



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:32 PM GMT

PDB ID : 1KRE  
Title : STRUCTURE OF P. CITRINUM ALPHA 1,2-MANNOSIDASE REVEALS  
THE BASIS FOR DIFFERENCES IN SPECIFICITY OF THE ER AND  
GOLGI CLASS I ENZYMES  
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Deposited on : 2002-01-09  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

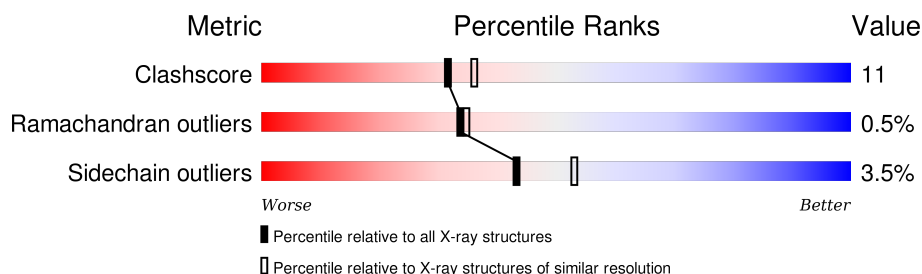
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	511	
1	B	511	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	601	X	-	-	-
2	NAG	A	801	X	-	-	-
2	NAG	B	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	801	X	-	-	-
3	NAG	A	701	X	-	-	-
3	MAN	A	702	X	-	-	-
3	NAG	B	701	X	-	-	-
3	MAN	B	702	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7904 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 Mannosyl-oligosaccharide alpha-1,2-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3724	2359	619	738	8			
1	B	475	Total	C	N	O	S	0	0	0
			3724	2359	619	738	8			

- Molecule 2 is a polymer of unknown type called SUGAR (NAG-NAG).

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

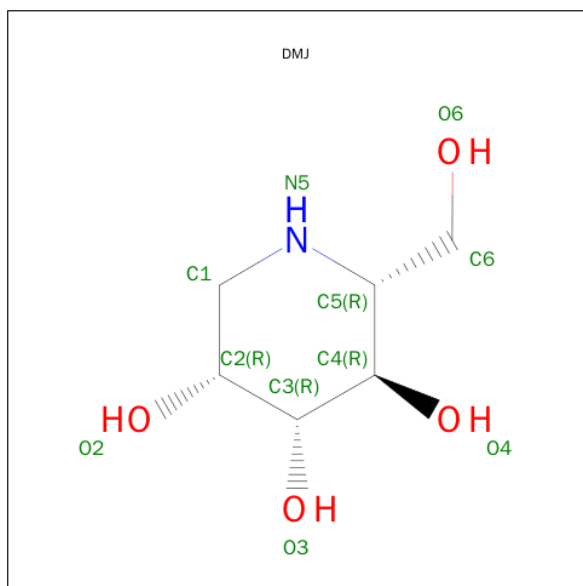
- Molecule 3 is a polymer of unknown type called SUGAR (NAG-NAG-MAN-MAN-MAN).

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 1-DEOXYMANNOJIRIMYCIN (three-letter code: DMJ) (formula:  $C_6H_{13}NO_4$ ).



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

- Molecule 6 is water.

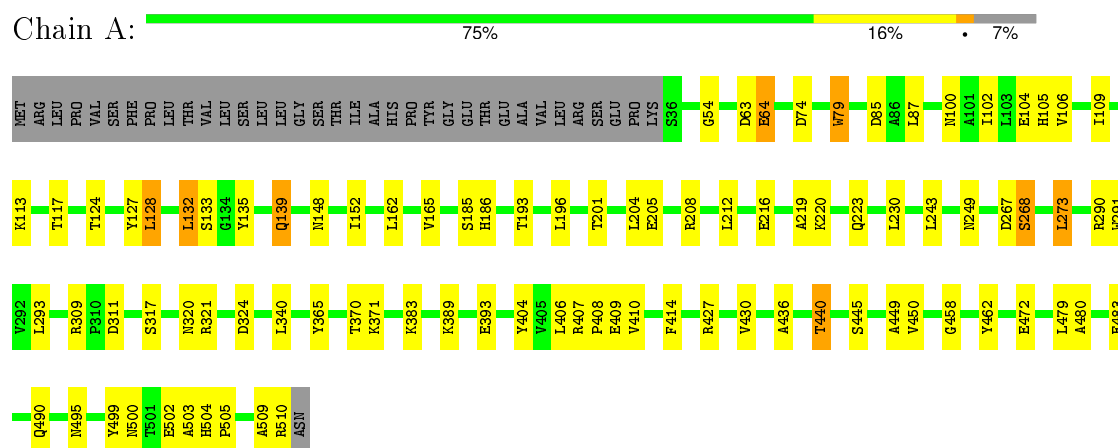
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	141	Total	O	0	0
			141	141		
6	B	57	Total	O	0	0
			57	57		

