



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 11:49 AM BST

PDB ID : 2PNC  
Title : Crystal Structure of Bovine Plasma Copper-Containing Amine Oxidase in Complex with Clonidine  
Authors : Cendron, L.; Holt, A.; Smith, D.J.; Zanutti, G.; Rigo, A.; Di Paolo, M.L.  
Deposited on : 2007-04-24  
Resolution : 2.40 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](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.

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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 : 2.13.1  
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

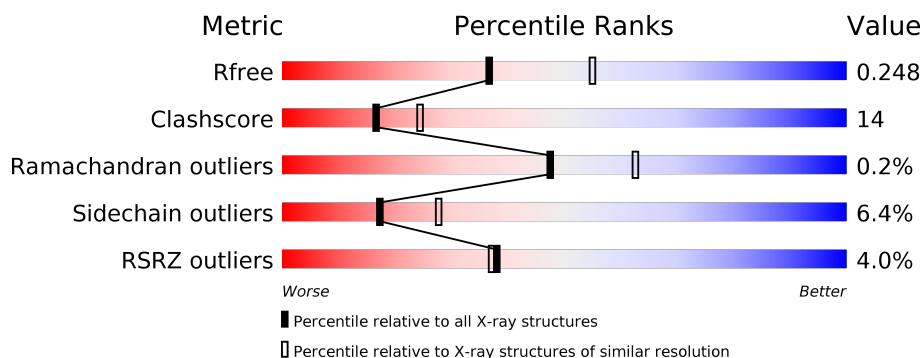
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	746	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>22%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	746	<div> <div>3%</div> <div> <div></div> <div>59%</div> <div>22%</div> <div>•</div> <div>16%</div> </div> </div>
2	C	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
2	D	3	<div> <div></div> <div>100%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	3	-	-	-	X
2	NAG	D	3	-	-	-	X

## 2 Entry composition [i](#)

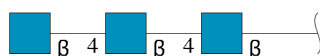
There are 7 unique types of molecules in this entry. The entry contains 10304 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Copper amine oxidase, liver isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	0	0	0
			4926	3156	846	905	19			
1	B	623	Total	C	N	O	S	0	0	0
			4926	3156	846	905	19			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	C	3	Total	C	N	O	0	0	0
			42	24	3	15			
2	D	3	Total	C	N	O	0	0	0
			42	24	3	15			

- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Ca	0	0
			2	2		

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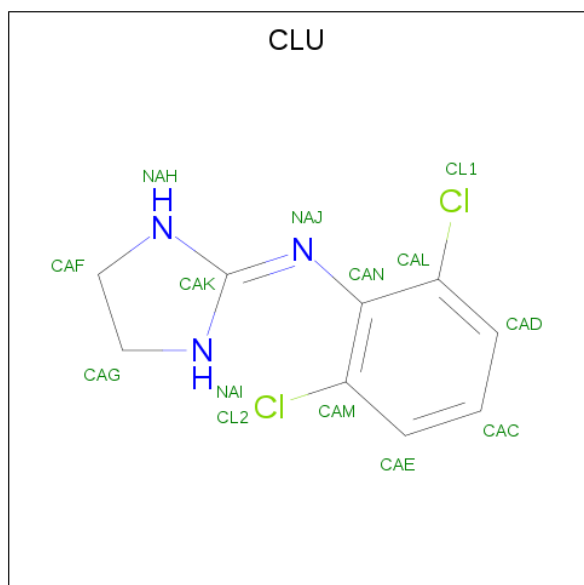
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 2,6-DICHLORO-N-IMIDAZOLIDIN-2-YLIDENEANILINE (three-letter code: CLU) (formula: C<sub>9</sub>H<sub>9</sub>Cl<sub>2</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	0	0
			14	9	2	3		
6	B	1	Total	C	Cl	N	0	0
			14	9	2	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	173	Total	O	0	0
			173	173		

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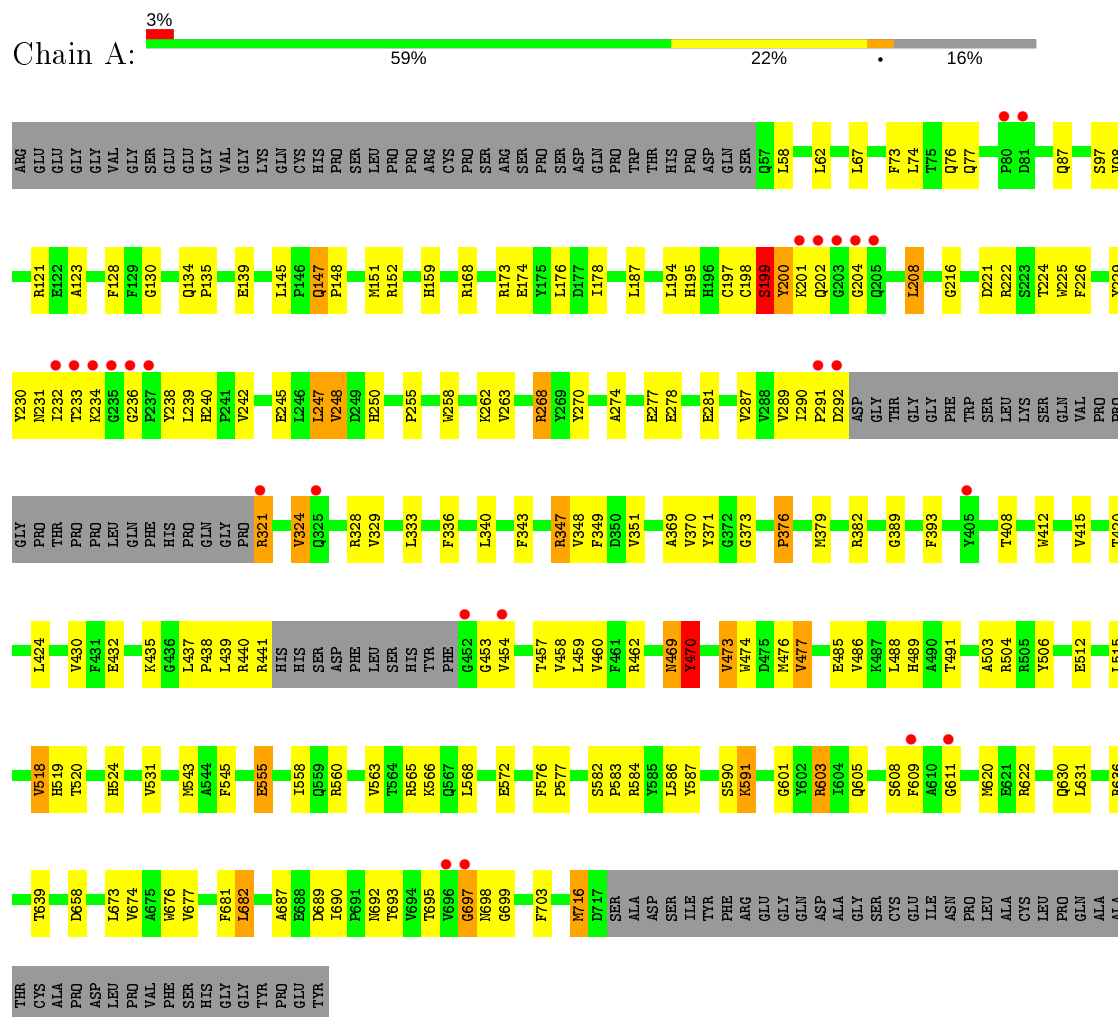
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	158	Total	O	0	0
			158	158		

