



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:12 PM UTC

PDB ID : 1PU4 / pdb_00001pu4
Title : Crystal structure of human vascular adhesion protein-1
Authors : Salminen, T.A.; Airenne, T.T.
Deposited on : 2003-06-24
Resolution : 3.20 Å(reported)

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

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

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

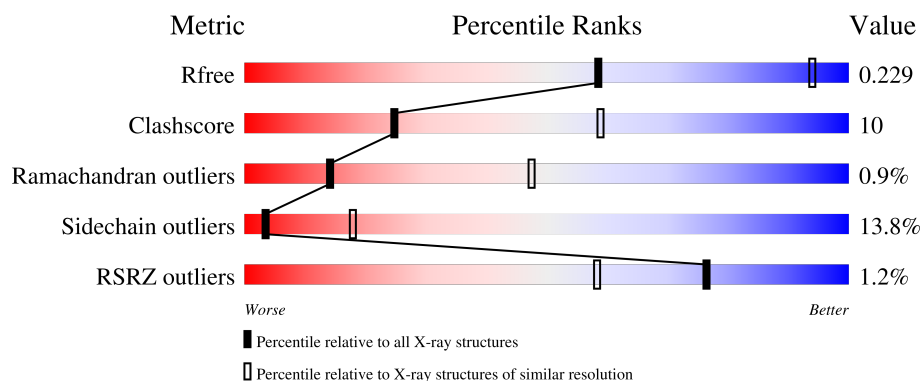
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	763	% 64% 24% •• 8%
1	B	763	% 66% 22% • 8%
2	C	2	100%
2	D	2	100%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11153 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 Membrane copper amine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	704	Total	C	N	O	S	0	0	0
			5545	3560	953	1012	20			
1	B	699	Total	C	N	O	S	0	0	0
			5518	3543	950	1005	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	TPQ	TYR	modified residue	UNP Q16853
B	471	TPQ	TYR	modified residue	UNP Q16853

- Molecule 2 is an oligosaccharide called 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	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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	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		

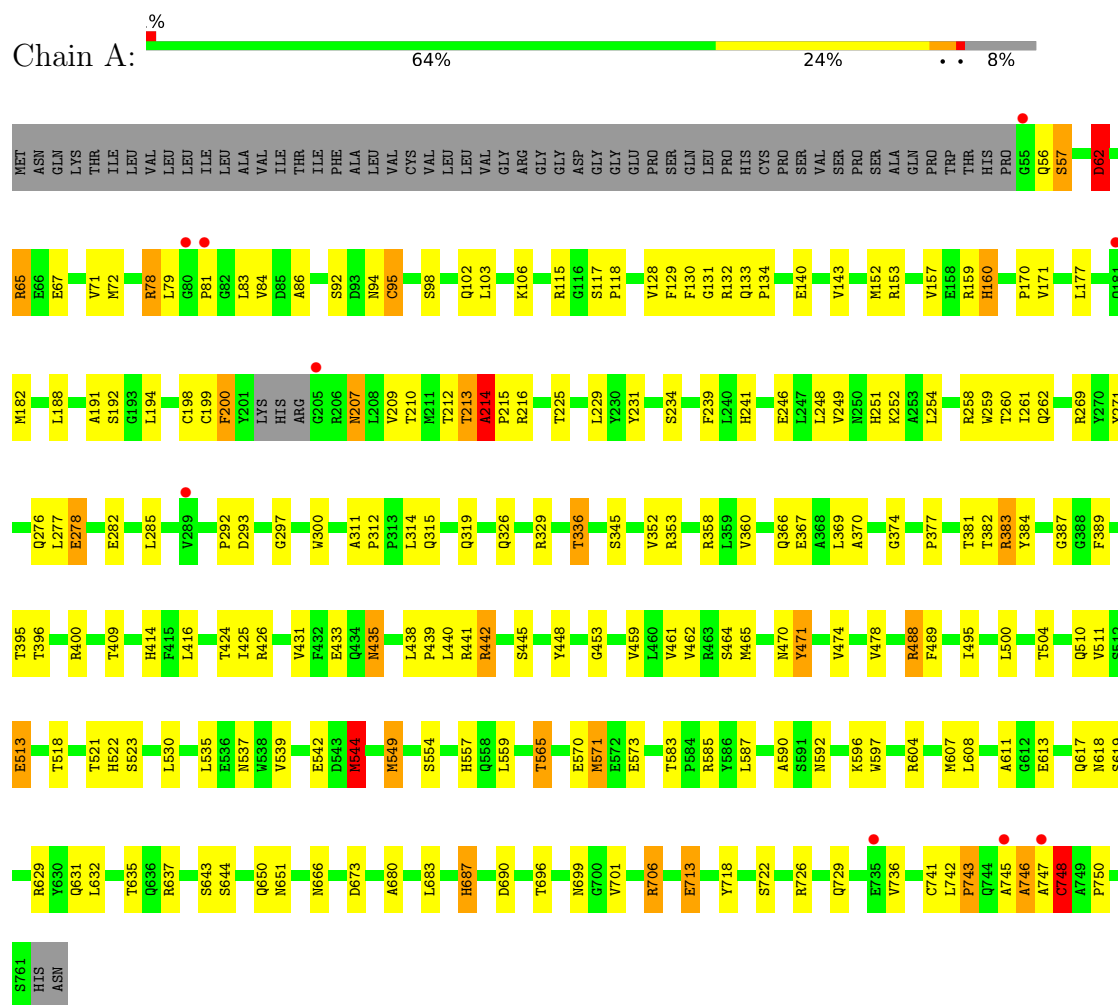
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

