



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:08 PM UTC

PDB ID : 1TU5 / pdb_00001tu5
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

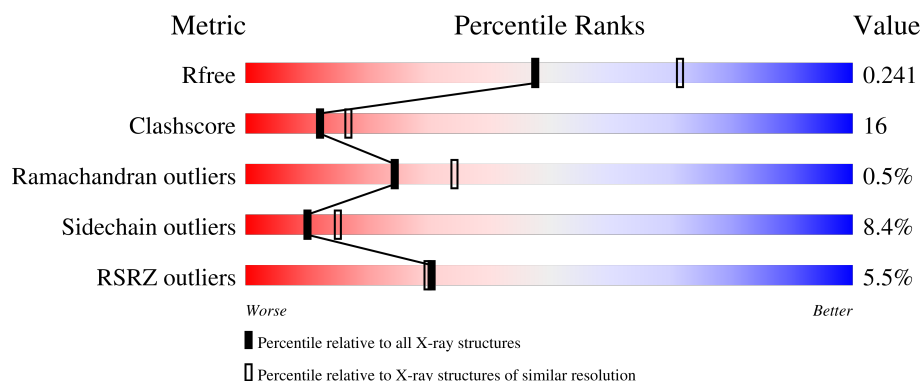
1 Overall quality at a glance

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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 of 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	4% 54% 25% 5% 15%
1	B	746	5% 57% 23% 5% 15%
2	C	3	33% 67%
2	D	3	67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	1	X	-	-	-
3	NAG	A	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.

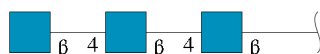
- Molecule 1 is a protein called Copper amine oxidase, liver isozyme.

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 (CCD ID: 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 (CCD ID: CU) (formula: Cu).

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is water.

