



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:06 PM BST

PDB ID : 6TT9
Title : rTBL Recombinant Lectin From Tepary Bean
Authors : Martinez Alarcon, D.; Varrot, A.
Deposited on : 2019-12-26
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

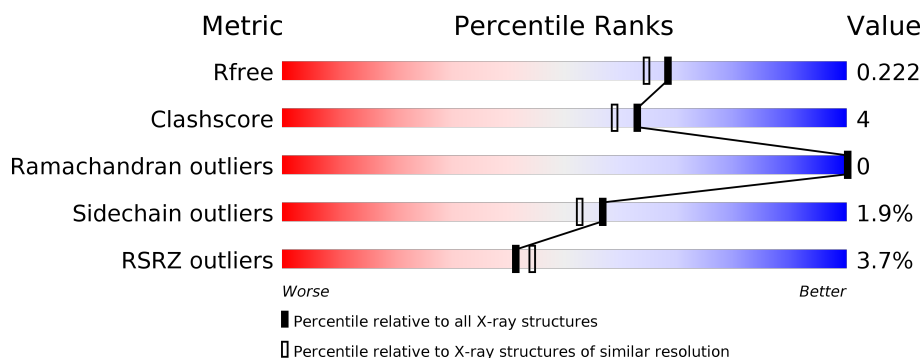
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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




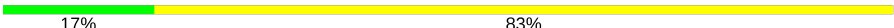
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 on 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	AAA	255	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>9%</div> </div> </div>
1	BBB	255	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	CCC	255	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	DDD	255	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>11%</div> </div> </div>
2	A	8	<div> <div></div> <div> <div>50%</div> <div>38%</div> <div>13%</div> </div> </div>
3	B	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	2	 50%50%
4	D	6	 17%83%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7916 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 Phytohemagglutinin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	AAA	233	Total	C	N	O	0	4	0
			1805	1139	300	366			
1	BBB	230	Total	C	N	O	0	4	0
			1779	1129	293	357			
1	CCC	233	Total	C	N	O	0	5	0
			1805	1138	300	367			
1	DDD	228	Total	C	N	O	0	3	0
			1747	1106	289	352			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-4	GLU	-	expression tag	UNP Q40750
AAA	-3	ALA	-	expression tag	UNP Q40750
AAA	-2	GLU	-	expression tag	UNP Q40750
AAA	-1	ALA	-	expression tag	UNP Q40750
AAA	0	ALA	-	expression tag	UNP Q40750
AAA	1	ALA	-	expression tag	UNP Q40750
AAA	117	LYS	ARG	conflict	UNP Q40750
AAA	158	VAL	GLY	conflict	UNP Q40750
AAA	159	ASN	GLN	conflict	UNP Q40750
AAA	206	SER	ARG	conflict	UNP Q40750
AAA	216	SER	THR	conflict	UNP Q40750
AAA	245	HIS	-	expression tag	UNP Q40750
AAA	246	HIS	-	expression tag	UNP Q40750
AAA	247	HIS	-	expression tag	UNP Q40750
AAA	248	HIS	-	expression tag	UNP Q40750
AAA	249	HIS	-	expression tag	UNP Q40750
AAA	250	HIS	-	expression tag	UNP Q40750
BBB	-4	GLU	-	expression tag	UNP Q40750
BBB	-3	ALA	-	expression tag	UNP Q40750
BBB	-2	GLU	-	expression tag	UNP Q40750
BBB	-1	ALA	-	expression tag	UNP Q40750

