



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:51 PM BST

PDB ID : 1TU5
Title : Crystal structure of bovine plasma copper-containing amine oxidase
Authors : Lunelli, M.; Di Paolo, M.L.; Biadene, M.; Calderone, V.; Scarpa, M.; Battistutta, R.; Rigo, A.; Zanotti, G.
Deposited on : 2004-06-24
Resolution : 2.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

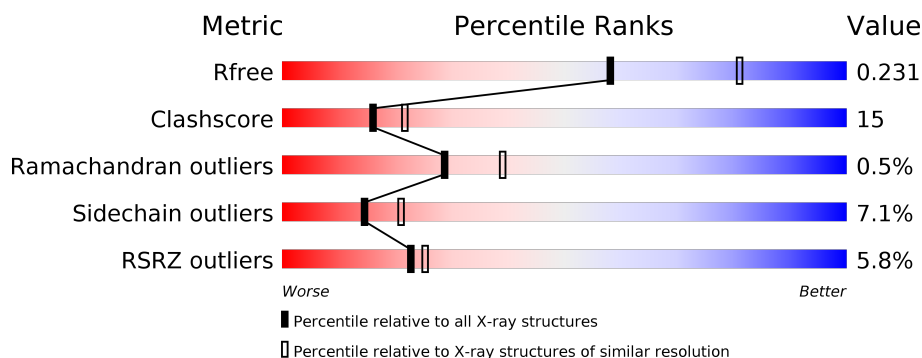
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	746	<div> <div>5%</div> <div> <div></div> <div>59%</div> <div>22%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	746	<div> <div>5%</div> <div> <div></div> <div>61%</div> <div>21%</div> <div>•</div> <div>15%</div> </div> </div>
2	C	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
2	D	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </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	1	X	-	-	-
2	NAG	D	3	-	-	-	X
3	NAG	A	803	-	-	-	X
3	NAG	A	804	X	-	-	X
3	NAG	B	804	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10581 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.

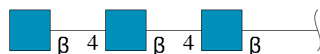
- Molecule 1 is a protein called Copper amine oxidase, liver isozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			5018	3217	862	920	19			
1	B	633	Total	C	N	O	S	0	0	0
			5018	3217	862	920	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	470	TPQ	TYR	modified residue	UNP Q29437
B	470	TPQ	TYR	modified residue	UNP Q29437

- 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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

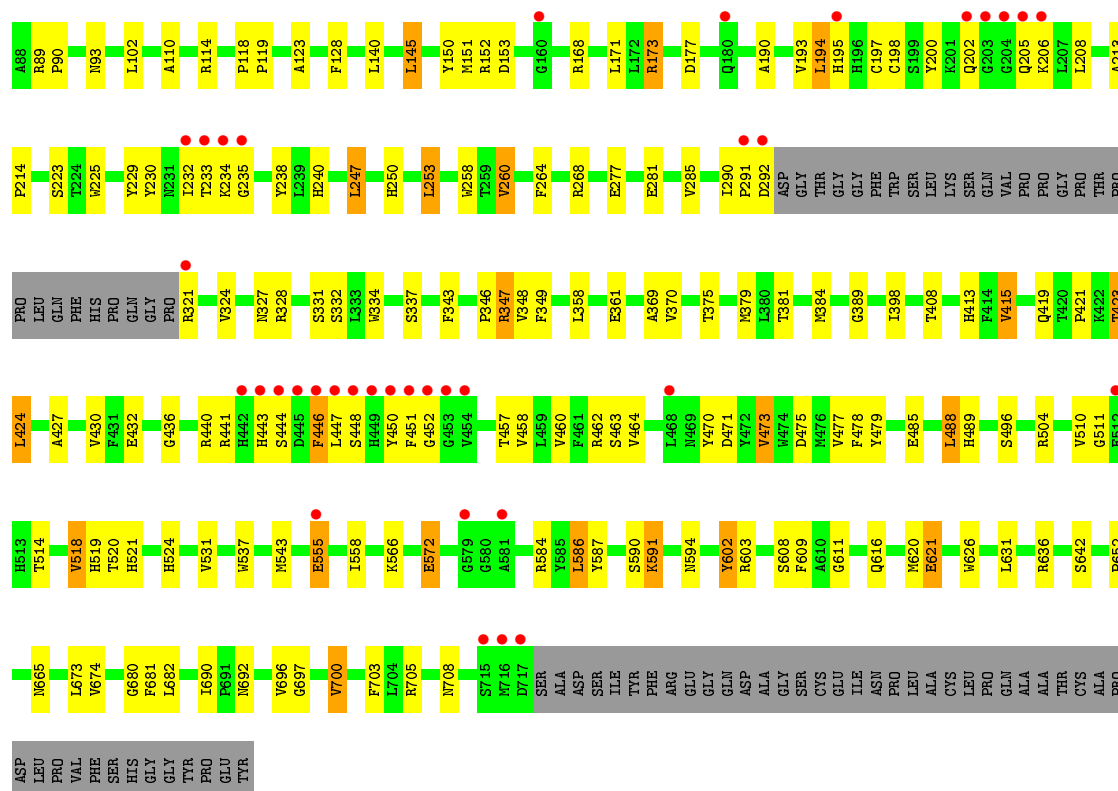
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total	O	0	0
			209	209		
7	B	201	Total	O	0	0
			201	201		

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.

- [illegible]

- [illegible]



- 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: 33% 67%



- 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: 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.68Å 131.19Å 134.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.37 27.85 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.7 (25.00-2.37) 93.8 (27.85-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.237 0.203 , 0.231	Depositor DCC
R_{free} test set	3719 reflections (7.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10581	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.57	2/5156 (0.0%)	0.83	7/7025 (0.1%)
1	B	0.55	0/5156	0.79	6/7025 (0.1%)
All	All	0.56	2/10312 (0.0%)	0.81	13/14050 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	142	VAL	CB-CG1	-6.81	1.38	1.52
1	A	142	VAL	CB-CG2	5.38	1.64	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	SER	N-CA-C	-9.93	84.20	111.00
1	A	446	PHE	N-CA-C	8.70	134.49	111.00
1	A	447	LEU	CA-CB-CG	-8.53	95.69	115.30
1	B	448	SER	N-CA-C	-8.41	88.30	111.00
1	B	446	PHE	N-CA-C	6.98	129.84	111.00
1	A	145	LEU	CA-CB-CG	-6.36	100.68	115.30
1	A	142	VAL	CG1-CB-CG2	6.10	120.66	110.90
1	A	145	LEU	CB-CG-CD2	-5.96	100.87	111.00
1	A	518	VAL	CB-CA-C	-5.78	100.41	111.40
1	B	145	LEU	CA-CB-CG	-5.57	102.50	115.30
1	B	518	VAL	CB-CA-C	-5.55	100.86	111.40
1	B	384	MET	N-CA-C	-5.35	96.56	111.00
1	B	145	LEU	C-N-CD	-5.12	109.34	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5018	0	4801	163	0
1	B	5018	0	4802	138	0
2	C	42	0	37	2	0
2	D	42	0	37	5	0
3	A	28	0	26	4	0
3	B	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
7	A	209	0	0	5	0
7	B	201	0	0	3	0
All	All	10581	0	9716	289	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 15.