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

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 25.00 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.7 (25.00-2.37) 93.7 (25.00-2.37)	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 0.215 , 0.241	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 , 46.5	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.67	3/5156 (0.1%)	1.16	40/7025 (0.6%)
1	B	0.65	1/5156 (0.0%)	1.12	37/7025 (0.5%)
All	All	0.66	4/10312 (0.0%)	1.14	77/14050 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	PRO	CG-CD	-6.34	1.34	1.51
1	B	151	MET	SD-CE	-6.14	1.64	1.79
1	A	144	PRO	CB-CG	-5.61	1.29	1.51
1	A	117	PRO	CA-C	5.18	1.54	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	PHE	N-CA-C	15.49	134.49	109.24
1	B	446	PHE	N-CA-C	12.24	129.84	109.76
1	A	448	SER	N-CA-C	-12.04	84.20	107.44
1	B	448	SER	N-CA-C	-9.21	88.30	107.37
1	A	79	GLY	CA-C-N	9.07	129.67	119.32
1	A	79	GLY	C-N-CA	9.07	129.67	119.32
1	B	684	ILE	N-CA-C	-7.93	99.12	107.60
1	A	518	VAL	CB-CA-C	-7.26	100.41	111.08
1	A	684	ILE	N-CA-C	-7.22	99.88	107.60
1	B	518	VAL	CB-CA-C	-6.95	100.86	111.08
1	B	626	TRP	N-CA-C	-6.45	104.67	112.54
1	B	460	VAL	N-CA-C	6.43	117.17	108.17
1	B	385	ASP	N-CA-C	6.41	119.96	111.75
1	A	626	TRP	N-CA-C	-6.39	104.75	112.54
1	A	195	HIS	N-CA-C	-6.33	104.30	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	PHE	N-CA-C	-6.33	103.46	112.13
1	B	381	THR	N-CA-C	6.27	119.45	110.10
1	B	388	PHE	N-CA-C	-6.16	104.74	112.93
1	A	517	PRO	N-CA-C	6.06	120.70	111.19
1	A	363	SER	N-CA-C	6.01	118.20	109.07
1	A	381	THR	N-CA-C	5.89	118.88	110.10
1	A	447	LEU	CA-CB-CG	-5.89	95.69	116.30
1	A	101	GLN	N-CA-C	-5.86	99.18	108.73
1	A	281	GLU	N-CA-C	-5.81	104.86	111.07
1	B	101	GLN	N-CA-C	-5.78	99.31	108.73
1	B	630	GLN	N-CA-C	-5.75	104.61	111.69
1	A	145	LEU	CA-C-N	5.71	140.71	127.00
1	A	145	LEU	C-N-CA	5.71	140.71	127.00
1	B	195	HIS	N-CA-C	-5.70	104.68	111.69
1	A	630	GLN	N-CA-C	-5.64	105.12	112.23
1	B	534	LEU	N-CA-C	5.63	117.22	111.14
1	B	629	TYR	N-CA-C	5.61	118.70	109.72
1	B	334	TRP	N-CA-C	5.58	118.67	109.85
1	B	168	ARG	CA-C-N	-5.56	114.23	119.85
1	B	168	ARG	C-N-CA	-5.56	114.23	119.85
1	A	576	PHE	CA-C-N	5.56	125.83	119.83
1	A	576	PHE	C-N-CA	5.56	125.83	119.83
1	A	165	TYR	N-CA-C	5.55	117.33	111.28
1	A	460	VAL	N-CA-C	5.48	115.84	108.17
1	A	516	GLY	CA-C-N	5.46	125.22	119.76
1	A	516	GLY	C-N-CA	5.46	125.22	119.76
1	B	702	PHE	N-CA-C	5.45	116.42	108.14
1	B	77	GLN	N-CA-C	5.40	119.03	112.23
1	A	646	VAL	N-CA-C	-5.39	104.31	111.05
1	A	534	LEU	N-CA-C	5.37	116.94	111.14
1	B	344	SER	N-CA-C	5.37	118.04	111.82
1	A	168	ARG	CA-C-N	-5.34	114.46	119.85
1	A	168	ARG	C-N-CA	-5.34	114.46	119.85
1	A	487	LYS	N-CA-C	5.33	117.29	109.24
1	B	517	PRO	N-CA-C	5.32	119.55	111.19
1	A	514	THR	N-CA-C	5.32	117.57	108.90
1	B	487	LYS	N-CA-C	5.30	117.24	109.24
1	B	145	LEU	N-CA-C	-5.29	102.46	110.39
1	A	334	TRP	N-CA-C	5.28	118.19	109.85
1	B	531	VAL	N-CA-C	5.24	115.14	108.12
1	B	672	ASP	N-CA-C	-5.22	101.27	109.25
1	A	629	TYR	N-CA-C	5.19	118.03	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	649	GLN	N-CA-C	5.18	117.33	111.11
1	B	516	GLY	N-CA-C	-5.18	101.77	112.34
1	A	137	VAL	N-CA-C	-5.15	101.06	108.53
1	A	704	LEU	N-CA-C	-5.12	100.07	108.41
1	B	145	LEU	C-N-CD	-5.12	109.34	120.60
1	B	704	LEU	N-CA-C	-5.11	100.09	108.41
1	B	614	MET	N-CA-C	-5.09	103.37	109.83
1	B	516	GLY	CA-C-N	5.07	124.83	119.76
1	B	516	GLY	C-N-CA	5.07	124.83	119.76
1	B	362	ILE	N-CA-C	-5.06	100.23	107.78
1	A	464	VAL	N-CA-C	5.05	115.39	108.12
1	A	505	ARG	N-CA-C	-5.04	106.64	112.89
1	B	152	ARG	N-CA-C	5.04	116.74	108.52
1	B	132	GLN	CA-C-N	5.03	125.06	119.32
1	B	132	GLN	C-N-CA	5.03	125.06	119.32
1	A	232	ILE	N-CA-C	5.03	115.55	108.36
1	A	143	GLY	CA-C-N	5.01	139.03	127.00
1	A	143	GLY	C-N-CA	5.01	139.03	127.00
1	A	611	GLY	N-CA-C	5.01	124.19	115.62
1	B	137	VAL	N-CA-C	-5.01	101.27	108.48

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	173	0
1	B	5018	0	4802	148	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	309	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 16.