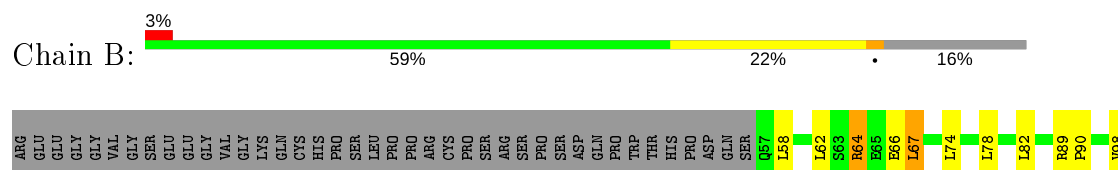
### 3 Residue-property plots [i](#)

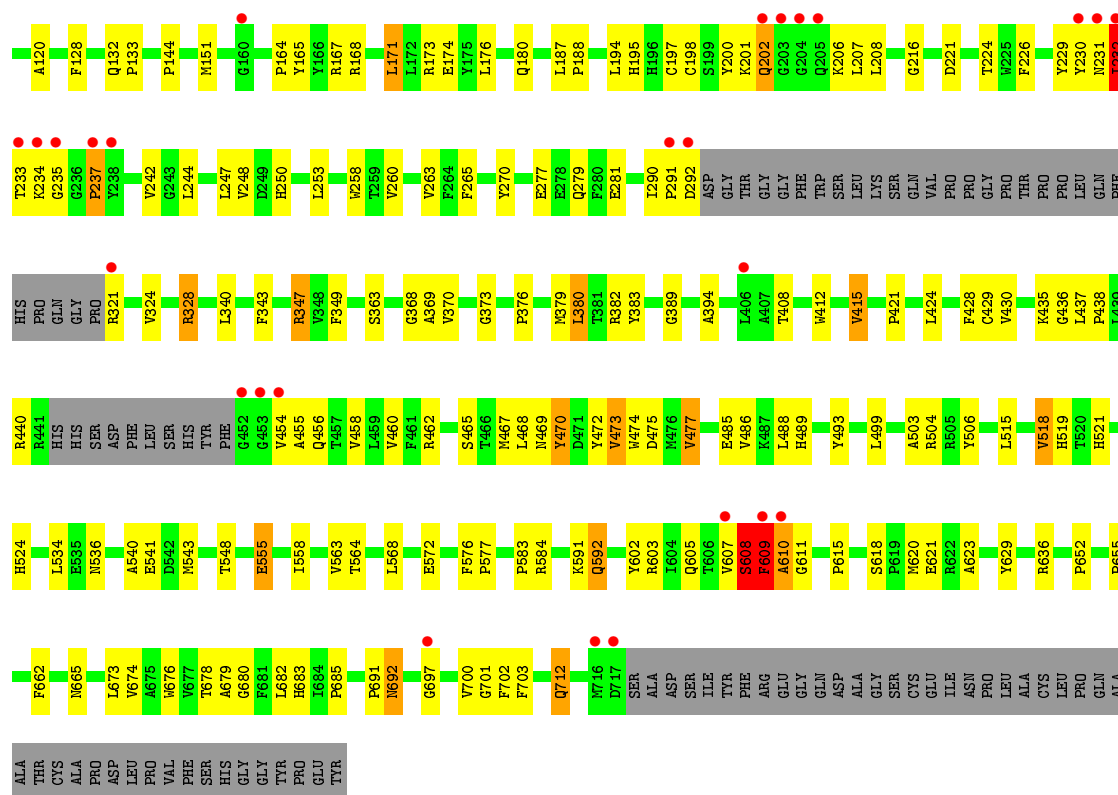
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Copper amine oxidase, liver isozyme





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

Chain C: 67% 33%

MAG1  
MAG2  
MAG3

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

Chain D: 100%

MAG1  
MAG2  
MAG3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.36 Å 131.96 Å 134.16 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.11 – 2.40 29.11 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.5 (29.11-2.40) 86.5 (29.11-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.237 , 0.252 0.236 , 0.248	Depositor DCC
$R_{free}$ test set	2429 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, CA, TPQ, CLU, CU

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	0.25	0/5057	0.46	3/6889 (0.0%)
1	B	0.24	0/5057	0.50	6/6889 (0.1%)
All	All	0.25	0/10114	0.48	9/13778 (0.1%)

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
1	A	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	610	ALA	N-CA-CB	-15.43	88.49	110.10
1	B	609	PHE	CB-CA-C	-8.66	93.07	110.40
1	A	200	TYR	N-CA-CB	-8.18	95.87	110.60
1	A	199	SER	CB-CA-C	-7.48	95.89	110.10
1	B	610	ALA	N-CA-C	6.84	129.47	111.00
1	A	697	GLY	N-CA-C	-6.32	97.31	113.10
1	B	608	SER	N-CA-CB	-5.44	102.33	110.50
1	B	232	ILE	CB-CA-C	5.16	121.92	111.60
1	B	232	ILE	N-CA-C	-5.09	97.24	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	470	TPQ	Peptide