### 3 Residue-property plots

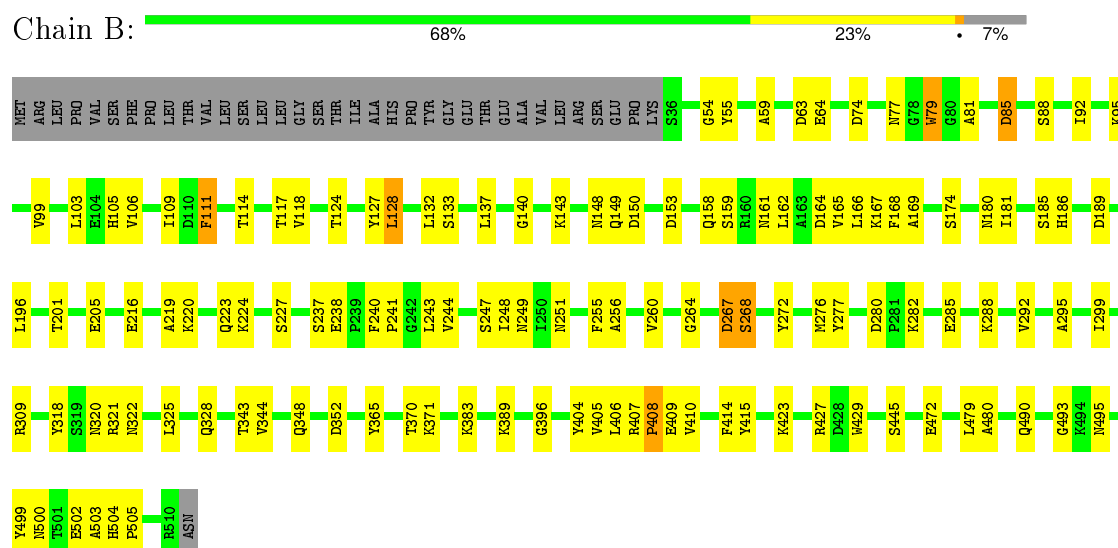
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: Mannosyl-oligosaccharide alpha-1,2-mannosidase



- Molecule 1: Mannosyl-oligosaccharide alpha-1,2-mannosidase



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.49Å 111.00Å 86.23Å 90.00° 99.17° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.20)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.198 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.36	0/3819	0.60	0/5190
1	B	0.30	0/3819	0.55	0/5190
All	All	0.33	0/7638	0.57	0/10380

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	2	0
2	B	2	0
3	A	2	0
3	B	2	0
All	All	8	0

There are no bond length outliers.

There are no bond angle outliers.

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	NAG	C1
3	A	701	NAG	C1
3	A	702	MAN	C1
2	A	801	NAG	C1
2	B	601	NAG	C1
3	B	701	NAG	C1
3	B	702	MAN	C1
2	B	801	NAG	C1



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	3724	0	3522	60	0
1	B	3724	0	3523	96	0
2	A	56	0	50	1	0
2	B	56	0	50	1	0
3	A	61	0	52	1	0
3	B	61	0	52	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	11	0	13	1	0
5	B	11	0	13	0	0
6	A	141	0	0	5	0
6	B	57	0	0	2	0
All	All	7904	0	7275	160	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 11.

