



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2023 – 07:48 PM EDT

PDB ID : 1VB9  
Title : Crystal structure of Thermoactinomyces vulgaris R-47 alpha-amylase II (TVA II) complexed with transglycosylated product  
Authors : Mizuno, M.; Tonozuka, T.; Uechi, A.; Ohtaki, A.; Ichikawa, K.; Kamitori, S.; Nishikawa, A.; Sakano, Y.  
Deposited on : 2004-02-25  
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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

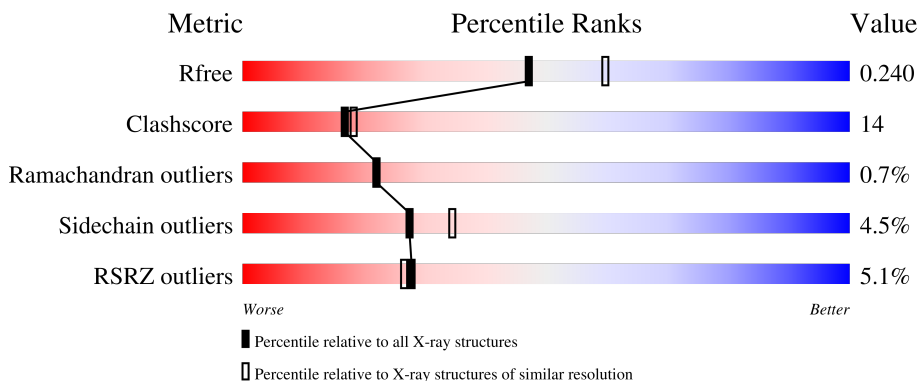
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	585	
1	B	585	
2	C	6	
2	D	6	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10196 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.

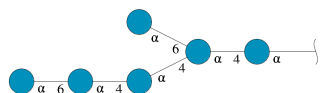
- Molecule 1 is a protein called alpha-amylase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	585	4776	3056	832	873	15	0	0	0
1	B	585	4776	3056	832	873	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASN	ASP	engineered mutation	UNP Q08751
B	325	ASN	ASP	engineered mutation	UNP Q08751

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	6	67	36	31	0	0	0
2	D	6	67	36	31	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

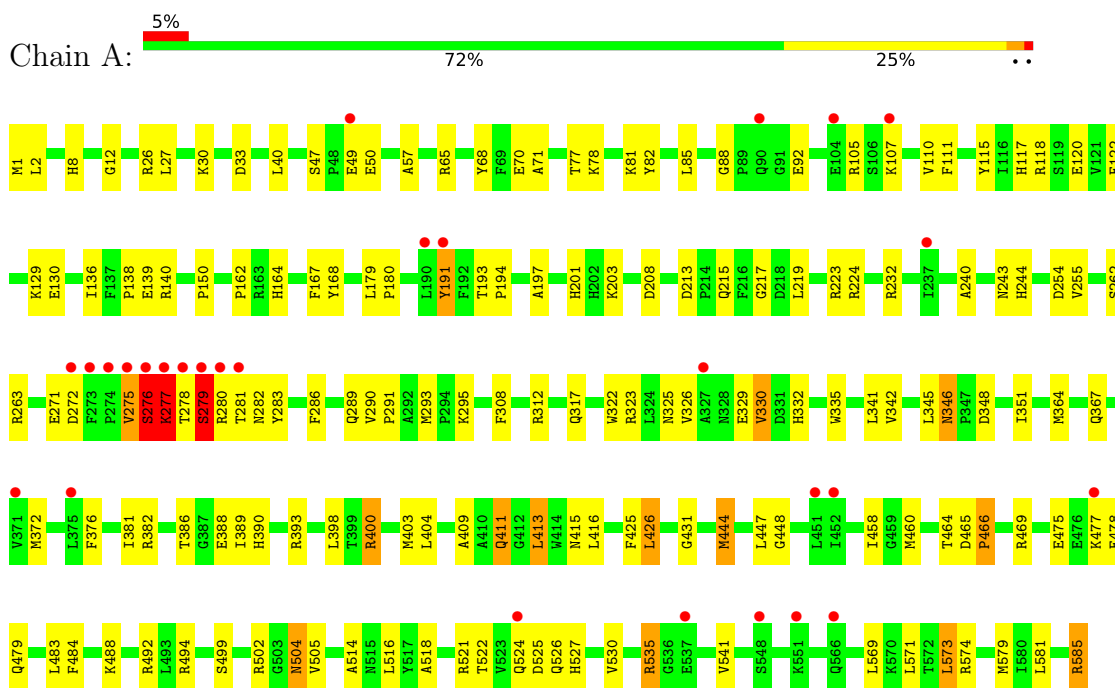
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total 249	O 249	0	0
4	B	259	Total 259	O 259	0	0

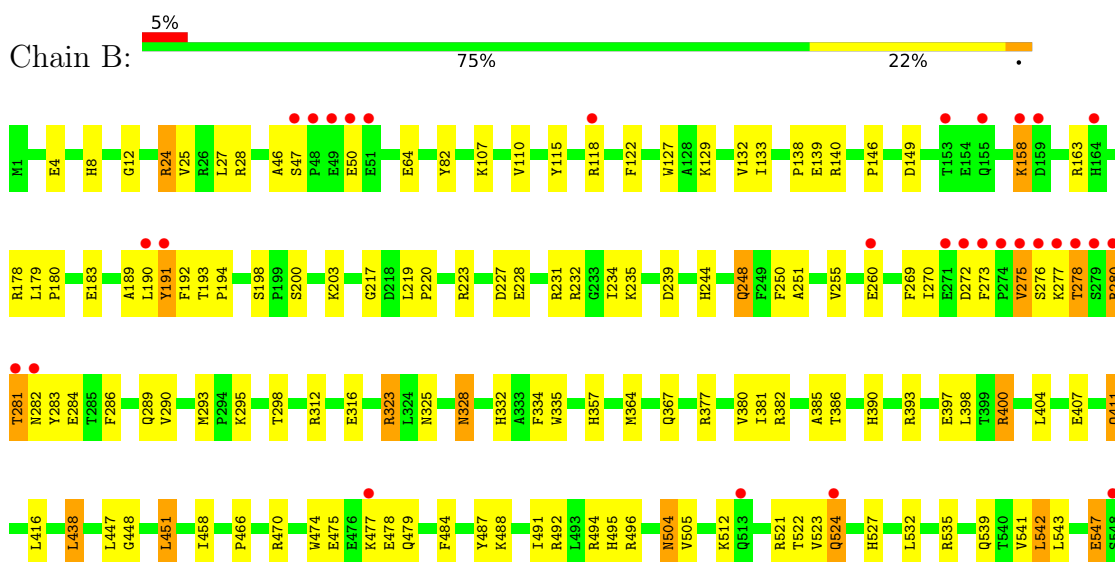
### 3 Residue-property plots [i](#)

