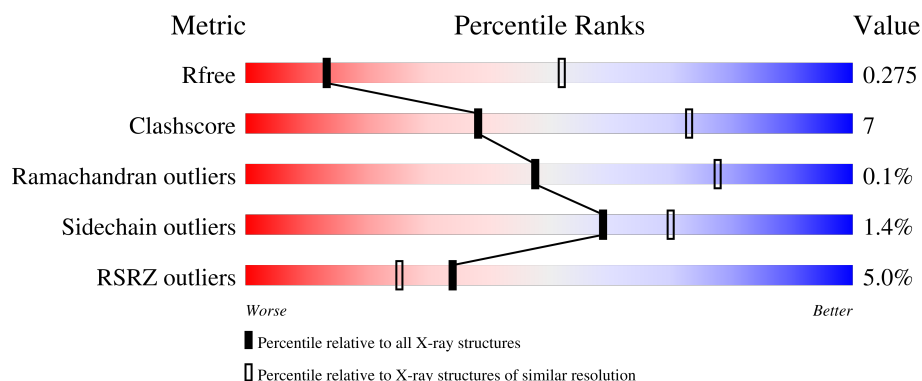
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	181	 83% 15% ..
1	F	181	 4% 87% 12% .
1	K	181	 2% 86% 14% .
1	P	181	 2% 90% 9% .
2	B	188	 6% 72% 18% . 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	188	
2	L	188	
2	Q	188	
3	C	15	
3	H	15	
3	M	15	
3	R	15	
4	D	207	
4	I	207	
4	N	207	
4	S	207	
5	E	243	
5	J	243	
5	O	243	
5	T	243	
6	U	4	
7	V	4	
8	W	3	
8	X	3	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 26248 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 HLA class II histocompatibility antigen, DP alpha 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1473	953	238	277	5			
1	F	180	Total	C	N	O	S	0	0	0
			1473	953	238	277	5			
1	K	180	Total	C	N	O	S	0	0	0
			1473	953	238	277	5			
1	P	180	Total	C	N	O	S	0	0	0
			1473	953	238	277	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DP beta 1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	0	0
			1397	876	248	265	8			
2	G	168	Total	C	N	O	S	0	0	0
			1367	855	243	261	8			
2	L	178	Total	C	N	O	S	0	0	0
			1460	918	258	276	8			
2	Q	177	Total	C	N	O	S	0	0	0
			1451	912	256	275	8			

- Molecule 3 is a protein called Pneumolysin-derived peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	14	Total	C	N	O	0	0	0
			126	85	20	21			
3	H	14	Total	C	N	O	0	0	0
			126	85	20	21			
3	M	14	Total	C	N	O	0	0	0
			126	85	20	21			
3	R	14	Total	C	N	O	0	0	0
			126	85	20	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	cloning artifact	UNP Q04IN8
C	-2	ALA	-	cloning artifact	UNP Q04IN8
H	-3	GLY	-	cloning artifact	UNP Q04IN8
H	-2	ALA	-	cloning artifact	UNP Q04IN8
M	-3	GLY	-	cloning artifact	UNP Q04IN8
M	-2	ALA	-	cloning artifact	UNP Q04IN8
R	-3	GLY	-	cloning artifact	UNP Q04IN8
R	-2	ALA	-	cloning artifact	UNP Q04IN8

- Molecule 4 is a protein called T cell receptor, B1, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	201	Total	C	N	O	S	0	0	0
			1597	1003	259	328	7			
4	I	201	Total	C	N	O	S	0	0	0
			1597	1003	259	328	7			
4	N	199	Total	C	N	O	S	0	0	0
			1575	985	257	326	7			
4	S	199	Total	C	N	O	S	0	0	0
			1575	985	257	326	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	176	CYS	THR	engineered mutation	UNP P01848
I	176	CYS	THR	engineered mutation	UNP P01848
N	176	CYS	THR	engineered mutation	UNP P01848
S	176	CYS	THR	engineered mutation	UNP P01848

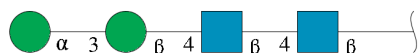
- Molecule 5 is a protein called T cell receptor, B1, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	235	Total	C	N	O	S	0	0	0
			1869	1178	328	358	5			
5	J	237	Total	C	N	O	S	0	0	0
			1883	1187	330	361	5			
5	O	238	Total	C	N	O	S	0	0	0
			1892	1192	332	363	5			
5	T	238	Total	C	N	O	S	0	0	0
			1892	1192	332	363	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	184	CYS	SER	engineered mutation	UNP P01850
E	202	ALA	CYS	engineered mutation	UNP P01850
J	184	CYS	SER	engineered mutation	UNP P01850
J	202	ALA	CYS	engineered mutation	UNP P01850
O	184	CYS	SER	engineered mutation	UNP P01850
O	202	ALA	CYS	engineered mutation	UNP P01850
T	184	CYS	SER	engineered mutation	UNP P01850
T	202	ALA	CYS	engineered mutation	UNP P01850

- Molecule 6 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.



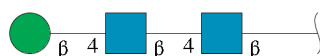
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	U	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 7 is an oligosaccharide called 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.



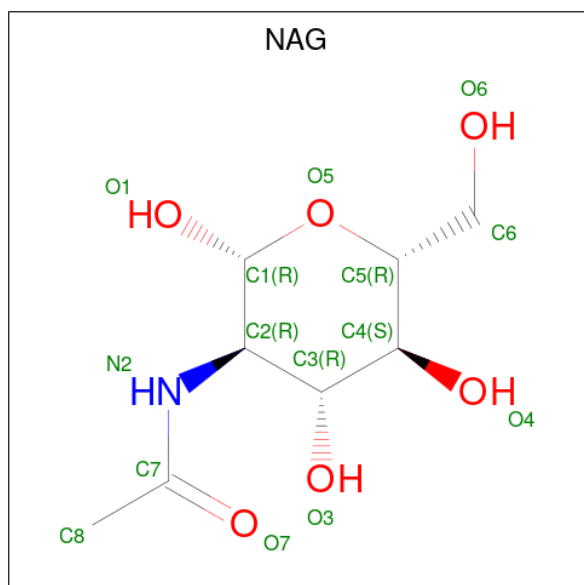
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	V	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 8 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
8	W	3	Total	C	N	O	0	0	0
			39	22	2	15			
8	X	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	F	1	Total	C	N	O	0	0
			14	8	1	5		
9	G	1	Total	C	N	O	0	0
			14	8	1	5		
9	K	1	Total	C	N	O	0	0
			14	8	1	5		
9	L	1	Total	C	N	O	0	0
			14	8	1	5		
9	P	1	Total	C	N	O	0	0
			14	8	1	5		
9	Q	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total 1	O 1	0	0
10	C	1	Total 1	O 1	0	0
10	F	1	Total 1	O 1	0	0
10	E	3	Total 3	O 3	0	0
10	I	1	Total 1	O 1	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

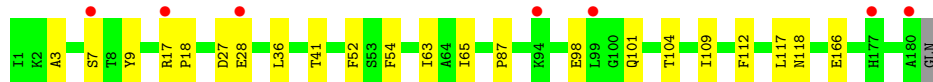
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

Chain A: 



- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

Chain F: 



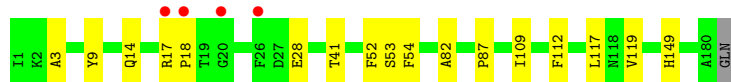
- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

Chain K: 



- Molecule 1: HLA class II histocompatibility antigen, DP alpha 1 chain

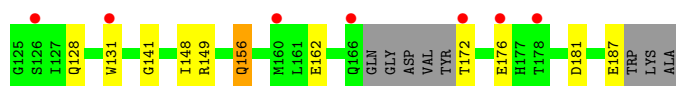
Chain P: 



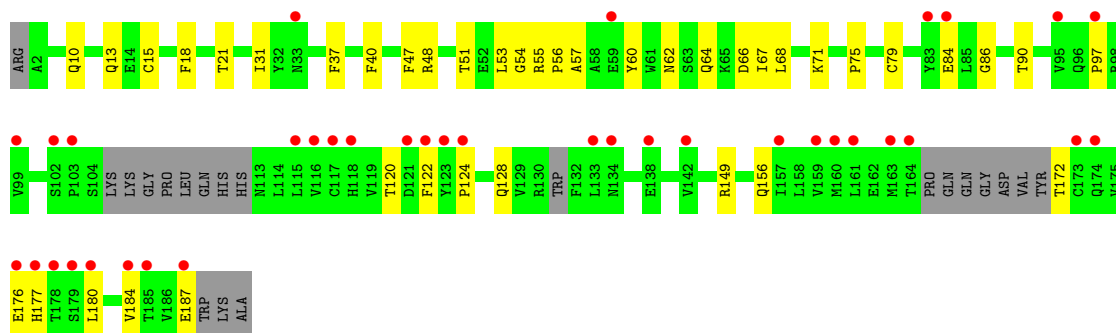
- Molecule 2: HLA class II histocompatibility antigen, DP beta 1 chain

Chain B: 

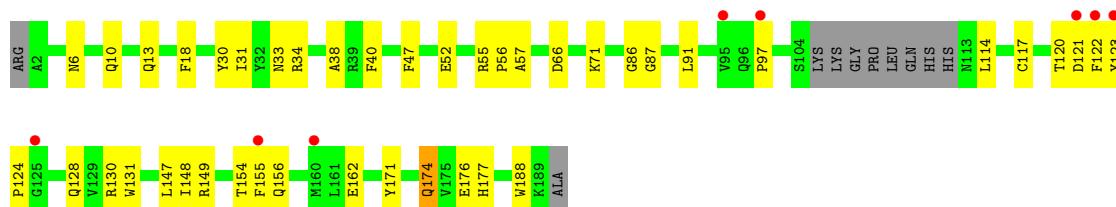




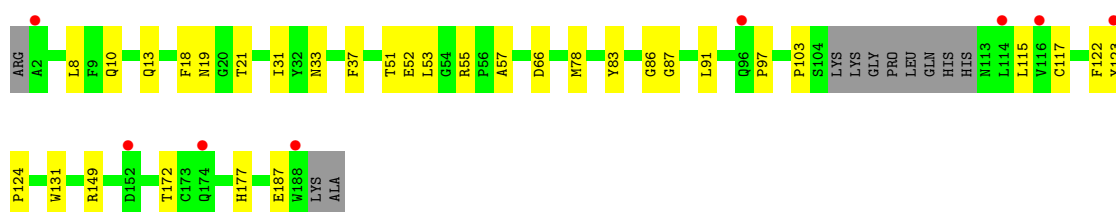
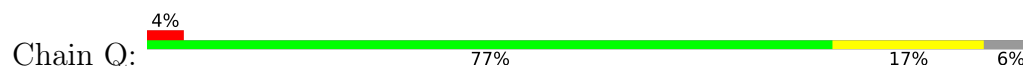
- Molecule 2: HLA class II histocompatibility antigen, DP beta 1 chain



- Molecule 2: HLA class II histocompatibility antigen, DP beta 1 chain



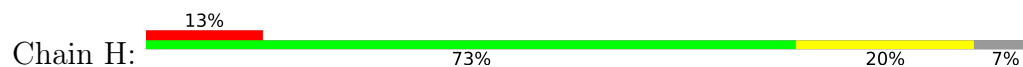
- Molecule 2: HLA class II histocompatibility antigen, DP beta 1 chain



- Molecule 3: Pneumolysin-derived peptide



- Molecule 3: Pneumolysin-derived peptide





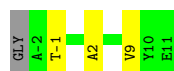
- Molecule 3: Pneumolysin-derived peptide

Chain M: 80% 13% 7%



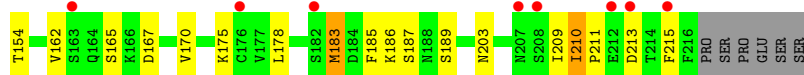
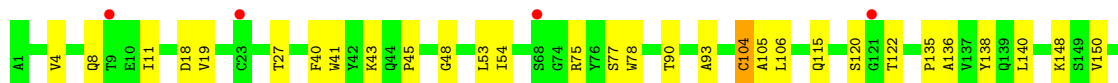
- Molecule 3: Pneumolysin-derived peptide

Chain R: 73% 20% 7%



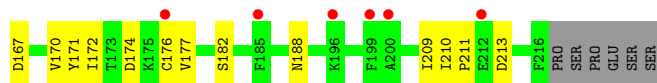
- Molecule 4: T cell receptor, B1, alpha chain

Chain D: 6% 74% 22% . .