All (289) 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:591:LYS:N	1:A:591:LYS:HD3	1.63	1.09
1:B:232:ILE:HG12	1:B:240:HIS:CD2	1.87	1.08
1:B:591:LYS:H	1:B:591:LYS:CD	1.62	1.07
1:B:591:LYS:HD2	1:B:591:LYS:N	1.65	1.07
1:A:591:LYS:CD	1:A:591:LYS:H	1.63	1.02
1:B:477:VAL:HG22	1:B:485:GLU:HB3	1.40	1.01
1:B:110:ALA:HB2	1:B:114:ARG:HH11	1.25	1.00
1:B:591:LYS:HD2	1:B:591:LYS:H	0.84	0.98
1:A:591:LYS:HD3	1:A:591:LYS:H	0.80	0.95
1:A:477:VAL:HG22	1:A:485:GLU:HB3	1.49	0.94
2:D:2:NAG:H61	2:D:3:NAG:H83	1.53	0.90
1:B:324:VAL:HG11	1:B:408:THR:HG21	1.54	0.89
1:A:110:ALA:HA	1:A:114:ARG:NH1	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ARG:HG3	1:A:475:ASP:OD1	1.75	0.87
1:A:324:VAL:HG11	1:A:408:THR:HG21	1.55	0.87
1:B:87:GLN:HA	1:B:173:ARG:HD2	1.56	0.86
1:B:110:ALA:HA	1:B:114:ARG:HE	1.41	0.85
1:B:324:VAL:CG1	1:B:408:THR:HG21	2.09	0.83
1:B:67:LEU:HG	1:B:415:VAL:HG12	1.61	0.83
1:B:74:LEU:HD23	1:B:151:MET:HE2	1.59	0.82
1:B:110:ALA:CB	1:B:114:ARG:HH11	1.93	0.81
1:B:477:VAL:CG2	1:B:485:GLU:HB3	2.11	0.81
1:A:477:VAL:CG2	1:A:485:GLU:HB3	2.11	0.80
1:B:110:ALA:HB2	1:B:114:ARG:NH1	1.96	0.80
1:A:324:VAL:CG1	1:A:408:THR:HG21	2.11	0.79
1:B:462:ARG:HG3	1:B:475:ASP:OD1	1.82	0.79
1:A:87:GLN:HA	1:A:173:ARG:HD2	1.66	0.78
1:A:89:ARG:NH1	1:A:173:ARG:HD3	2.00	0.75
2:D:2:NAG:C6	2:D:3:NAG:H83	2.17	0.75
1:A:110:ALA:HA	1:A:114:ARG:HH11	1.51	0.74
1:A:347:ARG:HG3	1:A:349:PHE:CE1	2.25	0.72
1:A:424:LEU:HD13	1:A:427:ALA:HB2	1.72	0.72
1:A:347:ARG:HD3	7:A:1064:HOH:O	1.89	0.71
1:A:616:GLN:HA	1:A:621:GLU:HG2	1.73	0.70
1:A:58:LEU:HD23	1:A:58:LEU:H	1.59	0.67
1:A:413:HIS:CD2	1:A:423:THR:HB	2.29	0.67
1:B:213:ALA:HA	1:B:214:PRO:O	1.95	0.67
2:D:2:NAG:H61	2:D:3:NAG:C8	2.25	0.66
1:A:277:GLU:O	1:A:281:GLU:HG2	1.96	0.66
1:B:321:ARG:NH1	1:B:457:THR:HG21	2.12	0.65
1:A:74:LEU:HD23	1:A:151:MET:HE2	1.78	0.65
1:A:611:GLY:O	1:B:543:MET:SD	2.55	0.65
1:A:321:ARG:NH2	1:A:432:GLU:OE2	2.29	0.65
1:A:67:LEU:HG	1:A:415:VAL:HG12	1.79	0.64
1:A:347:ARG:HG3	1:A:349:PHE:HE1	1.61	0.64
1:B:232:ILE:CG1	1:B:240:HIS:CD2	2.76	0.63
1:B:347:ARG:HG3	1:B:349:PHE:CE1	2.33	0.63
1:A:213:ALA:HA	1:A:214:PRO:O	1.98	0.63
1:A:557:GLN:HB2	7:A:1077:HOH:O	1.97	0.63
1:A:74:LEU:HD23	1:A:151:MET:CE	2.29	0.63
1:B:89:ARG:NH1	1:B:173:ARG:HD3	2.13	0.63
1:B:555:GLU:CD	1:B:555:GLU:H	2.00	0.62
2:C:3:NAG:H83	2:C:3:NAG:O3	1.99	0.62
1:A:510:VAL:CG2	1:A:690:ILE:HD11	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:O	1:A:93:ASN:HB2	1.98	0.62
1:B:277:GLU:O	1:B:281:GLU:HG2	1.99	0.62
1:B:230:TYR:HE1	1:B:290:ILE:HG22	1.65	0.61
1:A:402:ASP:OD1	1:B:441:ARG:HD2	2.01	0.61
1:A:58:LEU:H	1:A:58:LEU:CD2	2.14	0.60
1:A:584:ARG:NE	1:B:611:GLY:HA2	2.16	0.60
1:A:558:ILE:HD11	1:B:379:MET:O	2.02	0.60
1:B:74:LEU:CD2	1:B:151:MET:HE2	2.32	0.60
1:A:596:TRP:CZ2	1:B:511:GLY:HA2	2.37	0.60
1:B:58:LEU:H	1:B:58:LEU:HD23	1.65	0.59
1:A:506:TYR:O	1:A:518:VAL:HG22	2.02	0.59
1:B:537:TRP:HZ3	1:B:591:LYS:HG3	1.65	0.59
1:A:74:LEU:CD2	1:A:151:MET:HE2	2.31	0.59
1:A:268:ARG:HH21	1:A:268:ARG:HG3	1.66	0.59
1:A:473:VAL:HG13	1:A:489:HIS:HB2	1.84	0.59
1:A:555:GLU:CD	1:A:555:GLU:H	2.06	0.58
1:B:102:LEU:HD21	1:B:347:ARG:NH2	2.18	0.58
1:A:572:GLU:HG2	3:A:804:NAG:O6	2.03	0.58
1:A:543:MET:SD	1:B:611:GLY:O	2.62	0.58
1:B:424:LEU:HD13	1:B:427:ALA:HB2	1.85	0.58
1:A:462:ARG:NH2	1:B:436:GLY:O	2.37	0.58
1:A:413:HIS:HD2	1:A:423:THR:HB	1.67	0.57
1:B:232:ILE:C	1:B:234:LYS:H	2.06	0.57
1:B:473:VAL:HG13	1:B:489:HIS:HB2	1.87	0.57
1:B:636:ARG:HH11	1:B:636:ARG:HG3	1.68	0.57
1:A:232:ILE:HG22	1:A:234:LYS:H	1.69	0.57
1:B:636:ARG:HB2	1:B:674:VAL:CG2	2.34	0.57
1:B:531:VAL:O	1:B:590:SER:HB3	2.03	0.56
1:B:587:TYR:HB3	1:B:603:ARG:HB3	1.86	0.56
1:B:324:VAL:HG11	1:B:408:THR:CG2	2.31	0.56
1:B:74:LEU:HD23	1:B:151:MET:CE	2.33	0.56
1:A:636:ARG:HB2	1:A:674:VAL:HG23	1.87	0.56
1:A:424:LEU:HD13	1:A:427:ALA:CB	2.35	0.56
1:B:268:ARG:NH2	1:B:285:VAL:HG22	2.21	0.56
1:B:620:MET:HB2	1:B:652:PRO:HB2	1.88	0.56
1:A:130:GLY:HA2	1:A:135:PRO:HB3	1.87	0.56
1:A:370:VAL:O	1:A:519:HIS:HA	2.06	0.56
1:A:587:TYR:HB3	1:A:603:ARG:HB3	1.88	0.56
1:A:531:VAL:O	1:A:590:SER:HB3	2.07	0.55
1:B:510:VAL:CG2	1:B:690:ILE:HD11	2.36	0.55
3:A:803:NAG:H3	3:A:803:NAG:O7	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:616:GLN:HA	1:B:621:GLU:HG2	1.89	0.55
1:A:105:LYS:HE3	1:A:360:TYR:CG	2.41	0.55