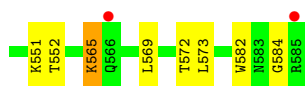
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: alpha-amylase II

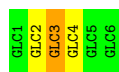


- Molecule 1: alpha-amylase II

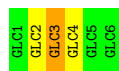




- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.05Å 118.27Å 112.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.99 – 2.20 33.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.99-2.20) 99.9 (33.98-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.29 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.194 , 0.233 0.202 , 0.240	Depositor DCC
$R_{free}$ test set	7737 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtrriage
Anisotropy	0.397	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 49.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.35	0/4906	0.62	3/6641 (0.0%)
1	B	0.35	0/4906	0.60	1/6641 (0.0%)
All	All	0.35	0/9812	0.61	4/13282 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	LYS	N-CA-C	-7.84	89.83	111.00
1	A	276	SER	N-CA-C	5.99	127.18	111.00
1	A	279	SER	N-CA-C	-5.39	96.45	111.00
1	B	323	ARG	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4776	0	4609	143	0
1	B	4776	0	4609	129	0
2	C	67	0	57	4	0
2	D	67	0	57	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	249	0	0	6	0
4	B	259	0	0	14	0
All	All	10196	0	9332	269	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 14.

All (269) 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:342:VAL:HG11	1:A:351:ILE:HD11	1.46	0.97
1:B:293:MET:HE1	2:D:4:GLC:H62	1.45	0.97
1:A:293:MET:HE1	2:C:4:GLC:H62	1.48	0.94
1:A:585:ARG:HH11	1:A:585:ARG:HB3	1.35	0.89
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.57	0.87
1:B:293:MET:CE	2:D:4:GLC:H62	2.05	0.86
1:A:140:ARG:HG2	1:A:469:ARG:O	1.77	0.84
1:A:290:VAL:HG11	1:A:293:MET:CE	2.06	0.84
1:A:293:MET:CE	2:C:4:GLC:H62	2.07	0.84
1:A:280:ARG:HA	1:A:289:GLN:OE1	1.79	0.81
1:B:290:VAL:HG11	1:B:293:MET:HE3	1.64	0.80
1:B:46:ALA:HB1	1:B:50:GLU:HG3	1.63	0.80
1:B:523:VAL:HG22	1:B:524:GLN:NE2	1.97	0.79
1:A:290:VAL:HG11	1:A:293:MET:HE2	1.65	0.78
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.32	0.76
1:A:447:LEU:HB2	1:A:505:VAL:HG21	1.66	0.76
1:A:484:PHE:CE1	1:A:488:LYS:HD2	2.21	0.76
1:B:470:ARG:HG3	4:B:741:HOH:O	1.85	0.75
1:A:504:ASN:C	1:A:504:ASN:HD22	1.91	0.73
1:B:505:VAL:HG12	1:B:521:ARG:CD	2.18	0.73
1:A:191:TYR:CZ	1:A:323:ARG:HD3	2.22	0.73
1:B:275:VAL:O	1:B:282:ASN:ND2	2.23	0.72
1:B:290:VAL:HG11	1:B:293:MET:CE	2.20	0.72
1:B:139:GLU:HB3	1:B:140:ARG:HH11	1.56	0.71
1:A:341:LEU:O	1:A:345:LEU:HD13	1.90	0.71
1:A:390:HIS:HD2	1:A:393:ARG:H	1.39	0.71
1:A:569:LEU:HG	1:A:571:LEU:HD13	1.72	0.71
1:A:277:LYS:O	1:A:277:LYS:HG3	1.91	0.70
1:B:328:ASN:N	1:B:328:ASN:HD22	1.89	0.70
1:A:194:PRO:HB2	1:A:203:LYS:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:TYR:O	1:B:491:ILE:HG12	1.93	0.69
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.74	0.69
1:A:330:VAL:HG22	1:A:335:TRP:NE1	2.08	0.69
1:A:271:GLU:HG3	1:A:272:ASP:H	1.58	0.68
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.23	0.68
1:A:400:ARG:CB	1:A:400:ARG:HH21	2.07	0.68
1:B:547:GLU:HG2	1:B:551:LYS:HE2	1.76	0.67
1:B:139:GLU:HB3	1:B:140:ARG:NH1	2.09	0.66
1:A:290:VAL:HG11	1:A:293:MET:HE3	1.76	0.66
1:A:224:ARG:HE	1:A:224:ARG:HA	1.59	0.66
1:A:477:LYS:N	1:A:477:LYS:HD2	2.11	0.65
1:B:492:ARG:O	1:B:496:ARG:HG3	1.98	0.64
1:A:275:VAL:HG12	1:A:275:VAL:O	1.97	0.64
1:B:255:VAL:HG11	1:B:270:ILE:HD11	1.78	0.63
1:B:400:ARG:O	1:B:404:LEU:HD13	1.98	0.63
1:B:504:ASN:C	1:B:504:ASN:HD22	2.02	0.62
1:A:386:THR:OG1	1:A:388:GLU:HG3	2.00	0.62
1:B:183:GLU:OE2	1:B:232:ARG:HD2	2.00	0.62
1:B:523:VAL:HG22	1:B:524:GLN:HE22	1.64	0.62
1:A:118:ARG:HG2	4:B:727:HOH:O	1.99	0.61
1:B:328:ASN:HD22	1:B:328:ASN:H	1.47	0.61
1:A:271:GLU:HG3	1:A:272:ASP:N	2.14	0.61
1:A:129:LYS:HD2	1:A:502:ARG:HH12	1.66	0.60
1:A:390:HIS:CD2	1:A:393:ARG:H	2.19	0.60
1:B:64:GLU:HB2	4:B:816:HOH:O	2.00	0.60
1:A:224:ARG:HA	1:A:224:ARG:NE	2.17	0.60
1:B:484:PHE:CE1	1:B:488:LYS:HD2	2.36	0.60
1:A:129:LYS:HB3	1:A:411:GLN:OE1	2.02	0.59
1:B:260:GLU:HB2	1:B:273:PHE:CD2	2.38	0.59
1:B:133:ILE:HB	1:B:451:LEU:HD23	1.85	0.59
1:A:129:LYS:HD2	1:A:502:ARG:NH1	2.17	0.59
1:A:409:ALA:O	1:A:413:LEU:HD13	2.04	0.58
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.39	0.58
1:B:390:HIS:NE2	1:B:512:LYS:HE2	2.19	0.57
1:B:447:LEU:HB2	1:B:505:VAL:CG1	2.34	0.57
1:A:382:ARG:HG2	1:A:389:ILE:HG23	1.86	0.57
1:B:505:VAL:HG12	1:B:521:ARG:HD2	1.86	0.56
1:B:312:ARG:O	1:B:316:GLU:HG3	2.04	0.56