All (309) 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:HD3	1:A:591:LYS:N	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:H	1:A:591:LYS:CD	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:H	1:B:591:LYS:HD2	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
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:B:71:MET:HE2	1:B:419:GLN:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:210:MET:HE1	1:A:495:SER:HB2	1.71	0.71
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:74:LEU:HD23	1:A:151:MET:HE2	1.74	0.69
1:A:58:LEU:H	1:A:58:LEU:HD23	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
1:B:555:GLU:CD	1:B:555:GLU:H	2.00	0.66
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: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:A:74:LEU:CD2	1:A:151:MET:HE2	2.28	0.64
1:B:232:ILE:CG1	1:B:240:HIS:CD2	2.76	0.63
1:A:555:GLU:CD	1:A:555:GLU:H	2.06	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:232:ILE:C	1:B:234:LYS:H	2.06	0.62
2:C:3:NAG:O3	2:C:3:NAG:H83	1.99	0.62
1:A:410:MET:HE1	1:A:430:VAL:HG23	1.81	0.62
1:A:81:ASP:O	1:A:93:ASN:HB2	1.98	0.62
1:A:510:VAL:CG2	1:A:690:ILE:HD11	2.30	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:A:596:TRP:CZ2	1:B:511:GLY:HA2	2.37	0.60
1:B:210:MET:HE1	1:B:495:SER:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LEU:CD2	1:B:151:MET:HE2	2.32	0.60
1:B:58:LEU:HD23	1:B:58:LEU:H	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: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: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: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:O7	3:A:803:NAG:H3	2.06	0.55
1:A:71:MET:HE2	1:A:419:GLN:HA	1.88	0.55
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:B:213:ALA:HA	1:B:214:PRO:C	2.32	0.54
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:B:410:MET:HE1	1:B:430:VAL:HG23	1.89	0.53
1:A:398:ILE:HD13	1:B:452:GLY:HA2	1.90	0.53
1:B:208:LEU:C	1:B:208:LEU:HD12	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:MET:HE1	1:A:95:VAL:HB	1.89	0.53
1:B:210:MET:HE1	1:B:495:SER:CB	2.38	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:HH11	1:A:114:ARG:HG3	1.74	0.52
1:B:128:PHE:CZ	1:B:168:ARG:HB2	2.44	0.52
1:A:67:LEU:HB3	1:A:421:PRO:HG3	1.91	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:B:225:TRP:CE2	1:B:247:LEU:HG	2.45	0.52
1:A:213:ALA:HA	1:A:214:PRO:C	2.35	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:NH1	1:A:114:ARG:HG3	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:210:MET:HE2	1:B:468:LEU:HD21	1.91	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:424:LEU:HD13	1:B:427:ALA:CB	2.41	0.50
1:A:90:PRO:HB2	1:A:253:LEU:HA	1.94	0.50
1:A:446:PHE:HB3	1:A:447:LEU:HD22	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:A:611:GLY:HA2	1:B:584:ARG:NE	2.26	0.49
1:B:343:PHE:HA	1:B:389:GLY:HA2	1.95	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD23	1:B:153:ASP:HA	1.95	0.49
1:B:385:ASP:HB3	1:B:467:MET:HE2	1.94	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: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: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:596:TRP:O	1:B:504:ARG:NH2	2.47	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:B:232:ILE:C	1:B:234:LYS:N	2.72	0.48
1:A:230:TYR:HE1	1:A:290:ILE:HG22	1.78	0.47
1:A:340:LEU:HD12	1:A:345:GLY:C	2.39	0.47
1:B:591:LYS:CD	1:B:591:LYS:N	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:A:689:ASP:CG	1:A:693:THR:HG22	2.40	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:210:MET:HE1	1:A:495:SER:CB	2.43	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:HD22	1:B:447:LEU:N	2.29	0.47
1:A:560:ARG:HG3	7:A:929:HOH:O	2.15	0.46
1:B:358:LEU:HD22	1:B:602:TYR:CE1	2.50	0.46
1:B:524:HIS:HB2	1:B:626:TRP:CE3	2.51	0.46
1:A:452:GLY:HA2	1:B:398:ILE:HD13	1.98	0.46
1:B:223:SER:HB3	1:B:247:LEU:HD22	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:197:CYS:C	1:B:198:CYS:SG	2.99	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:58:LEU:HD23	1:A:58:LEU:N	2.25	0.46
1:A:140:LEU:HD23	1:A:153:ASP:HA	1.98	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:A:379:MET:O	1:B:558:ILE:HD11	2.17	0.45
1:B:464:VAL:HG22	1:B:473:VAL:HB	1.98	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:A:81:ASP:HB2	1:A:93:ASN:HD22	1.82	0.44
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:OD2	1:A:81:ASP:C	2.60	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:281:GLU:C	1:A:283:GLY:H	2.25	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:232:ILE:C	1:A:234:LYS:H	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ALA:HA	1:B:114:ARG:NE	2.21	0.43
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:67:LEU:HD12	1:B:67:LEU:HA	1.92	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:A:477:VAL:HG23	1:A:479:TYR:CE1	2.53	0.43
1:B:467:MET:HE3	1:B:467:MET:HB3	1.91	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: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: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:A:467:MET:HE3	1:A:467:MET:HB3	1.86	0.42
1:B:385:ASP:CG	1:B:467:MET:HE2	2.45	0.42
1:B:512:GLU:CD	1:B:512:GLU:H	2.28	0.42
1:B:586:LEU:HD22	1:B:631:LEU:CD2	2.49	0.42
1:B:616:GLN:HA	1:B:621:GLU:CG	2.48	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:58:LEU:HD23	1:B:58:LEU:N	2.33	0.42
1:B:268:ARG:HH21	1:B:285:VAL:HG22	1.83	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:CD1	1:A:478:PHE:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:PHE:CD2	1:B:361:GLU:HB2	2.55	0.42
1:B:60:ALA:HB2	1:B:327:ASN:CG	2.44	0.42
1:A:208:LEU:C	1:A:208:LEU:HD12	2.45	0.41
1:A:281:GLU:OE1	1:A:281:GLU:HA	2.20	0.41
1:B:327:ASN:O	1:B:337:SER:HA	2.20	0.41
1:B:385:ASP:CB	1:B:467:MET:HE2	2.50	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: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:HG3	1:A:268:ARG:NH2	2.32	0.41
1:A:62:LEU:HD11	1:A:123:ALA:HB2	2.02	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:587:TYR:HB3	1:A:603:ARG:CB	2.51	0.41
1:A:136:ASN:OD1	1:A:136:ASN:C	2.65	0.40
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:81:ASP:O	1:A:81:ASP:OD2	2.38	0.40
1:A:608:SER:HA	1:A:700:VAL:CG2	2.51	0.40
1:A:271:GLU:HB2	1:A:275:GLN:OE1	2.22	0.40
1:A:384:MET:HE1	1:A:652:PRO:HB3	2.03	0.40
1:A:114:ARG:HH11	1:A:114:ARG:CG	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 [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	628/746 (84%)	592 (94%)	33 (5%)	3 (0%)	24	34
1	B	628/746 (84%)	594 (95%)	31 (5%)	3 (0%)	24	34
All	All	1256/1492 (84%)	1186 (94%)	64 (5%)	6 (0%)	24	34