1:A:229:TYR:CD2	1:A:238:TYR:HA	2.42	0.54
1:B:58:LEU:H	1:B:58:LEU:CD2	2.20	0.54
1:B:64:ARG:NH1	1:B:423:THR:HG22	2.22	0.54
1:B:443:HIS:ND1	1:B:444:SER:N	2.55	0.53
1:A:398:ILE:HD13	1:B:452:GLY:HA2	1.90	0.53
1:B:370:VAL:O	1:B:519:HIS:HA	2.09	0.53
1:B:510:VAL:HB	1:B:690:ILE:HD12	1.91	0.53
1:A:570:THR:HG21	3:A:804:NAG:C8	2.39	0.52
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.74	0.52
1:B:128:PHE:CZ	1:B:168:ARG:HB2	2.44	0.52
1:A:321:ARG:NH2	1:A:457:THR:CG2	2.73	0.52
1:A:620:MET:HB2	1:A:652:PRO:HB2	1.91	0.52
1:A:67:LEU:HB3	1:A:421:PRO:HG3	1.91	0.52
1:B:225:TRP:CE2	1:B:247:LEU:HG	2.45	0.52
1:A:436:GLY:O	1:B:462:ARG:NH2	2.43	0.52
1:A:443:HIS:ND1	1:A:444:SER:N	2.57	0.52
1:B:78:LEU:HD12	1:B:82:LEU:HD11	1.92	0.52
1:A:114:ARG:HG3	1:A:114:ARG:NH1	2.25	0.51
1:A:636:ARG:HB2	1:A:674:VAL:CG2	2.40	0.51
1:B:229:TYR:CD2	1:B:238:TYR:HA	2.45	0.51
1:A:223:SER:HB3	1:A:247:LEU:HD22	1.92	0.51
1:A:347:ARG:HG2	1:A:347:ARG:O	2.09	0.51
1:B:81:ASP:O	1:B:93:ASN:HB2	2.11	0.51
1:B:67:LEU:HB3	1:B:421:PRO:HG3	1.94	0.50
1:B:446:PHE:HB3	1:B:447:LEU:HD22	1.92	0.50
1:B:510:VAL:HB	1:B:690:ILE:CD1	2.41	0.50
1:A:689:ASP:CB	1:A:693:THR:HG22	2.42	0.50
1:A:324:VAL:HG11	1:A:408:THR:CG2	2.36	0.50
1:A:328:ARG:NH1	1:A:330:ALA:HB2	2.27	0.50
1:B:213:ALA:HA	1:B:214:PRO:C	2.32	0.50
1:B:424:LEU:HD13	1:B:427:ALA:CB	2.41	0.50
1:A:446:PHE:HB3	1:A:447:LEU:HD22	1.94	0.50
1:A:90:PRO:HB2	1:A:253:LEU:HA	1.94	0.50
1:B:572:GLU:OE2	1:B:665:ASN:N	2.44	0.50
1:A:499:LEU:HD12	1:A:515:LEU:HB2	1.94	0.49
1:B:347:ARG:HG3	1:B:349:PHE:HE1	1.77	0.49
1:A:128:PHE:CZ	1:A:168:ARG:HB2	2.47	0.49
1:B:343:PHE:HA	1:B:389:GLY:HA2	1.95	0.49
1:A:611:GLY:HA2	1:B:584:ARG:NE	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:SER:HA	1:B:700:VAL:HG22	1.95	0.49
1:A:291:PRO:O	1:A:292:ASP:HB2	2.12	0.49
1:B:346:PRO:HG3	1:B:463:SER:OG	2.12	0.49
1:B:90:PRO:HB2	1:B:253:LEU:HA	1.93	0.49
1:B:140:LEU:HD23	1:B:153:ASP:HA	1.95	0.49
1:A:616:GLN:HA	1:A:621:GLU:CG	2.41	0.49
1:B:413:HIS:CD2	1:B:423:THR:HB	2.47	0.49
1:A:67:LEU:HD12	1:A:98:VAL:HG22	1.94	0.49
1:A:464:VAL:HG22	1:A:473:VAL:HB	1.95	0.48
1:B:208:LEU:C	1:B:208:LEU:HD12	2.33	0.48
1:A:321:ARG:NH2	1:A:457:THR:HG23	2.27	0.48
1:B:488:LEU:HD12	1:B:489:HIS:N	2.28	0.48
2:D:2:NAG:H61	2:D:3:NAG:C7	2.44	0.48
1:A:64:ARG:HD2	1:A:421:PRO:HB2	1.95	0.48
1:A:410:MET:HE1	1:A:430:VAL:HG23	1.94	0.48
1:B:110:ALA:CA	1:B:114:ARG:HH11	2.26	0.48
1:B:477:VAL:HG23	1:B:479:TYR:CE1	2.48	0.48
1:A:609:PHE:O	1:A:681:PHE:HA	2.13	0.48
1:A:447:LEU:HD13	1:A:447:LEU:N	2.25	0.48
1:A:703:PHE:CZ	1:B:697:GLY:HA2	2.48	0.48
1:B:62:LEU:HD11	1:B:123:ALA:HB2	1.94	0.48
1:A:596:TRP:O	1:B:504:ARG:NH2	2.47	0.48
1:A:230:TYR:HE1	1:A:290:ILE:HG22	1.78	0.47
1:B:591:LYS:N	1:B:591:LYS:CD	2.42	0.47
1:A:697:GLY:HA2	1:B:703:PHE:CZ	2.49	0.47
1:B:232:ILE:O	1:B:234:LYS:N	2.46	0.47
1:B:321:ARG:HD3	1:B:432:GLU:OE1	2.14	0.47
1:B:334:TRP:CE2	1:B:478:PHE:HB3	2.49	0.47
1:A:87:GLN:CA	1:A:173:ARG:HD2	2.41	0.47
1:A:334:TRP:CE2	1:A:478:PHE:HB3	2.49	0.47
1:B:173:ARG:NH1	1:B:177:ASP:OD1	2.48	0.47
1:B:190:ALA:HB1	1:B:193:VAL:CG1	2.45	0.47
1:B:195:HIS:ND1	1:B:200:TYR:O	2.47	0.47
1:A:96:PHE:CZ	1:A:169:PRO:HG2	2.50	0.47
1:A:213:ALA:HA	1:A:214:PRO:C	2.35	0.47
1:B:190:ALA:O	1:B:194:LEU:HB2	2.13	0.47
1:A:430:VAL:HA	1:A:460:VAL:O	2.14	0.47
1:B:447:LEU:N	1:B:447:LEU:HD22	2.29	0.47
1:A:560:ARG:HG3	7:A:929:HOH:O	2.15	0.46
1:B:524:HIS:HB2	1:B:626:TRP:CE3	2.51	0.46
1:B:358:LEU:HD22	1:B:602:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:SER:HB3	1:B:247:LEU:HD22	1.95	0.46
1:A:452:GLY:HA2	1:B:398:ILE:HD13	1.98	0.46
1:A:596:TRP:CH2	1:B:511:GLY:HA2	2.51	0.46
1:B:608:SER:HA	1:B:700:VAL:CG2	2.45	0.46
1:A:496:SER:HB3	1:A:514:THR:HG23	1.98	0.46
1:A:696:VAL:O	1:B:705:ARG:NH2	2.44	0.46
1:B:250:HIS:HA	1:B:258:TRP:CD1	2.51	0.46
1:B:369:ALA:HA	1:B:520:THR:O	2.15	0.46
1:A:548:THR:HG22	1:A:549:ALA:O	2.16	0.46
3:A:803:NAG:O7	3:A:803:NAG:C3	2.64	0.46
1:B:636:ARG:HB2	1:B:674:VAL:HG23	1.98	0.46
1:A:140:LEU:HD23	1:A:153:ASP:HA	1.98	0.46
1:A:58:LEU:HD23	1:A:58:LEU:N	2.25	0.46
1:B:441:ARG:HA	1:B:452:GLY:O	2.16	0.46
1:B:586:LEU:HD22	1:B:631:LEU:HD21	1.98	0.45
1:A:190:ALA:HB1	1:A:193:VAL:CG1	2.46	0.45
1:B:79:GLY:N	1:B:80:PRO:HD2	2.31	0.45
1:A:327:ASN:O	1:A:337:SER:HA	2.17	0.45
1:B:464:VAL:HG22	1:B:473:VAL:HB	1.98	0.45