1:B:448:GLY:O	1:B:494:ARG:NH2	2.38	0.56
1:B:28:ARG:HD2	4:B:819:HOH:O	2.04	0.56
1:B:328:ASN:H	1:B:328:ASN:ND2	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:VAL:HG22	1:A:521:ARG:NE	2.21	0.55
1:A:26:ARG:HD3	1:A:70:GLU:OE2	2.05	0.55
1:B:190:LEU:HD13	1:B:234:ILE:CG2	2.36	0.55
1:B:416:LEU:HD23	1:B:416:LEU:H	1.70	0.55
1:A:254:ASP:OD2	1:A:262:SER:HB2	2.06	0.55
1:A:201:HIS:HE1	1:A:469:ARG:HH11	1.53	0.55
1:A:411:GLN:HG2	4:A:909:HOH:O	2.06	0.55
1:B:382:ARG:NH1	1:B:397:GLU:OE1	2.39	0.55
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.88	0.55
1:B:129:LYS:HG2	1:B:411:GLN:NE2	2.22	0.54
1:A:115:TYR:CZ	1:B:295:LYS:HE2	2.43	0.54
1:B:277:LYS:O	1:B:278:THR:OG1	2.23	0.54
1:A:139:GLU:OE2	1:A:140:ARG:NH1	2.41	0.54
1:A:504:ASN:C	1:A:504:ASN:ND2	2.59	0.54
1:A:514:ALA:O	1:A:535:ARG:HG3	2.08	0.54
1:B:572:THR:C	1:B:573:LEU:HD23	2.27	0.53
1:B:522:THR:OG1	1:B:527:HIS:HD2	1.90	0.53
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.42	0.53
1:A:275:VAL:O	1:A:276:SER:CB	2.56	0.53
1:B:328:ASN:N	1:B:328:ASN:ND2	2.56	0.53
1:B:255:VAL:HG11	1:B:270:ILE:CD1	2.38	0.52
1:B:541:VAL:HG22	1:B:543:LEU:HD12	1.91	0.52
1:A:162:PRO:HB3	1:A:168:TYR:HE2	1.75	0.52
1:B:190:LEU:HD13	1:B:234:ILE:HG21	1.91	0.52
1:A:281:THR:HG23	1:A:283:TYR:CE2	2.44	0.52
1:B:193:THR:HB	1:B:194:PRO:HD2	1.91	0.52
1:A:416:LEU:H	1:A:416:LEU:HD23	1.73	0.52
1:A:8:HIS:HD2	1:A:26:ARG:O	1.93	0.52
1:B:393:ARG:HH21	1:B:393:ARG:HG3	1.75	0.52
1:B:280:ARG:NH2	1:B:289:GLN:NE2	2.58	0.51
1:A:400:ARG:HH21	1:A:400:ARG:HB3	1.75	0.51
1:A:65:ARG:HB2	1:B:4:GLU:HG3	1.92	0.51
1:B:325:ASN:HD21	2:D:3:GLC:C1	2.24	0.51
1:B:447:LEU:HB2	1:B:505:VAL:HG11	1.92	0.51
1:A:275:VAL:O	1:A:276:SER:HB2	2.10	0.51
1:A:129:LYS:HG2	1:A:411:GLN:NE2	2.26	0.51
1:A:201:HIS:CE1	1:A:469:ARG:HH11	2.29	0.51
1:B:107:LYS:HE3	4:B:845:HOH:O	2.10	0.51
1:B:200:SER:O	1:B:203:LYS:HD2	2.11	0.50
1:B:504:ASN:HB2	4:B:751:HOH:O	2.11	0.50
1:B:332:HIS:HD2	1:B:367:GLN:OE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.93	0.50
1:B:228:GLU:O	1:B:232:ARG:HG2	2.12	0.50
1:A:574:ARG:NH1	1:A:574:ARG:HB2	2.27	0.50
1:B:47:SER:HB3	1:B:50:GLU:HG2	1.93	0.50
1:B:357:HIS:HD2	4:B:719:HOH:O	1.94	0.50
1:A:458:ILE:CD1	1:A:460:MET:HG3	2.42	0.50
1:A:522:THR:OG1	1:A:527:HIS:HD2	1.95	0.50
1:B:12:GLY:O	1:B:364:MET:HE1	2.12	0.50
1:A:213:ASP:OD1	1:A:215:GLN:HG2	2.12	0.49
1:A:346:ASN:ND2	1:A:348:ASP:H	2.10	0.49
1:A:488:LYS:O	1:A:492:ARG:HG3	2.12	0.49
1:A:140:ARG:HH12	1:A:201:HIS:HB2	1.78	0.49
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.95	0.49
1:A:346:ASN:HD22	1:A:346:ASN:C	2.15	0.49
1:A:382:ARG:HG3	1:A:388:GLU:HB2	1.95	0.49
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.78	0.49
1:A:82:TYR:N	1:A:110:VAL:CG2	2.76	0.48
1:A:281:THR:HG22	1:A:283:TYR:H	1.77	0.48
1:B:275:VAL:O	1:B:282:ASN:CG	2.51	0.48
1:B:504:ASN:C	1:B:504:ASN:ND2	2.66	0.48
1:A:162:PRO:HB3	1:A:168:TYR:CE2	2.48	0.48
1:A:323:ARG:HD2	1:A:372:MET:SD	2.54	0.48
1:B:248:GLN:HB2	4:B:783:HOH:O	2.12	0.48
1:A:448:GLY:O	1:A:494:ARG:NH2	2.47	0.48
1:A:255:VAL:HG12	1:A:275:VAL:HG21	1.95	0.48
1:A:68:TYR:CD2	1:A:403:MET:HG3	2.49	0.48
1:B:535:ARG:HD3	1:B:539:GLN:CD	2.34	0.48
1:A:585:ARG:HB3	1:A:585:ARG:NH1	2.17	0.48
1:B:82:TYR:N	1:B:110:VAL:HG22	2.29	0.47
1:B:158:LYS:HG2	1:B:478:GLU:OE2	2.14	0.47
1:A:505:VAL:HG22	1:A:521:ARG:CD	2.44	0.47
1:A:193:THR:HB	1:A:194:PRO:CD	2.45	0.47
1:A:179:LEU:N	1:A:180:PRO:CD	2.78	0.47
1:B:277:LYS:O	1:B:277:LYS:HD3	2.14	0.47
1:A:326:VAL:HG12	1:A:329:GLU:HB2	1.97	0.47
1:A:293:MET:HE2	2:C:4:GLC:H62	1.95	0.47
1:B:393:ARG:HG3	1:B:393:ARG:NH2	2.29	0.47
1:B:477:LYS:NZ	1:B:477:LYS:HB3	2.30	0.47
1:B:547:GLU:CG	1:B:551:LYS:HE2	2.45	0.47
1:A:275:VAL:O	1:A:275:VAL:CG1	2.63	0.47
1:B:223:ARG:HH21	1:B:223:ARG:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:C	1:A:282:ASN:OD1	2.54	0.46
1:A:2:LEU:HD12	1:A:30:LYS:CD	2.45	0.46
1:A:77:THR:O	1:A:78:LYS:HB2	2.16	0.46
1:A:140:ARG:NH2	4:A:751:HOH:O	2.48	0.46
1:B:276:SER:HB2	1:B:283:TYR:HE2	1.80	0.46
1:A:217:GLY:HA2	4:A:745:HOH:O	2.16	0.46
1:B:127:TRP:CG	1:B:235:LYS:HE3	2.51	0.46
1:B:504:ASN:HD21	1:B:522:THR:HB	1.80	0.46
1:A:197:ALA:HB3	1:A:208:ASP:HB3	1.97	0.46
1:B:277:LYS:O	1:B:278:THR:HG23	2.16	0.46
1:B:381:ILE:O	1:B:385:ALA:HB3	2.16	0.46
1:A:40:LEU:N	1:A:40:LEU:HD22	2.31	0.46
1:A:232:ARG:NE	4:A:896:HOH:O	2.41	0.45
1:A:330:VAL:HG22	1:A:335:TRP:CE2	2.51	0.45
1:A:475:GLU:O	1:A:479:GLN:HG3	2.16	0.45
1:A:488:LYS:NZ	1:A:488:LYS:HB3	2.30	0.45
1:B:377:ARG:O	1:B:380:VAL:HG22	2.17	0.45
1:A:136:ILE:O	1:A:138:PRO:HD3	2.16	0.45
1:A:244:HIS:CD2	1:A:286:PHE:HB2	2.51	0.45