## 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	4926	0	4727	154	0
1	B	4926	0	4728	145	0
2	C	42	0	37	1	0
2	D	42	0	37	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
6	A	14	0	9	0	0
6	B	14	0	9	5	0
7	A	173	0	0	2	0
7	B	158	0	0	7	0
All	All	10304	0	9547	277	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 (277) 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:268:ARG:HH21	1:A:268:ARG:HG2	1.23	0.99
1:A:605:GLN:NE2	1:B:609:PHE:CE1	2.37	0.92
1:A:477:VAL:HG13	1:A:485:GLU:HB3	1.52	0.92
1:B:328:ARG:HH11	1:B:328:ARG:CG	1.84	0.90
1:B:328:ARG:HG2	1:B:328:ARG:HH11	1.36	0.88
1:B:473:VAL:HG13	1:B:489:HIS:HB2	1.60	0.83
1:A:87:GLN:HA	1:A:173:ARG:HD3	1.61	0.82
1:A:268:ARG:NH2	1:A:268:ARG:HG2	1.92	0.81
1:A:199:SER:HB3	1:A:204:GLY:HA3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:HIS:CE1	1:B:202:GLN:HB2	2.18	0.79
1:B:291:PRO:O	1:B:292:ASP:HB2	1.81	0.78
1:B:328:ARG:HG2	1:B:328:ARG:NH1	1.94	0.78
1:B:467:MET:HE2	6:B:809:CLU:HAF1	1.66	0.77
1:A:379:MET:O	1:B:558:ILE:HD11	1.85	0.77
1:A:543:MET:SD	1:B:611:GLY:O	2.43	0.77
1:B:263:VAL:CG2	1:B:270:TYR:HB2	2.15	0.77
1:A:147:GLN:HA	1:A:147:GLN:HE21	1.52	0.75
1:B:242:VAL:HA	1:B:290:ILE:HD13	1.66	0.75
1:A:473:VAL:HG13	1:A:489:HIS:HB2	1.68	0.75
1:A:233:THR:HG22	1:A:233:THR:O	1.86	0.74
1:B:58:LEU:H	1:B:58:LEU:HD23	1.50	0.74
1:A:232:ILE:O	1:A:233:THR:HB	1.90	0.71
1:A:531:VAL:HG11	1:A:601:GLY:HA2	1.74	0.69
1:A:198:CYS:HA	1:A:230:TYR:OH	1.93	0.69
1:B:472:TYR:HE2	7:B:901:HOH:O	1.74	0.68
1:B:277:GLU:O	1:B:281:GLU:HG2	1.93	0.68
1:A:194:LEU:HB3	1:A:200:TYR:HB2	1.75	0.68
1:A:173:ARG:HH12	1:A:176:LEU:HB2	1.59	0.68
1:A:347:ARG:HD3	1:A:349:PHE:HE1	1.59	0.68
1:A:440:ARG:HG2	1:A:454:VAL:HG12	1.77	0.67
1:A:437:LEU:HD12	1:A:438:PRO:HD2	1.76	0.67
1:A:489:HIS:CE1	1:A:699:GLY:H	2.12	0.67
1:A:563:VAL:HG22	1:B:518:VAL:HG11	1.77	0.66
1:B:437:LEU:HD12	1:B:438:PRO:HD2	1.78	0.65
1:A:74:LEU:HD23	1:A:151:MET:HE2	1.77	0.65
1:B:67:LEU:HG	1:B:415:VAL:HG12	1.78	0.65
1:A:58:LEU:HD23	1:A:58:LEU:H	1.61	0.65
1:B:458:VAL:HG11	1:B:477:VAL:HG23	1.79	0.65
1:B:176:LEU:O	1:B:180:GLN:HG2	1.97	0.64
7:A:924:HOH:O	1:B:610:ALA:HB1	1.95	0.64
1:A:208:LEU:HD23	1:A:231:ASN:ND2	2.13	0.64
1:A:173:ARG:HA	1:A:173:ARG:HH11	1.62	0.63
1:A:168:ARG:O	1:A:222:ARG:NH2	2.30	0.63
1:A:584:ARG:NE	1:B:610:ALA:O	2.32	0.63
1:B:343:PHE:HA	1:B:389:GLY:HA2	1.81	0.63
1:A:232:ILE:HG22	1:A:234:LYS:HB3	1.80	0.62
1:B:458:VAL:CG1	1:B:477:VAL:HG23	2.29	0.62
1:A:370:VAL:O	1:A:519:HIS:HA	2.00	0.62
1:B:263:VAL:HG22	1:B:270:TYR:HB2	1.81	0.62
1:A:376:PRO:O	1:A:379:MET:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:GLY:HA2	1:B:703:PHE:CZ	2.36	0.61
1:B:469:ASN:C	1:B:470:TPQ:O	2.37	0.61
1:B:521:HIS:HB3	7:B:901:HOH:O	1.99	0.61
1:A:489:HIS:HE1	1:A:698:ASN:HA	1.66	0.61
1:B:230:TYR:HB3	1:B:232:ILE:HG22	1.83	0.61
1:B:74:LEU:HA	1:B:151:MET:HE1	1.82	0.61
1:B:435:LYS:HB2	1:B:456:GLN:HB3	1.82	0.60
1:B:194:LEU:HB3	1:B:200:TYR:CB	2.31	0.60
1:B:347:ARG:HG3	1:B:349:PHE:CE1	2.37	0.60
1:A:199:SER:CB	1:A:204:GLY:HA3	2.32	0.60
1:A:233:THR:CG2	1:A:233:THR:O	2.50	0.59
1:A:692:ASN:HD21	1:B:440:ARG:HB2	1.68	0.59
1:A:609:PHE:O	1:A:681:PHE:HA	2.02	0.59
1:A:703:PHE:CZ	1:B:697:GLY:HA2	2.38	0.59
1:B:462:ARG:HG3	1:B:475:ASP:OD1	2.03	0.59
1:A:586:LEU:HD22	1:A:631:LEU:HD21	1.83	0.59
1:A:608:SER:OG	1:A:630:GLN:NE2	2.31	0.59
1:B:173:ARG:O	1:B:173:ARG:HD3	2.02	0.59
1:B:237:PRO:HD3	1:B:493:TYR:CD1	2.38	0.58
1:B:67:LEU:HB3	1:B:421:PRO:HG3	1.86	0.58
1:A:473:VAL:CG1	1:A:489:HIS:HB2	2.34	0.58
1:A:147:GLN:NE2	1:A:147:GLN:HA	2.17	0.57
1:B:347:ARG:HB2	1:B:363:SER:HB3	1.86	0.57
1:B:265:PHE:HB2	7:B:1008:HOH:O	2.04	0.57
1:B:470:TPQ:HB2	6:B:809:CLU:CAD	2.34	0.56
1:A:277:GLU:O	1:A:281:GLU:HG2	2.05	0.56
1:A:324:VAL:CG1	1:A:408:THR:HG21	2.35	0.56
1:B:90:PRO:HB2	1:B:253:LEU:HA	1.85	0.56
1:A:563:VAL:HG22	1:B:518:VAL:CG1	2.34	0.56
1:B:474:TRP:CZ3	1:B:488:LEU:HD13	2.41	0.56
1:A:130:GLY:HA2	1:A:135:PRO:HB3	1.88	0.55
1:A:576:PHE:CE2	1:A:586:LEU:HD13	2.42	0.55
1:B:521:HIS:ND1	7:B:901:HOH:O	2.33	0.55
1:A:174:GLU:O	1:A:178:ILE:HG13	2.05	0.55
1:A:605:GLN:NE2	1:B:609:PHE:HE1	1.99	0.55
1:A:336:PHE:HB2	1:A:348:VAL:HG13	1.89	0.55
1:A:232:ILE:HG13	1:A:240:HIS:CE1	2.43	0.54
1:A:232:ILE:O	1:A:233:THR:CB	2.56	0.54
1:A:76:GLN:NE2	1:A:77:GLN:OE1	2.37	0.54
1:B:380:LEU:O	1:B:382:ARG:HD2	2.08	0.54
1:A:197:CYS:SG	1:A:198:CYS:N	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:HH21	1:A:268:ARG:CG	2.07	0.54
1:A:458:VAL:HB	1:A:477:VAL:HG23	1.90	0.54
1:A:582:SER:HB2	1:A:583:PRO:HD2	1.90	0.53
1:B:521:HIS:CE1	6:B:809:CLU:HAE	2.42	0.53
1:A:121:ARG:HG2	1:A:145:LEU:HD12	1.90	0.53
1:A:489:HIS:CE1	1:A:699:GLY:N	2.77	0.53
1:B:197:CYS:SG	1:B:198:CYS:N	2.81	0.53
1:A:236:GLY:HA3	1:A:239:LEU:HD13	1.89	0.53
1:B:328:ARG:CG	1:B:328:ARG:NH1	2.52	0.53
1:B:458:VAL:HG11	1:B:477:VAL:CG2	2.39	0.53
1:B:503:ALA:HB1	1:B:515:LEU:HD22	1.91	0.53
1:B:467:MET:HB2	6:B:809:CLU:CL1	2.46	0.53
1:B:235:GLY:HA2	1:B:493:TYR:OH	2.09	0.53
1:A:173:ARG:NH1	1:A:176:LEU:HB2	2.23	0.52
1:A:432:GLU:HA	1:A:458:VAL:O	2.08	0.52
1:B:499:LEU:HD12	1:B:515:LEU:HB2	1.91	0.52
1:A:274:ALA:O	1:A:278:GLU:HG3	2.09	0.52
1:A:636:ARG:HB2	1:A:674:VAL:HG23	1.91	0.52
1:A:208:LEU:HD23	1:A:231:ASN:HD22	1.74	0.52
1:B:524:HIS:CE1	1:B:676:TRP:HB3	2.45	0.52
1:B:629:TYR:O	1:B:678:THR:HB	2.10	0.51
1:A:639:THR:O	1:A:639:THR:HG22	2.10	0.51
1:A:343:PHE:HA	1:A:389:GLY:HA2	1.92	0.51
1:B:195:HIS:HE1	1:B:202:GLN:HB2	1.73	0.51
1:A:348:VAL:HG12	1:A:351:VAL:HG22	1.92	0.51
1:A:198:CYS:SG	1:A:242:VAL:HG13	2.51	0.51
1:A:250:HIS:CD2	1:A:250:HIS:H	2.29	0.50
1:B:208:LEU:HD12	1:B:229:TYR:HB2	1.93	0.50
1:A:187:LEU:HD22	1:A:194:LEU:HD21	1.92	0.50
1:B:98:VAL:HG22	1:B:415:VAL:CG1	2.41	0.50
1:A:462:ARG:NH2	1:B:436:GLY:O	2.44	0.50
1:A:232:ILE:CG2	1:A:234:LYS:HB3	2.42	0.50
1:A:609:PHE:CE2	1:B:605:GLN:HG2	2.46	0.50
1:A:689:ASP:HB3	1:A:693:THR:HG22	1.94	0.50
1:B:198:CYS:SG	1:B:242:VAL:HG13	2.52	0.50
1:B:607:VAL:HG23	1:B:702:PHE:HA	1.93	0.50
1:B:618:SER:HB3	1:B:621:GLU:HB2	1.93	0.49
1:B:691:PRO:HG2	1:B:692:ASN:ND2	2.28	0.49
1:B:486:VAL:O	1:B:701:GLY:HA3	2.12	0.49
1:A:491:THR:HB	1:A:695:THR:HG23	1.94	0.49
1:A:98:VAL:HB	1:A:415:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:GLU:HA	1:B:564:THR:O	2.11	0.49
2:C:1:NAG:H61	2:C:2:NAG:C1	2.43	0.49
1:A:208:LEU:CD1	1:A:229:TYR:HB2	2.43	0.49
1:A:329:VAL:HG11	1:A:459:LEU:HD21	1.94	0.49