All (160) 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:A:490:GLN:H	1:A:495:ASN:HD21	1.26	0.82
1:A:201:THR:OG1	1:A:268:SER:HB3	1.80	0.81
1:A:79:TRP:HD1	1:A:127:TYR:CZ	1.98	0.81
1:B:77:ASN:ND2	1:B:118:VAL:HG12	2.03	0.74
1:B:79:TRP:HD1	1:B:127:TYR:CZ	2.06	0.73
1:A:450:VAL:HG13	1:A:458:GLY:O	1.87	0.73
1:A:490:GLN:H	1:A:495:ASN:ND2	1.86	0.72
1:A:436:ALA:O	1:A:440:THR:HG23	1.90	0.71
1:B:63:ASP:HB2	1:B:74:ASP:HA	1.72	0.70
1:B:490:GLN:H	1:B:495:ASN:HD21	1.39	0.70
1:B:243:LEU:HB3	1:B:260:VAL:HG21	1.75	0.69
1:A:311:ASP:OD2	3:A:701:NAG:H81	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:TYR:CE2	1:B:505:PRO:HG3	2.30	0.66
1:B:180:ASN:HB2	1:B:189:ASP:HB2	1.78	0.66
1:A:499:TYR:CE2	1:A:505:PRO:HG3	2.30	0.65
1:B:427:ARG:HD3	1:B:480:ALA:O	1.96	0.65
1:A:193:THR:HG22	1:A:249:ASN:HD22	1.62	0.64
1:B:264:GLY:H	1:B:328:GLN:HE22	1.43	0.64
1:B:111:PHE:CD2	1:B:162:LEU:HD13	2.33	0.64
2:A:600:NAG:H62	2:A:601:NAG:H82	1.80	0.63
1:B:370:THR:O	1:B:371:LYS:HB2	1.98	0.63
1:B:111:PHE:HD2	1:B:162:LEU:HD13	1.64	0.62
1:A:162:LEU:O	1:A:165:VAL:HG12	2.00	0.62
1:B:264:GLY:H	1:B:328:GLN:NE2	1.98	0.61
1:A:510:ARG:NE	1:A:510:ARG:HA	2.16	0.61
1:A:100:ASN:O	1:A:104:GLU:HG3	1.99	0.61
1:A:63:ASP:HB2	1:A:74:ASP:HA	1.81	0.60
1:A:273:LEU:HB3	1:A:291:TRP:HB2	1.84	0.60
1:B:103:LEU:O	1:B:106:VAL:HG12	2.02	0.60
1:A:427:ARG:HD3	1:A:480:ALA:O	2.02	0.60
1:B:490:GLN:H	1:B:495:ASN:ND2	2.00	0.59
1:B:133:SER:O	1:B:137:LEU:HD23	2.03	0.58
1:B:238:GLU:OE2	1:B:241:PRO:HA	2.04	0.58
1:B:365:TYR:CE1	1:B:410:VAL:HG21	2.38	0.58
1:A:290:ARG:HD3	6:A:920:HOH:O	2.04	0.57
1:B:248:ILE:N	1:B:248:ILE:HD12	2.19	0.57
1:A:509:ALA:O	1:A:510:ARG:HB2	2.04	0.57
1:A:389:LYS:O	1:A:393:GLU:HG3	2.05	0.56
1:B:158:GLN:HA	1:B:161:ASN:HD22	1.70	0.56
1:A:117:THR:HG22	6:A:1024:HOH:O	2.06	0.55
1:B:423:LYS:HE3	3:B:704:MAN:H61	1.89	0.55
1:B:277:TYR:CE1	1:B:288:LYS:HD3	2.42	0.55
1:B:267:ASP:CG	1:B:268:SER:H	2.09	0.54
1:B:238:GLU:HG2	1:B:240:PHE:O	2.07	0.54
1:A:449:ALA:HB3	1:A:462:TYR:HB2	1.88	0.54
1:A:383:LYS:NZ	1:B:383:LYS:HE3	2.22	0.54
1:B:472:GLU:HG2	1:B:503:ALA:HB3	1.90	0.54
1:B:95:LYS:O	1:B:99:VAL:HG23	2.08	0.53
1:A:128:LEU:HD22	1:A:132:LEU:HD22	1.89	0.53
1:B:247:SER:OG	1:B:256:ALA:HB3	2.08	0.53
1:B:185:SER:O	1:B:186:HIS:HB2	2.09	0.53
1:A:185:SER:O	1:A:186:HIS:HB2	2.09	0.52
1:A:436:ALA:O	1:A:440:THR:CG2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ALA:O	1:B:223:GLN:HG3	2.09	0.52
1:A:79:TRP:HD1	1:A:127:TYR:CE1	2.27	0.52
1:B:415:TYR:CE2	1:B:479:LEU:HB3	2.45	0.52