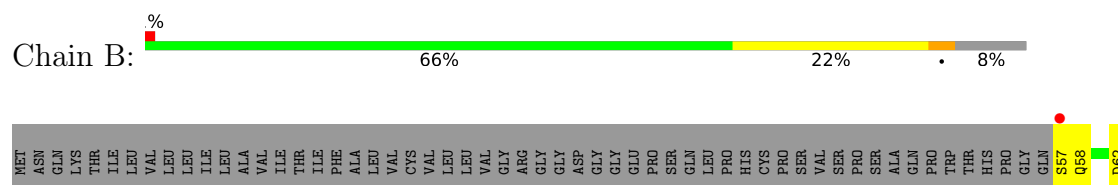
3 Residue-property plots

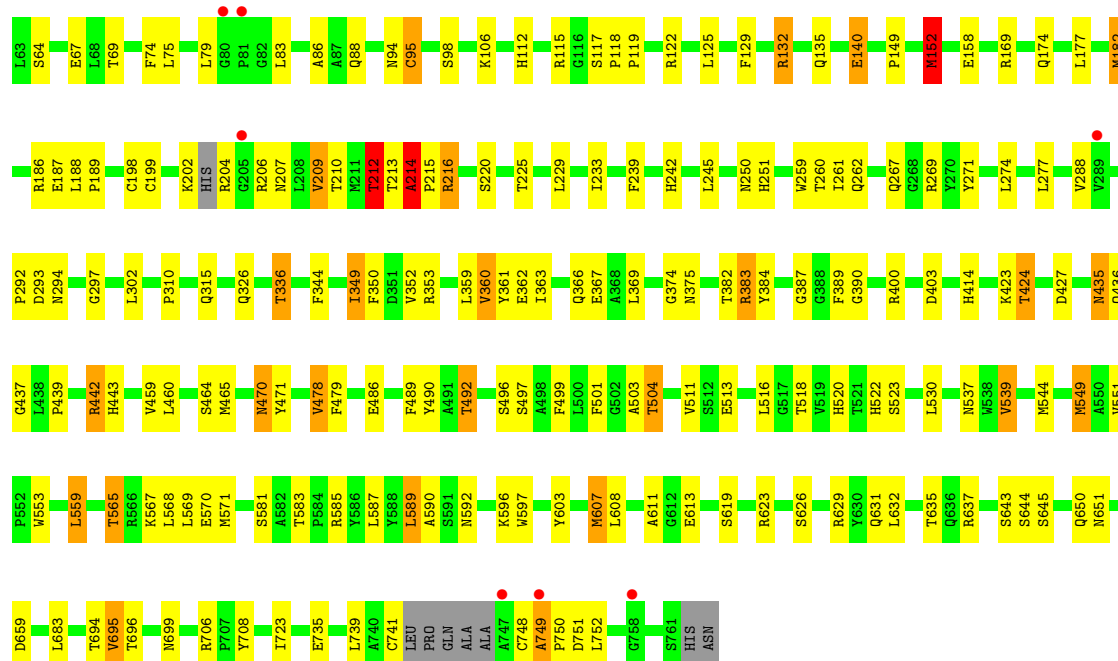
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: Membrane copper amine oxidase





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

Chain C: 100%

MAG1
MAG2

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

Chain D: 100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	225.92Å 225.92Å 218.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20 20.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-3.20) 95.9 (20.00-3.20)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.75 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.254 0.193 , 0.229	Depositor DCC
R_{free} test set	2619 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 17.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11153	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 3.78% 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, CA, NAG, 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	1.01	5/5705 (0.1%)	1.12	9/7779 (0.1%)
1	B	0.99	5/5676 (0.1%)	1.11	7/7735 (0.1%)
All	All	1.00	10/11381 (0.1%)	1.12	16/15514 (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	4
1	B	0	7
All	All	0	11

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	549	MET	SD-CE	10.60	2.06	1.79
1	A	571	MET	SD-CE	10.15	2.04	1.79
1	B	571	MET	SD-CE	8.52	2.00	1.79
1	B	607	MET	SD-CE	7.06	1.97	1.79
1	A	544	MET	SD-CE	-6.93	1.62	1.79
1	B	182	MET	SD-CE	6.79	1.96	1.79
1	A	549	MET	SD-CE	6.71	1.96	1.79
1	A	214	ALA	CA-CB	-6.31	1.43	1.53
1	B	152	MET	SD-CE	5.33	1.92	1.79
1	A	62	ASP	CG-OD2	5.13	1.35	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	ASN	N-CA-C	-8.26	102.23	111.07
1	B	592	ASN	N-CA-C	-8.01	101.25	111.02
1	B	119	PRO	CA-C-O	-7.28	115.66	120.90
1	B	374	GLY	N-CA-C	7.06	120.87	110.63
1	A	133	GLN	N-CA-C	7.04	114.46	108.13
1	A	374	GLY	N-CA-C	6.34	119.83	110.63
1	A	293	ASP	N-CA-C	-6.24	104.88	113.18
1	A	81	PRO	N-CA-C	-5.47	102.64	111.77
1	B	58	GLN	N-CA-C	5.47	117.54	110.65
1	A	57	SER	CA-C-N	5.42	129.59	122.06
1	A	57	SER	C-N-CA	5.42	129.59	122.06
1	B	212	THR	N-CA-C	5.40	117.51	110.43
1	A	249	VAL	CB-CA-C	-5.33	104.30	110.91
1	B	504	THR	CA-C-N	-5.30	117.14	123.44
1	B	504	THR	C-N-CA	-5.30	117.14	123.44
1	A	513	GLU	N-CA-C	-5.20	102.16	109.96

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	THR	Peptide
1	A	214	ALA	Peptide
1	A	292	PRO	Peptide
1	A	750	PRO	Peptide
1	B	213	THR	Peptide
1	B	214	ALA	Peptide
1	B	292	PRO	Peptide
1	B	293	ASP	Peptide
1	B	57	SER	Peptide
1	B	748	CYS	Peptide
1	B	94	ASN	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	5545	0	5293	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5518	0	5271	122	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
3	A	14	0	13	0	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
All	All	11153	0	10640	213	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 10.