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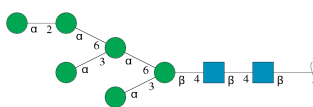
Chain	Residue	Modelled	Actual	Comment	Reference
BBB	0	ALA	-	expression tag	UNP Q40750
BBB	1	ALA	-	expression tag	UNP Q40750
BBB	117	LYS	ARG	conflict	UNP Q40750
BBB	158	VAL	GLY	conflict	UNP Q40750
BBB	159	ASN	GLN	conflict	UNP Q40750
BBB	206	SER	ARG	conflict	UNP Q40750
BBB	216	SER	THR	conflict	UNP Q40750
BBB	245	HIS	-	expression tag	UNP Q40750
BBB	246	HIS	-	expression tag	UNP Q40750
BBB	247	HIS	-	expression tag	UNP Q40750
BBB	248	HIS	-	expression tag	UNP Q40750
BBB	249	HIS	-	expression tag	UNP Q40750
BBB	250	HIS	-	expression tag	UNP Q40750
CCC	-4	GLU	-	expression tag	UNP Q40750
CCC	-3	ALA	-	expression tag	UNP Q40750
CCC	-2	GLU	-	expression tag	UNP Q40750
CCC	-1	ALA	-	expression tag	UNP Q40750
CCC	0	ALA	-	expression tag	UNP Q40750
CCC	1	ALA	-	expression tag	UNP Q40750
CCC	117	LYS	ARG	conflict	UNP Q40750
CCC	158	VAL	GLY	conflict	UNP Q40750
CCC	159	ASN	GLN	conflict	UNP Q40750
CCC	206	SER	ARG	conflict	UNP Q40750
CCC	216	SER	THR	conflict	UNP Q40750
CCC	245	HIS	-	expression tag	UNP Q40750
CCC	246	HIS	-	expression tag	UNP Q40750
CCC	247	HIS	-	expression tag	UNP Q40750
CCC	248	HIS	-	expression tag	UNP Q40750
CCC	249	HIS	-	expression tag	UNP Q40750
CCC	250	HIS	-	expression tag	UNP Q40750
DDD	-4	GLU	-	expression tag	UNP Q40750
DDD	-3	ALA	-	expression tag	UNP Q40750
DDD	-2	GLU	-	expression tag	UNP Q40750
DDD	-1	ALA	-	expression tag	UNP Q40750
DDD	0	ALA	-	expression tag	UNP Q40750
DDD	1	ALA	-	expression tag	UNP Q40750
DDD	117	LYS	ARG	conflict	UNP Q40750
DDD	158	VAL	GLY	conflict	UNP Q40750
DDD	159	ASN	GLN	conflict	UNP Q40750
DDD	206	SER	ARG	conflict	UNP Q40750
DDD	216	SER	THR	conflict	UNP Q40750
DDD	245	HIS	-	expression tag	UNP Q40750

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	246	HIS	-	expression tag	UNP Q40750
DDD	247	HIS	-	expression tag	UNP Q40750
DDD	248	HIS	-	expression tag	UNP Q40750
DDD	249	HIS	-	expression tag	UNP Q40750
DDD	250	HIS	-	expression tag	UNP Q40750

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[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.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	A	8	Total	C	N	O	0	0	0
			94	52	2	40			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-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
4	D	6	Total	C	N	O	0	0	0
			72	40	2	30			

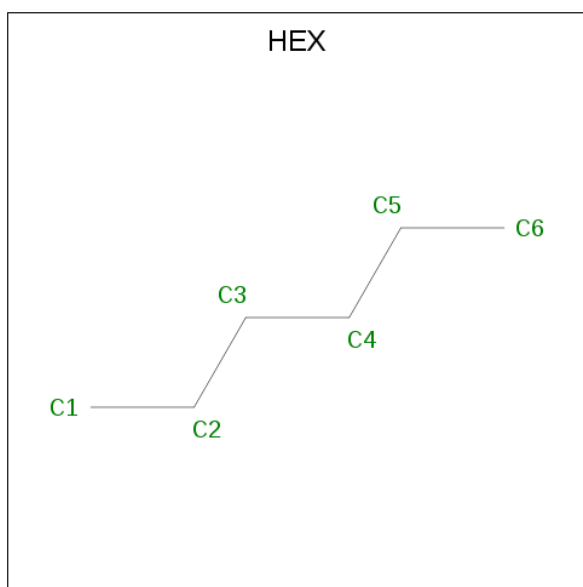
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	CCC	1	Total	Ca	0	0
			1	1		
5	BBB	1	Total	Ca	0	0
			1	1		
5	DDD	1	Total	Ca	0	0
			1	1		
5	AAA	1	Total	Ca	0	0
			1	1		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	CCC	1	Total	Mn	0	0
			1	1		
6	BBB	1	Total	Mn	0	0
			1	1		
6	DDD	1	Total	Mn	0	0
			1	1		
6	AAA	1	Total	Mn	0	0
			1	1		

- Molecule 7 is HEXANE (three-letter code: HEX) (formula: C₆H₁₄).