1:A:416:LEU:H	1:A:416:LEU:CD2	2.29	0.45
1:B:118:ARG:NH1	4:B:786:HOH:O	2.49	0.45
1:B:293:MET:HE2	2:D:4:GLC:H62	1.96	0.45
1:A:569:LEU:HG	1:A:571:LEU:CD1	2.42	0.45
1:A:271:GLU:HG2	1:A:282:ASN:O	2.17	0.45
1:A:444:MET:O	1:A:494:ARG:NH1	2.45	0.45
1:B:191:TYR:CE1	1:B:323:ARG:HG3	2.52	0.45
1:A:223:ARG:HD3	1:A:317:GLN:OE1	2.17	0.45
1:B:132:VAL:HG11	1:B:491:ILE:HD12	1.99	0.45
1:A:585:ARG:HH11	1:A:585:ARG:CB	2.18	0.45
1:B:133:ILE:HD13	1:B:189:ALA:HB3	1.99	0.45
1:B:223:ARG:HB3	1:B:223:ARG:CZ	2.46	0.45
1:B:535:ARG:HD3	1:B:539:GLN:NE2	2.32	0.45
1:A:129:LYS:CB	1:A:411:GLN:OE1	2.65	0.44
1:B:133:ILE:CD1	1:B:189:ALA:HB3	2.47	0.44
1:B:416:LEU:H	1:B:416:LEU:CD2	2.31	0.44
1:B:138:PRO:HD2	1:B:193:THR:OG1	2.18	0.44
1:B:447:LEU:HB2	1:B:505:VAL:HG13	2.00	0.44
1:B:251:ALA:O	1:B:255:VAL:HG23	2.17	0.44
1:B:298:THR:HB	1:B:334:PHE:CD2	2.52	0.44
1:A:323:ARG:HH12	1:A:325:ASN:HD22	1.65	0.44
1:B:232:ARG:HG3	1:B:232:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASP:OD2	1:B:282:ASN:ND2	2.50	0.44
1:B:280:ARG:HA	1:B:280:ARG:HD2	1.87	0.44
1:A:280:ARG:O	1:A:280:ARG:HG3	2.18	0.43
1:B:491:ILE:O	1:B:495:HIS:ND1	2.51	0.43
1:A:504:ASN:HD21	1:A:522:THR:HB	1.83	0.43
1:A:524:GLN:HB3	1:A:525:ASP:H	1.58	0.43
1:B:582:TRP:CZ2	1:B:584:GLY:HA2	2.53	0.43
1:A:81:LYS:HB2	1:A:110:VAL:HG21	1.99	0.43
1:B:382:ARG:HA	1:B:386:THR:OG1	2.19	0.43
1:B:438:LEU:CD2	1:B:532:LEU:HD22	2.48	0.43
1:A:105:ARG:HG2	1:A:105:ARG:HH21	1.83	0.43
1:A:223:ARG:HA	1:A:223:ARG:NE	2.33	0.43
1:A:332:HIS:HE1	4:B:906:HOH:O	2.02	0.43
1:A:381:ILE:HD13	1:A:425:PHE:CE1	2.53	0.43
1:A:477:LYS:N	1:A:477:LYS:CD	2.81	0.43
1:B:227:ASP:O	1:B:231:ARG:HG2	2.18	0.43
1:B:275:VAL:HG12	1:B:276:SER:N	2.34	0.43
1:B:277:LYS:HD3	1:B:277:LYS:C	2.39	0.43
1:A:107:LYS:HD3	4:A:947:HOH:O	2.18	0.43
1:A:110:VAL:HG22	1:A:111:PHE:O	2.19	0.42
1:A:478:GLU:OE2	1:A:478:GLU:HA	2.20	0.42
1:B:269:PHE:HB2	1:B:284:GLU:HB3	2.01	0.42
1:A:518:ALA:HA	1:A:530:VAL:O	2.19	0.42
1:B:565:LYS:HE3	4:B:831:HOH:O	2.19	0.42
1:A:82:TYR:C	1:A:110:VAL:HG23	2.40	0.42
1:A:330:VAL:CG2	1:A:335:TRP:CE2	3.03	0.42
1:B:8:HIS:CE1	1:B:25:VAL:HG13	2.55	0.42
1:B:178:ARG:HG3	1:B:474:TRP:CZ2	2.55	0.42
1:A:82:TYR:O	1:A:110:VAL:HG23	2.19	0.42
1:A:499:SER:OG	1:A:526:GLN:HG2	2.20	0.42
1:B:458:ILE:HD12	1:B:479:GLN:HG2	2.01	0.42
1:B:523:VAL:O	1:B:523:VAL:HG13	2.19	0.42
1:A:308:PHE:O	1:A:312:ARG:HG3	2.20	0.42
1:A:325:ASN:HD21	2:C:3:GLC:C1	2.33	0.42
1:A:464:THR:O	1:A:465:ASP:C	2.59	0.42
1:B:24:ARG:HG3	1:B:407:GLU:OE1	2.19	0.42
1:B:217:GLY:HA2	4:B:867:HOH:O	2.20	0.42
1:A:107:LYS:HE2	1:A:107:LYS:HB3	1.86	0.42
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.55	0.42
1:B:477:LYS:HB3	1:B:477:LYS:HZ3	1.85	0.42
1:A:12:GLY:HA2	1:A:364:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:O	1:A:282:ASN:OD1	2.38	0.41
1:A:335:TRP:HA	1:A:335:TRP:CE3	2.56	0.41
1:A:278:THR:HG23	1:A:291:PRO:CG	2.50	0.41
1:A:164:HIS:CE1	1:A:466:PRO:HD3	2.56	0.41
1:A:426:LEU:HD22	1:A:431:GLY:HA2	2.01	0.41
1:A:88:GLY:HA3	1:A:92:GLU:OE1	2.21	0.41
1:A:117:HIS:HB2	1:A:120:GLU:HG3	2.02	0.41
1:B:541:VAL:HG22	1:B:542:LEU:N	2.36	0.41
1:A:330:VAL:HG22	1:A:335:TRP:HE1	1.83	0.41
1:B:163:ARG:HH11	1:B:163:ARG:HG3	1.86	0.41
1:B:179:LEU:N	1:B:180:PRO:CD	2.83	0.41
1:B:543:LEU:HD12	1:B:543:LEU:N	2.35	0.41
1:B:27:LEU:HD23	1:B:27:LEU:C	2.41	0.41
1:B:192:PHE:O	1:B:239:ASP:HB2	2.21	0.41
1:B:280:ARG:HG3	1:B:280:ARG:O	2.21	0.41
1:A:332:HIS:HD2	1:A:367:GLN:OE1	2.04	0.41
1:A:574:ARG:CB	1:A:574:ARG:HH11	2.34	0.41
1:B:477:LYS:NZ	1:B:477:LYS:CB	2.84	0.41
1:A:1:MET:HB3	4:A:846:HOH:O	2.20	0.41
1:A:150:PRO:HG2	1:A:167:PHE:CD2	2.56	0.41
1:B:244:HIS:CD2	1:B:286:PHE:HB2	2.56	0.41
1:B:277:LYS:O	1:B:278:THR:CB	2.69	0.41
1:B:146:PRO:HA	1:B:149:ASP:OD1	2.21	0.40
1:A:27:LEU:C	1:A:27:LEU:HD23	2.41	0.40
1:A:130:GLU:H	1:A:130:GLU:HG2	1.81	0.40
1:A:376:PHE:CE1	1:A:415:ASN:HB3	2.56	0.40
1:B:250:PHE:CG	1:B:251:ALA:N	2.89	0.40
1:B:325:ASN:HB3	4:B:728:HOH:O	2.20	0.40
1:B:335:TRP:HA	1:B:335:TRP:CE3	2.56	0.40
1:B:400:ARG:HG3	1:B:400:ARG:NH2	2.37	0.40
1:A:30:LYS:O	1:A:33:ASP:HB2	2.22	0.40
1:A:573:LEU:CD1	1:A:579:MET:HG3	2.51	0.40
1:B:282:ASN:OD1	1:B:282:ASN:O	2.39	0.40
1:B:475:GLU:HG2	4:B:846:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	583/585 (100%)	556 (95%)	24 (4%)	3 (0%)	29	31
1	B	583/585 (100%)	556 (95%)	22 (4%)	5 (1%)	17	16
All	All	1166/1170 (100%)	1112 (95%)	46 (4%)	8 (1%)	22	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	SER
1	B	275	VAL
1	B	278	THR
1	A	275	VAL
1	B	281	THR
1	B	547	GLU
1	B	280	ARG
1	A	276	SER