1:B:620:MET:HB2	1:B:652:PRO:HB2	1.94	0.49
1:B:467:MET:CE	6:B:809:CLU:HAF1	2.40	0.49
1:A:347:ARG:HD3	1:A:349:PHE:CE1	2.44	0.49
1:B:216:GLY:HA3	1:B:221:ASP:HB3	1.95	0.49
1:B:78:LEU:HD12	1:B:82:LEU:HD11	1.94	0.49
1:A:199:SER:O	1:A:200:TYR:C	2.51	0.49
1:A:292:ASP:O	7:A:1023:HOH:O	2.20	0.49
1:B:610:ALA:O	1:B:611:GLY:C	2.50	0.49
1:A:518:VAL:HG21	1:B:563:VAL:HG23	1.95	0.48
1:B:472:TYR:CD2	1:B:488:LEU:HD11	2.47	0.48
1:B:132:GLN:HB2	1:B:133:PRO:HD2	1.95	0.48
1:A:173:ARG:HH12	1:A:176:LEU:CB	2.25	0.48
1:A:98:VAL:H	1:A:415:VAL:HG23	1.78	0.48
1:A:558:ILE:HD11	1:B:380:LEU:HA	1.96	0.48
1:B:58:LEU:H	1:B:58:LEU:CD2	2.23	0.48
1:A:232:ILE:HG22	1:A:234:LYS:H	1.79	0.48
1:A:195:HIS:HB3	1:A:202:GLN:HE22	1.79	0.48
1:B:472:TYR:CE2	7:B:901:HOH:O	2.55	0.48
1:A:195:HIS:ND1	1:A:202:GLN:CD	2.67	0.48
1:B:195:HIS:ND1	1:B:202:GLN:HB2	2.28	0.48
1:B:608:SER:HB2	1:B:679:ALA:HB1	1.96	0.48
1:B:608:SER:HB2	1:B:700:VAL:HG13	1.96	0.48
1:A:622:ARG:HG2	1:A:658:ASP:OD2	2.14	0.47
1:A:584:ARG:NH2	1:B:610:ALA:O	2.47	0.47
1:A:62:LEU:HD11	1:A:123:ALA:HB2	1.96	0.47
1:B:194:LEU:HB3	1:B:200:TYR:HB2	1.94	0.47
1:B:250:HIS:HA	1:B:258:TRP:CD1	2.49	0.47
1:A:239:LEU:HD21	1:A:690:ILE:HG23	1.97	0.47
1:B:679:ALA:HB1	1:B:700:VAL:HG13	1.95	0.47
1:A:262:LYS:HG3	1:A:270:TYR:O	2.14	0.47
1:B:584:ARG:O	1:B:603:ARG:NH1	2.47	0.47
1:A:584:ARG:O	1:A:603:ARG:NH1	2.47	0.47
1:B:120:ALA:HB1	1:B:144:PRO:HB3	1.96	0.47
1:B:521:HIS:CG	7:B:901:HOH:O	2.66	0.47
1:A:524:HIS:CE1	1:A:676:TRP:HB3	2.50	0.46
1:B:128:PHE:HE1	1:B:171:LEU:HD13	1.81	0.46
1:A:518:VAL:CG2	1:B:563:VAL:HG23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:VAL:CG1	1:B:408:THR:HG21	2.45	0.46
1:B:340:LEU:HD23	1:B:412:TRP:CD2	2.50	0.46
1:B:609:PHE:O	1:B:680:GLY:O	2.33	0.46
1:A:128:PHE:CZ	1:A:168:ARG:HB2	2.49	0.46
1:A:224:THR:HB	1:A:226:PHE:CE2	2.50	0.46
1:A:373:GLY:HA2	1:A:506:TYR:CB	2.45	0.46
1:A:476:MET:HG2	1:A:486:VAL:HG22	1.98	0.46
1:A:520:THR:HG22	1:A:682:LEU:HD23	1.98	0.46
1:B:468:LEU:O	1:B:469:ASN:HB2	2.16	0.46
1:B:576:PHE:HA	1:B:577:PRO:HD3	1.85	0.46
1:A:139:GLU:OE1	1:A:159:HIS:NE2	2.49	0.46
1:A:340:LEU:HD23	1:A:412:TRP:CD2	2.50	0.46
1:A:382:ARG:HG3	1:A:620:MET:SD	2.56	0.46
1:B:376:PRO:HA	1:B:379:MET:HE3	1.98	0.46
1:A:639:THR:O	1:A:639:THR:CG2	2.63	0.45
1:B:194:LEU:HD11	1:B:244:LEU:HD22	1.98	0.45
1:B:64:ARG:NH2	1:B:421:PRO:O	2.49	0.45
1:B:683:HIS:O	1:B:685:PRO:HD3	2.15	0.45
1:B:473:VAL:HG13	1:B:489:HIS:CB	2.40	0.45
1:A:73:PHE:HE1	1:A:151:MET:HB2	1.81	0.45
1:B:408:THR:O	1:B:429:CYS:HA	2.17	0.45
1:A:611:GLY:O	1:B:543:MET:SD	2.75	0.45
1:B:607:VAL:HG21	1:B:703:PHE:HD1	1.81	0.45
1:B:368:GLY:HA2	1:B:383:TYR:O	2.16	0.45
1:A:687:ALA:O	1:B:712:GLN:HA	2.16	0.45
1:A:62:LEU:HD11	1:A:123:ALA:CB	2.47	0.45
1:B:636:ARG:HB2	1:B:674:VAL:CG2	2.47	0.45
1:A:255:PRO:HA	1:A:258:TRP:CE2	2.52	0.45
1:A:572:GLU:N	1:A:572:GLU:OE2	2.50	0.45
1:B:454:VAL:HG22	1:B:455:ALA:N	2.33	0.45
1:A:225:TRP:CE2	1:A:247:LEU:HG	2.52	0.44
1:B:165:TYR:O	1:B:168:ARG:HD3	2.17	0.44
1:A:151:MET:HG2	1:A:151:MET:O	2.18	0.44
1:A:590:SER:HB2	1:A:591:LYS:HZ3	1.83	0.44
1:B:328:ARG:HG3	1:B:328:ARG:HH11	1.76	0.44
1:A:321:ARG:NH2	1:A:457:THR:OG1	2.50	0.44
1:A:558:ILE:CD1	1:B:380:LEU:HA	2.47	0.44
1:B:370:VAL:O	1:B:519:HIS:HA	2.18	0.44
1:B:208:LEU:HD23	1:B:231:ASN:ND2	2.33	0.44
1:A:491:THR:HB	1:A:695:THR:CG2	2.48	0.44
1:B:430:VAL:HA	1:B:460:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:CYS:HB3	1:A:287:VAL:CG1	2.48	0.43
1:A:98:VAL:HB	1:A:415:VAL:CG2	2.48	0.43
1:B:662:PHE:CD1	1:B:662:PHE:N	2.86	0.43
1:A:584:ARG:CZ	1:B:610:ALA:O	2.67	0.43
1:A:576:PHE:HA	1:A:577:PRO:HD3	1.88	0.43
1:B:373:GLY:HA2	1:B:506:TYR:CB	2.48	0.43
1:B:572:GLU:OE2	1:B:665:ASN:HA	2.18	0.43
1:B:712:GLN:HB3	1:B:712:GLN:HE21	1.59	0.43
1:A:565:ARG:NH1	1:B:504:ARG:O	2.39	0.43
1:A:555:GLU:CD	1:A:555:GLU:H	2.22	0.43
1:A:698:ASN:HD21	1:B:435:LYS:NZ	2.16	0.43
1:B:234:LYS:HB3	1:B:235:GLY:H	1.64	0.43
1:B:555:GLU:CD	1:B:555:GLU:H	2.22	0.43
1:A:147:GLN:HA	1:A:148:PRO:HD3	1.82	0.43
1:B:477:VAL:HG13	1:B:485:GLU:HB3	2.01	0.43
1:B:540:ALA:HB1	1:B:583:PRO:HG2	2.01	0.43
1:B:609:PHE:CD2	1:B:609:PHE:N	2.74	0.43
1:A:503:ALA:HB1	1:A:515:LEU:HD22	2.00	0.42
1:B:174:GLU:HA	7:B:945:HOH:O	2.18	0.42
1:B:691:PRO:HG2	1:B:692:ASN:HD21	1.84	0.42
1:A:147:GLN:CA	1:A:147:GLN:HE21	2.20	0.42
1:A:208:LEU:HD12	1:A:229:TYR:HB2	2.02	0.42
1:A:631:LEU:HD13	1:A:677:VAL:HG22	2.01	0.42
1:B:224:THR:HB	1:B:226:PHE:CE2	2.54	0.42
1:B:394:ALA:HA	1:B:465:SER:HA	2.00	0.42
1:A:587:TYR:HB3	1:A:603:ARG:CB	2.50	0.42
1:A:371:TYR:CD2	1:A:519:HIS:HB3	2.55	0.42
1:A:389:GLY:O	1:A:393:PHE:HB2	2.20	0.42
1:A:373:GLY:HA2	1:A:506:TYR:HB3	2.01	0.42
1:A:250:HIS:HA	1:A:258:TRP:CD1	2.55	0.42
1:B:260:VAL:HG23	1:B:260:VAL:O	2.20	0.42
1:A:545:PHE:CD1	1:B:615:PRO:HD3	2.55	0.42
1:B:164:PRO:HB2	1:B:167:ARG:HG3	2.01	0.42
1:B:592:GLN:HE21	1:B:592:GLN:HB2	1.65	0.42
1:A:194:LEU:HA	1:A:197:CYS:SG	2.60	0.41
1:A:216:GLY:HA3	1:A:221:ASP:HB3	2.01	0.41
1:A:197:CYS:HA	1:A:289:VAL:HA	2.02	0.41
1:A:531:VAL:O	1:A:590:SER:HB3	2.20	0.41
1:B:187:LEU:HD22	1:B:194:LEU:HD21	2.02	0.41
1:B:187:LEU:N	1:B:188:PRO:CD	2.83	0.41
1:B:369:ALA:HB3	1:B:383:TYR:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:HD2	1:A:248:VAL:CG1	2.33	0.41
1:B:279:GLN:HB3	1:B:279:GLN:HE21	1.76	0.41
1:B:347:ARG:HB2	1:B:363:SER:CB	2.50	0.41
1:A:470:TPQ:H6	1:A:470:TPQ:HA	1.73	0.41
1:A:582:SER:HB2	1:A:583:PRO:CD	2.50	0.41
1:B:200:TYR:O	1:B:201:LYS:HB2	2.21	0.41
1:A:369:ALA:HA	1:A:520:THR:O	2.21	0.41
1:A:430:VAL:HA	1:A:460:VAL:O	2.20	0.41
1:A:474:TRP:CZ3	1:A:488:LEU:HD13	2.54	0.41
1:A:97:SER:HA	1:A:415:VAL:O	2.20	0.41
1:A:198:CYS:SG	1:A:242:VAL:CG1	3.09	0.41
1:B:62:LEU:HA	1:B:66:GLU:OE1	2.20	0.41
1:A:245:GLU:OE2	1:A:376:PRO:HB2	2.21	0.41
1:A:435:LYS:HA	1:A:435:LYS:HD2	1.92	0.41
1:A:333:LEU:HD21	1:A:716:MET:HA	2.03	0.41
1:B:340:LEU:HB2	1:B:428:PHE:CE2	2.56	0.41
1:A:441:ARG:HA	1:A:453:GLY:HA3	2.03	0.40
1:B:340:LEU:HB2	1:B:428:PHE:CZ	2.56	0.40
1:B:623:ALA:HA	1:B:655:PRO:HB3	2.02	0.40
1:A:290:ILE:HA	1:A:291:PRO:HD2	1.77	0.40
1:A:689:ASP:CB	1:A:693:THR:HG22	2.50	0.40
1:A:439:LEU:HB3	1:A:454:VAL:HG13	2.03	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	616/746 (83%)	580 (94%)	34 (6%)	2 (0%)	41	55
1	B	616/746 (83%)	582 (94%)	33 (5%)	1 (0%)	47	62
All	All	1232/1492 (83%)	1162 (94%)	67 (5%)	3 (0%)	47	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	237	PRO
1	A	376	PRO
1	A	469	ASN