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 [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	530/623 (85%)	483 (91%)	47 (9%)	9	13
1	B	530/623 (85%)	488 (92%)	42 (8%)	11	17
All	All	1060/1246 (85%)	971 (92%)	89 (8%)	10	15

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	82	LEU
1	A	98	VAL
1	A	102	LEU
1	A	171	LEU
1	A	173	ARG
1	A	194	LEU
1	A	205	GLN
1	A	242	VAL
1	A	247	LEU
1	A	248	VAL
1	A	253	LEU
1	A	260	VAL
1	A	262	LYS
1	A	263	VAL
1	A	286	ASN
1	A	328	ARG
1	A	331	SER
1	A	332	SER
1	A	335	THR
1	A	347	ARG
1	A	348	VAL
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	458	VAL
1	A	462	ARG
1	A	473	VAL
1	A	477	VAL
1	A	488	LEU
1	A	512	GLU
1	A	518	VAL
1	A	534	LEU
1	A	555	GLU
1	A	560	ARG
1	A	566	LYS
1	A	572	GLU
1	A	591	LYS
1	A	621	GLU
1	A	639	THR

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Mol	Chain	Res	Type
1	A	642	SER
1	A	673	LEU
1	A	682	LEU
1	A	700	VAL
1	B	67	LEU
1	B	98	VAL
1	B	102	LEU
1	B	171	LEU
1	B	173	ARG
1	B	194	LEU
1	B	202	GLN
1	B	205	GLN
1	B	242	VAL
1	B	247	LEU
1	B	248	VAL
1	B	253	LEU
1	B	260	VAL
1	B	263	VAL
1	B	328	ARG
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	447	LEU
1	B	458	VAL
1	B	473	VAL
1	B	477	VAL
1	B	488	LEU
1	B	512	GLU
1	B	518	VAL
1	B	534	LEU
1	B	555	GLU
1	B	566	LYS
1	B	572	GLU
1	B	586	LEU
1	B	591	LYS
1	B	621	GLU
1	B	642	SER
1	B	646	VAL

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Mol	Chain	Res	Type
1	B	673	LEU
1	B	682	LEU
1	B	692	ASN
1	B	700	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) 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	442	HIS
1	A	456	GLN
1	A	513	HIS
1	A	616	GLN
1	A	712	GLN
1	B	184	ASN
1	B	205	GLN
1	B	231	ASN
1	B	279	GLN
1	B	413	HIS
1	B	425	HIS
1	B	442	HIS
1	B	456	GLN
1	B	489	HIS
1	B	513	HIS
1	B	559	GLN
1	B	567	GLN
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	13,14,15	2.93	7 (53%)	13,19,21	0.98	0
1	TPQ	B	470	1	13,14,15	2.89	7 (53%)	13,19,21	1.18	1 (7%)