### 5.3.2 Protein sidechains [i](#)

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	493/493 (100%)	468 (95%)	25 (5%)	24	29
1	B	493/493 (100%)	474 (96%)	19 (4%)	32	41
All	All	986/986 (100%)	942 (96%)	44 (4%)	27	34

All (44) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	49	GLU
1	A	85	LEU
1	A	122	PHE
1	A	191	TYR
1	A	219	LEU
1	A	263	ARG
1	A	276	SER
1	A	277	LYS
1	A	279	SER
1	A	330	VAL
1	A	346	ASN
1	A	398	LEU
1	A	400	ARG
1	A	404	LEU
1	A	411	GLN
1	A	413	LEU
1	A	426	LEU
1	A	444	MET
1	A	466	PRO
1	A	483	LEU
1	A	504	ASN
1	A	535	ARG
1	A	573	LEU
1	A	581	LEU
1	A	585	ARG
1	B	24	ARG
1	B	122	PHE
1	B	158	LYS
1	B	191	TYR
1	B	248	GLN
1	B	281	THR
1	B	328	ASN
1	B	398	LEU
1	B	400	ARG
1	B	411	GLN
1	B	438	LEU
1	B	451	LEU
1	B	466	PRO
1	B	504	ASN
1	B	524	GLN
1	B	542	LEU
1	B	552	THR
1	B	565	LYS

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Mol	Chain	Res	Type
1	B	569	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	90	GLN
1	A	135	GLN
1	A	164	HIS
1	A	201	HIS
1	A	244	HIS
1	A	261	GLN
1	A	325	ASN
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS
1	A	504	ASN
1	A	527	HIS
1	A	563	HIS
1	B	135	GLN
1	B	243	ASN
1	B	244	HIS
1	B	257	GLN
1	B	261	GLN
1	B	289	GLN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	367	GLN
1	B	411	GLN
1	B	504	ASN
1	B	509	HIS
1	B	524	GLN
1	B	527	HIS
1	B	568	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