1:A:379:MET:O	1:B:558:ILE:HD11	2.17	0.45
1:A:129:PHE:CG	2:C:1:NAG:H62	2.51	0.45
1:A:321:ARG:CZ	1:A:432:GLU:OE1	2.65	0.45
1:B:71:MET:HE2	1:B:419:GLN:HA	1.99	0.45
1:A:128:PHE:HE1	1:A:171:LEU:HD13	1.81	0.44
1:A:321:ARG:HH22	1:A:457:THR:HG23	1.81	0.44
1:A:81:ASP:HB2	1:A:93:ASN:HD22	1.82	0.44
1:A:268:ARG:NH2	7:A:1100:HOH:O	2.50	0.44
1:A:343:PHE:HA	1:A:389:GLY:HA2	1.98	0.44
1:A:349:PHE:CD2	1:A:361:GLU:HB2	2.53	0.44
1:A:447:LEU:HD12	1:A:447:LEU:HA	1.60	0.44
1:A:689:ASP:OD1	1:A:693:THR:HG22	2.17	0.44
1:B:521:HIS:O	1:B:680:GLY:HA3	2.17	0.44
1:A:90:PRO:HB2	1:A:253:LEU:O	2.17	0.44
1:A:448:SER:HB3	1:A:450:TYR:CE1	2.52	0.44
1:B:587:TYR:HB3	1:B:603:ARG:CB	2.47	0.44
1:A:631:LEU:HD13	1:A:677:VAL:HG22	2.00	0.44
1:A:447:LEU:HD13	1:A:447:LEU:H	1.81	0.44
1:A:510:VAL:O	1:A:690:ILE:HD12	2.18	0.44
1:A:245:GLU:OE2	1:A:376:PRO:HB2	2.18	0.43
1:A:622:ARG:HH12	1:A:655:PRO:HD2	1.83	0.43
1:B:110:ALA:HA	1:B:114:ARG:NE	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:PHE:CZ	1:B:375:THR:HG22	2.53	0.43
1:A:208:LEU:HD23	1:A:231:ASN:ND2	2.33	0.43
1:A:619:PRO:HD2	7:B:2011:HOH:O	2.17	0.43
1:B:537:TRP:CZ3	1:B:591:LYS:HG3	2.49	0.43
1:B:291:PRO:O	1:B:292:ASP:HB2	2.17	0.43
1:B:430:VAL:HA	1:B:460:VAL:O	2.17	0.43
1:A:471:ASP:OD2	1:B:441:ARG:NE	2.50	0.43
1:B:205:GLN:NE2	1:B:206:LYS:H	2.17	0.43
1:B:213:ALA:O	1:B:381:THR:HA	2.18	0.43
1:B:67:LEU:HA	1:B:67:LEU:HD12	1.92	0.43
1:A:477:VAL:HG23	1:A:479:TYR:CE1	2.53	0.43
1:B:232:ILE:C	1:B:234:LYS:N	2.72	0.43
1:A:397:LEU:HD13	1:A:429:CYS:HB3	1.99	0.43
1:B:150:TYR:CD1	1:B:152:ARG:HD2	2.54	0.43
1:A:80:PRO:O	1:A:82:LEU:N	2.47	0.43
1:B:496:SER:HB3	1:B:514:THR:HG23	2.00	0.43
1:A:340:LEU:HD12	1:A:345:GLY:C	2.39	0.43
1:A:481:ASN:ND2	1:B:696:VAL:HG21	2.34	0.43
1:A:357:ARG:HD2	7:A:947:HOH:O	2.19	0.42
1:A:689:ASP:CG	1:A:693:THR:HG22	2.40	0.42
1:A:173:ARG:NH1	1:A:177:ASP:OD1	2.51	0.42
1:A:462:ARG:NH1	1:A:475:ASP:OD2	2.52	0.42
1:A:98:VAL:O	1:A:415:VAL:HG13	2.20	0.42
1:A:399:ARG:HG2	1:A:409:TYR:CZ	2.55	0.42
1:A:441:ARG:HA	1:A:452:GLY:O	2.19	0.42
1:A:521:HIS:O	1:A:680:GLY:HA3	2.19	0.42
1:A:230:TYR:CE1	1:A:290:ILE:HG22	2.53	0.42
1:B:616:GLN:HA	1:B:621:GLU:CG	2.48	0.42
1:B:586:LEU:HD22	1:B:631:LEU:CD2	2.49	0.42
1:A:462:ARG:CG	1:A:475:ASP:OD1	2.58	0.42
1:A:608:SER:HA	1:A:700:VAL:HG22	2.02	0.42
1:B:268:ARG:HH21	1:B:285:VAL:HG22	1.83	0.42
1:B:58:LEU:N	1:B:58:LEU:HD23	2.33	0.42
1:B:609:PHE:O	1:B:681:PHE:HA	2.18	0.42
2:D:3:NAG:O7	2:D:3:NAG:C1	2.67	0.42
1:B:347:ARG:HD3	7:B:2079:HOH:O	2.20	0.42
1:A:478:PHE:N	1:A:478:PHE:CD1	2.88	0.42
1:A:250:HIS:HA	1:A:258:TRP:CD1	2.55	0.42
1:A:594:ASN:HB3	1:A:708:ASN:O	2.20	0.42
1:B:349:PHE:CD2	1:B:361:GLU:HB2	2.55	0.42
1:A:281:GLU:HA	1:A:281:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ASN:O	1:B:337:SER:HA	2.20	0.41
1:A:437:LEU:HD11	1:B:489:HIS:CD2	2.55	0.41
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.65	0.41
1:A:213:ALA:O	1:A:381:THR:HA	2.21	0.41
1:A:462:ARG:HG3	1:A:462:ARG:HH11	1.85	0.41
1:B:590:SER:HB2	1:B:591:LYS:HD2	2.01	0.41
1:A:386:SER:O	1:A:646:VAL:HG13	2.21	0.41
1:A:77:GLN:HB2	1:A:151:MET:HE1	2.01	0.41
1:B:197:CYS:C	1:B:198:CYS:SG	2.99	0.41
1:A:232:ILE:HD12	1:A:240:HIS:CD2	2.56	0.41
1:A:128:PHE:CD1	1:A:168:ARG:HD2	2.55	0.41
1:A:268:ARG:NH2	1:A:268:ARG:HG3	2.32	0.41
1:A:98:VAL:HG22	1:A:415:VAL:CG1	2.51	0.41
1:A:321:ARG:HH22	1:A:457:THR:CG2	2.34	0.41
1:A:62:LEU:HD11	1:A:123:ALA:HB2	2.02	0.41
1:A:587:TYR:HB3	1:A:603:ARG:CB	2.51	0.41
1:A:234:LYS:HB3	1:A:235:GLY:H	1.52	0.40
1:A:689:ASP:HB3	1:A:693:THR:HG22	2.02	0.40
1:B:118:PRO:HA	1:B:119:PRO:HD3	1.95	0.40
1:A:608:SER:HA	1:A:700:VAL:CG2	2.51	0.40
1:A:81:ASP:O	1:A:81:ASP:OD2	2.38	0.40
1:A:271:GLU:HB2	1:A:275:GLN:OE1	2.22	0.40
1:A:114:ARG:CG	1:A:114:ARG:HH11	2.34	0.40
1:A:542:ASP:OD1	1:A:584:ARG:NH1	2.47	0.40
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.84	0.40
1:A:369:ALA:HA	1:A:520:THR:O	2.22	0.40
1:A:388:PHE:HB3	1:A:393:PHE:CE2	2.56	0.40
1:B:260:VAL:HG13	7:B:1960:HOH:O	2.21	0.40
1:B:496:SER:HB3	1:B:514:THR:CG2	2.52	0.40
1:B:594:ASN:HB3	1:B:708:ASN:O	2.21	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	628/746 (84%)	592 (94%)	33 (5%)	3 (0%)	29	39
1	B	628/746 (84%)	594 (95%)	31 (5%)	3 (0%)	29	39
All	All	1256/1492 (84%)	1186 (94%)	64 (5%)	6 (0%)	29	39