- Molecule 4: T cell receptor, B1, alpha chain

Chain I: 5% 77% 19% . .

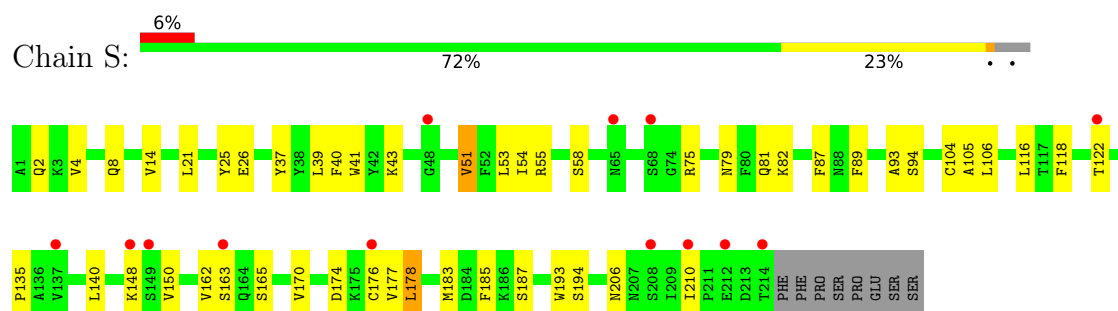


- Molecule 4: T cell receptor, B1, alpha chain

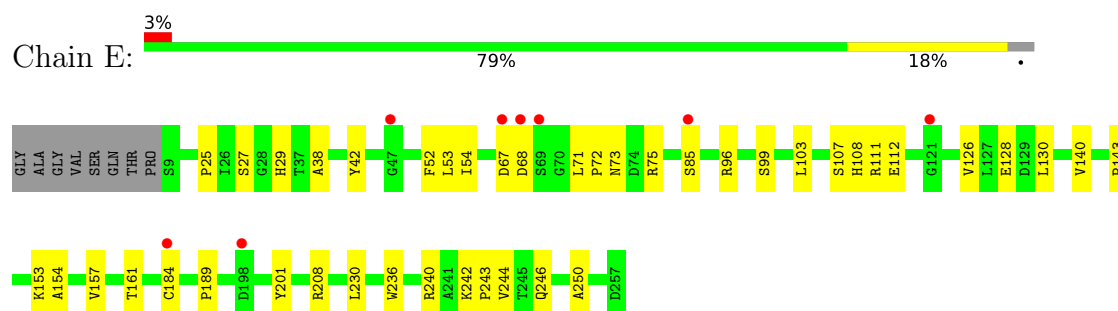
Chain N: 5% 74% 21% . .



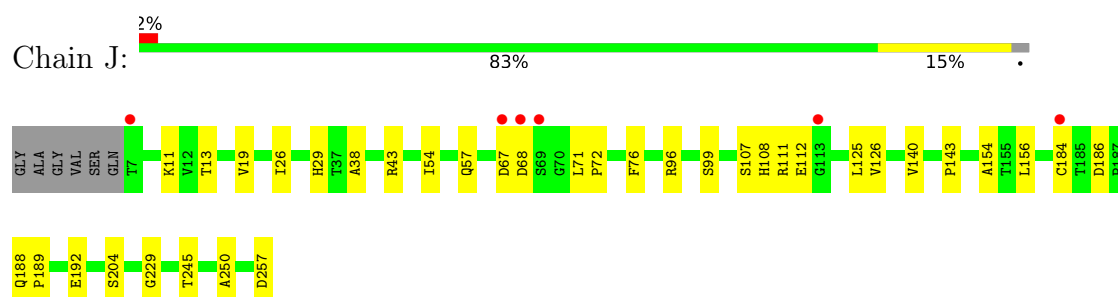
- Molecule 4: T cell receptor, B1, alpha chain



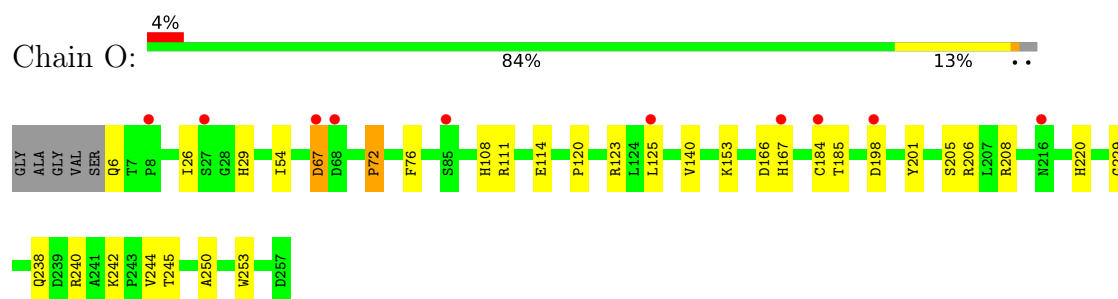
- Molecule 5: T cell receptor, B1, beta chain



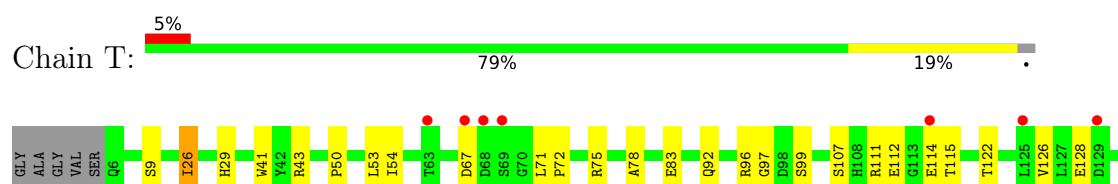
- Molecule 5: T cell receptor, B1, beta chain

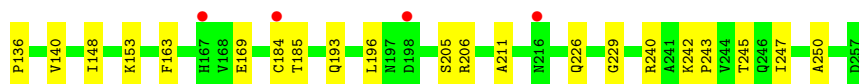


- Molecule 5: T cell receptor, B1, beta chain



- Molecule 5: T cell receptor, B1, beta chain





- Molecule 6: 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

Chain U: 50% 50%



- Molecule 7: 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 V: 50% 50%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 67% 33%



- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.71Å 193.57Å 236.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.40 – 3.40 33.40 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.40-3.40) 99.4 (33.40-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 3.39Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.236 , 0.271 0.243 , 0.275	Depositor DCC
R_{free} test set	5047 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	91.9	Xtrriage
Anisotropy	0.571	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26248	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7578e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.08	0/1521	0.26	0/2076
1	F	0.18	0/1521	0.36	0/2076
1	K	0.09	0/1521	0.27	0/2076
1	P	0.09	0/1521	0.28	0/2076
2	B	0.10	0/1428	0.29	0/1936
2	G	0.10	0/1394	0.28	0/1886
2	L	0.10	0/1495	0.31	0/2029
2	Q	0.11	0/1486	0.29	0/2018
3	C	0.08	0/132	0.30	0/182
3	H	0.09	0/132	0.36	0/182
3	M	0.10	0/132	0.33	0/182
3	R	0.08	0/132	0.32	0/182
4	D	0.13	0/1631	0.31	0/2215
4	I	0.12	0/1631	0.32	0/2215
4	N	0.17	0/1607	0.37	0/2183
4	S	0.09	0/1607	0.29	0/2183
5	E	0.10	0/1920	0.31	0/2610
5	J	0.10	0/1935	0.30	0/2632
5	O	0.09	0/1944	0.28	0/2644
5	T	0.10	0/1944	0.31	0/2644
All	All	0.11	0/26634	0.30	0/36227