12 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	GLC	C	1	2	12,12,12	0.46	0	17,17,17	0.36	0
2	GLC	C	2	2	11,11,12	0.66	0	15,15,17	0.67	1 (6%)
2	GLC	C	3	2	11,11,12	0.71	0	15,15,17	1.57	2 (13%)
2	GLC	C	4	2	11,11,12	0.52	0	15,15,17	0.67	0
2	GLC	C	5	2	11,11,12	0.47	0	15,15,17	0.56	0
2	GLC	C	6	2	11,11,12	0.49	0	15,15,17	0.53	0
2	GLC	D	1	2	12,12,12	0.40	0	17,17,17	0.34	0
2	GLC	D	2	2	11,11,12	0.59	0	15,15,17	0.71	1 (6%)
2	GLC	D	3	2	11,11,12	0.50	0	15,15,17	1.14	2 (13%)
2	GLC	D	4	2	11,11,12	0.55	0	15,15,17	0.60	0
2	GLC	D	5	2	11,11,12	0.47	0	15,15,17	0.50	0
2	GLC	D	6	2	11,11,12	0.49	0	15,15,17	0.59	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
2	GLC	C	1	2	-	1/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	1/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
2	GLC	C	6	2	-	0/2/19/22	0/1/1/1
2	GLC	D	1	2	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	2/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
2	GLC	D	6	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	GLC	C1-O5-C5	3.85	117.41	112.19
2	C	3	GLC	C1-C2-C3	-2.83	106.19	109.67
2	D	3	GLC	C1-O5-C5	2.62	115.74	112.19
2	D	3	GLC	C1-C2-C3	-2.42	106.69	109.67
2	C	2	GLC	C1-O5-C5	2.17	115.13	112.19
2	D	2	GLC	C1-O5-C5	2.12	115.07	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

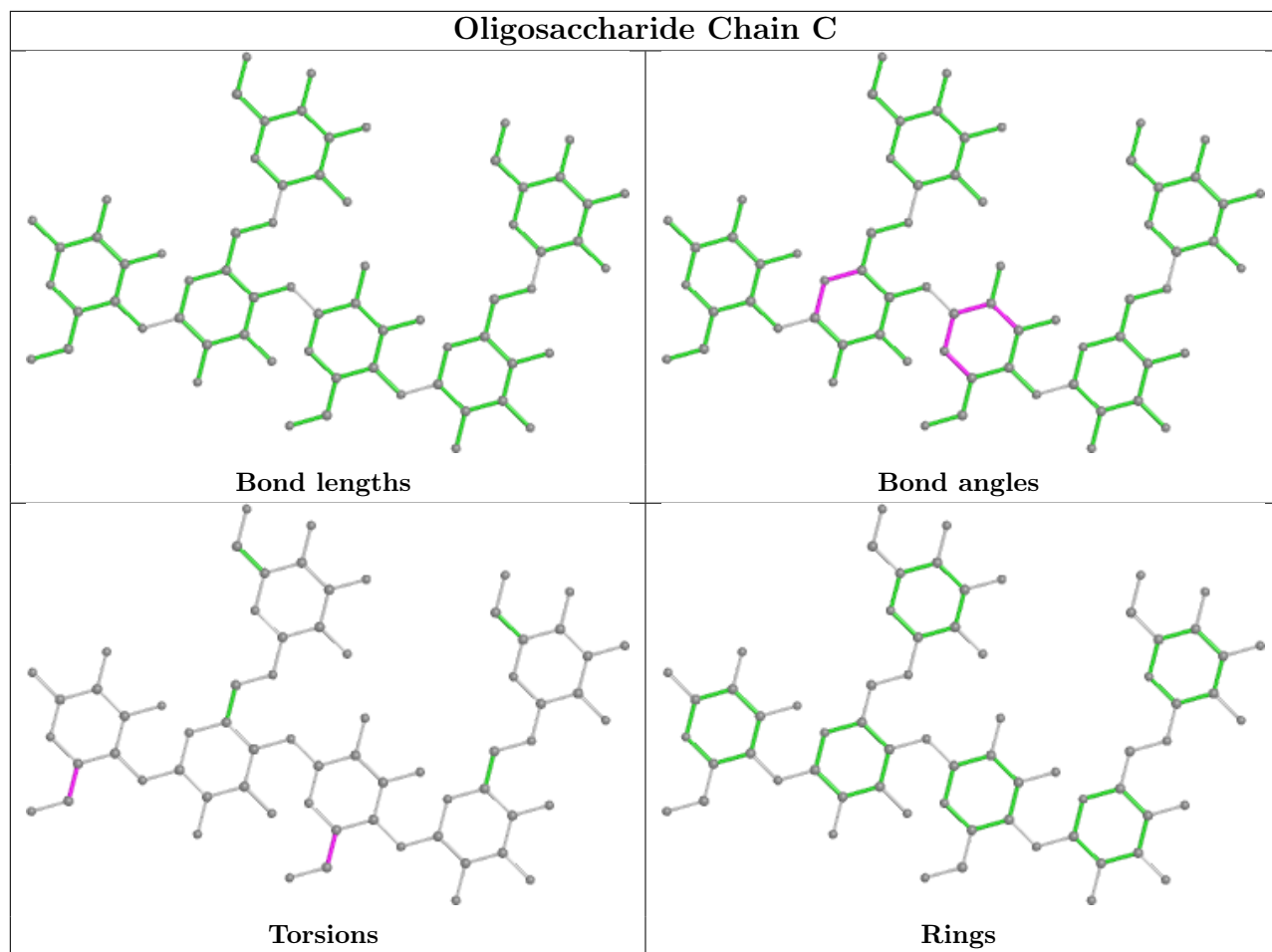
Mol	Chain	Res	Type	Atoms
2	D	1	GLC	C4-C5-C6-O6
2	D	3	GLC	O5-C5-C6-O6
2	D	1	GLC	O5-C5-C6-O6
2	D	3	GLC	C4-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6