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	-	2/5/22/24	0/1/1/1
1	TPQ	B	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	-7.90	1.38	1.49
1	A	470	TPQ	C1-C2	-7.76	1.38	1.49
1	A	470	TPQ	O5-C5	3.35	1.33	1.24
1	B	470	TPQ	O5-C5	3.24	1.33	1.24
1	A	470	TPQ	O2-C2	3.22	1.33	1.24
1	B	470	TPQ	O2-C2	3.06	1.32	1.24
1	A	470	TPQ	C4-C5	-2.89	1.38	1.47
1	A	470	TPQ	C6-C5	-2.44	1.38	1.44
1	B	470	TPQ	C4-C5	-2.43	1.40	1.47
1	B	470	TPQ	C6-C5	-2.25	1.38	1.44
1	A	470	TPQ	C3-C2	-2.11	1.39	1.44
1	B	470	TPQ	C3-C2	-2.10	1.39	1.44
1	B	470	TPQ	C6-C1	2.08	1.39	1.34
1	A	470	TPQ	C6-C1	2.03	1.39	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	470	TPQ	C6-C1-C2	2.31	120.30	118.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	470	TPQ	N-CA-CB-C1
1	B	470	TPQ	N-CA-CB-C1
1	B	470	TPQ	C-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 [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	2,1	14,14,15	0.58	0	17,19,21	1.02	1 (5%)
2	NAG	C	2	2	14,14,15	0.71	0	17,19,21	0.63	0
2	NAG	C	3	2	14,14,15	1.12	1 (7%)	17,19,21	1.05	1 (5%)
2	NAG	D	1	2,1	14,14,15	0.84	1 (7%)	17,19,21	1.19	2 (11%)
2	NAG	D	2	2	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
2	NAG	D	3	2	14,14,15	0.75	0	17,19,21	0.87	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	2,1	-	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	2,1	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	3.67	1.57	1.52
2	D	1	NAG	O5-C5	2.11	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	3.04	116.26	112.19
2	C	1	NAG	C1-C2-N2	-2.64	106.28	110.43
2	D	2	NAG	C2-N2-C7	-2.50	119.55	122.90
2	C	3	NAG	C3-C4-C5	-2.47	105.75	110.23
2	D	1	NAG	C2-N2-C7	-2.28	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:

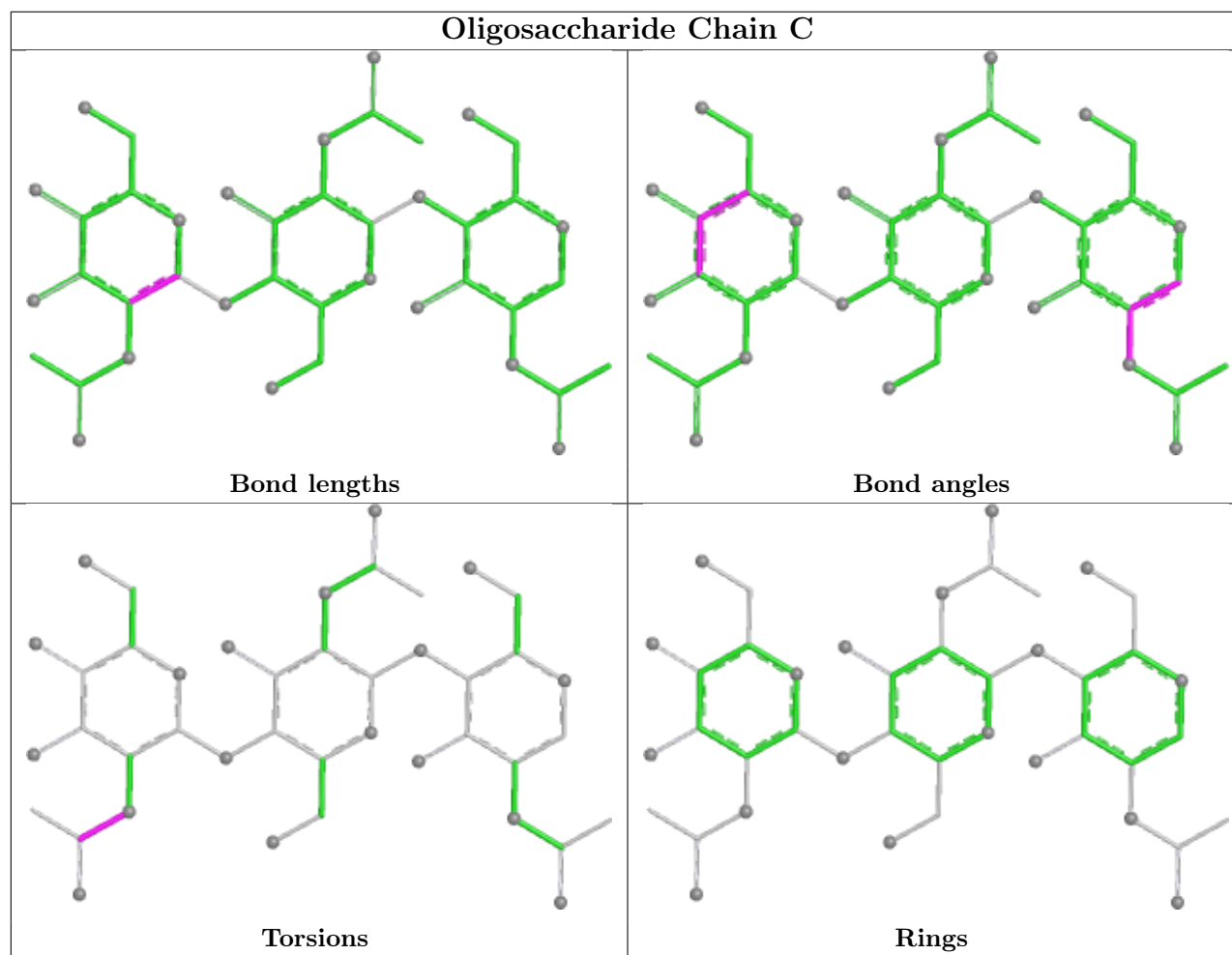
Mol	Chain	Res	Type	Atoms
2	C	3	NAG	C8-C7-N2-C2
2	C	3	NAG	O7-C7-N2-C2
2	D	3	NAG	C1-C2-N2-C7
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	3	NAG	C4-C5-C6-O6
2	D	3	NAG	O5-C5-C6-O6
2	D	3	NAG	C8-C7-N2-C2
2	D	3	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2