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	1473	0	1375	19	0
1	F	1473	0	1375	15	0
1	K	1473	0	1375	16	0
1	P	1473	0	1375	13	0
2	B	1397	0	1326	23	0
2	G	1367	0	1300	29	0
2	L	1460	0	1383	29	0
2	Q	1451	0	1370	24	0
3	C	126	0	113	3	0
3	H	126	0	113	3	0
3	M	126	0	113	2	0
3	R	126	0	113	3	0
4	D	1597	0	1505	33	0
4	I	1597	0	1506	33	0
4	N	1575	0	1488	31	0
4	S	1575	0	1488	38	0
5	E	1869	0	1774	26	0
5	J	1883	0	1789	29	0
5	O	1892	0	1797	24	0
5	T	1892	0	1797	32	0
6	U	50	0	43	0	0
7	V	50	0	43	0	0
8	W	39	0	34	1	0
8	X	39	0	34	0	0
9	A	14	0	13	0	0
9	B	14	0	13	0	0
9	F	14	0	13	0	0
9	G	14	0	13	0	0
9	K	14	0	13	0	0
9	L	14	0	13	0	0
9	P	14	0	13	0	0
9	Q	14	0	13	1	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
10	E	3	0	0	0	0
10	F	1	0	0	0	0
10	I	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	26248	0	24733	351	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 (351) 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)
4:I:176:CYS:CB	5:J:184:CYS:SG	2.27	1.22
4:S:176:CYS:CB	5:T:184:CYS:SG	2.34	1.14
4:N:176:CYS:SG	5:O:184:CYS:CB	2.37	1.12
4:N:176:CYS:CB	5:O:184:CYS:SG	2.40	1.08
4:S:176:CYS:SG	5:T:184:CYS:CB	2.64	0.84
4:S:176:CYS:HG	5:T:184:CYS:CB	1.92	0.83
2:Q:52:GLU:HG2	2:Q:55:ARG:HH22	1.52	0.75
5:J:229:GLY:H	5:J:245:THR:HG22	1.51	0.74
4:I:176:CYS:HB3	5:J:184:CYS:SG	2.25	0.73
4:S:37:TYR:H	4:S:58:SER:HB2	1.52	0.73
4:I:165:SER:HB3	4:I:172:ILE:HG22	1.70	0.72
4:I:56:ARG:HB2	4:I:87:PHE:HZ	1.54	0.72
1:P:9:TYR:HB2	2:Q:13:GLN:HB2	1.71	0.72
2:L:52:GLU:HG2	2:L:55:ARG:HH21	1.56	0.69
2:G:51:THR:HG23	2:G:53:LEU:H	1.58	0.68
2:L:97:PRO:HB3	2:L:122:PHE:HB3	1.74	0.68
1:P:3:ALA:HA	2:Q:18:PHE:HB2	1.75	0.68
4:I:114:ARG:HD2	5:J:112:GLU:HB2	1.75	0.67
1:P:87:PRO:HB3	1:P:112:PHE:HB3	1.76	0.67
1:F:9:TYR:HB2	2:G:13:GLN:HB2	1.76	0.67
5:O:153:LYS:HD2	5:O:208:ARG:HD3	1.77	0.67
4:D:210:ILE:HG13	4:D:211:PRO:HD3	1.77	0.66
1:K:9:TYR:HB2	2:L:13:GLN:HB2	1.76	0.66
4:D:40:PHE:HB2	4:D:105:ALA:HB3	1.76	0.66
2:B:128:GLN:NE2	2:B:176:GLU:OE1	2.29	0.65
1:F:118:ASN:HB2	1:F:166:GLU:HB2	1.78	0.65
1:A:87:PRO:HB3	1:A:112:PHE:HB3	1.78	0.65
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.79	0.65
4:D:77:SER:HB2	4:D:90:THR:HB	1.78	0.64
4:D:178:LEU:HG	5:E:184:CYS:HB2	1.79	0.64
4:N:209:ILE:HG22	4:N:211:PRO:HD2	1.79	0.64
2:L:10:GLN:HG3	2:L:31:ILE:HB	1.80	0.64
1:A:9:TYR:HB2	2:B:13:GLN:HB2	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:82:ALA:HB2	2:Q:33:ASN:HB3	1.79	0.63
5:J:29:HIS:HA	5:J:108:HIS:HA	1.81	0.63
4:S:135:PRO:HB2	4:S:210:ILE:HD13	1.81	0.62
2:G:62:ASN:HA	2:G:68:LEU:HD21	1.82	0.62
4:I:160:THR:HB	4:I:209:ILE:HD11	1.81	0.62
4:S:105:ALA:HB1	4:S:116:LEU:HD12	1.81	0.62
5:O:54:ILE:HG13	5:O:67:ASP:HB3	1.81	0.61
5:T:54:ILE:HG13	5:T:67:ASP:HB3	1.81	0.61
4:N:167:ASP:HB3	4:N:170:VAL:HG13	1.83	0.61
4:I:176:CYS:C	5:J:184:CYS:SG	2.85	0.60
5:J:99:SER:HB3	5:J:126:VAL:H	1.66	0.60
4:N:41:TRP:HZ3	4:N:102:TYR:HB3	1.67	0.60
1:F:87:PRO:HB3	1:F:112:PHE:HB3	1.84	0.60
1:A:36:LEU:HD21	1:A:63:ILE:HG13	1.84	0.60
1:K:82:ALA:HB2	2:L:33:ASN:HB3	1.84	0.60
1:A:27:ASP:O	2:B:149:ARG:NH2	2.35	0.59
2:Q:19:ASN:ND2	9:Q:201:NAG:O7	2.36	0.58
2:Q:172:THR:HG22	2:Q:187:GLU:HG2	1.85	0.58
1:F:109:ILE:HG21	1:F:117:LEU:HD21	1.85	0.58
1:F:27:ASP:O	2:G:149:ARG:NH2	2.37	0.58
4:N:75:ARG:NH1	4:N:93:ALA:O	2.36	0.58
2:G:86:GLY:O	2:G:90:THR:N	2.37	0.57
4:N:49:GLU:HG2	5:O:120:PRO:HA	1.85	0.57
1:F:3:ALA:HA	2:G:18:PHE:HB2	1.87	0.57
2:Q:10:GLN:HG3	2:Q:31:ILE:HB	1.87	0.57
4:D:27:THR:HB	4:D:106:LEU:HD21	1.86	0.56
2:L:57:ALA:HB2	3:M:9:VAL:HG13	1.87	0.56
5:T:9:SER:HB3	5:T:122:THR:HG22	1.87	0.56
2:B:71:LYS:NZ	3:C:5:TRP:O	2.39	0.56
4:D:41:TRP:HB2	4:D:54:ILE:HG22	1.88	0.56
4:I:165:SER:HB2	4:I:170:VAL:HG23	1.87	0.56
5:T:54:ILE:HD13	5:T:78:ALA:HB3	1.87	0.56
5:E:230:LEU:HD12	5:E:243:PRO:HD2	1.87	0.56
4:D:150:VAL:HG21	5:E:157:VAL:HG11	1.87	0.56
1:F:36:LEU:HD21	1:F:63:ILE:HG13	1.86	0.55
1:P:14:GLN:HB3	2:Q:8:LEU:HD12	1.87	0.55
4:N:178:LEU:HD21	5:O:206:ARG:HB2	1.88	0.55
1:P:82:ALA:H	2:Q:33:ASN:HD22	1.54	0.55
5:O:229:GLY:H	5:O:245:THR:HG22	1.72	0.55
2:Q:57:ALA:HB2	3:R:9:VAL:HG13	1.88	0.55
4:S:41:TRP:HB2	4:S:54:ILE:HG22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:13:THR:HG21	5:J:19:VAL:HG22	1.89	0.55
4:S:177:VAL:N	5:T:184:CYS:SG	2.80	0.55
1:F:7:SER:HB2	2:G:15:CYS:HB2	1.88	0.55
5:O:242:LYS:HB3	5:O:244:VAL:HG13	1.88	0.54
2:Q:51:THR:HG23	2:Q:53:LEU:H	1.72	0.54
4:S:162:VAL:HG21	4:S:174:ASP:HA	1.89	0.54
2:G:71:LYS:NZ	3:H:5:TRP:O	2.40	0.54
5:E:54:ILE:HG13	5:E:67:ASP:HB3	1.88	0.54
4:I:27:THR:HG21	4:I:106:LEU:HD22	1.90	0.54
1:K:96:PRO:HD3	2:L:120:THR:HG21	1.89	0.54
5:T:240:ARG:HH22	5:T:243:PRO:HG3	1.71	0.54
5:J:186:ASP:OD2	5:J:204:SER:OG	2.24	0.54
4:N:25:TYR:HB2	4:N:106:LEU:HD12	1.90	0.53
2:B:57:ALA:HB2	3:C:9:VAL:HG13	1.90	0.53
2:G:97:PRO:HB3	2:G:122:PHE:HB3	1.89	0.53
1:A:85:ASP:OD2	2:B:34:ARG:NH1	2.41	0.53
4:I:56:ARG:HB2	4:I:87:PHE:CZ	2.40	0.53
5:J:143:PRO:HD3	5:J:156:LEU:HG	1.89	0.53
4:N:75:ARG:HD2	4:N:93:ALA:HB3	1.90	0.53
5:T:140:VAL:HG23	5:T:250:ALA:HB3	1.90	0.53
5:T:193:GLN:HB3	5:T:196:LEU:HD13	1.89	0.53
1:F:98:GLU:HG2	1:F:101:GLN:HB3	1.89	0.53
4:I:41:TRP:HE1	4:I:87:PHE:HB3	1.72	0.53
5:O:185:THR:HG23	5:O:205:SER:HB2	1.91	0.53
8:W:2:NAG:H3	8:W:2:NAG:H83	1.90	0.53
4:D:167:ASP:HB3	4:D:170:VAL:HG22	1.90	0.53
5:J:54:ILE:HG13	5:J:67:ASP:HB3	1.90	0.52
4:S:41:TRP:HE1	4:S:87:PHE:HD1	1.57	0.52
5:T:229:GLY:H	5:T:245:THR:HG22	1.74	0.52
2:G:60:TYR:HE2	5:J:111:ARG:HD3	1.74	0.52
5:T:169:GLU:HB2	5:T:226:GLN:HB3	1.92	0.52
4:D:43:LYS:HB2	4:D:53:LEU:HD11	1.92	0.52
5:T:185:THR:HG23	5:T:205:SER:HB2	1.92	0.52
5:E:38:ALA:HB3	5:E:107:SER:HB3	1.92	0.52
2:Q:37:PHE:HA	2:Q:51:THR:HG22	1.92	0.52
4:N:148:LYS:HD2	4:N:193:TRP:HD1	1.74	0.51
2:Q:87:GLY:HA2	2:Q:91:LEU:HD13	1.92	0.51
5:O:29:HIS:HA	5:O:108:HIS:HA	1.93	0.51
2:L:128:GLN:NE2	2:L:176:GLU:OE1	2.43	0.51
4:D:135:PRO:HG2	4:D:209:ILE:HG21	1.93	0.51
4:S:40:PHE:HB2	4:S:105:ALA:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:162:VAL:HG21	4:I:174:ASP:HA	1.92	0.50
5:T:114:GLU:HG2	5:T:115:THR:H	1.76	0.50
1:K:27:ASP:O	2:L:149:ARG:NH2	2.44	0.50
5:O:198:ASP:OD1	5:O:198:ASP:N	2.44	0.50
2:Q:122:PHE:HB2	2:Q:177:HIS:CE1	2.47	0.50
4:S:21:LEU:HD12	4:S:89:PHE:HD2	1.76	0.50
5:T:111:ARG:NH1	5:T:112:GLU:O	2.44	0.50
4:D:4:VAL:HG11	4:D:104:CYS:HB3	1.93	0.50
2:L:71:LYS:NZ	3:M:5:TRP:O	2.44	0.50
4:N:189:SER:HB2	5:O:206:ARG:HD3	1.93	0.50
4:I:41:TRP:HZ3	4:I:102:TYR:HB3	1.77	0.50
4:N:107:SER:HB2	4:N:116:LEU:HD12	1.92	0.50
1:A:17:ARG:HB3	1:A:18:PRO:HD3	1.94	0.50
2:L:124:PRO:HD2	2:L:177:HIS:HE1	1.76	0.50
5:O:6:GLN:HG3	5:O:120:PRO:HG3	1.94	0.50
4:S:79:ASN:HD21	4:S:81:GLN:HE21	1.59	0.50
1:K:85:ASP:OD2	2:L:34:ARG:NH1	2.45	0.49
2:G:75:PRO:HA	2:G:79:CYS:HB2	1.94	0.49
4:D:183:MET:O	4:D:185:PHE:N	2.43	0.49
2:G:10:GLN:HG3	2:G:31:ILE:HB	1.95	0.49
2:G:128:GLN:HG3	2:G:176:GLU:HB2	1.92	0.49
2:L:148:ILE:HB	2:L:156:GLN:HB2	1.94	0.49
2:Q:18:PHE:O	2:Q:21:THR:HG22	2.12	0.49
4:S:25:TYR:HB2	4:S:106:LEU:HD22	1.93	0.49
2:B:181:ASP:OD1	2:B:181:ASP:N	2.46	0.49
4:I:167:ASP:HB3	4:I:170:VAL:HG22	1.94	0.49
4:S:183:MET:SD	5:T:153:LYS:NZ	2.85	0.49
1:A:58:GLY:O	1:A:62:ASN:ND2	2.46	0.49
5:T:99:SER:HB3	5:T:126:VAL:H	1.77	0.49
2:B:141:GLY:HA3	2:B:162:GLU:HB2	1.95	0.49
1:P:109:ILE:HG21	1:P:117:LEU:HD21	1.94	0.49
2:Q:83:TYR:CZ	2:Q:91:LEU:HD21	2.47	0.49
5:E:140:VAL:HG23	5:E:250:ALA:HB3	1.94	0.49
4:S:170:VAL:HA	4:S:194:SER:HB2	1.95	0.48
4:N:25:TYR:HH	4:N:37:TYR:HH	1.51	0.48
4:N:140:LEU:HB2	4:N:150:VAL:HG13	1.95	0.48
1:F:17:ARG:HB2	1:F:18:PRO:HD3	1.96	0.48
2:Q:66:ASP:OD1	5:T:111:ARG:NH2	2.46	0.48
4:S:43:LYS:HB3	4:S:51:VAL:HG22	1.96	0.48
2:G:66:ASP:OD1	5:J:111:ARG:NH2	2.46	0.48
4:N:41:TRP:CZ3	4:N:102:TYR:HB3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:124:PRO:HB2	2:G:177:HIS:HE2	1.78	0.48
2:B:10:GLN:HG3	2:B:31:ILE:HB	1.96	0.48
2:B:37:PHE:HA	2:B:51:THR:HG22	1.96	0.47
1:P:119:VAL:HB	1:P:149:HIS:CE1	2.48	0.47
4:I:115:GLN:NE2	5:J:68:ASP:OD2	2.46	0.47
4:N:106:LEU:HD23	4:N:107:SER:N	2.29	0.47
1:F:41:THR:HG21	1:F:54:PHE:HB3	1.95	0.47
4:D:54:ILE:HB	4:D:78:TRP:CZ2	2.50	0.47
4:S:8:GLN:O	4:S:122:THR:HG22	2.15	0.47
2:B:148:ILE:HB	2:B:156:GLN:HB3	1.97	0.47
4:I:2:GLN:HA	4:I:27:THR:HG22	1.96	0.47
2:L:124:PRO:HD2	2:L:177:HIS:CE1	2.50	0.47
1:K:15:THR:OG1	2:L:6:ASN:HA	2.15	0.47
2:L:171:TYR:HB2	2:L:188:TRP:HB3	1.96	0.47
4:N:13:VAL:HG21	4:N:19:VAL:HB	1.97	0.47
4:N:27:THR:HG21	4:N:106:LEU:HD22	1.97	0.47
2:L:66:ASP:OD1	5:O:111:ARG:NH2	2.48	0.47
2:G:120:THR:HG22	2:G:156:GLN:HG2	1.97	0.47
1:P:17:ARG:HB3	1:P:18:PRO:HD3	1.97	0.47
5:T:96:ARG:NH1	5:T:128:GLU:OE1	2.48	0.47
2:B:30:TYR:HB2	2:B:38:ALA:HB3	1.97	0.47
5:J:11:LYS:HE2	5:J:19:VAL:HG13	1.97	0.47
2:G:37:PHE:HA	2:G:51:THR:HG22	1.97	0.46
2:G:57:ALA:HB2	3:H:9:VAL:HG13	1.98	0.46
5:E:143:PRO:HG3	5:E:154:ALA:HB1	1.97	0.46
4:I:136:ALA:HB2	4:I:213:ASP:HB3	1.98	0.46
5:J:38:ALA:HB3	5:J:107:SER:HB3	1.97	0.46
2:L:30:TYR:HB2	2:L:38:ALA:HB3	1.97	0.46
5:O:123:ARG:HD3	5:O:167:HIS:ND1	2.30	0.46
4:D:140:LEU:HB2	4:D:150:VAL:HG13	1.97	0.46
4:I:76:TYR:HB3	4:I:78:TRP:CH2	2.51	0.46
4:I:209:ILE:HG22	4:I:211:PRO:HD2	1.98	0.46
1:A:96:PRO:HD3	2:B:120:THR:HG21	1.98	0.46
5:E:236:TRP:HB2	5:E:242:LYS:HE2	1.96	0.46
5:E:244:VAL:O	5:E:246:GLN:HG3	2.16	0.46
4:I:115:GLN:N	4:I:115:GLN:OE1	2.46	0.46
5:J:43:ARG:HH21	5:J:72:PRO:HG3	1.80	0.46
1:K:16:HIS:HB3	1:K:17:ARG:H	1.56	0.46
2:L:130:ARG:HD2	2:L:174:GLN:HE21	1.81	0.46
4:S:37:TYR:HE2	4:S:82:LYS:HE3	1.80	0.46
4:I:128:PRO:O	4:I:158:SER:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:148:LYS:HD3	4:S:193:TRP:CD1	2.51	0.46
4:S:178:LEU:HD21	5:T:206:ARG:HB2	1.98	0.46
4:I:210:ILE:HG23	4:I:211:PRO:HD3	1.96	0.46
2:Q:117:CYS:HB2	2:Q:131:TRP:CZ2	2.51	0.46
2:L:121:ASP:HA	2:L:154:THR:HB	1.97	0.45
5:E:73:ASN:OD1	5:E:75:ARG:NH2	2.50	0.45
5:E:112:GLU:H	5:E:112:GLU:CD	2.23	0.45
4:S:4:VAL:HG11	4:S:104:CYS:HB3	1.98	0.45
4:I:6:GLN:HB3	4:I:122:THR:HG23	1.99	0.45
1:P:41:THR:HG21	1:P:54:PHE:HB3	1.98	0.45
1:K:17:ARG:HB2	1:K:18:PRO:HD3	1.97	0.45
1:F:28:GLU:HB2	2:G:149:ARG:CZ	2.46	0.45
5:J:143:PRO:HG3	5:J:154:ALA:HB1	1.98	0.45
2:Q:97:PRO:HB3	2:Q:122:PHE:HB3	1.99	0.45
5:T:229:GLY:N	5:T:245:THR:HG22	2.31	0.45
5:J:99:SER:HB2	5:J:125:LEU:HA	1.99	0.45
5:J:140:VAL:HG23	5:J:250:ALA:HB3	1.99	0.45
4:N:25:TYR:OH	4:N:37:TYR:OH	2.25	0.45
5:E:96:ARG:HD3	5:E:128:GLU:HG2	1.98	0.45
4:N:37:TYR:OH	4:N:82:LYS:HD3	2.17	0.45
4:D:115:GLN:HG3	5:E:52:PHE:CG	2.52	0.45
5:E:29:HIS:HA	5:E:108:HIS:HA	1.98	0.45
5:E:42:TYR:O	5:E:103:LEU:N	2.49	0.45
5:E:189:PRO:HB2	5:E:201:TYR:HB3	1.98	0.45
5:O:238:GLN:HG2	5:O:240:ARG:H	1.82	0.45
4:S:165:SER:OG	4:S:170:VAL:O	2.33	0.45
2:G:180:LEU:HD13	2:G:184:VAL:HG23	1.97	0.44
1:A:117:LEU:HD13	1:A:119:VAL:HG23	1.99	0.44
2:L:117:CYS:HB2	2:L:131:TRP:CZ2	2.52	0.44
4:N:183:MET:O	4:N:185:PHE:N	2.48	0.44
4:D:138:TYR:HA	4:D:215:PHE:HE1	1.82	0.44
4:I:18:ASP:N	4:I:18:ASP:OD1	2.48	0.44
5:T:26:ILE:HD12	5:T:29:HIS:CE1	2.53	0.44
1:A:84:ASN:HD21	2:B:3:THR:HG21	1.82	0.44
5:O:26:ILE:HD12	5:O:29:HIS:NE2	2.32	0.44
4:N:152:LEU:HD11	4:N:189:SER:HB3	2.00	0.44
1:P:52:PHE:CZ	2:Q:86:GLY:HA2	2.53	0.44
4:S:2:GLN:HA	4:S:26:GLU:O	2.18	0.44
1:A:103:ASN:OD1	1:A:104:THR:N	2.48	0.44
1:F:52:PHE:CZ	2:G:86:GLY:HA2	2.52	0.44
5:T:41:TRP:HB2	5:T:54:ILE:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:185:PHE:CE2	4:D:187:SER:HB3	2.53	0.44
2:B:67:ILE:HG12	3:C:7:ARG:NH2	2.33	0.44
4:S:118:PHE:CD1	5:T:50:PRO:HG2	2.53	0.44
4:D:75:ARG:NH1	4:D:93:ALA:O	2.50	0.44
4:N:15:GLU:HG2	4:N:16:LYS:HG3	2.00	0.44
4:S:116:LEU:HD13	4:S:116:LEU:HA	1.87	0.44
2:B:172:THR:HG22	2:B:187:GLU:HG2	2.00	0.43
5:T:136:PRO:HB3	5:T:163:PHE:HB3	1.99	0.43
2:L:55:ARG:HB3	2:L:56:PRO:HD3	1.99	0.43
5:O:72:PRO:HG2	5:O:76:PHE:CD1	2.53	0.43
5:T:43:ARG:NH2	5:T:97:GLY:O	2.51	0.43
1:A:82:ALA:HB2	2:B:33:ASN:HB3	2.00	0.43
4:D:209:ILE:HG13	4:D:211:PRO:HD2	2.01	0.43
4:I:171:TYR:HE1	5:J:192:GLU:HA	1.83	0.43
5:O:166:ASP:HB3	5:O:201:TYR:CZ	2.53	0.43
4:S:75:ARG:HD2	4:S:93:ALA:HB3	1.99	0.43
2:B:60:TYR:HE2	5:E:111:ARG:HD3	1.81	0.43
4:D:185:PHE:CG	5:E:153:LYS:HE2	2.52	0.43
4:N:77:SER:HB2	4:N:90:THR:HB	1.99	0.43
5:T:75:ARG:HD2	5:T:92:GLN:O	2.19	0.43
1:F:65:ILE:HD13	5:J:57:GLN:HG2	2.01	0.43
5:J:96:ARG:HA	5:J:126:VAL:HB	2.01	0.43
5:T:107:SER:OG	5:T:111:ARG:O	2.32	0.43
1:K:105:LEU:HB2	1:K:153:PHE:CE1	2.53	0.43
1:K:123:CYS:O	1:K:126:GLU:HG2	2.19	0.43
4:S:40:PHE:CE1	4:S:55:ARG:HG3	2.54	0.43
4:D:175:LYS:HA	4:D:189:SER:O	2.19	0.43
4:S:140:LEU:HB2	4:S:150:VAL:HG13	2.00	0.43
4:I:49:GLU:H	4:I:49:GLU:CD	2.26	0.42
2:G:18:PHE:O	2:G:21:THR:HG22	2.19	0.42
5:E:130:LEU:HD13	5:E:230:LEU:HD22	2.01	0.42
1:K:87:PRO:HD2	1:K:170:LEU:HG	2.01	0.42
5:E:25:PRO:HD2	5:E:85:SER:O	2.20	0.42
4:D:8:GLN:HB3	4:D:11:ILE:HD11	2.00	0.42
4:S:14:VAL:O	4:S:94:SER:OG	2.36	0.42
5:T:242:LYS:HA	5:T:243:PRO:HD3	1.94	0.42
4:D:115:GLN:NE2	5:E:68:ASP:OD2	2.34	0.42
4:I:127:LEU:HD12	4:I:127:LEU:HA	1.85	0.42
2:L:114:LEU:HG	2:L:162:GLU:HA	2.01	0.42
4:N:54:ILE:HD12	4:N:54:ILE:HA	1.88	0.42
5:O:140:VAL:HG23	5:O:250:ALA:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:220:HIS:HB2	5:O:253:TRP:CZ3	2.54	0.42
4:S:43:LYS:HB2	4:S:53:LEU:HD11	2.01	0.42
5:T:71:LEU:HA	5:T:72:PRO:HD3	1.90	0.42
1:A:31:MET:HE2	1:A:32:PHE:HD2	1.84	0.42
5:J:26:ILE:HD12	5:J:29:HIS:NE2	2.35	0.42
4:N:154:THR:OG1	5:O:208:ARG:NH2	2.53	0.42
1:P:53:SER:N	3:R:-1:THR:O	2.47	0.42
2:Q:78:MET:HG3	3:R:2:ALA:HB3	2.00	0.42
2:G:55:ARG:HB3	2:G:56:PRO:HD3	2.02	0.42
2:Q:103:PRO:HA	2:Q:115:LEU:HD12	2.01	0.42
1:P:28:GLU:HB2	2:Q:149:ARG:NH2	2.35	0.42
1:A:47:GLU:H	1:A:47:GLU:HG2	1.61	0.42
4:D:154:THR:OG1	5:E:208:ARG:NH2	2.52	0.42
4:I:8:GLN:HB2	4:I:122:THR:HG22	2.02	0.42
4:D:209:ILE:HD12	4:D:209:ILE:HA	1.96	0.41
4:N:56:ARG:NH1	4:N:64:GLN:O	2.53	0.41
1:A:87:PRO:HD2	1:A:170:LEU:HG	2.01	0.41
4:D:138:TYR:HA	4:D:215:PHE:CE1	2.56	0.41
4:I:156:PHE:CZ	4:I:188:ASN:HB3	2.55	0.41
4:D:18:ASP:N	4:D:18:ASP:OD1	2.54	0.41
4:D:165:SER:HB2	4:D:170:VAL:HG23	2.02	0.41
5:E:99:SER:HB3	5:E:126:VAL:H	1.85	0.41
1:K:3:ALA:HA	2:L:18:PHE:HB2	2.01	0.41
1:A:118:ASN:HB2	1:A:166:GLU:HB2	2.02	0.41
2:G:172:THR:HG22	2:G:187:GLU:HG2	2.02	0.41
4:I:54:ILE:HG12	4:I:78:TRP:CE2	2.55	0.41
2:L:123:TYR:HB3	2:L:124:PRO:HD3	2.02	0.41
4:D:8:GLN:O	4:D:122:THR:HG22	2.20	0.41
5:E:240:ARG:HH12	5:E:243:PRO:HG3	1.85	0.41
4:I:177:VAL:N	5:J:184:CYS:SG	2.92	0.41
2:L:40:PHE:HB2	2:L:47:PHE:CD2	2.55	0.41
5:J:188:GLN:HA	5:J:189:PRO:HD3	1.91	0.41
2:L:147:LEU:HD22	2:L:155:PHE:HD2	1.85	0.41
4:S:40:PHE:HE2	4:S:116:LEU:HD21	1.85	0.41
4:N:80:PHE:HB2	4:N:87:PHE:HE1	1.86	0.41
5:O:123:ARG:HD3	5:O:167:HIS:CE1	2.56	0.41
4:S:176:CYS:C	5:T:184:CYS:SG	3.04	0.41
5:T:148:ILE:HG23	5:T:211:ALA:HB1	2.03	0.41
2:B:52:GLU:HG2	2:B:55:ARG:NH2	2.35	0.41
2:G:37:PHE:HD2	2:G:54:GLY:HA3	1.86	0.41
4:D:45:PRO:HG2	4:D:48:GLY:HA3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:LYS:HE3	5:E:161:THR:HG21	2.03	0.41
4:I:209:ILE:HG22	4:I:211:PRO:CD	2.51	0.41
5:J:71:LEU:HD22	5:J:76:PHE:HB3	2.01	0.41
1:K:52:PHE:CE1	2:L:86:GLY:HA2	2.56	0.41
4:N:185:PHE:CE2	4:N:187:SER:HB3	2.55	0.41
4:S:37:TYR:H	4:S:58:SER:CB	2.27	0.41
4:S:163:SER:HB3	4:S:206:ASN:HB2	2.03	0.41
1:A:70:LEU:HD13	2:B:9:PHE:HB2	2.03	0.41
2:G:67:ILE:HG12	3:H:7:ARG:NH1	2.35	0.41
1:K:14:GLN:NE2	1:K:115:PRO:HG2	2.36	0.41
1:K:140:ARG:HB3	1:K:142:ASP:OD1	2.20	0.41
2:Q:123:TYR:HB3	2:Q:124:PRO:HD3	2.03	0.41
1:A:41:THR:HG21	1:A:54:PHE:HB3	2.03	0.41
4:D:178:LEU:O	4:D:186:LYS:HA	2.21	0.41
4:S:54:ILE:HD12	4:S:54:ILE:HA	1.92	0.41
2:G:66:ASP:CG	5:J:111:ARG:HH22	2.29	0.40
1:K:41:THR:HG21	1:K:54:PHE:HB3	2.03	0.40
4:N:170:VAL:HB	4:N:194:SER:HB2	2.02	0.40
2:G:64:GLN:HG3	5:J:111:ARG:HE	1.86	0.40
1:A:33:TYR:CG	1:A:136:LEU:HD11	2.56	0.40
2:B:40:PHE:HB2	2:B:47:PHE:CE1	2.56	0.40
5:E:71:LEU:HA	5:E:72:PRO:HD3	1.95	0.40
5:O:125:LEU:HD21	5:O:167:HIS:CE1	2.56	0.40
4:S:39:LEU:HG	4:S:106:LEU:HD13	2.02	0.40
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.57	0.40
1:F:17:ARG:HA	1:F:17:ARG:NH2	2.37	0.40
2:G:40:PHE:HB2	2:G:47:PHE:CE2	2.57	0.40
4:D:136:ALA:HB2	4:D:213:ASP:HB3	2.02	0.40
4:I:41:TRP:CZ3	4:I:102:TYR:HB3	2.55	0.40
2:L:87:GLY:HA2	2:L:91:LEU:HD13	2.04	0.40
4:S:185:PHE:CE2	4:S:187:SER:HB3	2.56	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	178/181 (98%)	175 (98%)	3 (2%)	0	100	100
1	F	178/181 (98%)	171 (96%)	7 (4%)	0	100	100
1	K	178/181 (98%)	173 (97%)	5 (3%)	0	100	100
1	P	178/181 (98%)	172 (97%)	6 (3%)	0	100	100
2	B	165/188 (88%)	157 (95%)	8 (5%)	0	100	100
2	G	160/188 (85%)	156 (98%)	4 (2%)	0	100	100
2	L	174/188 (93%)	169 (97%)	5 (3%)	0	100	100
2	Q	173/188 (92%)	163 (94%)	10 (6%)	0	100	100
3	C	12/15 (80%)	12 (100%)	0	0	100	100
3	H	12/15 (80%)	12 (100%)	0	0	100	100
3	M	12/15 (80%)	12 (100%)	0	0	100	100
3	R	12/15 (80%)	12 (100%)	0	0	100	100
4	D	199/207 (96%)	187 (94%)	11 (6%)	1 (0%)	24	54
4	I	199/207 (96%)	180 (90%)	18 (9%)	1 (0%)	24	54
4	N	197/207 (95%)	186 (94%)	11 (6%)	0	100	100
4	S	197/207 (95%)	188 (95%)	9 (5%)	0	100	100
5	E	233/243 (96%)	223 (96%)	9 (4%)	1 (0%)	30	59
5	J	235/243 (97%)	229 (97%)	6 (3%)	0	100	100
5	O	236/243 (97%)	224 (95%)	11 (5%)	1 (0%)	30	59
5	T	236/243 (97%)	224 (95%)	12 (5%)	0	100	100
All	All	3164/3336 (95%)	3025 (96%)	135 (4%)	4 (0%)	48	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	27	SER
4	D	120	SER
4	I	182	SER
5	O	72	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	161/162 (99%)	160 (99%)	1 (1%)	78	80
1	F	161/162 (99%)	160 (99%)	1 (1%)	78	80
1	K	161/162 (99%)	159 (99%)	2 (1%)	63	72
1	P	161/162 (99%)	161 (100%)	0	100	100
2	B	153/167 (92%)	151 (99%)	2 (1%)	61	71
2	G	150/167 (90%)	148 (99%)	2 (1%)	61	71
2	L	159/167 (95%)	158 (99%)	1 (1%)	78	80
2	Q	158/167 (95%)	158 (100%)	0	100	100
3	C	11/11 (100%)	11 (100%)	0	100	100
3	H	11/11 (100%)	11 (100%)	0	100	100
3	M	11/11 (100%)	11 (100%)	0	100	100
3	R	11/11 (100%)	11 (100%)	0	100	100
4	D	184/190 (97%)	178 (97%)	6 (3%)	33	57
4	I	184/190 (97%)	177 (96%)	7 (4%)	29	54
4	N	182/190 (96%)	174 (96%)	8 (4%)	25	51
4	S	182/190 (96%)	180 (99%)	2 (1%)	65	74
5	E	201/206 (98%)	200 (100%)	1 (0%)	81	81
5	J	203/206 (98%)	202 (100%)	1 (0%)	81	81
5	O	204/206 (99%)	202 (99%)	2 (1%)	68	75
5	T	204/206 (99%)	200 (98%)	4 (2%)	48	65
All	All	2852/2944 (97%)	2812 (99%)	40 (1%)	59	70