1:B:105:HIS:CE1	1:B:109:ILE:HD11	2.45	0.52
1:B:164:ASP:HA	1:B:167:LYS:HD3	1.92	0.51
1:B:288:LYS:O	1:B:292:VAL:HG23	2.10	0.51
1:B:502:GLU:O	1:B:502:GLU:HG3	2.11	0.51
1:A:124:THR:HG22	1:A:205:GLU:HG3	1.92	0.50
1:B:260:VAL:HG12	1:B:318:TYR:HB3	1.92	0.50
3:B:700:NAG:H61	3:B:701:NAG:HN2	1.77	0.50
2:B:800:NAG:H61	2:B:801:NAG:O7	2.11	0.50
1:B:404:TYR:CE2	1:B:406:LEU:HA	2.46	0.50
1:B:79:TRP:CD1	1:B:127:TYR:CZ	2.95	0.50
1:B:493:GLY:HA2	6:B:911:HOH:O	2.10	0.50
1:B:118:VAL:CG2	1:B:181:ILE:HG13	2.42	0.49
1:B:249:ASN:HD21	1:B:256:ALA:HB2	1.78	0.49
1:B:162:LEU:O	1:B:165:VAL:HG22	2.12	0.49
1:B:81:ALA:O	1:B:85:ASP:HB2	2.12	0.49
1:B:132:LEU:HD11	1:B:159:SER:HB3	1.94	0.49
1:B:407:ARG:HB3	1:B:409:GLU:OE2	2.12	0.49
1:A:162:LEU:O	1:A:165:VAL:CG1	2.61	0.48
1:B:128:LEU:HD23	1:B:132:LEU:HD13	1.95	0.48
1:B:105:HIS:O	1:B:109:ILE:HG13	2.13	0.48
1:B:111:PHE:CE2	1:B:162:LEU:HD22	2.49	0.48
1:B:106:VAL:HA	1:B:109:ILE:CD1	2.44	0.47
1:A:133:SER:HB2	1:A:504:HIS:HB3	1.96	0.47
1:A:79:TRP:CZ3	1:A:113:LYS:O	2.68	0.47
1:B:106:VAL:HA	1:B:109:ILE:HD12	1.95	0.47
1:B:348:GLN:HE21	1:B:352:ASP:CG	2.18	0.47
1:A:370:THR:O	1:A:371:LYS:HB2	2.15	0.47
1:B:243:LEU:CB	1:B:260:VAL:HG21	2.44	0.47
1:A:105:HIS:CE1	1:A:109:ILE:HD11	2.50	0.46
1:B:309:ARG:HG3	1:B:396:GLY:HA3	1.96	0.46
1:A:320:ASN:O	1:A:321:ARG:HB2	2.16	0.46
1:B:244:VAL:HB	1:B:255:PHE:CE2	2.50	0.46
1:A:124:THR:CG2	1:A:205:GLU:HG3	2.46	0.46
1:A:79:TRP:O	1:A:105:HIS:HE1	1.98	0.46
1:A:205:GLU:H	1:A:205:GLU:CD	2.19	0.46
1:B:88:SER:HB2	6:B:931:HOH:O	2.14	0.46
1:B:54:GLY:HA3	1:B:445:SER:O	2.16	0.46
1:B:295:ALA:O	1:B:299:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:GLU:HG2	1:B:503:ALA:CB	2.46	0.45
3:B:700:NAG:H61	3:B:701:NAG:N2	2.32	0.45
1:A:472:GLU:HG2	1:A:503:ALA:HB3	1.97	0.45
1:A:54:GLY:HA3	1:A:445:SER:O	2.16	0.45
1:B:99:VAL:O	1:B:103:LEU:HG	2.17	0.45
1:B:272:TYR:O	1:B:276:MET:HG2	2.17	0.45
1:B:237:SER:OG	1:B:255:PHE:HB2	2.16	0.45
1:B:404:TYR:CZ	1:B:406:LEU:HA	2.51	0.45
1:B:405:VAL:HG23	1:B:407:ARG:HG3	1.99	0.45
1:A:317:SER:HB2	1:A:324:ASP:HB3	1.98	0.45
1:B:389:LYS:O	1:B:389:LYS:HD3	2.17	0.45
1:B:162:LEU:HD11	1:B:166:LEU:HD11	1.98	0.44
1:B:148:ASN:OD1	1:B:150:ASP:HB2	2.17	0.44
1:B:149:GLN:HG3	1:B:153:ASP:OD2	2.17	0.44
1:B:124:THR:CG2	1:B:205:GLU:HG3	2.47	0.44
1:B:280:ASP:OD1	1:B:282:LYS:HB3	2.18	0.44
1:B:79:TRP:CH2	1:B:114:THR:HB	2.52	0.44
1:A:309:ARG:HG3	1:A:309:ARG:HH11	1.83	0.44
1:A:230:LEU:O	1:A:290:ARG:HD2	2.18	0.44
1:A:139:GLN:HE22	1:A:152:ILE:HG21	1.82	0.44