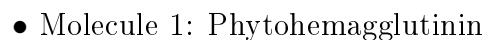
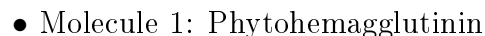
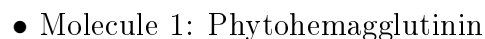


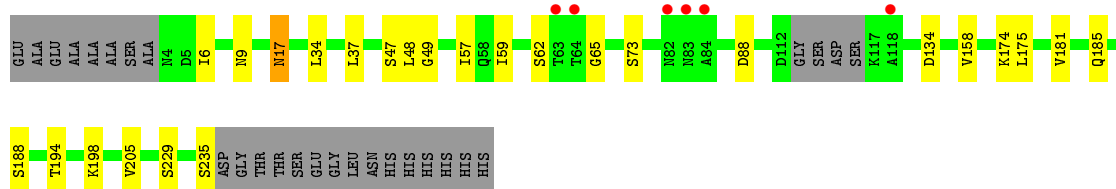
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	1	Total C 6 6	0	0
7	BBB	1	Total C 6 6	0	0
7	CCC	1	Total C 6 6	0	0
7	CCC	1	Total C 6 6	0	0
7	DDD	1	Total C 6 6	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	AAA	128	Total O 129 129	0	1
8	BBB	127	Total O 131 131	0	4
8	CCC	131	Total O 136 136	0	5
8	DDD	118	Total O 124 124	0	6

- Molecule 1: Phytohemagglutinin





- Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[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 A: 50% 38% 13%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 50% 50%



- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-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 D: 17% 83%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.57Å 64.47Å 67.59Å 96.35° 101.95° 97.27°	Depositor
Resolution (Å)	32.73 – 1.90 32.73 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.73-1.90) 99.7 (32.73-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.169 , 0.213 0.177 , 0.222	Depositor DCC
R_{free} test set	3646 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7916	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	AAA	0.90	2/1847 (0.1%)	0.96	1/2520 (0.0%)
1	BBB	0.91	2/1820 (0.1%)	0.98	1/2482 (0.0%)
1	CCC	0.87	2/1844 (0.1%)	0.99	1/2517 (0.0%)
1	DDD	0.89	1/1785 (0.1%)	0.97	1/2437 (0.0%)
All	All	0.89	7/7296 (0.1%)	0.98	4/9956 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	15	GLU	CD-OE1	7.44	1.33	1.25
1	AAA	15[A]	GLU	CD-OE2	7.32	1.33	1.25
1	AAA	15[B]	GLU	CD-OE2	7.32	1.33	1.25
1	CCC	15	GLU	CD-OE1	6.66	1.32	1.25
1	CCC	15	GLU	CD-OE2	6.16	1.32	1.25
1	DDD	47	SER	CA-CB	-5.99	1.44	1.52
1	BBB	118	ALA	C-O	5.29	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	235	SER	CA-C-O	-6.44	106.57	120.10
1	DDD	134	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	AAA	104	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	BBB	134	ASP	CB-CG-OD2	5.13	122.91	118.30