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
2	B	21	THR
2	B	156	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	104	THR
2	G	48	ARG
2	G	84	GLU
4	D	19	VAL
4	D	104	CYS
4	D	162	VAL
4	D	183	MET
4	D	203	ASN
4	D	210	ILE
5	E	53	LEU
4	I	14	VAL
4	I	18	ASP
4	I	39	LEU
4	I	67	ILE
4	I	104	CYS
4	I	122	THR
4	I	127	LEU
5	J	257	ASP
1	K	19	THR
1	K	73	LEU
2	L	174	GLN
4	N	95	GLN
4	N	97	VAL
4	N	104	CYS
4	N	162	VAL
4	N	170	VAL
4	N	183	MET
4	N	201	CYS
4	N	214	THR
5	O	67	ASP
5	O	114	GLU
4	S	51	VAL
4	S	178	LEU
5	T	26	ILE
5	T	53	LEU
5	T	83	GLU
5	T	247	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	75	GLN
2	B	100	ASN
1	F	67	ASN
1	F	75	GLN
4	D	2	GLN
4	D	8	GLN
4	D	81	GLN
5	E	108	HIS
5	E	175	ASN
5	E	220	HIS
4	I	2	GLN
4	I	161	ASN
5	J	220	HIS
5	J	238	GLN
5	J	246	GLN
1	K	14	GLN
1	K	67	ASN
1	K	68	ASN
1	K	79	HIS
2	L	150	ASN
4	N	57	ASN
1	P	68	ASN
2	Q	6	ASN
4	S	44	GLN
4	S	65	ASN
4	S	81	GLN
4	S	161	ASN
5	T	226	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 ⓘ