All (213) 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:B:549:MET:SD	1:B:549:MET:CE	2.06	1.44
1:A:571:MET:SD	1:A:571:MET:CE	2.04	1.43
1:A:441:ARG:HA	1:B:492:THR:HG21	1.56	0.87
1:A:495:ILE:H	1:A:495:ILE:HD12	1.41	0.85
1:A:216:ARG:HD2	1:A:651:ASN:OD1	1.76	0.83
1:B:749:ALA:HB3	1:B:750:PRO:HD3	1.62	0.80
1:A:500:LEU:HD22	1:A:510:GLN:HG3	1.66	0.75
1:A:680:ALA:HB1	1:A:701:VAL:CG1	2.16	0.74
1:B:360:VAL:HG12	1:B:530:LEU:HD23	1.70	0.73
1:B:250:ASN:HB2	1:B:262:GLN:NE2	2.06	0.71
1:B:607:MET:HE1	1:B:631:GLN:HB3	1.70	0.71
1:A:336:THR:HG22	1:A:353:ARG:HB2	1.71	0.70
1:B:723:ILE:HD11	1:B:739:LEU:HG	1.73	0.70
1:A:315:GLN:NE2	1:B:315:GLN:HE21	1.90	0.69
1:A:212:THR:CG2	1:A:216:ARG:NH2	2.56	0.69
1:A:212:THR:HG21	1:A:216:ARG:NH2	2.07	0.69
1:B:202:LYS:O	1:B:204:ARG:HA	1.91	0.69
1:B:435:ASN:C	1:B:435:ASN:HD22	2.01	0.69
1:B:214:ALA:CB	1:B:382:THR:HA	2.25	0.67
1:A:78:ARG:HB3	1:A:152:MET:HE1	1.77	0.66
1:A:369:LEU:HD12	1:A:384:TYR:O	1.96	0.66
1:B:212:THR:CG2	1:B:216:ARG:NH2	2.59	0.66
1:A:194:LEU:HD23	1:A:277:LEU:HD21	1.78	0.65
1:A:611:ALA:O	1:B:585:ARG:NH1	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ILE:HD12	1:A:495:ILE:N	2.11	0.65
1:A:212:THR:HG21	1:A:216:ARG:HH22	1.63	0.63
1:B:360:VAL:HG21	1:B:363:ILE:HG13	1.79	0.63
1:A:212:THR:HG22	1:A:213:THR:N	2.13	0.63
1:B:214:ALA:CB	1:B:215:PRO:CD	2.77	0.62
1:B:435:ASN:C	1:B:435:ASN:ND2	2.57	0.62
1:B:492:THR:CG2	1:B:694:THR:O	2.47	0.62
1:A:214:ALA:CB	1:A:215:PRO:CD	2.77	0.62
1:B:375:ASN:ND2	1:B:501:PHE:O	2.30	0.62
1:B:214:ALA:HB1	1:B:383:ARG:H	1.66	0.61
1:B:436:GLN:HE21	1:B:436:GLN:HA	1.66	0.60
1:A:160:HIS:N	1:A:160:HIS:CD2	2.69	0.60
1:A:194:LEU:CD2	1:A:277:LEU:HD21	2.33	0.59
1:B:492:THR:HG23	1:B:694:THR:O	2.02	0.58
1:A:106:LYS:NZ	1:A:673:ASP:OD2	2.36	0.58
1:A:71:VAL:HG13	1:A:143:VAL:HG11	1.85	0.58
1:A:214:ALA:HB3	1:A:215:PRO:CD	2.34	0.58
1:B:212:THR:HG21	1:B:216:ARG:NH2	2.20	0.57
1:A:440:LEU:HG	1:B:695:VAL:HG12	1.86	0.56
1:B:182:MET:HE1	1:B:259:TRP:O	2.04	0.56
1:B:214:ALA:HB2	1:B:382:THR:HG23	1.88	0.56
1:B:250:ASN:C	1:B:250:ASN:ND2	2.63	0.56
1:B:125:LEU:HD21	1:B:140:GLU:HB3	1.87	0.56
1:B:212:THR:HG21	1:B:216:ARG:HH22	1.71	0.56
1:A:214:ALA:CB	1:A:382:THR:HA	2.36	0.56
1:A:159:ARG:HB3	1:A:160:HIS:CD2	2.41	0.56
1:A:495:ILE:H	1:A:495:ILE:CD1	2.16	0.56
1:A:544:MET:HE2	1:B:683:LEU:HD13	1.87	0.55
1:A:699:ASN:HD21	1:B:706:ARG:HH22	1.54	0.55
1:B:659:ASP:C	1:B:659:ASP:OD1	2.49	0.55
1:B:129:PHE:CE2	1:B:169:ARG:HG3	2.42	0.55
1:A:500:LEU:CD2	1:A:510:GLN:HG3	2.34	0.55
1:B:565:THR:HG22	1:B:565:THR:O	2.07	0.55
1:B:470:ASN:H	1:B:470:ASN:ND2	2.05	0.54
1:B:414:HIS:ND1	1:B:424:THR:OG1	2.35	0.54
1:B:64:SER:OG	1:B:67:GLU:HG3	2.08	0.54
1:B:359:LEU:HD13	1:B:603:TYR:CZ	2.43	0.54
1:B:214:ALA:HB3	1:B:215:PRO:CD	2.38	0.54
1:B:271:TYR:CE2	1:B:277:LEU:HD13	2.43	0.54
1:A:442:ARG:HH11	1:B:403:ASP:CG	2.17	0.53
1:B:95:CYS:HB3	1:B:129:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ALA:CB	1:A:215:PRO:HD3	2.38	0.53
1:A:442:ARG:NH1	1:B:403:ASP:OD2	2.40	0.53
1:A:489:PHE:C	1:A:489:PHE:CD1	2.86	0.53
1:A:706:ARG:HH22	1:B:699:ASN:HD21	1.56	0.53
1:A:214:ALA:HB1	1:A:215:PRO:HD3	1.90	0.53
1:B:750:PRO:HB2	1:B:752:LEU:HD21	1.91	0.52
1:A:441:ARG:HA	1:B:492:THR:CG2	2.33	0.52
1:B:539:VAL:HG22	1:B:569:LEU:HB2	1.91	0.52
1:B:216:ARG:HD2	1:B:651:ASN:OD1	2.09	0.52
1:B:214:ALA:HB3	1:B:215:PRO:HD2	1.91	0.52
1:B:369:LEU:HD12	1:B:384:TYR:O	2.10	0.51
1:A:381:THR:O	1:A:383:ARG:HD2	2.10	0.51
1:A:65:ARG:HD2	1:A:414:HIS:ND1	2.24	0.51
1:A:565:THR:HG22	1:A:565:THR:O	2.11	0.51
1:A:500:LEU:HD22	1:A:510:GLN:CG	2.37	0.51
1:A:241:HIS:HE1	1:A:300:TRP:CE2	2.28	0.51
1:B:749:ALA:CB	1:B:750:PRO:HD3	2.37	0.50
1:A:745:ALA:O	1:A:746:ALA:HB2	2.12	0.50
1:A:117:SER:HB3	1:A:118:PRO:HD2	1.94	0.49
1:B:352:VAL:HB	1:B:360:VAL:HG22	1.94	0.49
1:A:687:HIS:CD2	1:B:708:TYR:HD1	2.29	0.49
1:A:729:GLN:NE2	1:A:736:VAL:HG13	2.27	0.49
1:A:596:LYS:HD2	1:A:597:TRP:CH2	2.47	0.49
1:A:696:THR:HG21	1:B:439:PRO:O	2.12	0.49
1:A:117:SER:HB3	1:A:118:PRO:CD	2.42	0.49
1:B:212:THR:CG2	1:B:216:ARG:HH21	2.25	0.49
1:B:435:ASN:ND2	1:B:437:GLY:H	2.11	0.49
1:A:465:MET:SD	1:B:442:ARG:HD2	2.53	0.49
1:A:573:GLU:OE2	1:A:666:ASN:N	2.45	0.49
1:B:366:GLN:HE21	1:B:644:SER:H	1.60	0.49
1:B:250:ASN:HB2	1:B:262:GLN:HE21	1.78	0.48
1:A:171:VAL:HG21	1:A:216:ARG:CZ	2.44	0.48
1:A:248:LEU:HG	1:A:262:GLN:HB2	1.95	0.48
1:A:214:ALA:HB3	1:A:382:THR:HA	1.95	0.48
1:A:86:ALA:HA	1:A:95:CYS:SG	2.54	0.48
1:B:132:ARG:O	1:B:132:ARG:HG2	2.14	0.48
1:B:336:THR:HG22	1:B:353:ARG:HB2	1.96	0.48
1:A:251:HIS:HA	1:A:259:TRP:CD1	2.49	0.48
1:A:377:PRO:HB3	1:B:553:TRP:CZ3	2.49	0.48
1:A:438:LEU:HD11	1:B:490:TYR:CZ	2.48	0.48
1:B:187:GLU:HG3	1:B:274:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:LYS:C	1:B:204:ARG:N	2.72	0.48
1:A:199:CYS:HA	1:A:231:TYR:OH	2.14	0.47