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	AAA	1805	0	1732	17	0
1	BBB	1779	0	1723	20	0
1	CCC	1805	0	1729	17	0
1	DDD	1747	0	1662	15	0
2	A	94	0	79	1	0
3	B	28	0	25	0	0
3	C	28	0	25	1	0
4	D	72	0	61	0	0
5	AAA	1	0	0	0	0
5	BBB	1	0	0	0	0
5	CCC	1	0	0	0	0
5	DDD	1	0	0	0	0
6	AAA	1	0	0	0	0
6	BBB	1	0	0	0	0
6	CCC	1	0	0	0	0
6	DDD	1	0	0	0	0
7	AAA	6	0	14	0	0
7	BBB	6	0	14	0	0
7	CCC	12	0	28	0	0
7	DDD	6	0	14	0	0
8	AAA	129	0	0	1	0
8	BBB	131	0	0	2	0
8	CCC	136	0	0	0	0
8	DDD	124	0	0	0	0
All	All	7916	0	7106	62	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 4.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:38:ASN:HB3	1:CCC:44:THR:HG22	1.67	0.77
1:AAA:175:LEU:HD21	1:CCC:181[A]:VAL:HG21	1.66	0.75
1:AAA:37:LEU:HD11	1:AAA:222:THR:HG22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:181[B]:VAL:HG11	1:CCC:175:LEU:HD21	1.77	0.66
1:BBB:181[A]:VAL:HG21	1:DDD:175:LEU:HD21	1.77	0.65
1:BBB:67:VAL:CG2	1:BBB:198:LYS:HE3	2.33	0.58
1:AAA:175:LEU:HD21	1:CCC:181[A]:VAL:CG2	2.34	0.57
1:AAA:181[B]:VAL:CG1	1:CCC:175:LEU:HD21	2.35	0.57
1:DDD:62:SER:OG	3:C:2:NAG:H62	2.05	0.56
1:BBB:37:LEU:HD11	8:BBB:454:HOH:O	2.06	0.56
1:BBB:34:LEU:O	1:BBB:49:GLY:HA3	2.08	0.54
1:AAA:48:LEU:HD11	1:AAA:109:GLY:HA3	1.89	0.54
1:BBB:181[A]:VAL:CG2	1:DDD:175:LEU:HD21	2.36	0.53
1:DDD:34:LEU:O	1:DDD:49:GLY:HA3	2.07	0.53
1:AAA:181[A]:VAL:HG12	1:AAA:188:SER:HB3	1.90	0.52
1:AAA:34:LEU:O	1:AAA:49:GLY:HA3	2.10	0.52
1:BBB:6:ILE:HG22	1:BBB:232[A]:SER:OG	2.09	0.50
1:AAA:6:ILE:HG21	1:AAA:57:ILE:HD12	1.94	0.49
1:CCC:6:ILE:HG21	1:CCC:57:ILE:HD12	1.95	0.49
1:AAA:158:VAL:HG21	1:AAA:185:GLN:HG3	1.96	0.48
1:BBB:104:ARG:HB2	8:BBB:406:HOH:O	2.12	0.48
1:CCC:34:LEU:O	1:CCC:49:GLY:HA3	2.12	0.48
1:BBB:158:VAL:HG21	1:BBB:185:GLN:HG3	1.95	0.48
1:CCC:158:VAL:HG21	1:CCC:185:GLN:HG3	1.95	0.47
1:DDD:6:ILE:HG21	1:DDD:57:ILE:HD12	1.95	0.47
1:CCC:214:GLY:HA3	1:CCC:219:ASN:O	2.14	0.47
1:BBB:48:LEU:HD11	1:BBB:109:GLY:HA3	1.97	0.46
1:DDD:59:ILE:HG12	1:DDD:205:VAL:HG22	1.98	0.45
1:CCC:42:GLU:OE1	1:CCC:42:GLU:HA	2.17	0.44
1:DDD:65:GLY:HA2	1:DDD:198:LYS:NZ	2.33	0.44
1:AAA:17:ASN:HD22	1:AAA:17:ASN:C	2.20	0.43
1:BBB:67:VAL:HG22	1:BBB:198:LYS:HG3	2.00	0.43
1:CCC:48:LEU:HD11	1:CCC:109:GLY:HA3	2.00	0.43
1:AAA:80:VAL:HG21	1:AAA:86:PRO:HB3	2.00	0.43
1:BBB:203:GLU:OE2	2:A:1:NAG:O6	2.36	0.43
1:CCC:59:ILE:HG12	1:CCC:205:VAL:HG22	1.99	0.43
1:BBB:67:VAL:HG23	1:BBB:198:LYS:HE3	1.99	0.42
1:CCC:5[A]:ASP:OD1	1:DDD:9:ASN:HB3	2.19	0.42
1:DDD:158:VAL:HG21	1:DDD:185:GLN:HG3	2.00	0.42