14 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	U	1	1,6	14,14,15	0.25	0	17,19,21	0.55	0
6	NAG	U	2	6	14,14,15	0.14	0	17,19,21	0.64	0
6	BMA	U	3	6	11,11,12	0.65	0	15,15,17	0.93	1 (6%)
6	MAN	U	4	6	11,11,12	0.77	0	15,15,17	1.60	1 (6%)
7	NAG	V	1	1,7	14,14,15	0.20	0	17,19,21	0.59	0
7	NAG	V	2	7	14,14,15	0.39	0	17,19,21	0.62	0
7	BMA	V	3	7	11,11,12	1.09	1 (9%)	15,15,17	1.06	1 (6%)
7	MAN	V	4	7	11,11,12	1.69	3 (27%)	15,15,17	1.38	2 (13%)
8	NAG	W	1	8,1	14,14,15	0.23	0	17,19,21	0.49	0
8	NAG	W	2	8	14,14,15	0.36	0	17,19,21	1.36	2 (11%)
8	BMA	W	3	8	11,11,12	0.56	0	15,15,17	0.81	0
8	NAG	X	1	8,1	14,14,15	0.22	0	17,19,21	0.49	0
8	NAG	X	2	8	14,14,15	0.36	0	17,19,21	0.57	0
8	BMA	X	3	8	11,11,12	0.95	0	15,15,17	0.78	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	U	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	U	2	6	-	2/6/23/26	0/1/1/1
6	BMA	U	3	6	-	0/2/19/22	0/1/1/1
6	MAN	U	4	6	-	0/2/19/22	0/1/1/1
7	NAG	V	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	V	2	7	-	2/6/23/26	0/1/1/1
7	BMA	V	3	7	-	2/2/19/22	0/1/1/1
7	MAN	V	4	7	-	0/2/19/22	1/1/1/1
8	NAG	W	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	W	2	8	-	4/6/23/26	0/1/1/1
8	BMA	W	3	8	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	X	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	0/6/23/26	0/1/1/1
8	BMA	X	3	8	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	V	4	MAN	O5-C5	3.79	1.50	1.43
7	V	4	MAN	O5-C1	3.18	1.49	1.43
7	V	4	MAN	C1-C2	2.30	1.57	1.52
7	V	3	BMA	O5-C5	2.22	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	U	4	MAN	C1-O5-C5	5.16	119.11	112.19
8	W	2	NAG	C2-N2-C7	4.64	129.12	122.90
7	V	4	MAN	C1-O5-C5	3.79	117.26	112.19
7	V	3	BMA	O5-C5-C6	3.23	113.94	107.66
7	V	4	MAN	O2-C2-C3	-2.30	105.38	110.15
6	U	3	BMA	C1-O5-C5	2.26	115.22	112.19
8	W	2	NAG	C1-C2-N2	2.25	113.98	110.43