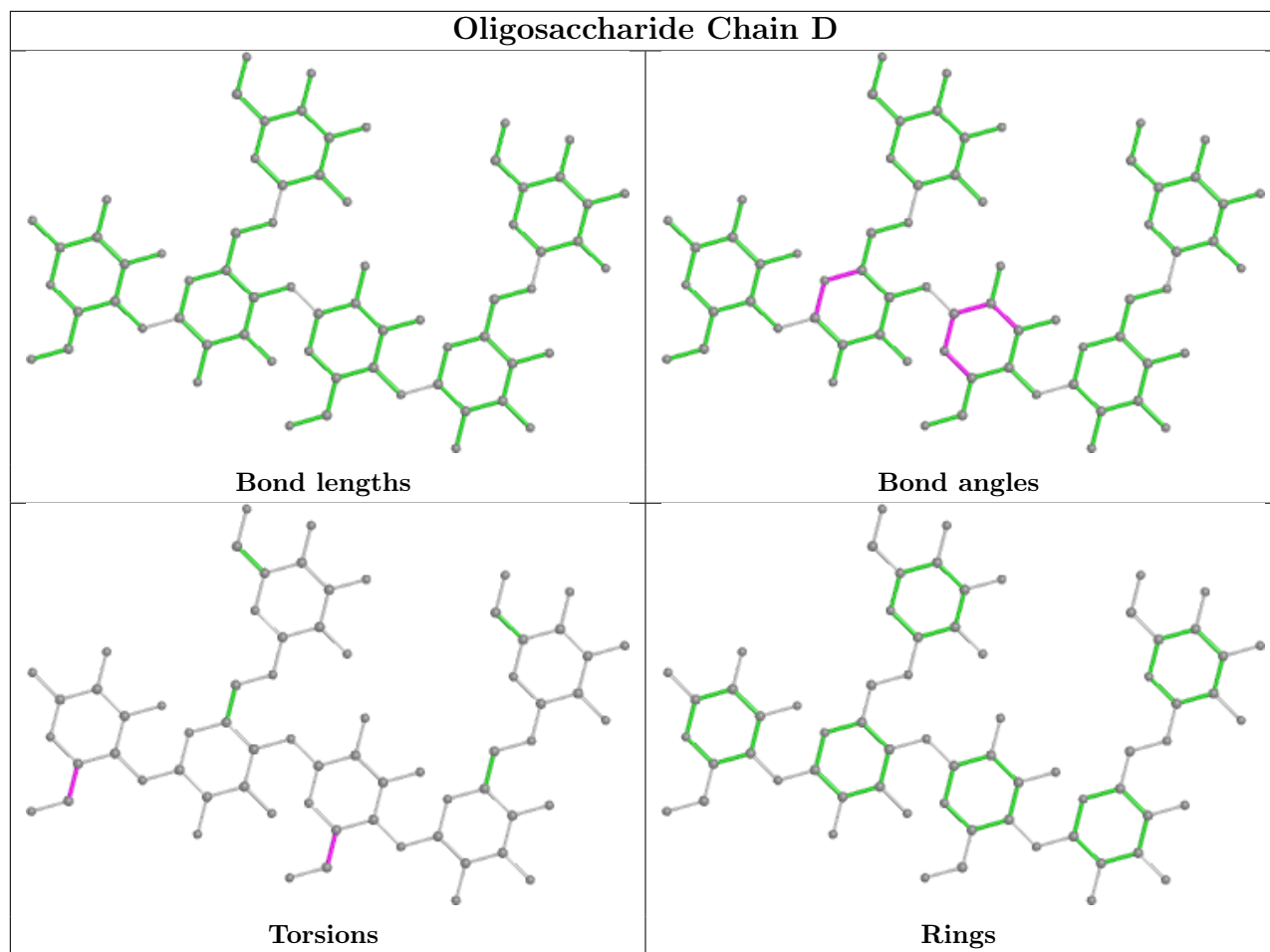
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	GLC	3	0
2	C	3	GLC	1	0
2	D	3	GLC	1	0
2	C	4	GLC	3	0

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





## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	585/585 (100%)	-0.02	28 (4%) 30 29	18, 28, 48, 96	0
1	B	585/585 (100%)	0.02	32 (5%) 25 24	19, 29, 51, 106	0
All	All	1170/1170 (100%)	0.00	60 (5%) 28 26	18, 28, 49, 106	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	SER	16.3
1	B	279	SER	14.5
1	B	273	PHE	11.5
1	B	280	ARG	9.4
1	B	277	LYS	8.9
1	B	272	ASP	8.8
1	B	274	PRO	8.3
1	A	280	ARG	7.7
1	B	278	THR	7.5
1	B	275	VAL	7.5
1	B	276	SER	7.1
1	A	278	THR	7.0
1	A	272	ASP	6.5
1	A	273	PHE	5.4
1	A	274	PRO	5.3
1	A	275	VAL	4.0
1	B	513	GLN	4.0
1	B	477	LYS	3.9
1	B	48	PRO	3.8
1	A	277	LYS	3.7
1	B	51	GLU	3.2
1	A	49	GLU	3.2
1	B	281	THR	3.2
1	A	281	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	49	GLU	3.0
1	A	107	LYS	2.9
1	B	282	ASN	2.9
1	A	451	LEU	2.9
1	A	551	LYS	2.8
1	B	548	SER	2.7
1	A	566	GLN	2.7
1	B	164	HIS	2.6
1	B	158	LYS	2.5
1	B	585	ARG	2.5
1	B	566	GLN	2.5
1	A	237	ILE	2.5
1	A	276	SER	2.4
1	A	477	LYS	2.4
1	B	155	GLN	2.4
1	A	548	SER	2.4
1	A	191	TYR	2.4
1	A	524	GLN	2.4
1	B	159	ASP	2.3
1	B	47	SER	2.3
1	A	375	LEU	2.3
1	A	537	GLU	2.3
1	B	153	THR	2.2
1	A	371	VAL	2.2
1	A	452	ILE	2.2
1	B	50	GLU	2.2
1	A	104	GLU	2.2
1	B	191	TYR	2.2
1	B	118	ARG	2.1
1	A	190	LEU	2.1
1	B	190	LEU	2.1
1	B	271	GLU	2.1
1	A	90	GLN	2.1
1	B	524	GLN	2.1
1	A	327	ALA	2.0
1	B	260	GLU	2.0