### 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	520/623 (84%)	487 (94%)	33 (6%)	18	28
1	B	520/623 (84%)	486 (94%)	34 (6%)	17	27
All	All	1040/1246 (84%)	973 (94%)	67 (6%)	17	28

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	134	GLN
1	A	147	GLN
1	A	152	ARG
1	A	199	SER
1	A	201	LYS
1	A	208	LEU
1	A	238	TYR
1	A	247	LEU
1	A	248	VAL
1	A	263	VAL
1	A	268	ARG
1	A	321	ARG
1	A	324	VAL
1	A	328	ARG
1	A	347	ARG
1	A	420	THR
1	A	424	LEU
1	A	469	ASN
1	A	473	VAL

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Mol	Chain	Res	Type
1	A	477	VAL
1	A	504	ARG
1	A	512	GLU
1	A	518	VAL
1	A	555	GLU
1	A	560	ARG
1	A	566	LYS
1	A	568	LEU
1	A	591	LYS
1	A	603	ARG
1	A	673	LEU
1	A	682	LEU
1	A	716	MET
1	B	64	ARG
1	B	67	LEU
1	B	89	ARG
1	B	171	LEU
1	B	202	GLN
1	B	206	LYS
1	B	207	LEU
1	B	232	ILE
1	B	233	THR
1	B	247	LEU
1	B	248	VAL
1	B	321	ARG
1	B	328	ARG
1	B	347	ARG
1	B	380	LEU
1	B	415	VAL
1	B	424	LEU
1	B	473	VAL
1	B	477	VAL
1	B	518	VAL
1	B	534	LEU
1	B	536	ASN
1	B	548	THR
1	B	555	GLU
1	B	568	LEU
1	B	591	LYS
1	B	592	GLN
1	B	602	TYR
1	B	608	SER