1:AAA:3:ALA:N	8:AAA:411:HOH:O	2.51	0.42
1:CCC:86:PRO:HB2	1:CCC:127:THR:HB	2.00	0.42
1:DDD:17:ASN:C	1:DDD:17:ASN:HD22	2.23	0.42
1:BBB:6:ILE:HG21	1:BBB:57:ILE:HD12	2.02	0.42
1:DDD:73:SER:HG	1:DDD:229[B]:SER:HG	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:174:LYS:O	1:DDD:194:THR:HA	2.19	0.42
1:DDD:37:LEU:N	1:DDD:37:LEU:HD22	2.35	0.42
1:BBB:176:LEU:HD23	1:BBB:176:LEU:C	2.40	0.42
1:BBB:176:LEU:HD23	1:BBB:177:VAL:N	2.35	0.42
1:AAA:15[A]:GLU:CD	1:AAA:15[A]:GLU:H	2.24	0.41
1:AAA:174:LYS:O	1:AAA:194:THR:HA	2.20	0.41
1:BBB:65:GLY:O	1:BBB:198:LYS:CE	2.69	0.41
1:BBB:6:ILE:CG2	1:BBB:232[A]:SER:OG	2.68	0.41
1:BBB:4:ASN:C	1:BBB:5:ASP:OD1	2.58	0.41
1:CCC:12:ARG:HG3	1:CCC:30:GLY:HA3	2.02	0.41
1:AAA:59:ILE:HG12	1:AAA:205:VAL:HG22	2.02	0.41
1:BBB:59:ILE:HD13	1:BBB:59:ILE:HA	1.91	0.41
1:CCC:174:LYS:O	1:CCC:194:THR:HA	2.20	0.41
1:DDD:48:LEU:HD23	1:DDD:49:GLY:N	2.35	0.41
1:CCC:17:ASN:C	1:CCC:17:ASN:HD22	2.23	0.41
1:DDD:181:VAL:HG12	1:DDD:188:SER:HB3	2.02	0.40
1:AAA:181[A]:VAL:HG12	1:AAA:188:SER:CB	2.51	0.40
1:BBB:62:SER:N	1:BBB:203:GLU:OE1	2.53	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	AAA	236/255 (92%)	229 (97%)	7 (3%)	0	100	100
1	BBB	231/255 (91%)	224 (97%)	7 (3%)	0	100	100
1	CCC	235/255 (92%)	229 (97%)	6 (3%)	0	100	100
1	DDD	226/255 (89%)	220 (97%)	6 (3%)	0	100	100
All	All	928/1020 (91%)	902 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	202/216 (94%)	199 (98%)	3 (2%)	65	62
1	BBB	200/216 (93%)	195 (98%)	5 (2%)	47	41
1	CCC	202/216 (94%)	198 (98%)	4 (2%)	55	51
1	DDD	193/216 (89%)	190 (98%)	3 (2%)	62	60
All	All	797/864 (92%)	782 (98%)	15 (2%)	57	53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	6	ILE
1	AAA	17	ASN
1	AAA	235	SER
1	BBB	5	ASP
1	BBB	6	ILE
1	BBB	17	ASN
1	BBB	88	ASP
1	BBB	235	SER
1	CCC	6	ILE
1	CCC	17	ASN
1	CCC	151	LYS
1	CCC	235	SER
1	DDD	17	ASN
1	DDD	88	ASP
1	DDD	235	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAG	A	1	1,2	14,14,15	0.40	0	17,19,21	1.37	2 (11%)
2	NAG	A	2	2	14,14,15	0.57	0	17,19,21	0.66	0
2	BMA	A	3	2	11,11,12	0.67	0	15,15,17	0.78	0
2	MAN	A	4	2	11,11,12	0.61	0	15,15,17	0.64	0
2	MAN	A	5	2	11,11,12	0.84	0	15,15,17	1.05	0
2	MAN	A	6	2	11,11,12	1.29	2 (18%)	15,15,17	1.27	2 (13%)
2	MAN	A	7	2	11,11,12	1.15	1 (9%)	15,15,17	1.54	2 (13%)
2	MAN	A	8	2	11,11,12	1.10	1 (9%)	15,15,17	0.98	0
3	NAG	B	1	1,3	14,14,15	0.46	0	17,19,21	1.14	2 (11%)
3	NAG	B	2	3	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