1:A:214:ALA:HB1	1:A:383:ARG:H	1.79	0.47
1:B:188:LEU:N	1:B:189:PRO:CD	2.77	0.47
1:A:239:PHE:CD1	1:A:470:ASN:HB3	2.50	0.47
1:A:439:PRO:O	1:B:696:THR:HG21	2.15	0.47
1:A:747:ALA:O	1:A:748:CYS:HB2	2.14	0.47
1:B:74:PHE:CD1	1:B:149:PRO:HB2	2.50	0.47
1:B:537:ASN:HA	1:B:590:ALA:O	2.15	0.47
1:B:242:HIS:HD2	1:B:499:PHE:HB2	1.80	0.46
1:B:492:THR:HG22	1:B:694:THR:O	2.13	0.46
1:A:680:ALA:HB1	1:A:701:VAL:HG12	1.96	0.46
1:B:589:LEU:N	1:B:589:LEU:HD23	2.30	0.46
1:A:687:HIS:CD2	1:B:708:TYR:CD1	3.04	0.46
1:A:367:GLU:OE2	1:A:387:GLY:N	2.40	0.46
1:A:680:ALA:HB1	1:A:701:VAL:HG13	1.94	0.46
1:B:182:MET:HB2	1:B:186:ARG:NH2	2.30	0.46
1:A:607:MET:HE1	1:A:631:GLN:HB3	1.97	0.46
1:A:699:ASN:ND2	1:B:706:ARG:HH22	2.14	0.46
1:B:366:GLN:NE2	1:B:643:SER:OG	2.48	0.46
1:B:132:ARG:O	1:B:132:ARG:CG	2.63	0.46
1:A:687:HIS:HD2	1:B:708:TYR:HD1	1.64	0.45
1:B:117:SER:HB3	1:B:118:PRO:HD2	1.98	0.45
1:A:159:ARG:CB	1:A:160:HIS:HD2	2.28	0.45
1:B:344:PHE:HA	1:B:390:GLY:HA2	1.99	0.45
1:A:212:THR:HG22	1:A:213:THR:O	2.17	0.45
1:B:214:ALA:HB3	1:B:382:THR:HA	1.98	0.45
1:B:225:THR:OG1	1:B:251:HIS:HE1	2.00	0.45
1:B:366:GLN:HG3	1:B:644:SER:CB	2.47	0.45
1:A:67:GLU:O	1:A:71:VAL:HG23	2.17	0.45
1:A:453:GLY:HA3	1:B:302:LEU:HD13	1.99	0.45
1:B:460:LEU:HB3	1:B:479:PHE:HB2	1.97	0.45
1:A:191:ALA:HA	1:A:278:GLU:HG3	1.98	0.45
1:B:551:VAL:HG22	1:B:559:LEU:HB3	1.99	0.45
1:A:366:GLN:NE2	1:A:644:SER:H	2.15	0.45
1:A:246:GLU:OE1	1:A:377:PRO:HD2	2.17	0.45
1:B:520:HIS:CD2	1:B:522:HIS:NE2	2.84	0.45
1:A:495:ILE:HD11	1:A:690:ASP:O	2.17	0.44
1:A:128:VAL:HG11	1:A:130:PHE:CZ	2.52	0.44
1:A:170:PRO:HA	1:A:651:ASN:ND2	2.33	0.44
1:A:471:TPQ:H6	1:A:471:TPQ:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:HD2	1:B:465:MET:SD	2.58	0.44
1:B:367:GLU:OE2	1:B:387:GLY:N	2.48	0.44
1:A:94:ASN:HD22	1:A:131:GLY:H	1.65	0.44
1:A:95:CYS:HB3	1:A:129:PHE:HB2	2.00	0.44
1:A:214:ALA:HB2	1:A:382:THR:HG23	1.98	0.44
1:A:742:LEU:N	1:A:743:PRO:HD2	2.32	0.44
1:B:239:PHE:CD1	1:B:470:ASN:HB3	2.53	0.44
1:B:350:PHE:CE2	1:B:362:GLU:HG3	2.53	0.44
1:A:438:LEU:HD21	1:B:490:TYR:CE1	2.53	0.43
1:A:687:HIS:HD2	1:B:708:TYR:CD1	2.36	0.43
1:A:585:ARG:NH1	1:B:611:ALA:O	2.51	0.43
1:B:623:ARG:HD2	1:B:659:ASP:OD2	2.19	0.43
1:A:352:VAL:HB	1:A:360:VAL:CG2	2.48	0.43
1:A:587:LEU:HD22	1:A:632:LEU:HD21	1.99	0.43
1:B:86:ALA:HA	1:B:95:CYS:SG	2.59	0.43
1:A:488:ARG:HA	1:A:488:ARG:HD3	1.64	0.43
1:B:587:LEU:HD22	1:B:632:LEU:HD21	1.99	0.43
1:A:549:MET:HE2	1:A:549:MET:HB3	1.76	0.43
1:B:366:GLN:HG3	1:B:644:SER:HB2	2.00	0.43
1:A:200:PHE:N	1:A:200:PHE:CD2	2.87	0.43
1:A:438:LEU:HD11	1:B:490:TYR:CE2	2.54	0.43
1:B:442:ARG:HG2	1:B:443:HIS:N	2.32	0.42
1:A:102:GLN:HE21	1:A:103:LEU:N	2.17	0.42
1:A:160:HIS:N	1:A:160:HIS:HD2	2.14	0.42
1:B:233:ILE:N	1:B:233:ILE:HD13	2.34	0.42
1:A:683:LEU:HD13	1:B:544:MET:HE2	2.00	0.42
1:B:152:MET:O	1:B:152:MET:HG2	2.18	0.42
1:B:106:LYS:HG3	1:B:361:TYR:CZ	2.54	0.42
1:A:713:GLU:OE2	1:A:718:TYR:CE2	2.72	0.42
1:A:132:ARG:HE	1:A:132:ARG:HB2	1.61	0.42
1:A:352:VAL:HB	1:A:360:VAL:HG22	2.02	0.42
1:A:745:ALA:O	1:A:746:ALA:CB	2.67	0.42
1:B:478:VAL:HG22	1:B:486:GLU:HB3	2.01	0.42
1:A:435:ASN:C	1:A:435:ASN:HD22	2.28	0.42
1:B:596:LYS:HD2	1:B:597:TRP:CZ2	2.55	0.42
1:A:311:ALA:HA	1:A:312:PRO:HD3	1.91	0.41
1:A:370:ALA:HA	1:A:521:THR:O	2.20	0.41
1:B:349:ILE:HD12	1:B:352:VAL:HG21	2.02	0.41
1:B:389:PHE:CE1	1:B:650:GLN:OE1	2.73	0.41
1:A:471:TPQ:C3	1:A:522:HIS:HE1	2.34	0.41
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:HB1	1:B:215:PRO:HD3	2.01	0.41
1:B:88:GLN:C	1:B:174:GLN:HG3	2.46	0.41
1:B:596:LYS:HD2	1:B:597:TRP:CH2	2.56	0.41
1:A:215:PRO:HD3	1:A:383:ARG:H	1.85	0.41
1:A:225:THR:OG1	1:A:251:HIS:HE1	2.03	0.41
1:A:389:PHE:HE1	1:A:650:GLN:OE1	2.03	0.41
1:A:537:ASN:HA	1:A:590:ALA:O	2.19	0.41
1:A:554:SER:O	1:A:557:HIS:HB2	2.21	0.41
1:A:465:MET:HG2	1:A:474:VAL:HG22	2.03	0.41
1:B:229:LEU:HD13	1:B:245:LEU:HD23	2.03	0.41
1:B:389:PHE:HE1	1:B:650:GLN:OE1	2.04	0.41
1:B:723:ILE:CD1	1:B:739:LEU:HG	2.48	0.41
1:A:319:GLN:HE21	1:B:310:PRO:HA	1.86	0.41
1:A:706:ARG:HH22	1:B:699:ASN:ND2	2.19	0.41
1:B:504:THR:HG23	1:B:516:LEU:HD13	2.03	0.40
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.94	0.40
1:A:198:CYS:SG	1:A:199:CYS:N	2.94	0.40
1:A:212:THR:HG23	1:A:216:ARG:NH2	2.34	0.40
1:A:431:VAL:HA	1:A:461:VAL:O	2.21	0.40
1:A:207:ASN:H	1:A:207:ASN:HD22	1.69	0.40
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.92	0.40
1:A:448:TYR:CZ	1:B:209:VAL:HG22	2.56	0.40
1:B:400:ARG:NH2	1:B:427:ASP:OD1	2.54	0.40
1:B:435:ASN:ND2	1:B:437:GLY:N	2.69	0.40
1:B:489:PHE:CD1	1:B:489:PHE:C	2.97	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	699/763 (92%)	646 (92%)	46 (7%)	7 (1%)	12 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	692/763 (91%)	634 (92%)	53 (8%)	5 (1%)	18	52
All	All	1391/1526 (91%)	1280 (92%)	99 (7%)	12 (1%)	14	47