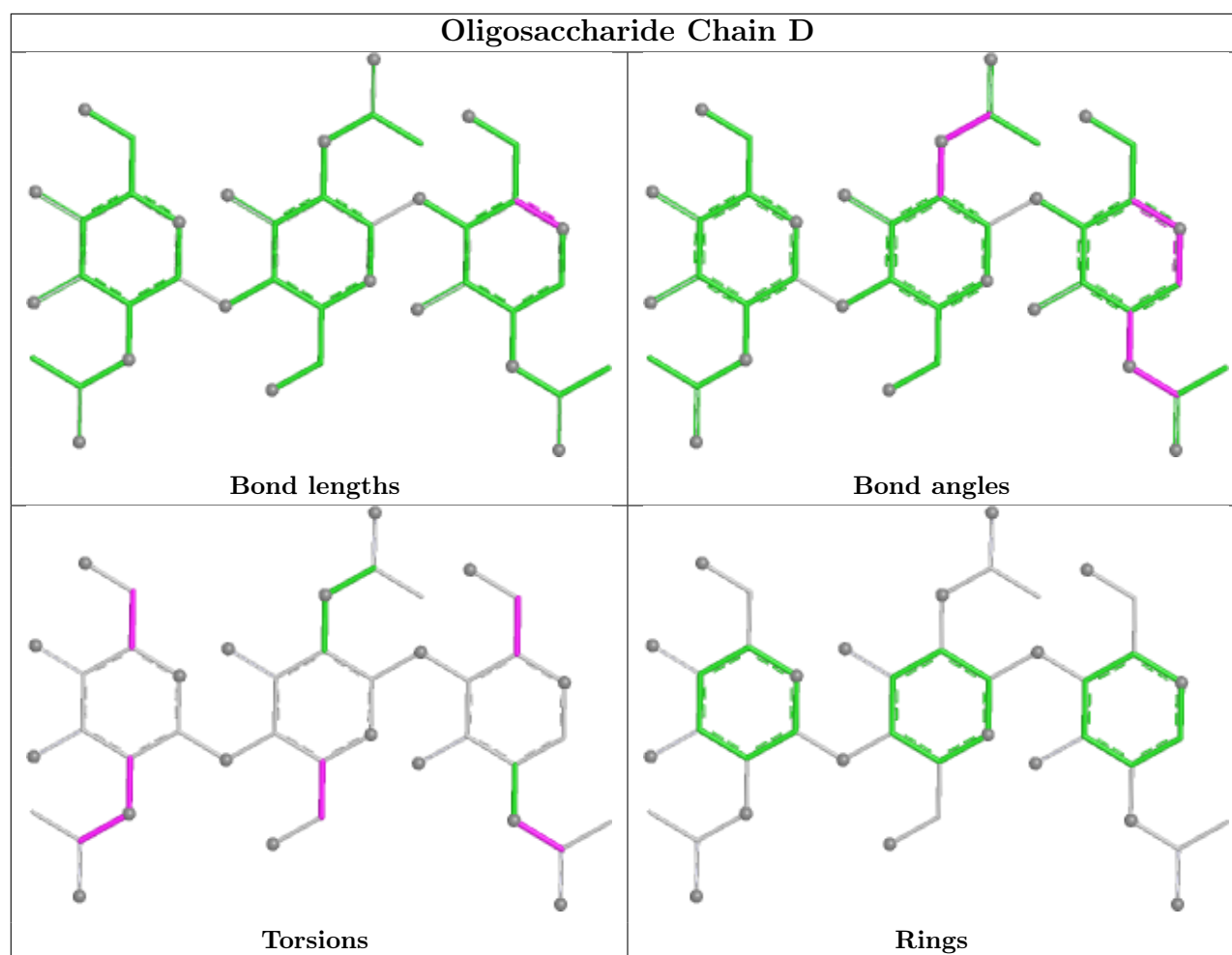
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	4	0
2	C	1	NAG	1	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	A	804	1	14,14,15	0.61	0	17,19,21	0.72	1 (5%)
3	NAG	A	803	1	14,14,15	0.73	0	17,19,21	1.07	1 (5%)
3	NAG	B	804	1	14,14,15	0.77	0	17,19,21	0.84	1 (5%)