3	NAG	C	1	1,3	14,14,15	0.48	0	17,19,21	1.24	3 (17%)
3	NAG	C	2	3	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
4	NAG	D	1	1,4	14,14,15	0.40	0	17,19,21	1.85	4 (23%)
4	NAG	D	2	4	14,14,15	0.55	0	17,19,21	1.31	2 (11%)
4	BMA	D	3	4	11,11,12	0.74	0	15,15,17	0.92	0
4	MAN	D	4	4	11,11,12	0.44	0	15,15,17	0.84	1 (6%)
4	MAN	D	5	4	11,11,12	0.95	0	15,15,17	1.17	2 (13%)
4	MAN	D	6	4	11,11,12	0.43	0	15,15,17	1.09	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2	2	-	0/6/23/26	0/1/1/1
2	BMA	A	3	2	-	0/2/19/22	0/1/1/1
2	MAN	A	4	2	-	0/2/19/22	0/1/1/1
2	MAN	A	5	2	-	1/2/19/22	0/1/1/1
2	MAN	A	6	2	-	1/2/19/22	0/1/1/1
2	MAN	A	7	2	-	0/2/19/22	0/1/1/1
2	MAN	A	8	2	-	2/2/19/22	0/1/1/1
3	NAG	B	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2	3	-	0/6/23/26	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	0/2/19/22	0/1/1/1
4	MAN	D	5	4	-	0/2/19/22	0/1/1/1
4	MAN	D	6	4	-	2/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	7	MAN	O5-C5	3.49	1.50	1.43
2	A	6	MAN	O5-C5	2.92	1.49	1.43
2	A	8	MAN	O5-C5	2.44	1.48	1.43
2	A	6	MAN	C4-C5	2.07	1.57	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	7	MAN	C1-C2-C3	5.03	115.85	109.67
4	D	1	NAG	O5-C1-C2	-4.39	104.36	111.29
4	D	1	NAG	O4-C4-C5	-3.24	101.25	109.30
4	D	2	NAG	O4-C4-C3	-2.95	103.53	110.35
4	D	1	NAG	C1-C2-N2	2.93	115.49	110.49
4	D	6	MAN	C1-C2-C3	2.83	113.15	109.67
2	A	1	NAG	C1-O5-C5	-2.56	108.72	112.19
3	B	1	NAG	O3-C3-C2	-2.54	104.21	109.47
4	D	5	MAN	C1-O5-C5	2.46	115.53	112.19
3	C	2	NAG	C2-N2-C7	2.45	126.39	122.90
3	C	1	NAG	O4-C4-C3	-2.45	104.69	110.35
3	C	1	NAG	C2-N2-C7	-2.38	119.52	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	NAG	C4-C3-C2	-2.34	107.59	111.02
2	A	6	MAN	C2-C3-C4	-2.29	106.93	110.89
4	D	2	NAG	C4-C3-C2	2.23	114.28	111.02
4	D	1	NAG	C1-O5-C5	-2.20	109.21	112.19
2	A	7	MAN	O2-C2-C3	-2.17	105.78	110.14
3	B	1	NAG	C4-C3-C2	2.10	114.10	111.02
3	C	1	NAG	C1-O5-C5	-2.10	109.35	112.19
2	A	1	NAG	O4-C4-C5	-2.09	104.10	109.30
4	D	4	MAN	C1-O5-C5	2.08	115.00	112.19
2	A	6	MAN	C1-C2-C3	-2.03	107.17	109.67
4	D	5	MAN	O2-C2-C3	-2.03	106.07	110.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	6	MAN	O5-C5-C6-O6
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
2	A	8	MAN	C4-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
4	D	6	MAN	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
2	A	8	MAN	O5-C5-C6-O6
2	A	6	MAN	O5-C5-C6-O6
4	D	2	NAG	O7-C7-N2-C2
2	A	5	MAN	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NAG	1	0
3	C	2	NAG	1	0