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

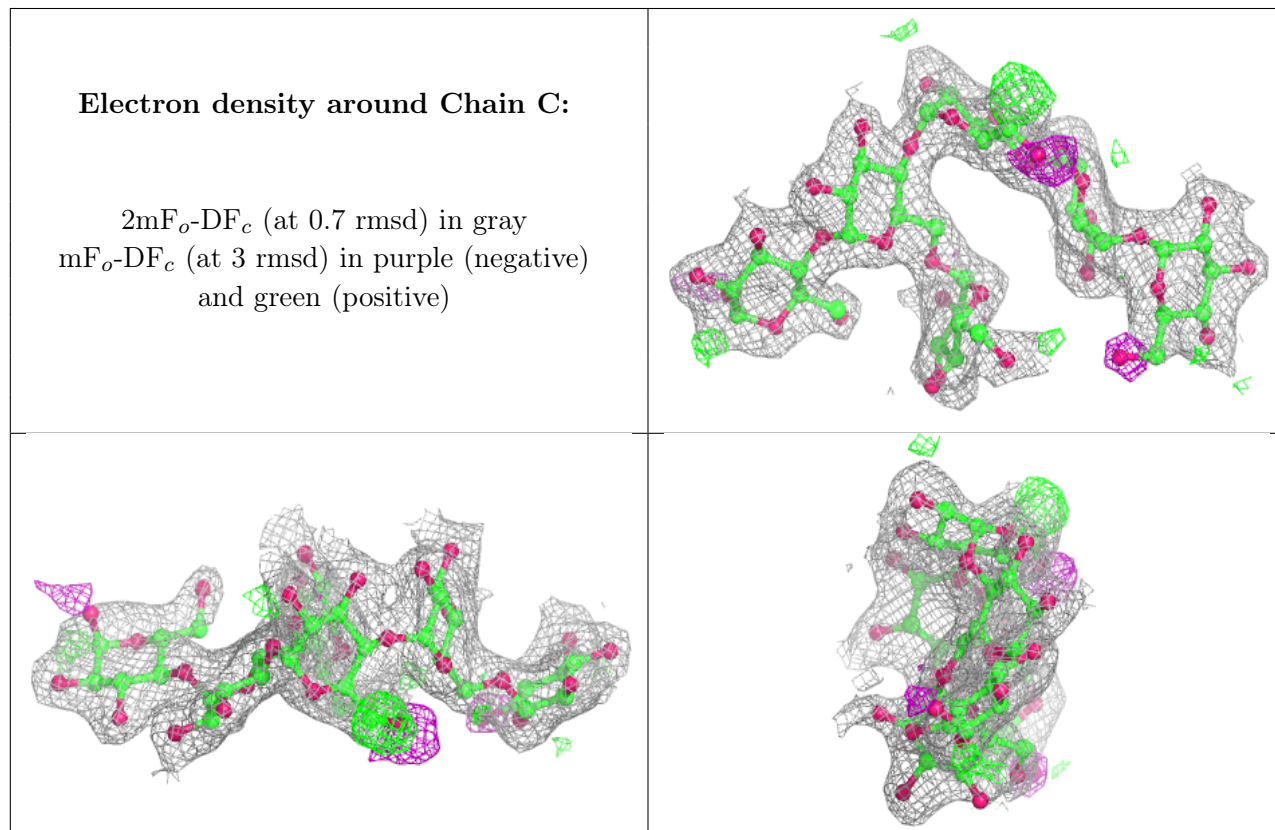
There are no non-standard protein/DNA/RNA residues in this entry.

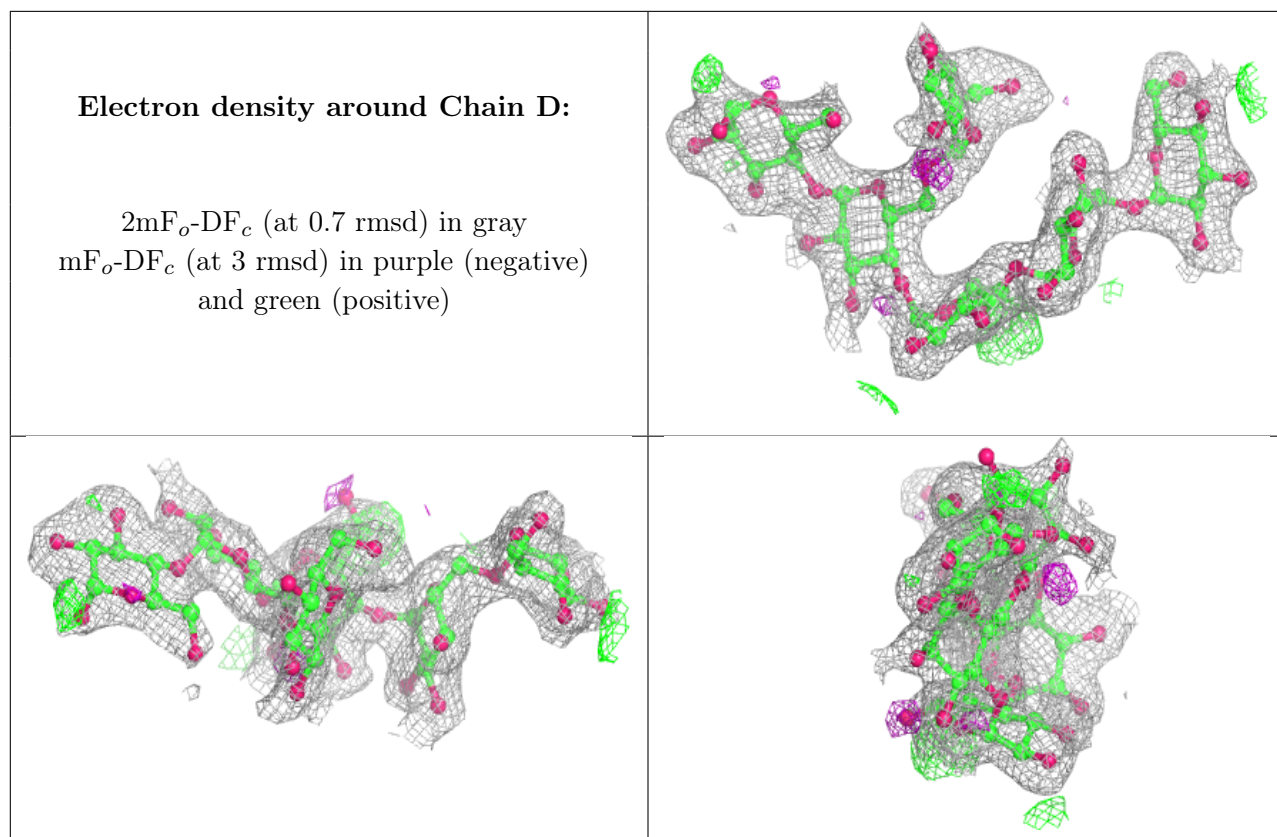
### 6.3 Carbohydrates i

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GLC	D	6	11/12	0.68	0.26	56,59,60,61	0
2	GLC	D	1	12/12	0.76	0.20	46,51,54,54	0
2	GLC	C	6	11/12	0.85	0.23	48,52,54,55	0
2	GLC	C	3	11/12	0.86	0.18	24,28,31,42	0
2	GLC	D	2	11/12	0.87	0.16	37,43,47,52	0
2	GLC	C	1	12/12	0.87	0.17	36,42,45,47	0
2	GLC	D	3	11/12	0.89	0.16	28,32,36,46	0
2	GLC	C	5	11/12	0.91	0.15	30,35,40,46	0
2	GLC	D	5	11/12	0.93	0.14	37,39,42,43	0
2	GLC	C	2	11/12	0.94	0.10	31,34,37,43	0
2	GLC	D	4	11/12	0.95	0.09	30,30,32,36	0
2	GLC	C	4	11/12	0.97	0.08	26,28,30,31	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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	CA	A	601	1/1	0.99	0.06	26,26,26,26	0
3	CA	B	602	1/1	0.99	0.04	34,34,34,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.