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	V	3	BMA	O5-C5-C6-O6
8	W	3	BMA	O5-C5-C6-O6
7	V	3	BMA	C4-C5-C6-O6
8	W	2	NAG	C8-C7-N2-C2
8	W	2	NAG	O7-C7-N2-C2
7	V	2	NAG	O5-C5-C6-O6
8	W	3	BMA	C4-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	U	2	NAG	C1-C2-N2-C7
8	W	2	NAG	C1-C2-N2-C7
8	W	2	NAG	C3-C2-N2-C7
7	V	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	X	3	BMA	C4-C5-C6-O6

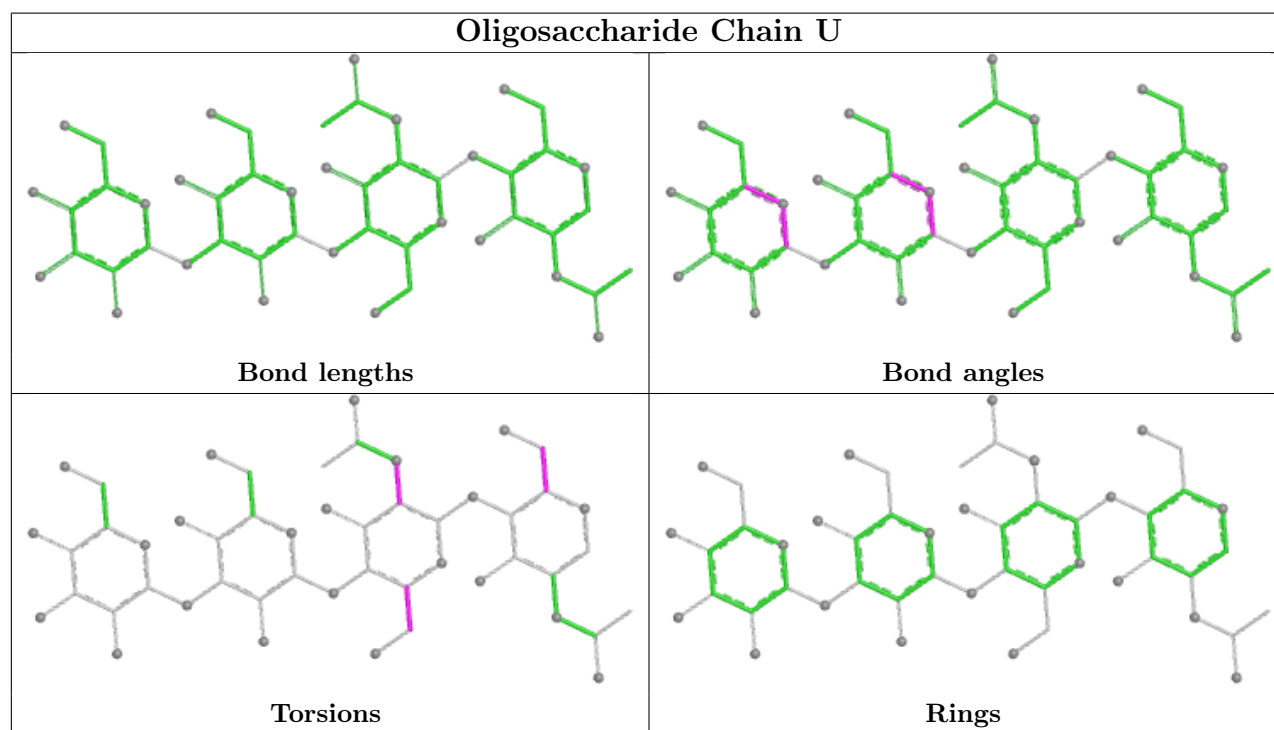
All (1) ring outliers are listed below:

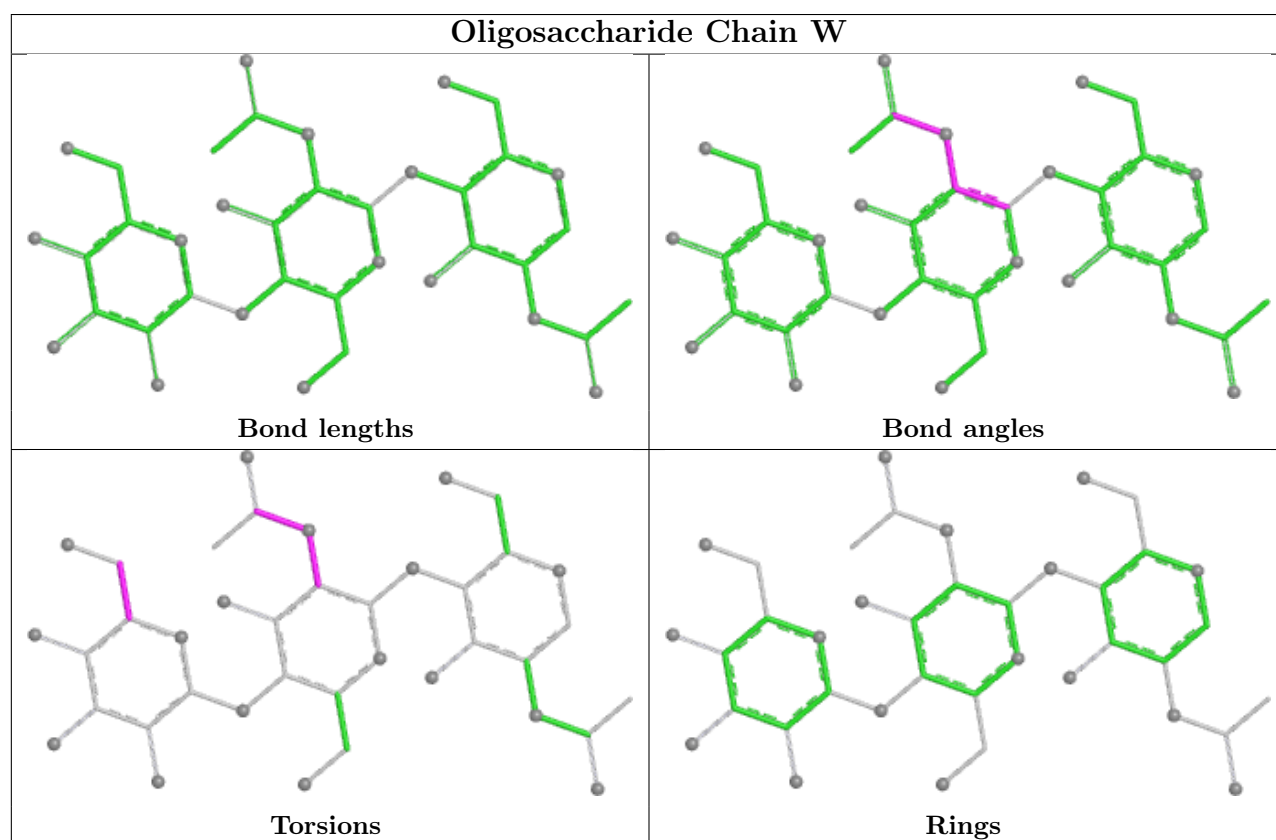
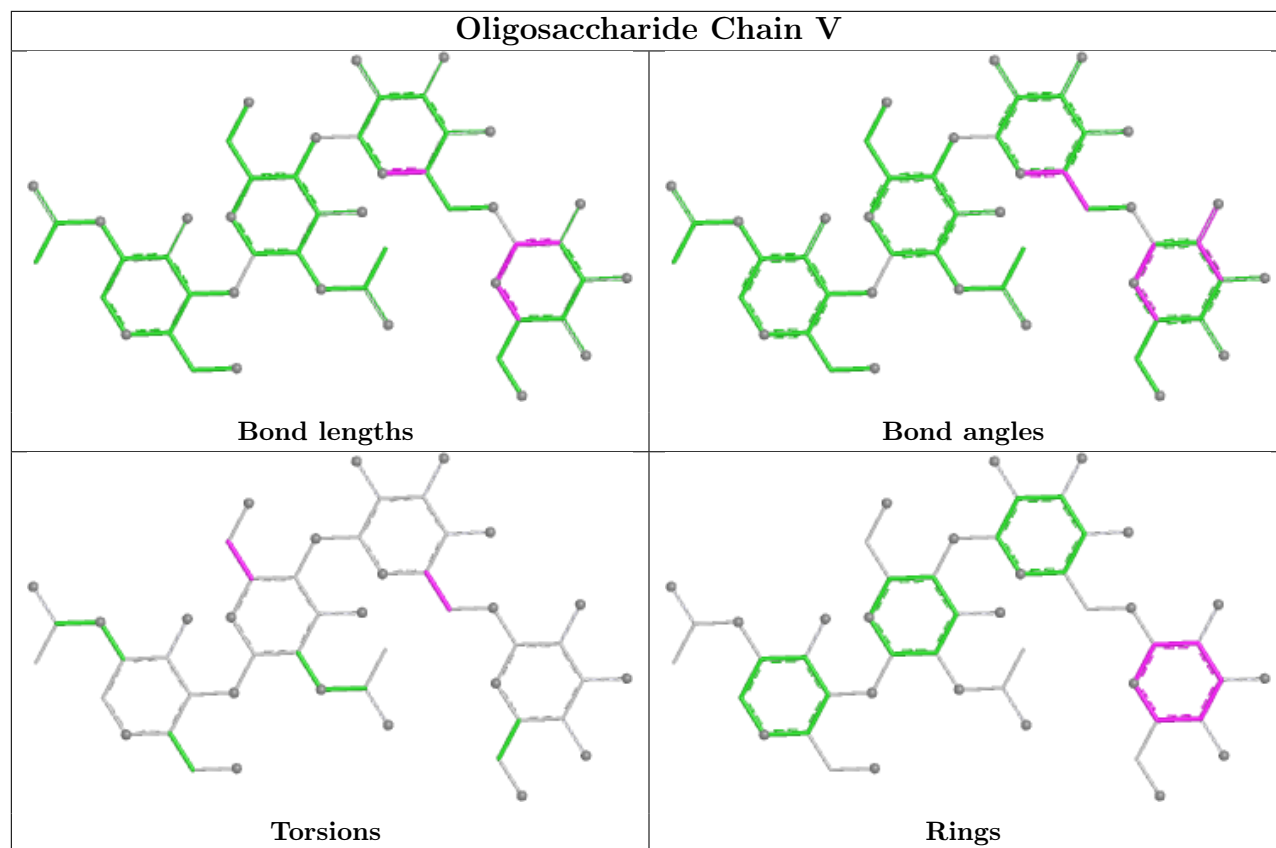
Mol	Chain	Res	Type	Atoms
7	V	4	MAN	C1-C2-C3-C4-C5-O5