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ALA
1	A	746	ALA
1	A	748	CYS
1	B	214	ALA
1	B	749	ALA
1	B	503	ALA
1	A	743	PRO
1	A	62	ASP
1	B	62	ASP
1	B	297	GLY
1	A	297	GLY
1	A	134	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	583/634 (92%)	491 (84%)	92 (16%)	2	13
1	B	581/634 (92%)	512 (88%)	69 (12%)	5	23
All	All	1164/1268 (92%)	1003 (86%)	161 (14%)	3	18

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	57	SER
1	A	62	ASP
1	A	65	ARG

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Mol	Chain	Res	Type
1	A	72	MET
1	A	78	ARG
1	A	83	LEU
1	A	84	VAL
1	A	92	SER
1	A	95	CYS
1	A	98	SER
1	A	115	ARG
1	A	140	GLU
1	A	153	ARG
1	A	157	VAL
1	A	160	HIS
1	A	177	LEU
1	A	182	MET
1	A	188	LEU
1	A	192	SER
1	A	200	PHE
1	A	207	ASN
1	A	209	VAL
1	A	210	THR
1	A	229	LEU
1	A	234	SER
1	A	252	LYS
1	A	254	LEU
1	A	258	ARG
1	A	260	THR
1	A	261	ILE
1	A	269	ARG
1	A	271	TYR
1	A	276	GLN
1	A	278	GLU
1	A	282	GLU
1	A	285	LEU
1	A	314	LEU
1	A	326	GLN
1	A	329	ARG
1	A	336	THR
1	A	345	SER
1	A	358	ARG
1	A	383	ARG
1	A	395	THR
1	A	396	THR