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	THR
1	A	81	ASP
1	A	235	GLY
1	A	233	THR
1	B	235	GLY
1	B	450	TYR

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	530/623 (85%)	491 (93%)	39 (7%)	13	19
1	B	530/623 (85%)	494 (93%)	36 (7%)	16	23
All	All	1060/1246 (85%)	985 (93%)	75 (7%)	14	21

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	LEU
1	A	67	LEU
1	A	82	LEU
1	A	171	LEU
1	A	173	ARG
1	A	194	LEU
1	A	247	LEU

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Mol	Chain	Res	Type
1	A	248	VAL
1	A	253	LEU
1	A	260	VAL
1	A	328	ARG
1	A	331	SER
1	A	332	SER
1	A	347	ARG
1	A	348	VAL
1	A	382	ARG
1	A	415	VAL
1	A	423	THR
1	A	424	LEU
1	A	441	ARG
1	A	445	ASP
1	A	447	LEU
1	A	451	PHE
1	A	458	VAL
1	A	473	VAL
1	A	488	LEU
1	A	518	VAL
1	A	542	ASP
1	A	555	GLU
1	A	560	ARG
1	A	572	GLU
1	A	591	LYS
1	A	621	GLU
1	A	639	THR
1	A	642	SER
1	A	673	LEU
1	A	682	LEU
1	A	692	ASN
1	A	700	VAL
1	B	58	LEU
1	B	67	LEU
1	B	171	LEU
1	B	173	ARG
1	B	194	LEU
1	B	202	GLN
1	B	247	LEU
1	B	253	LEU
1	B	260	VAL
1	B	328	ARG

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Mol	Chain	Res	Type
1	B	331	SER
1	B	332	SER
1	B	347	ARG
1	B	348	VAL
1	B	415	VAL
1	B	423	THR
1	B	424	LEU
1	B	440	ARG
1	B	451	PHE
1	B	458	VAL
1	B	471	ASP
1	B	473	VAL
1	B	488	LEU
1	B	518	VAL
1	B	555	GLU
1	B	566	LYS
1	B	572	GLU
1	B	586	LEU
1	B	591	LYS
1	B	602	TYR
1	B	621	GLU
1	B	642	SER
1	B	673	LEU
1	B	682	LEU
1	B	692	ASN
1	B	700	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	205	GLN
1	A	279	GLN
1	A	413	HIS
1	A	456	GLN
1	A	559	GLN
1	A	616	GLN
1	A	712	GLN
1	B	184	ASN
1	B	205	GLN
1	B	231	ASN
1	B	279	GLN