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Mol	Chain	Res	Type
1	B	609	PHE
1	B	673	LEU
1	B	682	LEU
1	B	692	ASN
1	B	712	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	76	GLN
1	A	77	GLN
1	A	132	GLN
1	A	147	GLN
1	A	180	GLN
1	A	184	ASN
1	A	196	HIS
1	A	202	GLN
1	A	205	GLN
1	A	240	HIS
1	A	286	ASN
1	A	456	GLN
1	A	469	ASN
1	A	489	HIS
1	A	556	HIS
1	A	559	GLN
1	A	665	ASN
1	A	692	ASN
1	A	698	ASN
1	B	57	GLN
1	B	134	GLN
1	B	195	HIS
1	B	231	ASN
1	B	279	GLN
1	B	434	ASN
1	B	489	HIS
1	B	559	GLN
1	B	592	GLN
1	B	692	ASN
1	B	698	ASN
1	B	712	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	TPQ	A	470	1,3	13,14,15	2.16	3 (23%)	15,19,21	0.93	0
1	TPQ	B	470	1,3	13,14,15	2.17	3 (23%)	15,19,21	0.97	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
1	TPQ	A	470	1,3	-	4/5/22/24	0/1/1/1
1	TPQ	B	470	1,3	-	4/5/22/24	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	TPQ	O2-C2	4.57	1.36	1.24
1	B	470	TPQ	O2-C2	4.55	1.36	1.24
1	A	470	TPQ	O5-C5	4.55	1.36	1.24
1	B	470	TPQ	O5-C5	4.50	1.36	1.24
1	B	470	TPQ	C3-C4	2.42	1.39	1.35
1	A	470	TPQ	C3-C4	2.37	1.39	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	470	TPQ	N-CA-CB-C1
1	A	470	TPQ	C-CA-CB-C1
1	A	470	TPQ	O-C-CA-CB
1	B	470	TPQ	N-CA-CB-C1
1	B	470	TPQ	C-CA-CB-C1
1	B	470	TPQ	C2-C1-CB-CA
1	A	470	TPQ	C2-C1-CB-CA
1	B	470	TPQ	C6-C1-CB-CA

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	470	TPQ	1	0
1	B	470	TPQ	2	0

## 5.5 Carbohydrates [i](#)

6 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	C	1	1,2	14,14,15	0.54	0	17,19,21	0.96	0
2	NAG	C	2	2	14,14,15	0.56	0	17,19,21	1.29	2 (11%)
2	NAG	C	3	2	14,14,15	0.51	0	17,19,21	1.13	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.55	0	17,19,21	1.05	2 (11%)
2	NAG	D	2	2	14,14,15	0.61	0	17,19,21	1.26	2 (11%)
2	NAG	D	3	2	14,14,15	0.66	0	17,19,21	1.28	2 (11%)

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	C	1	1,2	-	6/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	3	2	-	6/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	3	2	-	2/6/23/26	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	C	3	NAG	C1-O5-C5	4.04	117.67	112.19
2	D	3	NAG	C1-O5-C5	3.23	116.57	112.19
2	C	2	NAG	O5-C5-C6	3.19	112.20	107.20
2	D	2	NAG	C4-C3-C2	2.87	115.22	111.02
2	D	2	NAG	O5-C5-C6	2.74	111.50	107.20
2	C	2	NAG	C3-C4-C5	-2.60	105.60	110.24
2	D	1	NAG	C4-C3-C2	2.51	114.69	111.02
2	D	3	NAG	O5-C1-C2	2.36	115.01	111.29
2	D	1	NAG	O5-C1-C2	-2.21	107.81	111.29

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	NAG	O7-C7-N2-C2
2	D	3	NAG	C8-C7-N2-C2
2	D	3	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	3	NAG	C4-C5-C6-O6
2	C	3	NAG	C8-C7-N2-C2
2	C	3	NAG	O5-C5-C6-O6
2	C	3	NAG	C1-C2-N2-C7
2	C	1	NAG	O5-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2

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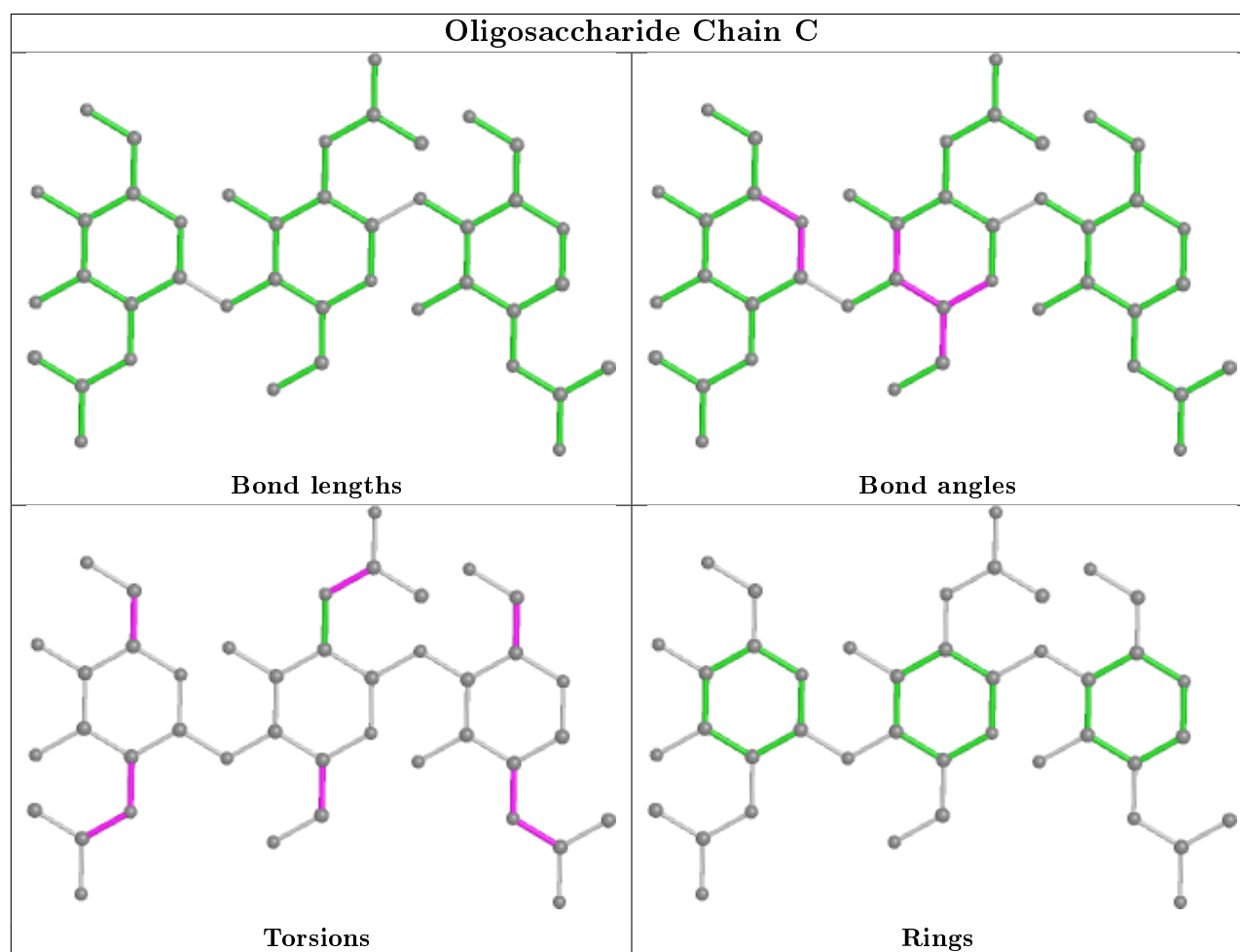
Mol	Chain	Res	Type	Atoms
2	C	3	NAG	C3-C2-N2-C7
2	D	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C1-C2-N2-C7
2	C	1	NAG	C3-C2-N2-C7