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Mol	Chain	Res	Type
1	A	400	ARG
1	A	409	THR
1	A	416	LEU
1	A	424	THR
1	A	425	ILE
1	A	426	ARG
1	A	433	GLU
1	A	435	ASN
1	A	442	ARG
1	A	445	SER
1	A	459	VAL
1	A	462	VAL
1	A	464	SER
1	A	478	VAL
1	A	488	ARG
1	A	504	THR
1	A	511	VAL
1	A	513	GLU
1	A	518	THR
1	A	523	SER
1	A	530	LEU
1	A	535	LEU
1	A	539	VAL
1	A	542	GLU
1	A	544	MET
1	A	559	LEU
1	A	565	THR
1	A	570	GLU
1	A	583	THR
1	A	604	ARG
1	A	608	LEU
1	A	613	GLU
1	A	617	GLN
1	A	618	ASN
1	A	619	SER
1	A	629	ARG
1	A	635	THR
1	A	637	ARG
1	A	643	SER
1	A	687	HIS
1	A	706	ARG
1	A	713	GLU

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Mol	Chain	Res	Type
1	A	722	SER
1	A	726	ARG
1	A	741	CYS
1	A	748	CYS
1	B	69	THR
1	B	83	LEU
1	B	95	CYS
1	B	98	SER
1	B	112	HIS
1	B	115	ARG
1	B	122	ARG
1	B	132	ARG
1	B	135	GLN
1	B	140	GLU
1	B	152	MET
1	B	158	GLU
1	B	177	LEU
1	B	198	CYS
1	B	199	CYS
1	B	206	ARG
1	B	207	ASN
1	B	209	VAL
1	B	210	THR
1	B	212	THR
1	B	216	ARG
1	B	220	SER
1	B	260	THR
1	B	261	ILE
1	B	267	GLN
1	B	269	ARG
1	B	288	VAL
1	B	294	ASN
1	B	326	GLN
1	B	336	THR
1	B	349	ILE
1	B	360	VAL
1	B	383	ARG
1	B	423	LYS
1	B	424	THR
1	B	435	ASN
1	B	442	ARG
1	B	459	VAL

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Mol	Chain	Res	Type
1	B	464	SER
1	B	470	ASN
1	B	478	VAL
1	B	492	THR
1	B	496	SER
1	B	497	SER
1	B	511	VAL
1	B	513	GLU
1	B	518	THR
1	B	523	SER
1	B	539	VAL
1	B	559	LEU
1	B	565	THR
1	B	567	LYS
1	B	568	LEU
1	B	570	GLU
1	B	581	SER
1	B	583	THR
1	B	589	LEU
1	B	608	LEU
1	B	613	GLU
1	B	619	SER
1	B	626	SER
1	B	629	ARG
1	B	635	THR
1	B	637	ARG
1	B	645	SER
1	B	695	VAL
1	B	735	GLU
1	B	741	CYS
1	B	751	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	135	GLN
1	A	174	GLN
1	A	207	ASN
1	A	241	HIS
1	A	242	HIS
1	A	250	ASN

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Mol	Chain	Res	Type
1	A	251	HIS
1	A	267	GLN
1	A	280	GLN
1	A	287	ASN
1	A	294	ASN
1	A	315	GLN
1	A	319	GLN
1	A	366	GLN
1	A	435	ASN
1	A	470	ASN
1	A	537	ASN
1	A	617	GLN
1	A	650	GLN
1	A	687	HIS
1	A	699	ASN
1	B	94	ASN
1	B	167	HIS
1	B	250	ASN
1	B	251	HIS
1	B	262	GLN
1	B	267	GLN
1	B	276	GLN
1	B	366	GLN
1	B	435	ASN
1	B	436	GLN
1	B	470	ASN
1	B	514	HIS
1	B	557	HIS
1	B	636	GLN
1	B	693	ASN
1	B	699	ASN

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	471	4,1	13,14,15	3.32	7 (53%)	13,19,21	2.69	6 (46%)
1	TPQ	A	471	4,1	13,14,15	3.29	8 (61%)	13,19,21	2.91	5 (38%)

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	471	4,1	-	4/5/22/24	0/1/1/1
1	TPQ	A	471	4,1	-	4/5/22/24	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	471	TPQ	C1-C2	-6.50	1.40	1.49
1	B	471	TPQ	O5-C5	5.26	1.38	1.24
1	B	471	TPQ	C3-C4	5.18	1.45	1.36
1	A	471	TPQ	O2-C2	5.13	1.38	1.24
1	B	471	TPQ	O2-C2	4.90	1.37	1.24
1	A	471	TPQ	C3-C4	4.56	1.44	1.36
1	B	471	TPQ	C1-C2	-4.42	1.43	1.49
1	B	471	TPQ	C6-C1	3.95	1.44	1.34
1	B	471	TPQ	O4-C4	3.84	1.43	1.33
1	A	471	TPQ	O5-C5	3.70	1.34	1.24
1	B	471	TPQ	CB-C1	3.46	1.56	1.50
1	A	471	TPQ	C6-C1	3.14	1.42	1.34
1	A	471	TPQ	O4-C4	3.09	1.41	1.33
1	A	471	TPQ	C4-C5	-3.04	1.38	1.47
1	A	471	TPQ	CB-C1	2.09	1.54	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	TPQ	C3-C4-C5	-6.78	114.31	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	TPQ	C4-C3-C2	5.59	126.34	120.30
1	B	471	TPQ	C3-C4-C5	-5.26	115.86	121.23
1	B	471	TPQ	C4-C3-C2	4.74	125.43	120.30
1	B	471	TPQ	CB-C1-C2	4.26	126.02	118.56
1	A	471	TPQ	CB-C1-C2	3.44	124.58	118.56
1	A	471	TPQ	C6-C1-C2	-3.02	116.51	118.66
1	B	471	TPQ	C6-C1-C2	-2.97	116.54	118.66
1	B	471	TPQ	O4-C4-C5	2.45	123.36	117.97
1	B	471	TPQ	O5-C5-C4	2.06	122.68	119.43
1	A	471	TPQ	C6-C5-C4	2.03	120.35	116.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	471	TPQ	C-CA-CB-C1
1	A	471	TPQ	C2-C1-CB-CA
1	A	471	TPQ	C6-C1-CB-CA
1	B	471	TPQ	C-CA-CB-C1
1	B	471	TPQ	C2-C1-CB-CA
1	B	471	TPQ	C6-C1-CB-CA
1	A	471	TPQ	N-CA-CB-C1
1	B	471	TPQ	N-CA-CB-C1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	471	TPQ	2	0