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Mol	Chain	Res	Type
1	B	413	HIS
1	B	442	HIS
1	B	456	GLN
1	B	489	HIS
1	B	559	GLN
1	B	692	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	B	470	1	13,14,15	2.77	7 (53%)	15,19,21	1.33	2 (13%)
1	TPQ	A	470	1	13,14,15	2.81	7 (53%)	15,19,21	1.22	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
1	TPQ	B	470	1	-	2/5/22/24	0/1/1/1
1	TPQ	A	470	1	-	2/5/22/24	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	470	TPQ	C1-C2	-7.27	1.38	1.49
1	A	470	TPQ	C1-C2	-7.13	1.38	1.49
1	A	470	TPQ	O5-C5	3.33	1.33	1.24
1	B	470	TPQ	O5-C5	3.22	1.33	1.24
1	A	470	TPQ	O2-C2	3.20	1.33	1.24
1	B	470	TPQ	O2-C2	3.04	1.32	1.24
1	A	470	TPQ	C4-C5	-2.82	1.38	1.47
1	B	470	TPQ	C4-C5	-2.38	1.40	1.47
1	A	470	TPQ	C3-C4	2.37	1.39	1.35
1	B	470	TPQ	C3-C4	2.36	1.39	1.35
1	A	470	TPQ	C6-C5	-2.35	1.38	1.44
1	B	470	TPQ	C6-C5	-2.17	1.38	1.44
1	A	470	TPQ	C3-C2	-2.04	1.39	1.44
1	B	470	TPQ	C3-C2	-2.03	1.39	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	TPQ	CB-CA-C	-3.02	105.81	111.47
1	B	470	TPQ	CB-CA-C	-2.86	106.10	111.47
1	B	470	TPQ	C6-C1-C2	2.16	120.30	118.64

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

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	0.57	0	17,19,21	0.98	1 (5%)
2	NAG	C	2	2	14,14,15	0.69	0	17,19,21	0.61	0
2	NAG	C	3	2	14,14,15	1.05	1 (7%)	17,19,21	1.07	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.82	1 (7%)	17,19,21	1.17	2 (11%)
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	0.91	1 (5%)
2	NAG	D	3	2	14,14,15	0.73	0	17,19,21	0.85	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	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	C	3	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	1/1/5/7	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	3	2	-	5/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	NAG	C1-C2	3.35	1.57	1.52
2	D	1	NAG	O5-C5	2.02	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	3.00	116.26	112.19
2	C	3	NAG	C3-C4-C5	-2.52	105.75	110.24
2	C	1	NAG	C1-C2-N2	-2.46	106.28	110.49
2	D	2	NAG	C2-N2-C7	-2.36	119.55	122.90
2	D	1	NAG	C2-N2-C7	-2.15	119.84	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	1	NAG	C1

All (13) torsion outliers are listed below:

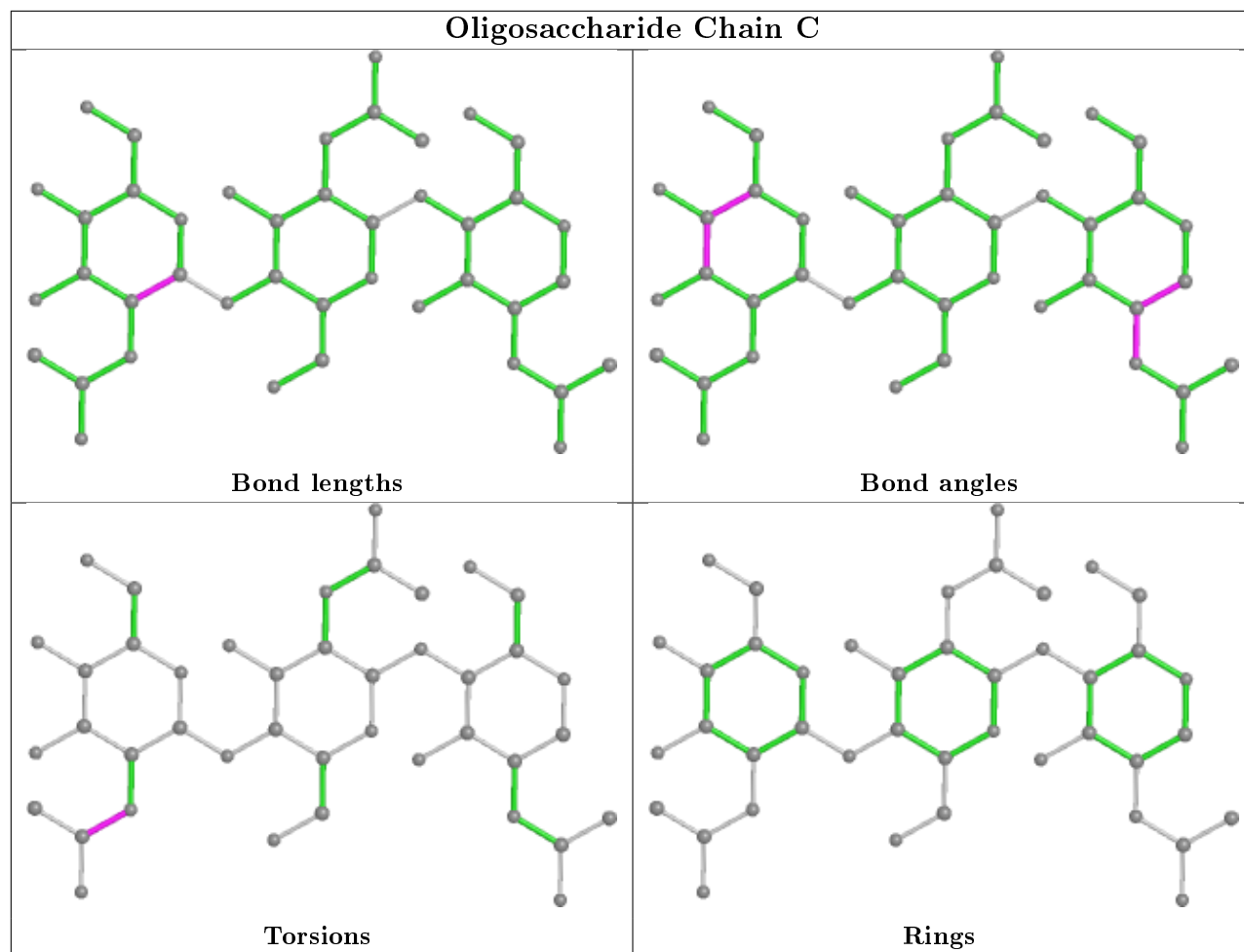
Mol	Chain	Res	Type	Atoms
2	C	3	NAG	C8-C7-N2-C2
2	C	3	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	3	NAG	C1-C2-N2-C7
2	D	2	NAG	C4-C5-C6-O6
2	D	3	NAG	C4-C5-C6-O6
2	D	3	NAG	C8-C7-N2-C2
2	D	3	NAG	O5-C5-C6-O6
2	D	3	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