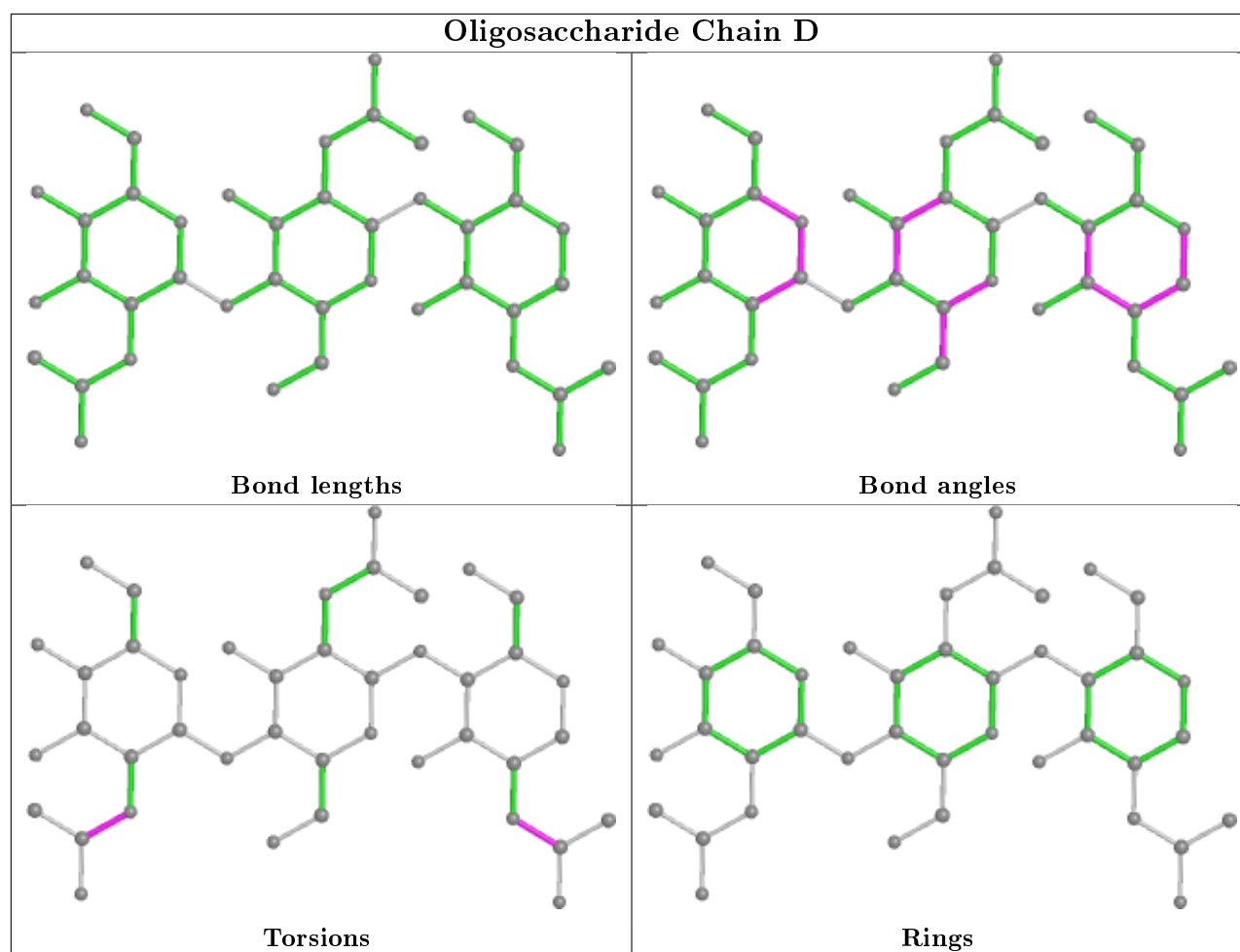
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	C	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](#)

Of 11 ligands modelled in this entry, 9 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	$\# Z  > 2$
6	CLU	A	808	-	15,15,15	2.10	5 (33%)	20,20,20	1.87	3 (15%)
6	CLU	B	809	-	15,15,15	2.09	5 (33%)	20,20,20	2.09	3 (15%)

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	CLU	A	808	-	-	0/4/11/11	0/2/2/2
6	CLU	B	809	-	-	0/4/11/11	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	808	CLU	CAN-NAJ	-5.66	1.33	1.42
6	B	809	CLU	CAN-NAJ	-5.46	1.34	1.42
6	B	809	CLU	CAK-NAJ	3.32	1.39	1.31
6	A	808	CLU	CAK-NAJ	3.24	1.39	1.31
6	B	809	CLU	CAK-NAH	2.71	1.39	1.35
6	B	809	CLU	CAL-CL1	2.63	1.79	1.73
6	B	809	CLU	CAM-CL2	2.63	1.79	1.73
6	A	808	CLU	CAM-CL2	2.63	1.79	1.73
6	A	808	CLU	CAL-CL1	2.60	1.79	1.73
6	A	808	CLU	CAK-NAH	2.50	1.39	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	809	CLU	CAN-NAJ-CAK	8.18	132.64	119.60
6	A	808	CLU	CAN-NAJ-CAK	6.70	130.27	119.60
6	A	808	CLU	NAH-CAK-NAI	-2.46	107.29	108.94
6	A	808	CLU	CAL-CAN-CAM	2.28	119.79	116.59
6	B	809	CLU	NAH-CAK-NAI	-2.24	107.43	108.94
6	B	809	CLU	CAL-CAN-CAM	2.16	119.62	116.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	809	CLU	5	0

## 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, 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	622/746 (83%)	-0.08	24 (3%) 39 38	9, 24, 56, 107	0
1	B	622/746 (83%)	-0.01	26 (4%) 36 35	8, 24, 57, 109	0
All	All	1244/1492 (83%)	-0.05	50 (4%) 38 37	8, 24, 57, 109	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	GLY	7.9
1	B	292	ASP	7.1
1	B	717	ASP	7.0
1	A	205	GLN	7.0
1	B	203	GLY	6.9
1	B	233	THR	6.5
1	B	716	MET	6.3
1	B	232	ILE	5.9
1	A	233	THR	5.8
1	B	234	LYS	5.2
1	B	202	GLN	5.1
1	A	609	PHE	4.9
1	B	609	PHE	4.8
1	A	235	GLY	4.7
1	A	234	LYS	4.7
1	B	237	PRO	4.2
1	A	292	ASP	4.1
1	A	204	GLY	4.1
1	B	160	GLY	4.0
1	B	231	ASN	4.0
1	B	238	TYR	3.9
1	B	452	GLY	3.8
1	A	203	GLY	3.8
1	B	610	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	291	PRO	3.7
1	A	232	ILE	3.6
1	B	453	GLY	3.5
1	A	80	PRO	3.5
1	A	611	GLY	3.4
1	A	405	TYR	3.3
1	B	230	TYR	3.3
1	B	205	GLN	3.2
1	A	696	VAL	3.2
1	B	235	GLY	3.2
1	A	291	PRO	2.9
1	B	321	ARG	2.9
1	B	607	VAL	2.7
1	A	697	GLY	2.7
1	A	201	LYS	2.6
1	A	81	ASP	2.6
1	A	237	PRO	2.4
1	A	454	VAL	2.4
1	A	202	GLN	2.3
1	B	697	GLY	2.2
1	B	454	VAL	2.1
1	A	452	GLY	2.1
1	B	406	LEU	2.1
1	A	325	GLN	2.1
1	A	236	GLY	2.0
1	A	321	ARG	2.0

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

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.