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	HEX	DDD	309	-	5,5,5	0.16	0	4,4,4	0.15	0
7	HEX	CCC	305	-	5,5,5	0.37	0	4,4,4	0.45	0
7	HEX	BBB	305	-	5,5,5	0.07	0	4,4,4	0.17	0
7	HEX	CCC	306	-	5,5,5	0.35	0	4,4,4	0.15	0
7	HEX	AAA	311	-	5,5,5	0.34	0	4,4,4	0.42	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
7	HEX	DDD	309	-	-	0/3/3/3	-
7	HEX	CCC	305	-	-	2/3/3/3	-
7	HEX	BBB	305	-	-	2/3/3/3	-
7	HEX	CCC	306	-	-	2/3/3/3	-
7	HEX	AAA	311	-	-	3/3/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	AAA	311	HEX	C2-C3-C4-C5
7	CCC	306	HEX	C2-C3-C4-C5
7	BBB	305	HEX	C3-C4-C5-C6
7	CCC	305	HEX	C1-C2-C3-C4
7	AAA	311	HEX	C3-C4-C5-C6
7	CCC	305	HEX	C3-C4-C5-C6
7	AAA	311	HEX	C1-C2-C3-C4
7	CCC	306	HEX	C3-C4-C5-C6
7	BBB	305	HEX	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AAA	233/255 (91%)	-0.15	10 (4%) 35 38	17, 28, 52, 67	0
1	BBB	230/255 (90%)	-0.12	9 (3%) 39 42	18, 28, 55, 78	4 (1%)
1	CCC	233/255 (91%)	-0.17	9 (3%) 39 42	18, 28, 49, 67	1 (0%)
1	DDD	228/255 (89%)	-0.12	6 (2%) 56 58	19, 30, 52, 70	0
All	All	924/1020 (90%)	-0.14	34 (3%) 41 44	17, 28, 52, 78	5 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	63	THR	5.6
1	CCC	63	THR	4.8
1	CCC	62	SER	4.5
1	DDD	118	ALA	4.5
1	CCC	64	THR	4.0
1	BBB	65	GLY	3.7
1	BBB	2	SER	3.7
1	CCC	65	GLY	3.5
1	CCC	235	SER	3.3
1	BBB	66	ALA	3.1
1	AAA	62	SER	3.0
1	CCC	83	ASN	3.0
1	AAA	235	SER	3.0
1	BBB	83	ASN	3.0
1	AAA	63	THR	2.9
1	DDD	84	ALA	2.9
1	DDD	83	ASN	2.9
1	BBB	235	SER	2.7
1	AAA	113	GLY	2.7
1	AAA	83	ASN	2.7
1	BBB	62	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	DDD	64	THR	2.6
1	BBB	3	ALA	2.5
1	AAA	64	THR	2.5
1	AAA	65	GLY	2.4
1	CCC	113	GLY	2.3
1	AAA	3	ALA	2.3
1	BBB	64	THR	2.3
1	DDD	82	ASN	2.3
1	DDD	63	THR	2.2
1	CCC	82	ASN	2.1
1	AAA	4	ASN	2.1
1	CCC	66	ALA	2.0
1	AAA	218	GLY	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(\AA^2)	Q<0.9
2	MAN	A	8	11/12	0.71	0.30	49,54,62,63	0
4	MAN	D	5	11/12	0.74	0.21	30,47,51,61	0
3	NAG	B	2	14/15	0.77	0.26	45,60,65,66	14
4	NAG	D	2	14/15	0.85	0.16	38,41,44,44	14
3	NAG	C	2	14/15	0.85	0.32	69,74,81,81	1
2	BMA	A	3	11/12	0.87	0.12	25,30,36,46	11
4	MAN	D	6	11/12	0.87	0.27	71,74,79,81	0
4	MAN	D	4	11/12	0.88	0.22	36,47,50,52	0
3	NAG	B	1	14/15	0.90	0.18	35,43,48,58	0
2	NAG	A	2	14/15	0.90	0.22	29,35,39,40	0
2	MAN	A	6	11/12	0.90	0.17	43,49,57,59	0
4	NAG	D	1	14/15	0.91	0.15	34,42,46,48	0
2	MAN	A	5	11/12	0.92	0.14	34,40,51,51	0
3	NAG	C	1	14/15	0.93	0.19	34,40,45,57	0
4	BMA	D	3	11/12	0.93	0.08	31,36,38,38	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	A	1	14/15	0.94	0.14	24,28,33,37	0
2	MAN	A	7	11/12	0.94	0.16	38,46,55,57	0
2	MAN	A	4	11/12	0.95	0.10	28,33,36,37	0

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(\AA^2)	Q<0.9
7	HEX	CCC	306	6/6	0.79	0.39	51,55,58,60	0
7	HEX	BBB	305	6/6	0.84	0.25	41,45,52,52	0
7	HEX	AAA	311	6/6	0.86	0.23	38,40,51,52	0
7	HEX	DDD	309	6/6	0.87	0.18	39,42,45,46	0
7	HEX	CCC	305	6/6	0.90	0.18	38,39,47,50	0
5	CA	DDD	307	1/1	0.98	0.05	26,26,26,26	0
5	CA	CCC	303	1/1	0.99	0.05	25,25,25,25	0
5	CA	AAA	309	1/1	0.99	0.05	26,26,26,26	0
6	MN	DDD	308	1/1	0.99	0.09	19,19,19,19	0
5	CA	BBB	303	1/1	0.99	0.04	27,27,27,27	0
6	MN	AAA	310	1/1	0.99	0.11	19,19,19,19	0
6	MN	CCC	304	1/1	1.00	0.10	19,19,19,19	0
6	MN	BBB	304	1/1	1.00	0.08	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.