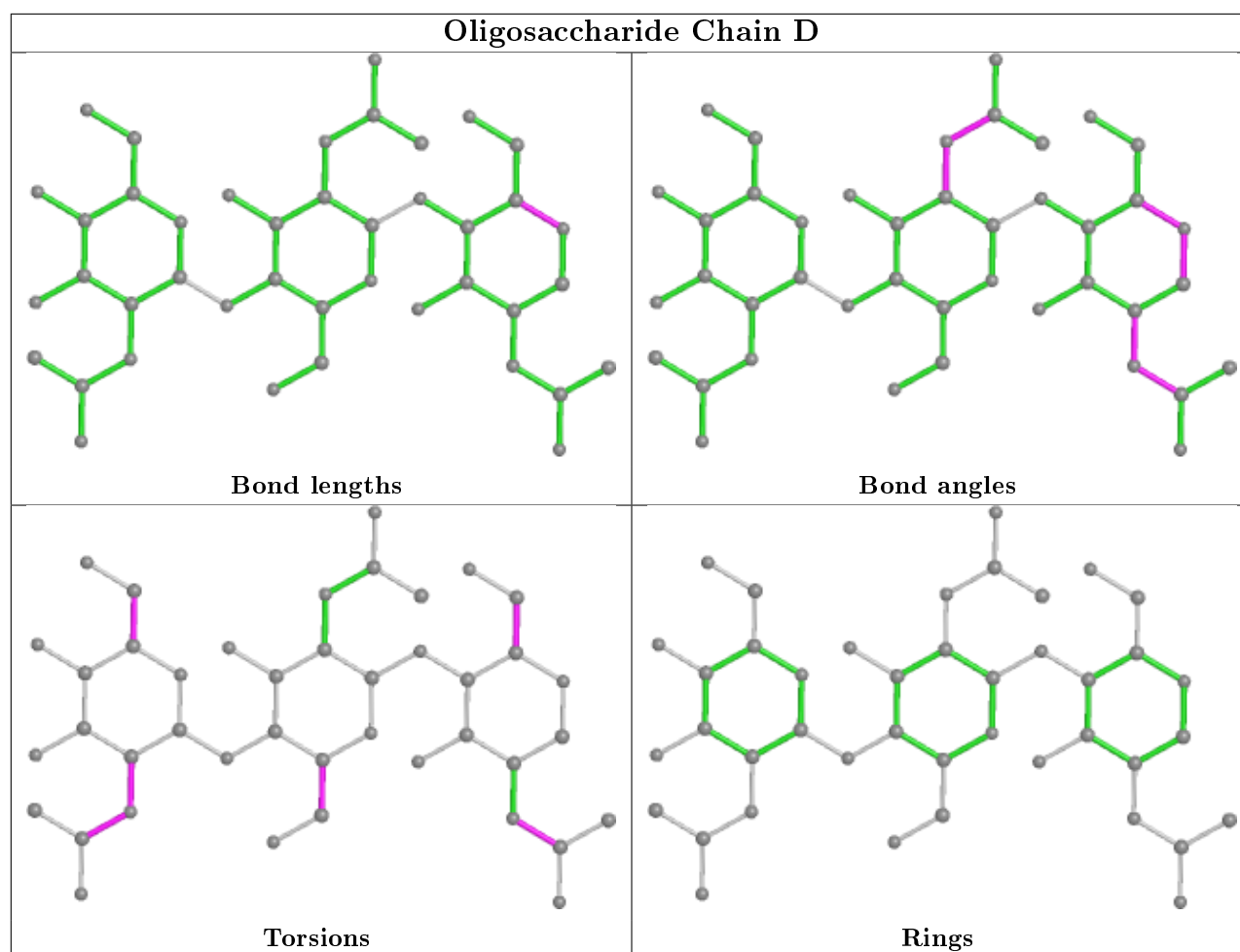
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	NAG	1	0
2	D	2	NAG	4	0
2	C	3	NAG	1	0
2	D	3	NAG	5	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 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 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	$\# Z > 2$
3	NAG	B	804	1	14,14,15	0.74	0	17,19,21	0.81	1 (5%)
3	NAG	A	803	1	14,14,15	0.72	0	17,19,21	1.04	1 (5%)
3	NAG	A	804	1	14,14,15	0.58	0	17,19,21	0.69	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
3	NAG	B	804	1	-	2/6/23/26	0/1/1/1
3	NAG	A	803	1	-	3/6/23/26	0/1/1/1
3	NAG	A	804	1	1/1/5/7	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	NAG	O5-C1-C2	-2.12	107.94	111.29
3	B	804	NAG	C2-N2-C7	-2.05	119.99	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	804	NAG	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	NAG	C8-C7-N2-C2
3	A	804	NAG	O7-C7-N2-C2
3	A	803	NAG	C3-C2-N2-C7
3	B	804	NAG	C8-C7-N2-C2
3	B	804	NAG	O7-C7-N2-C2
3	A	804	NAG	O5-C5-C6-O6
3	A	803	NAG	C4-C5-C6-O6
3	A	804	NAG	C4-C5-C6-O6
3	A	803	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	NAG	2	0
3	A	804	NAG	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	632/746 (84%)	0.30	37 (5%) 22 24	11, 25, 50, 114	0
1	B	632/746 (84%)	0.37	36 (5%) 23 26	9, 25, 48, 115	0
All	All	1264/1492 (84%)	0.33	73 (5%) 23 25	9, 25, 49, 115	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	PHE	16.7
1	A	447	LEU	15.1
1	B	451	PHE	14.7
1	A	444	SER	14.6
1	A	450	TYR	14.6
1	B	444	SER	14.2
1	A	448	SER	14.0
1	B	450	TYR	13.7
1	A	449	HIS	12.5
1	B	447	LEU	12.2
1	B	445	ASP	11.5
1	A	446	PHE	10.9
1	B	448	SER	10.9
1	A	451	PHE	10.3
1	B	233	THR	9.8
1	A	443	HIS	9.5
1	B	449	HIS	9.2
1	B	716	MET	7.8
1	B	203	GLY	7.4
1	B	443	HIS	7.0
1	A	235	GLY	6.9
1	A	445	ASP	6.9
1	A	442	HIS	6.8
1	B	717	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	233	THR	5.6
1	B	715	SER	5.6
1	A	452	GLY	4.7
1	B	234	LYS	4.5
1	B	204	GLY	4.4
1	B	292	ASP	4.3
1	B	235	GLY	4.2
1	B	453	GLY	4.1
1	B	232	ILE	3.7
1	A	232	ILE	3.6
1	A	234	LYS	3.6
1	A	453	GLY	3.6
1	A	81	ASP	3.6
1	B	442	HIS	3.5
1	A	512	GLU	3.3
1	B	202	GLN	3.3
1	B	555	GLU	3.3
1	A	321	ARG	3.3
1	B	160	GLY	3.3
1	A	282	ALA	3.2
1	A	80	PRO	3.2
1	A	117	PRO	3.1
1	B	291	PRO	3.0
1	B	454	VAL	2.9
1	B	579	GLY	2.9
1	B	180	GLN	2.9
1	B	321	ARG	2.8
1	A	611	GLY	2.8
1	B	452	GLY	2.7
1	B	206	LYS	2.7
1	B	205	GLN	2.7
1	A	493	TYR	2.6
1	A	115	GLY	2.6
1	A	581	ALA	2.5
1	B	581	ALA	2.4
1	A	133	PRO	2.4
1	A	116	SER	2.3
1	A	674	VAL	2.3
1	A	328	ARG	2.3
1	B	468	LEU	2.3
1	B	512	GLU	2.2
1	A	292	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	325	GLN	2.2
1	A	405	TYR	2.1
1	B	195	HIS	2.1
1	A	278	GLU	2.1
1	A	332	SER	2.1
1	A	134	GLN	2.0
1	A	256	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPQ	B	470	14/15	0.82	0.21	40,53,55,56	0
1	TPQ	A	470	14/15	0.85	0.18	40,50,52,52	0