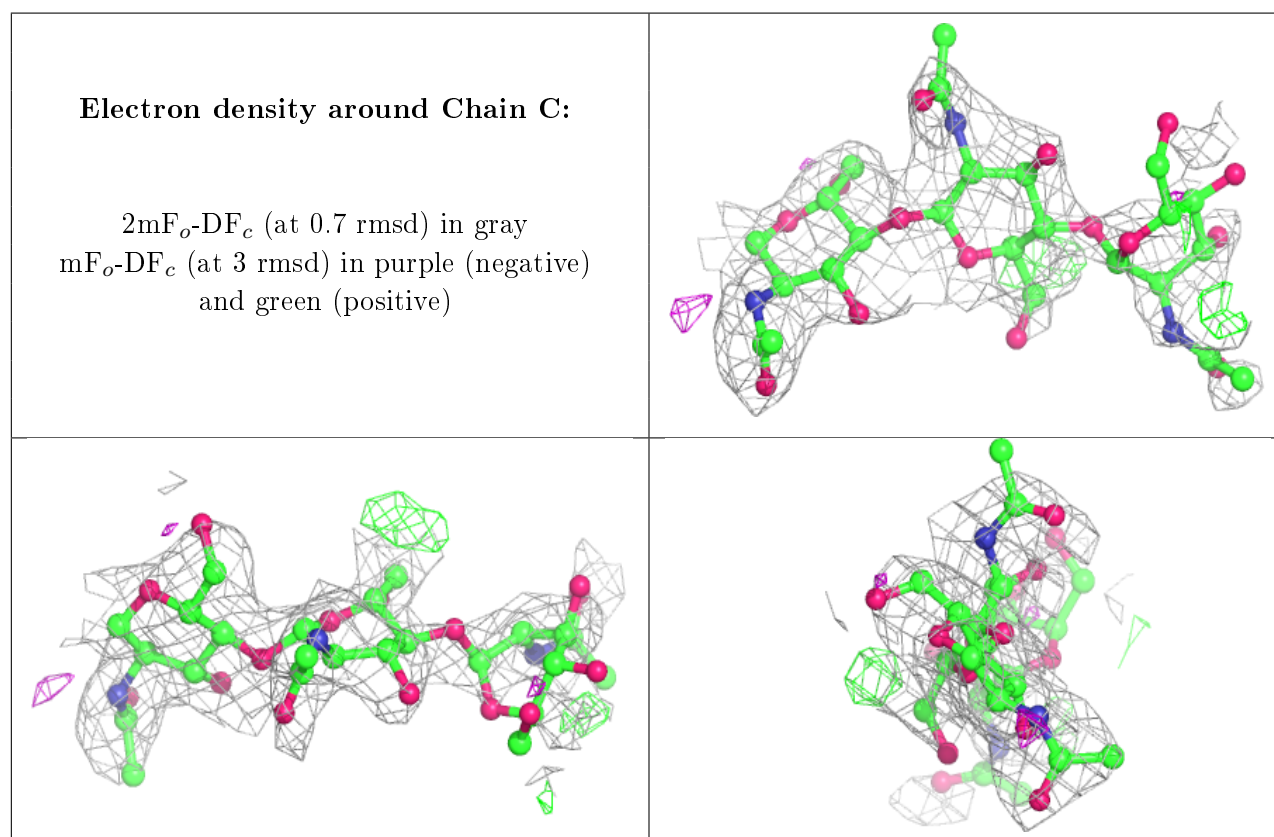
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TPQ	B	470	14/15	0.81	0.24	36,40,42,43	0
1	TPQ	A	470	14/15	0.85	0.21	34,36,39,39	0

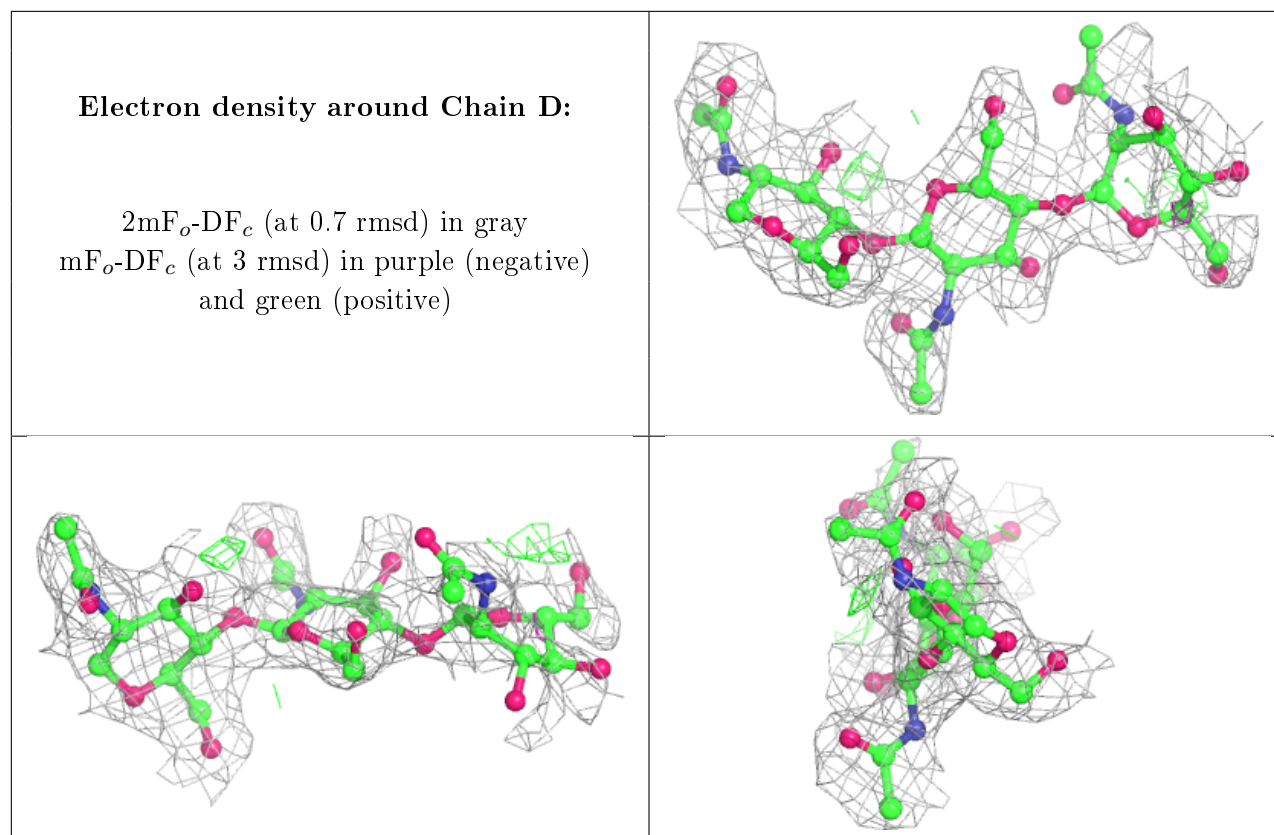
## 6.3 Carbohydrates ⓘ

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, 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	NAG	D	3	14/15	0.53	0.43	71,75,76,77	0
2	NAG	C	3	14/15	0.57	0.53	82,86,87,87	0
2	NAG	C	2	14/15	0.75	0.31	59,65,71,78	0
2	NAG	D	2	14/15	0.79	0.22	50,54,59,66	0
2	NAG	C	1	14/15	0.84	0.22	38,42,48,56	0
2	NAG	D	1	14/15	0.87	0.13	31,38,42,44	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( $\text{\AA}^2$ )	Q<0.9
4	CA	B	806	1/1	0.26	0.26	29,29,29,29	0
4	CA	A	806	1/1	0.55	0.23	28,28,28,28	0
5	CL	A	807	1/1	0.68	0.21	33,33,33,33	0
4	CA	A	805	1/1	0.76	0.17	20,20,20,20	0
6	CLU	A	808	14/14	0.77	0.23	30,40,42,43	0
4	CA	B	805	1/1	0.79	0.12	20,20,20,20	0
3	CU	A	804	1/1	0.80	0.09	29,29,29,29	0
6	CLU	B	809	14/14	0.88	0.21	34,43,43,44	0
3	CU	B	804	1/1	0.88	0.10	27,27,27,27	0
5	CL	B	808	1/1	0.95	0.16	27,27,27,27	0
5	CL	B	807	1/1	0.96	0.12	43,43,43,43	0

## 6.5 Other polymers

There are no such residues in this entry.