5:A:901:DMJ:H12	6:A:1027:HOH:O	2.18	0.44
1:A:414:PHE:HB3	1:A:430:VAL:HG23	2.00	0.44
1:A:407:ARG:HB3	1:A:409:GLU:OE2	2.17	0.44
1:B:201:THR:HG22	1:B:201:THR:O	2.18	0.43
1:A:321:ARG:NH1	1:A:321:ARG:HG3	2.34	0.43
1:B:320:ASN:O	1:B:321:ARG:HB2	2.18	0.43
1:B:320:ASN:C	1:B:322:ASN:H	2.22	0.43
1:B:174:SER:HB3	1:B:251:ASN:O	2.19	0.43
1:B:325:LEU:HD12	1:B:325:LEU:N	2.34	0.43
1:B:237:SER:CB	1:B:255:PHE:HB2	2.48	0.42
1:A:404:TYR:CE2	1:A:406:LEU:HA	2.54	0.42
1:A:219:ALA:O	1:A:223:GLN:HG3	2.19	0.42
1:A:502:GLU:O	1:A:502:GLU:HG3	2.19	0.42
1:B:216:GLU:O	1:B:220:LYS:HG3	2.19	0.42
1:B:133:SER:HB2	1:B:504:HIS:HB3	2.01	0.42
1:B:205:GLU:OE2	1:B:272:TYR:HE2	2.03	0.42
1:B:389:LYS:C	1:B:389:LYS:HD3	2.39	0.42
1:B:55:TYR:CD1	1:B:59:ALA:HB3	2.55	0.42
1:B:169:ALA:HB2	1:B:181:ILE:HD13	2.02	0.42
1:B:414:PHE:CE1	1:B:429:TRP:HB3	2.55	0.42
1:A:79:TRP:CD1	1:A:127:TYR:CZ	2.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ALA:O	1:A:510:ARG:CB	2.67	0.42
1:B:267:ASP:OD2	1:B:268:SER:N	2.45	0.42
1:B:118:VAL:HG22	1:B:181:ILE:HG13	2.02	0.42
1:B:140:GLY:O	1:B:143:LYS:HB2	2.20	0.41
1:A:105:HIS:HD2	6:A:951:HOH:O	2.02	0.41
1:A:404:TYR:CZ	1:A:406:LEU:HA	2.55	0.41
1:B:260:VAL:CG1	1:B:318:TYR:HB3	2.50	0.41
1:B:247:SER:O	1:B:255:PHE:HA	2.20	0.41
1:B:224:LYS:O	1:B:227:SER:OG	2.32	0.41
1:B:92:ILE:HG21	1:B:479:LEU:HD11	2.01	0.41
1:A:79:TRP:HZ3	1:A:113:LYS:O	2.03	0.41
1:A:321:ARG:HH11	1:A:321:ARG:HG3	1.86	0.41
1:A:208:ARG:NH2	1:A:212:LEU:HD21	2.35	0.41
1:B:201:THR:OG1	1:B:268:SER:HB3	2.20	0.41
1:A:124:THR:CG2	1:A:205:GLU:CG	2.98	0.41
1:A:102:ILE:O	1:A:106:VAL:HG23	2.21	0.41
1:B:168:PHE:C	1:B:168:PHE:CD1	2.94	0.41
1:B:77:ASN:HD21	1:B:118:VAL:HG12	1.80	0.41
1:A:135:TYR:O	1:A:139:GLN:HB2	2.21	0.41
1:A:216:GLU:O	1:A:220:LYS:HG3	2.20	0.41
1:B:128:LEU:O	1:B:132:LEU:HD13	2.21	0.40
1:B:285:GLU:OE1	1:B:288:LYS:HE3	2.21	0.40
1:A:365:TYR:CE1	1:A:410:VAL:HG21	2.56	0.40
1:A:64:GLU:HG3	6:A:947:HOH:O	2.22	0.40
1:B:343:THR:HG23	1:B:344:VAL:N	2.36	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	473/511 (93%)	461 (98%)	10 (2%)	2 (0%)	39 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	473/511 (93%)	445 (94%)	25 (5%)	3 (1%)	30	29
All	All	946/1022 (93%)	906 (96%)	35 (4%)	5 (0%)	34	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASP
1	B	267	ASP
1	B	111	PHE
1	A	148	ASN
1	B	408	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	400/432 (93%)	381 (95%)	19 (5%)	31	37
1	B	400/432 (93%)	391 (98%)	9 (2%)	58	71
All	All	800/864 (93%)	772 (96%)	28 (4%)	43	53