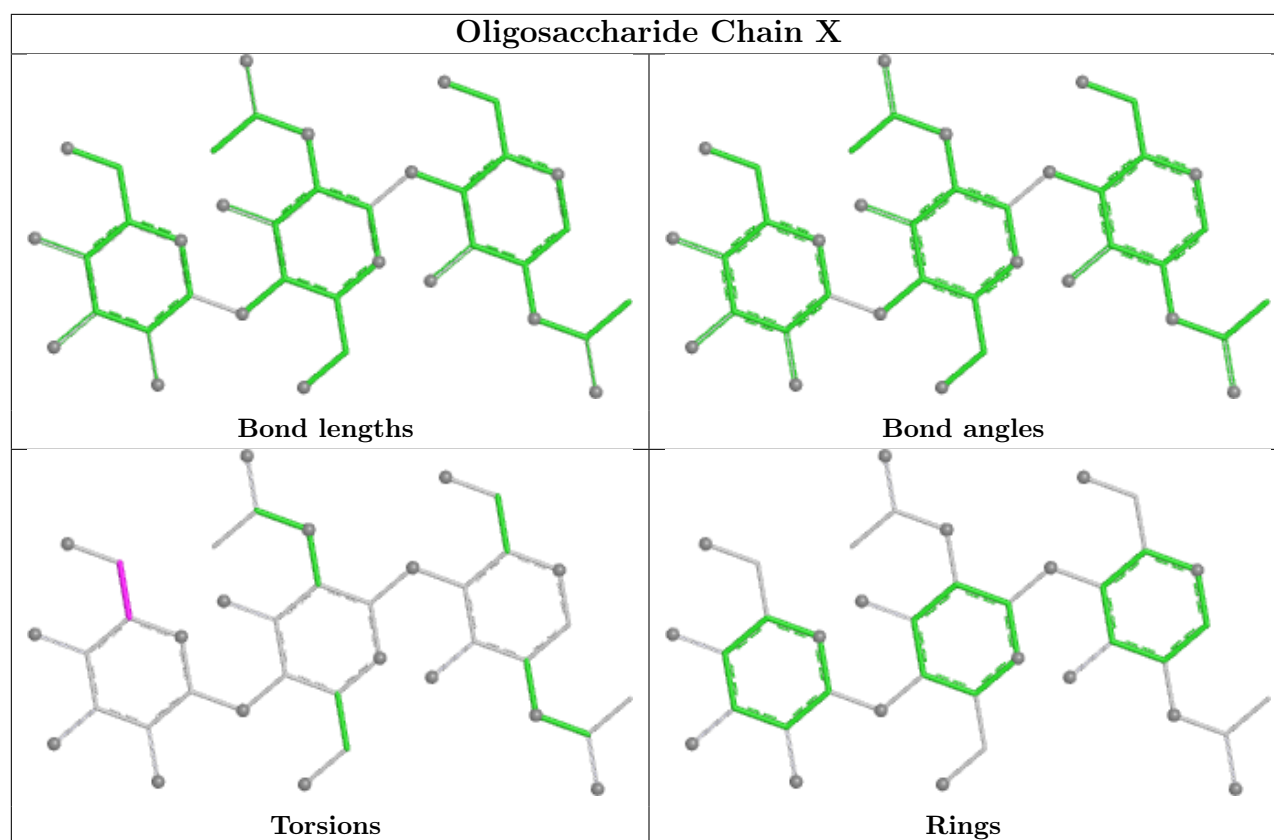
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	W	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.







5.6 Ligand geometry [i](#)

8 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$
9	NAG	A	201	1	14,14,15	0.25	0	17,19,21	0.45	0
9	NAG	Q	201	2	14,14,15	1.15	1 (7%)	17,19,21	1.13	1 (5%)
9	NAG	F	201	1	14,14,15	0.25	0	17,19,21	0.59	0
9	NAG	K	201	1	14,14,15	0.25	0	17,19,21	0.46	0
9	NAG	B	201	2	14,14,15	0.27	0	17,19,21	0.45	0
9	NAG	G	201	2	14,14,15	0.20	0	17,19,21	0.60	0
9	NAG	P	201	1	14,14,15	0.37	0	17,19,21	0.61	1 (5%)
9	NAG	L	201	2	14,14,15	0.28	0	17,19,21	0.47	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
9	NAG	A	201	1	-	0/6/23/26	0/1/1/1
9	NAG	Q	201	2	-	1/6/23/26	0/1/1/1
9	NAG	F	201	1	-	2/6/23/26	0/1/1/1
9	NAG	K	201	1	-	0/6/23/26	0/1/1/1
9	NAG	B	201	2	-	0/6/23/26	0/1/1/1
9	NAG	G	201	2	-	2/6/23/26	0/1/1/1
9	NAG	P	201	1	-	0/6/23/26	0/1/1/1
9	NAG	L	201	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	201	NAG	C1-C2	3.47	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	201	NAG	C2-N2-C7	3.30	127.32	122.90
9	P	201	NAG	C1-O5-C5	2.03	114.90	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	Q	201	NAG	C1-C2-N2-C7
9	L	201	NAG	O5-C5-C6-O6
9	F	201	NAG	C1-C2-N2-C7
9	G	201	NAG	C3-C2-N2-C7
9	G	201	NAG	C1-C2-N2-C7
9	F	201	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	Q	201	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	180/181 (99%)	0.07	0 100 100	61, 85, 114, 143	0
1	F	180/181 (99%)	0.38	7 (3%) 43 31	70, 98, 138, 176	0
1	K	180/181 (99%)	0.15	3 (1%) 69 54	65, 88, 128, 186	0
1	P	180/181 (99%)	0.22	4 (2%) 62 47	63, 88, 133, 189	0
2	B	171/188 (90%)	0.50	12 (7%) 22 18	67, 106, 176, 228	0
2	G	168/188 (89%)	1.34	37 (22%) 2 4	72, 117, 202, 234	8 (4%)
2	L	178/188 (94%)	0.49	8 (4%) 38 28	74, 112, 188, 222	0
2	Q	177/188 (94%)	0.48	8 (4%) 38 28	71, 110, 185, 224	0
3	C	14/15 (93%)	0.45	0 100 100	64, 75, 108, 113	0
3	H	14/15 (93%)	0.65	2 (14%) 6 8	73, 89, 121, 140	0
3	M	14/15 (93%)	0.40	0 100 100	70, 86, 122, 131	0
3	R	14/15 (93%)	0.28	0 100 100	65, 79, 108, 132	0
4	D	201/207 (97%)	0.61	12 (5%) 27 21	59, 93, 155, 196	0
4	I	201/207 (97%)	0.75	10 (4%) 34 25	64, 100, 159, 202	0
4	N	199/207 (96%)	0.69	10 (5%) 34 25	60, 101, 161, 193	0
4	S	199/207 (96%)	0.58	13 (6%) 25 20	60, 96, 162, 200	0
5	E	235/243 (96%)	0.22	8 (3%) 48 35	59, 83, 130, 173	0
5	J	237/243 (97%)	0.34	6 (2%) 58 43	63, 87, 125, 171	0
5	O	238/243 (97%)	0.43	10 (4%) 40 29	62, 98, 153, 185	0
5	T	238/243 (97%)	0.43	11 (4%) 37 27	61, 99, 151, 194	0
All	All	3218/3336 (96%)	0.47	161 (5%) 34 25	59, 95, 167, 234	8 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	161	LEU	9.9
2	G	117	CYS	8.8
2	G	173	CYS	8.4
2	G	160	MET	7.2
2	G	115	LEU	7.0
2	G	164	THR	6.4
2	G	97	PRO	5.5
2	G	133	LEU	5.4
5	O	184	CYS	5.2
5	T	184	CYS	5.2
2	G	142	VAL	5.1
5	O	85	SER	5.1
4	S	176	CYS	5.1
5	O	167	HIS	5.0
4	I	176	CYS	4.9
1	F	7	SER	4.9
1	F	180	ALA	4.8
5	T	68	ASP	4.8
5	J	184	CYS	4.8
5	O	68	ASP	4.7
2	G	187	GLU	4.7
4	N	176	CYS	4.6
2	G	159	VAL	4.6
2	G	123	TYR	4.5
4	D	176	CYS	4.4
5	E	184	CYS	4.1
4	I	148	LYS	4.0
2	G	122	PHE	3.9
5	T	67	ASP	3.8
4	I	200	ALA	3.7
4	N	207	ASN	3.6
5	J	67	ASP	3.5
4	N	121	GLY	3.5
2	G	118	HIS	3.4
4	D	207	ASN	3.4
5	E	69	SER	3.4
4	I	199	PHE	3.3
4	N	204	ALA	3.3
5	T	216	ASN	3.2
5	E	68	ASP	3.2
2	G	184	VAL	3.2
5	O	216	ASN	3.2
5	O	125	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	177	HIS	3.1
2	B	126	SER	3.1
4	D	121	GLY	3.0
2	Q	152	ASP	3.0
5	E	67	ASP	3.0
4	S	212	GLU	3.0
5	J	68	ASP	3.0
2	B	123	TYR	2.9
4	D	208	SER	2.9
2	Q	188	TRP	2.9
2	G	102	SER	2.9
2	Q	2	ALA	2.9
5	J	69	SER	2.9
5	T	69	SER	2.9
5	T	167	HIS	2.9
4	N	80	PHE	2.8
2	B	131	TRP	2.8
5	O	8	PRO	2.8
2	B	178	THR	2.8
2	Q	123	TYR	2.7
4	S	148	LYS	2.7
1	K	180	ALA	2.7
4	I	87	PHE	2.7
4	S	48	GLY	2.7
2	G	116	VAL	2.7
1	P	26	PHE	2.7
5	J	113	GLY	2.7
2	B	166	GLN	2.6
2	G	124	PRO	2.6
5	T	125	LEU	2.6
2	L	97	PRO	2.6
2	G	33	ASN	2.6
2	L	123	TYR	2.6
4	I	163	SER	2.6
5	O	198	ASP	2.6
3	H	-2	ALA	2.6
2	G	134	ASN	2.6
2	B	124	PRO	2.5
2	L	155	PHE	2.5
2	G	180	LEU	2.5
4	I	196	LYS	2.5
4	N	200	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	9	THR	2.5
5	T	114	GLU	2.5
1	K	28	GLU	2.4
4	N	163	SER	2.4
2	B	121	ASP	2.4
5	E	121	GLY	2.4
4	S	65	ASN	2.4
5	T	198	ASP	2.4
5	E	85	SER	2.4
2	B	116	VAL	2.4
2	G	121	ASP	2.3
2	G	59	GLU	2.3
2	G	176	GLU	2.3
2	G	99	VAL	2.3
2	B	172	THR	2.3
4	S	122	THR	2.3
5	E	198	ASP	2.3
2	B	92	GLN	2.3
1	K	7	SER	2.3
1	P	18	PRO	2.3
4	N	67	ILE	2.3
4	S	210	ILE	2.3
5	T	63	THR	2.3
1	F	177	HIS	2.3
2	G	83	TYR	2.3
5	T	129	ASP	2.3
1	F	99	LEU	2.3
4	D	215	PHE	2.3
2	B	176	GLU	2.2
2	G	103	PRO	2.2
2	Q	116	VAL	2.2
5	E	47	GLY	2.2
5	J	7	THR	2.2
4	D	163	SER	2.2
4	S	68	SER	2.2
1	F	28	GLU	2.2
3	H	1	LEU	2.2
1	P	17	ARG	2.2
4	I	212	GLU	2.2
1	P	20	GLY	2.2
4	D	23	CYS	2.2
4	S	214	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	S	163	SER	2.2
5	O	27	SER	2.2
2	G	84	GLU	2.2
4	D	212	GLU	2.2
4	S	149	SER	2.1
4	S	208	SER	2.1
2	L	125	GLY	2.1
2	L	121	ASP	2.1
5	O	67	ASP	2.1
2	G	179	SER	2.1
4	I	185	PHE	2.1
2	G	157	ILE	2.1
2	G	138	GLU	2.1
4	N	49	GLU	2.1
2	Q	114	LEU	2.1
4	N	23	CYS	2.1
2	G	178	THR	2.1
2	B	160	MET	2.1
2	G	174	GLN	2.1
2	G	95	VAL	2.1
4	I	166	LYS	2.1
2	Q	96	GLN	2.1
2	Q	174	GLN	2.1
2	L	122	PHE	2.1
1	F	94	LYS	2.0
4	S	137	VAL	2.0
4	D	68	SER	2.0
2	L	160	MET	2.0
4	D	213	ASP	2.0
2	L	95	VAL	2.0
4	D	182	SER	2.0
2	G	163	MET	2.0
2	G	185	THR	2.0
1	F	17	ARG	2.0