6.3 Carbohydrates [i](#)

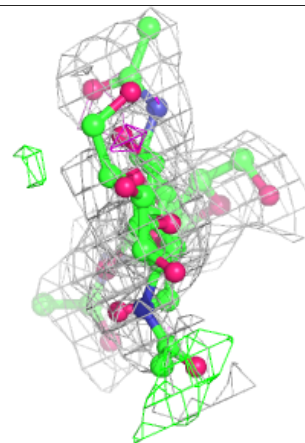
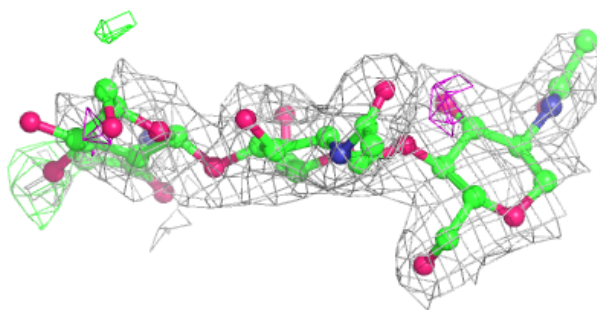
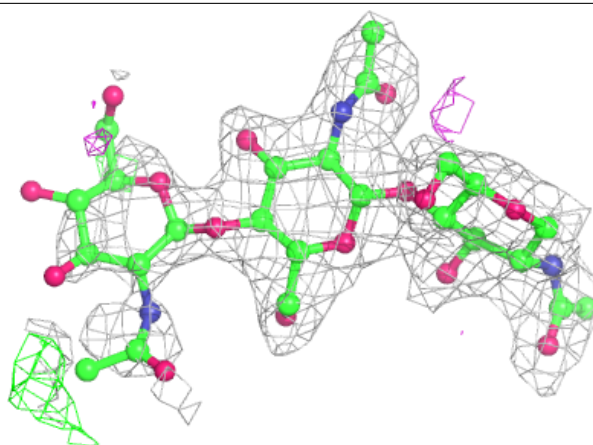
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	3	14/15	0.68	0.47	63,70,73,74	0
2	NAG	D	3	14/15	0.69	0.41	61,64,66,67	0
2	NAG	C	2	14/15	0.89	0.15	28,44,49,55	0
2	NAG	D	2	14/15	0.91	0.22	35,42,49,55	0
2	NAG	C	1	14/15	0.93	0.13	29,30,32,36	0
2	NAG	D	1	14/15	0.94	0.12	29,31,35,35	0

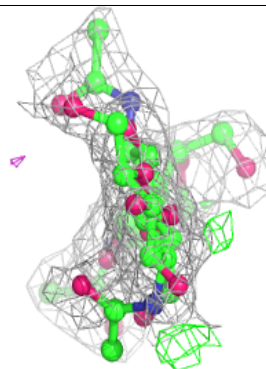
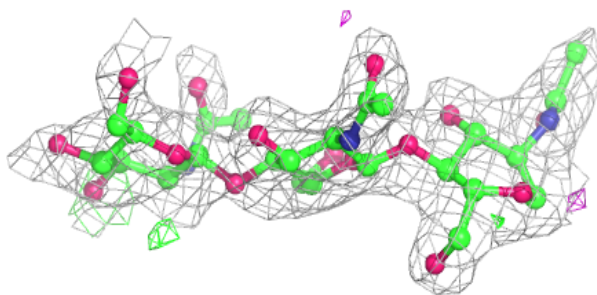
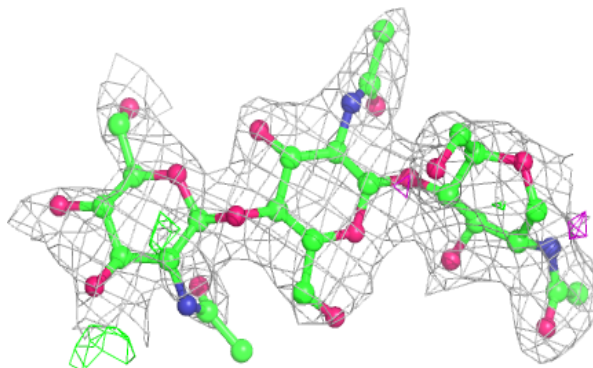
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

**Electron density around Chain D:**

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



6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	B	804	14/15	0.70	0.50	57,60,62,63	0
3	NAG	A	803	14/15	0.77	0.42	48,49,51,52	0
3	NAG	A	804	14/15	0.80	0.53	64,67,67,68	0
6	CL	A	904	1/1	0.94	0.08	32,32,32,32	0
6	CL	B	1904	1/1	0.98	0.09	32,32,32,32	0
6	CL	B	1905	1/1	0.98	0.10	25,25,25,25	0
5	CA	A	903	1/1	0.98	0.03	19,19,19,19	0
5	CA	A	902	1/1	0.99	0.10	18,18,18,18	0
4	CU	B	901	1/1	0.99	0.07	23,23,23,23	0
5	CA	B	1902	1/1	0.99	0.06	23,23,23,23	0
5	CA	B	1903	1/1	0.99	0.05	23,23,23,23	0
4	CU	A	901	1/1	1.00	0.08	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.