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	GLU
1	A	79	TRP
1	A	85	ASP
1	A	87	LEU
1	A	128	LEU
1	A	132	LEU
1	A	139	GLN
1	A	196	LEU
1	A	204	LEU
1	A	243	LEU
1	A	268	SER

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Mol	Chain	Res	Type
1	A	273	LEU
1	A	293	LEU
1	A	340	LEU
1	A	408	PRO
1	A	440	THR
1	A	479	LEU
1	A	483	GLU
1	A	500	ASN
1	B	64	GLU
1	B	79	TRP
1	B	85	ASP
1	B	117	THR
1	B	128	LEU
1	B	196	LEU
1	B	268	SER
1	B	408	PRO
1	B	500	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	105	HIS
1	A	139	GLN
1	A	144	ASN
1	A	149	GLN
1	A	223	GLN
1	A	249	ASN
1	A	305	HIS
1	A	418	HIS
1	A	432	ASN
1	A	490	GLN
1	A	495	ASN
1	B	37	ASN
1	B	38	GLN
1	B	139	GLN
1	B	149	GLN
1	B	161	ASN
1	B	223	GLN
1	B	249	ASN
1	B	251	ASN
1	B	328	GLN

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Mol	Chain	Res	Type
1	B	348	GLN
1	B	432	ASN
1	B	457	ASN
1	B	490	GLN
1	B	495	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