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	A	804	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	A	803	1	-	3/6/23/26	0/1/1/1
3	NAG	B	804	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	804	NAG	C2-N2-C7	-2.17	119.99	122.90
3	A	803	NAG	O5-C1-C2	-2.17	107.94	111.29
3	A	804	NAG	C2-N2-C7	-2.08	120.11	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	803	NAG	C3-C2-N2-C7
3	A	804	NAG	C8-C7-N2-C2
3	A	804	NAG	O7-C7-N2-C2
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	804	NAG	2	0
3	A	803	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.16	33 (5%)	33 32	11, 25, 50, 114	0
1	B	632/746 (84%)	0.19	37 (5%)	28 27	9, 25, 48, 115	0
All	All	1264/1492 (84%)	0.17	70 (5%)	30 30	9, 25, 49, 115	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	LEU	7.6
1	A	447	LEU	6.6
1	B	446	PHE	6.3
1	A	235	GLY	6.3
1	A	611	GLY	6.1
1	A	450	TYR	6.1
1	A	446	PHE	5.7
1	B	450	TYR	5.6
1	A	443	HIS	5.4
1	B	451	PHE	5.3
1	A	449	HIS	5.3
1	A	444	SER	5.1
1	B	235	GLY	5.1
1	B	448	SER	5.1
1	A	442	HIS	5.1
1	B	233	THR	4.9
1	B	444	SER	4.9
1	B	443	HIS	4.5
1	A	452	GLY	4.3
1	A	81	ASP	4.3
1	B	449	HIS	4.2
1	A	451	PHE	4.1
1	B	203	GLY	3.9
1	B	442	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	448	SER	3.6
1	B	715	SER	3.6
1	B	445	ASP	3.4
1	B	204	GLY	3.4
1	A	717	ASP	3.4
1	B	78	LEU	3.2
1	A	233	THR	3.2
1	A	232	ILE	3.2
1	B	452	GLY	3.1
1	B	195	HIS	3.0
1	B	281	GLU	3.0
1	A	453	GLY	3.0
1	B	234	LYS	2.9
1	A	695	THR	2.9
1	B	282	ALA	2.8
1	A	282	ALA	2.8
1	B	321	ARG	2.7
1	B	453	GLY	2.7
1	A	321	ARG	2.7
1	B	147	GLN	2.7
1	A	512	GLU	2.7
1	A	493	TYR	2.6
1	B	454	VAL	2.6
1	A	406	LEU	2.6
1	B	468	LEU	2.6
1	A	292	ASP	2.6
1	B	716	MET	2.6
1	B	232	ILE	2.6
1	B	611	GLY	2.5
1	B	292	ASP	2.5
1	B	717	ASP	2.5
1	B	202	GLN	2.4
1	A	380	LEU	2.4
1	A	692	ASN	2.4
1	A	328	ARG	2.4
1	A	234	LYS	2.3
1	B	455	ALA	2.3
1	A	440	ARG	2.2
1	A	716	MET	2.1
1	B	237	PRO	2.1
1	A	279	GLN	2.1
1	B	236	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	558	ILE	2.1
1	A	238	TYR	2.1
1	B	205	GLN	2.1
1	B	697	GLY	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	0.75	0.17	40,53,55,56	0
1	TPQ	A	470	14/15	0.81	0.15	40,50,52,52	0