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

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

6.3 Carbohydrates

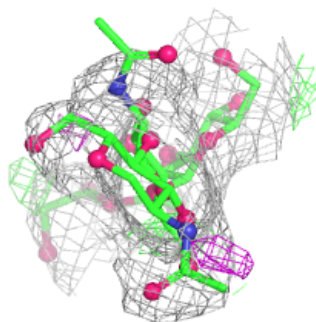
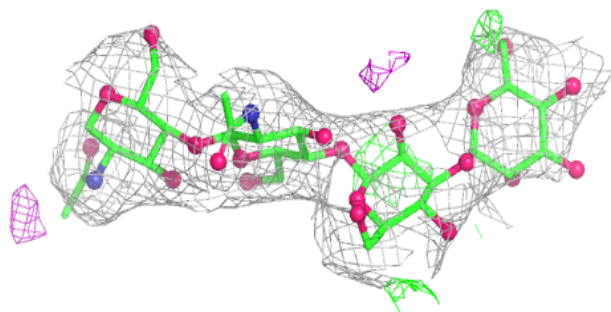
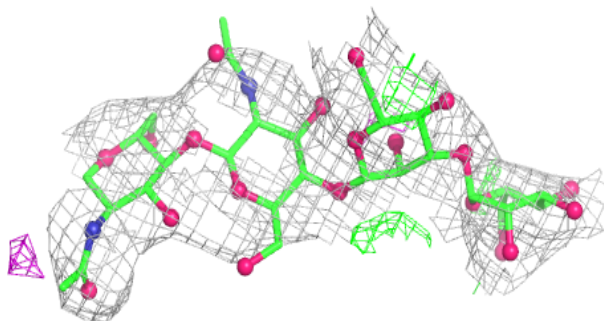
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MAN	V	4	11/12	0.51	0.20	203,210,217,219	0
8	BMA	X	3	11/12	0.58	0.14	148,157,178,195	0
8	BMA	W	3	11/12	0.64	0.10	121,151,163,164	0
7	BMA	V	3	11/12	0.64	0.14	162,164,177,182	0
8	NAG	W	2	14/15	0.66	0.12	136,159,176,177	0
6	BMA	U	3	11/12	0.67	0.17	120,148,156,158	0
7	NAG	V	2	14/15	0.70	0.19	122,138,154,160	0
6	MAN	U	4	11/12	0.73	0.17	151,193,202,219	0
8	NAG	X	2	14/15	0.76	0.13	136,142,160,168	0
6	NAG	U	2	14/15	0.88	0.13	107,124,139,144	0
8	NAG	X	1	14/15	0.93	0.09	100,107,133,138	0
7	NAG	V	1	14/15	0.93	0.11	89,101,130,133	0
8	NAG	W	1	14/15	0.93	0.08	91,115,136,141	0
6	NAG	U	1	14/15	0.95	0.07	75,99,111,116	0

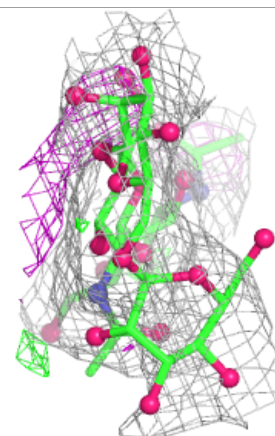
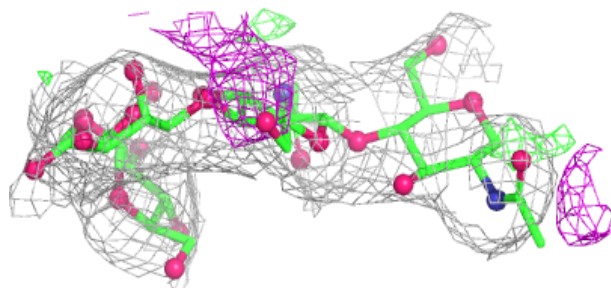
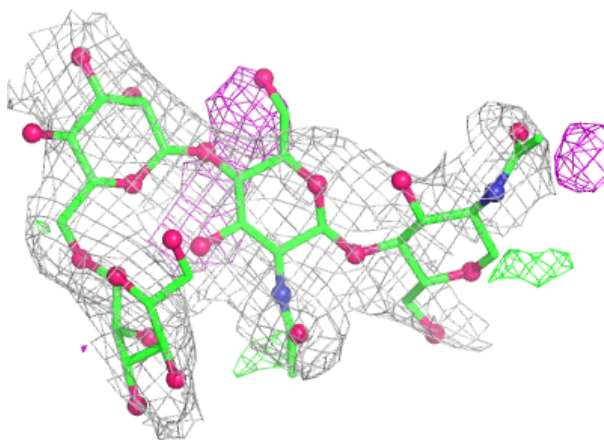
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain U:

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

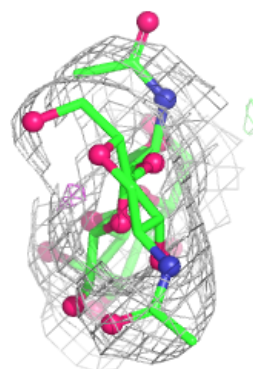
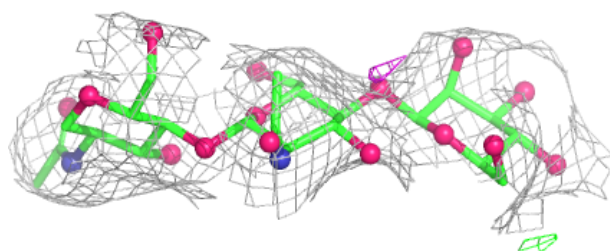
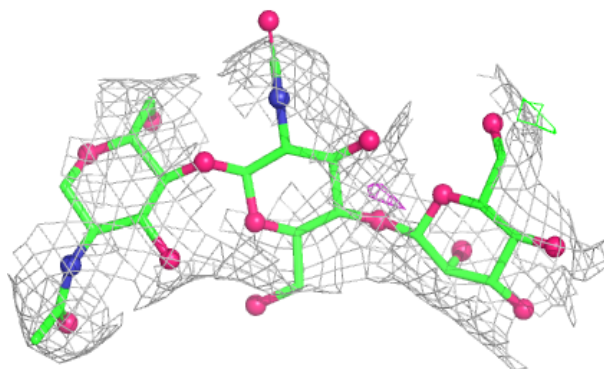
**Electron density around Chain V:**

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

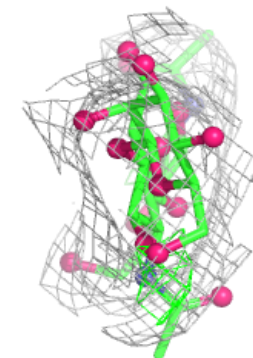
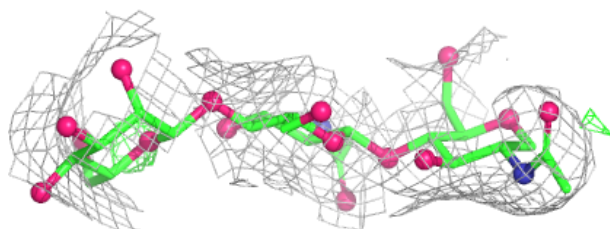
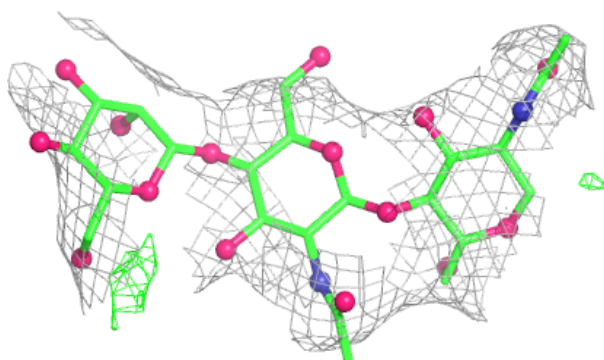


Electron density around Chain W:

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

**Electron density around Chain X:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	NAG	Q	201	14/15	0.46	0.12	133,187,193,196	0
9	NAG	L	201	14/15	0.47	0.12	158,178,195,196	0
9	NAG	G	201	14/15	0.49	0.13	132,183,192,195	0
9	NAG	F	201	14/15	0.71	0.12	147,167,180,181	0
9	NAG	B	201	14/15	0.71	0.12	126,170,183,188	0
9	NAG	P	201	14/15	0.76	0.13	144,166,180,181	0
9	NAG	A	201	14/15	0.78	0.11	119,138,155,158	0
9	NAG	K	201	14/15	0.80	0.12	146,156,172,173	0

6.5 Other polymers [i](#)

There are no such residues in this entry.