18 carbohydrates 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	600	1,2	14,14,15	0.46	0	15,19,21	0.82	1 (6%)
2	NAG	A	601	2	14,14,15	0.52	0	15,19,21	0.66	0
3	NAG	A	700	1,3	14,14,15	0.74	0	15,19,21	0.69	0
3	NAG	A	701	3	14,14,15	0.83	0	15,19,21	0.82	1 (6%)
3	MAN	A	702	3	11,11,12	0.51	0	14,15,17	0.44	0
3	MAN	A	703	3	11,11,12	0.41	0	14,15,17	0.64	0
3	MAN	A	704	3	11,11,12	0.42	0	14,15,17	0.57	0
2	NAG	A	800	1,2	14,14,15	0.40	0	15,19,21	0.72	1 (6%)
2	NAG	A	801	2	14,14,15	0.53	0	15,19,21	0.79	1 (6%)
2	NAG	B	600	1,2	14,14,15	0.50	0	15,19,21	0.66	0
2	NAG	B	601	2	14,14,15	0.51	0	15,19,21	0.80	1 (6%)
3	NAG	B	700	1,3	14,14,15	0.62	0	15,19,21	0.66	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	701	3	14,14,15	0.70	0	15,19,21	0.69	1 (6%)
3	MAN	B	702	3	11,11,12	0.62	0	14,15,17	0.40	0
3	MAN	B	703	3	11,11,12	0.50	0	14,15,17	0.59	0
3	MAN	B	704	3	11,11,12	0.46	0	14,15,17	0.72	1 (7%)
2	NAG	B	800	1,2	14,14,15	0.53	0	15,19,21	0.76	1 (6%)
2	NAG	B	801	2	14,14,15	0.64	0	15,19,21	0.69	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	600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	601	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	700	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	701	3	1/1/5/7	0/6/23/26	0/1/1/1
3	MAN	A	702	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	A	703	3	-	0/2/19/22	0/1/1/1
3	MAN	A	704	3	-	0/2/19/22	0/1/1/1
2	NAG	A	800	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	801	2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	601	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	700	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	701	3	1/1/5/7	0/6/23/26	0/1/1/1
3	MAN	B	702	3	1/1/4/5	0/2/19/22	0/1/1/1
3	MAN	B	703	3	-	0/2/19/22	0/1/1/1
3	MAN	B	704	3	-	0/2/19/22	0/1/1/1
2	NAG	B	800	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	801	2	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	NAG	C2-N2-C7	-2.71	119.56	123.04
3	A	701	NAG	C2-N2-C7	-2.49	119.84	123.04
2	B	800	NAG	C2-N2-C7	-2.34	120.04	123.04
2	A	801	NAG	C2-N2-C7	-2.29	120.09	123.04
2	B	601	NAG	C2-N2-C7	-2.21	120.20	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	NAG	C2-N2-C7	-2.20	120.22	123.04
2	B	801	NAG	C2-N2-C7	-2.06	120.39	123.04
3	B	701	NAG	C2-N2-C7	-2.02	120.45	123.04
3	B	704	MAN	C1-O5-C5	2.29	115.16	112.25

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	801	NAG	C1
3	B	701	NAG	C1
2	A	601	NAG	C1
2	B	601	NAG	C1
2	B	801	NAG	C1
3	A	701	NAG	C1
3	B	702	MAN	C1
3	A	702	MAN	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	NAG	1	0
2	A	601	NAG	1	0
3	A	701	NAG	1	0
3	B	700	NAG	2	0
3	B	701	NAG	2	0
3	B	704	MAN	1	0
2	B	800	NAG	1	0
2	B	801	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
5	DMJ	A	901	4	11,11,11	3.82	6 (54%)	11,15,15	3.66	3 (27%)
5	DMJ	B	902	4	11,11,11	3.70	6 (54%)	11,15,15	3.69	3 (27%)

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	DMJ	A	901	4	-	0/2/19/19	0/1/1/1
5	DMJ	B	902	4	-	0/2/19/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	DMJ	C6-C5	2.26	1.57	1.52
5	A	901	DMJ	C6-C5	2.35	1.57	1.52
5	A	901	DMJ	C4-C5	2.76	1.58	1.52
5	B	902	DMJ	C4-C5	2.77	1.58	1.52
5	A	901	DMJ	C3-C4	3.09	1.60	1.52
5	B	902	DMJ	C3-C4	3.14	1.60	1.52
5	A	901	DMJ	C1-C2	5.66	1.58	1.52
5	B	902	DMJ	C2-C3	5.92	1.60	1.52
5	B	902	DMJ	C1-C2	6.12	1.59	1.52
5	A	901	DMJ	C2-C3	6.29	1.61	1.52
5	B	902	DMJ	C5-N5	7.36	1.55	1.47
5	A	901	DMJ	C5-N5	8.02	1.56	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	DMJ	O4-C4-C3	-2.81	104.02	110.34
5	B	902	DMJ	O4-C4-C3	-2.74	104.18	110.34
5	A	901	DMJ	O4-C4-C5	-2.33	104.50	109.11
5	B	902	DMJ	O4-C4-C5	-2.18	104.80	109.11
5	A	901	DMJ	O6-C6-C5	11.16	141.02	111.12
5	B	902	DMJ	O6-C6-C5	11.38	141.60	111.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	DMJ	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.