6.3 Carbohydrates [i](#)

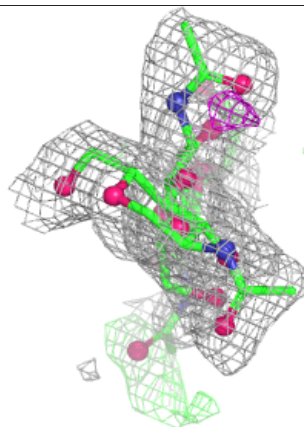
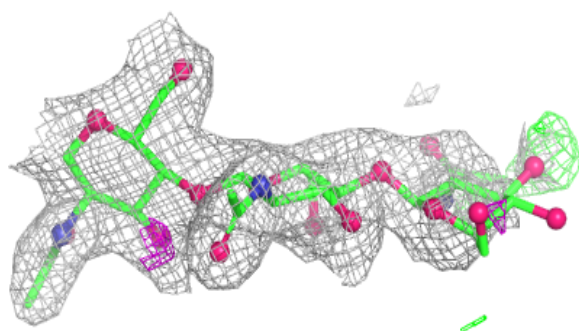
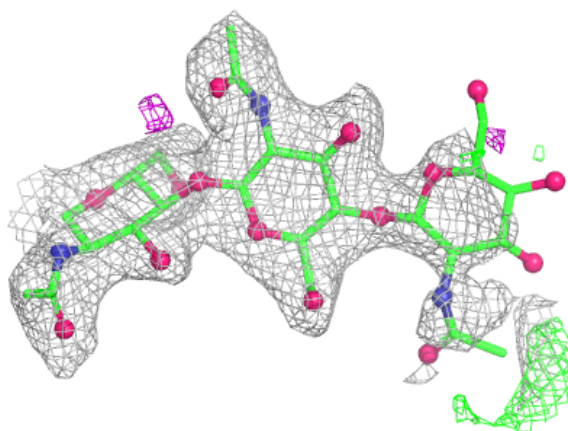
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.37	0.23	63,70,73,74	0
2	NAG	D	3	14/15	0.63	0.17	61,64,66,67	0
2	NAG	D	2	14/15	0.89	0.10	35,42,49,55	0
2	NAG	C	2	14/15	0.92	0.08	28,44,49,55	0
2	NAG	D	1	14/15	0.92	0.08	29,31,35,35	0
2	NAG	C	1	14/15	0.93	0.08	29,30,32,36	0

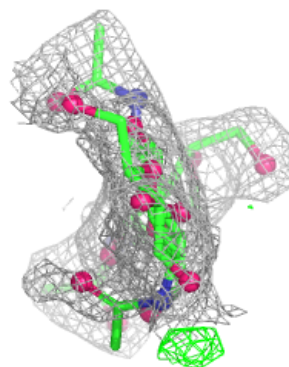
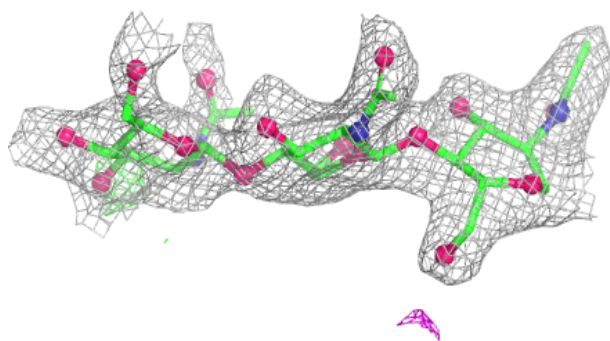
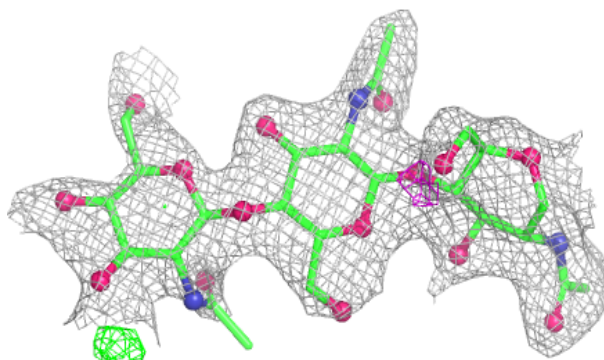
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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($\text{\AA}^2$)	Q<0.9
3	NAG	B	804	14/15	0.51	0.18	57,60,62,63	0
3	NAG	A	803	14/15	0.57	0.16	48,49,51,52	0
3	NAG	A	804	14/15	0.64	0.16	64,67,67,68	0
6	CL	A	904	1/1	0.95	0.06	32,32,32,32	0
6	CL	B	1905	1/1	0.97	0.05	25,25,25,25	0
5	CA	A	903	1/1	0.98	0.04	19,19,19,19	0
6	CL	B	1904	1/1	0.98	0.05	32,32,32,32	0
5	CA	B	1902	1/1	0.98	0.03	23,23,23,23	0
4	CU	B	901	1/1	0.99	0.02	23,23,23,23	0
5	CA	A	902	1/1	0.99	0.02	18,18,18,18	0
5	CA	B	1903	1/1	0.99	0.02	23,23,23,23	0
4	CU	A	901	1/1	1.00	0.01	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.