5.5 Carbohydrates

4 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	1.89	4 (23%)
2	NAG	C	2	2	14,14,15	0.91	0	17,19,21	2.01	5 (29%)
2	NAG	D	1	2,1	14,14,15	0.62	0	17,19,21	1.80	6 (35%)
2	NAG	D	2	2	14,14,15	0.97	1 (7%)	17,19,21	2.38	6 (35%)

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	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	4/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	NAG	C3-C2	2.65	1.58	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C1-O5-C5	5.35	119.35	112.19
2	C	1	NAG	C1-O5-C5	4.90	118.75	112.19
2	D	2	NAG	O3-C3-C2	4.63	119.02	109.40
2	C	2	NAG	C3-C4-C5	-3.95	103.06	110.23
2	D	2	NAG	O5-C1-C2	-3.72	105.54	111.29
2	D	1	NAG	O3-C3-C4	-3.50	102.11	110.38
2	C	2	NAG	O4-C4-C3	3.21	117.95	110.38
2	C	2	NAG	O7-C7-C8	-3.08	116.58	122.05
2	C	1	NAG	O3-C3-C2	3.06	115.75	109.40
2	D	1	NAG	C1-O5-C5	2.99	116.19	112.19
2	D	2	NAG	O4-C4-C5	2.89	116.43	109.32
2	C	2	NAG	O4-C4-C5	2.84	116.31	109.32
2	C	2	NAG	C1-O5-C5	2.81	115.95	112.19
2	D	1	NAG	C8-C7-N2	2.57	120.39	116.12
2	D	2	NAG	C1-C2-N2	-2.46	106.56	110.43
2	D	1	NAG	O5-C1-C2	-2.44	107.52	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C6-C5-C4	-2.39	107.16	113.02
2	C	1	NAG	O4-C4-C3	-2.26	105.04	110.38
2	C	1	NAG	C6-C5-C4	-2.23	107.55	113.02
2	D	2	NAG	O3-C3-C4	-2.18	105.24	110.38
2	D	1	NAG	O7-C7-C8	-2.15	118.22	122.05

There are no chirality outliers.

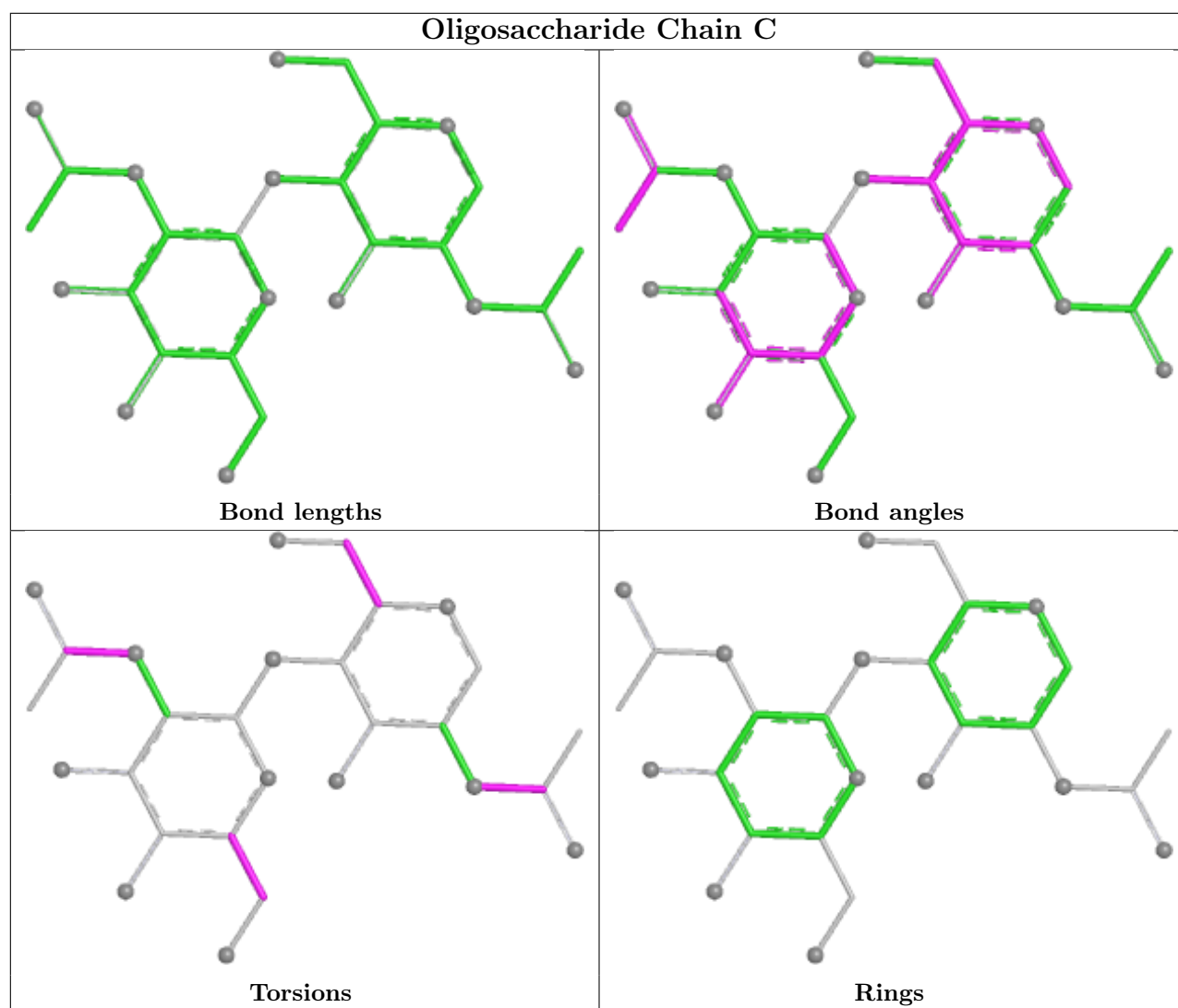
All (14) torsion outliers are listed below:

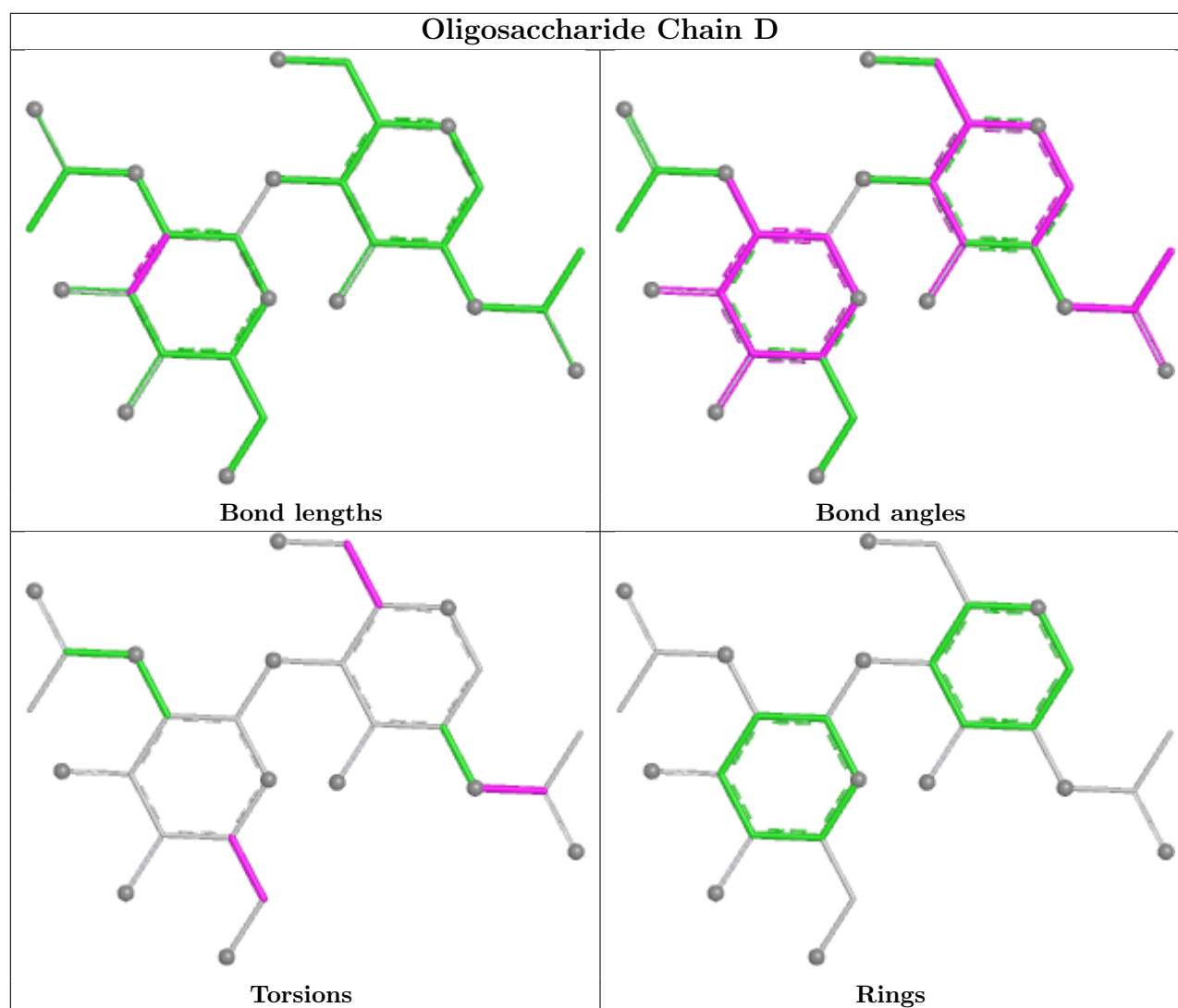
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
2	D	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C4-C5-C6-O6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

There are no ring outliers.

No monomer is involved in short contacts.

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 8 ligands modelled in this entry, 6 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	$\# Z > 2$
3	NAG	A	2781	1	14,14,15	0.82	0	17,19,21	1.60	4 (23%)
3	NAG	B	2781	1	14,14,15	1.02	1 (7%)	17,19,21	1.60	5 (29%)

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	2781	1	-	3/6/23/26	0/1/1/1
3	NAG	B	2781	1	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2781	NAG	C1-C2	2.31	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2781	NAG	C1-C2-N2	3.39	115.77	110.43
3	A	2781	NAG	C1-O5-C5	3.02	116.23	112.19
3	B	2781	NAG	O5-C5-C6	2.78	113.06	107.66
3	B	2781	NAG	C1-C2-N2	2.64	114.60	110.43
3	B	2781	NAG	C2-N2-C7	2.60	126.38	122.90
3	B	2781	NAG	C4-C3-C2	-2.35	107.57	111.02
3	A	2781	NAG	O7-C7-C8	-2.23	118.08	122.05
3	B	2781	NAG	C1-O5-C5	2.10	115.01	112.19
3	A	2781	NAG	C8-C7-N2	2.10	119.60	116.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2781	NAG	C1-C2-N2-C7
3	B	2781	NAG	C1-C2-N2-C7
3	B	2781	NAG	O5-C5-C6-O6
3	B	2781	NAG	O7-C7-N2-C2
3	A	2781	NAG	C4-C5-C6-O6
3	B	2781	NAG	C8-C7-N2-C2
3	A	2781	NAG	O5-C5-C6-O6
3	B	2781	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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	703/763 (92%)	-0.33	9 (1%) 75 55	15, 28, 45, 69	0
1	B	698/763 (91%)	-0.35	8 (1%) 78 61	16, 28, 45, 65	0
All	All	1401/1526 (91%)	-0.34	17 (1%) 76 58	15, 28, 45, 69	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	81	PRO	3.9
1	A	747	ALA	3.5
1	B	747	ALA	3.4
1	A	205	GLY	3.2
1	B	205	GLY	3.0
1	B	81	PRO	2.8
1	A	55	GLY	2.6
1	B	758	GLY	2.6
1	B	80	GLY	2.4
1	A	289	VAL	2.3
1	A	735	GLU	2.3
1	B	57	SER	2.2
1	B	289	VAL	2.1
1	A	745	ALA	2.1
1	A	80	GLY	2.1
1	B	749	ALA	2.1
1	A	181	GLN	2.1

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.

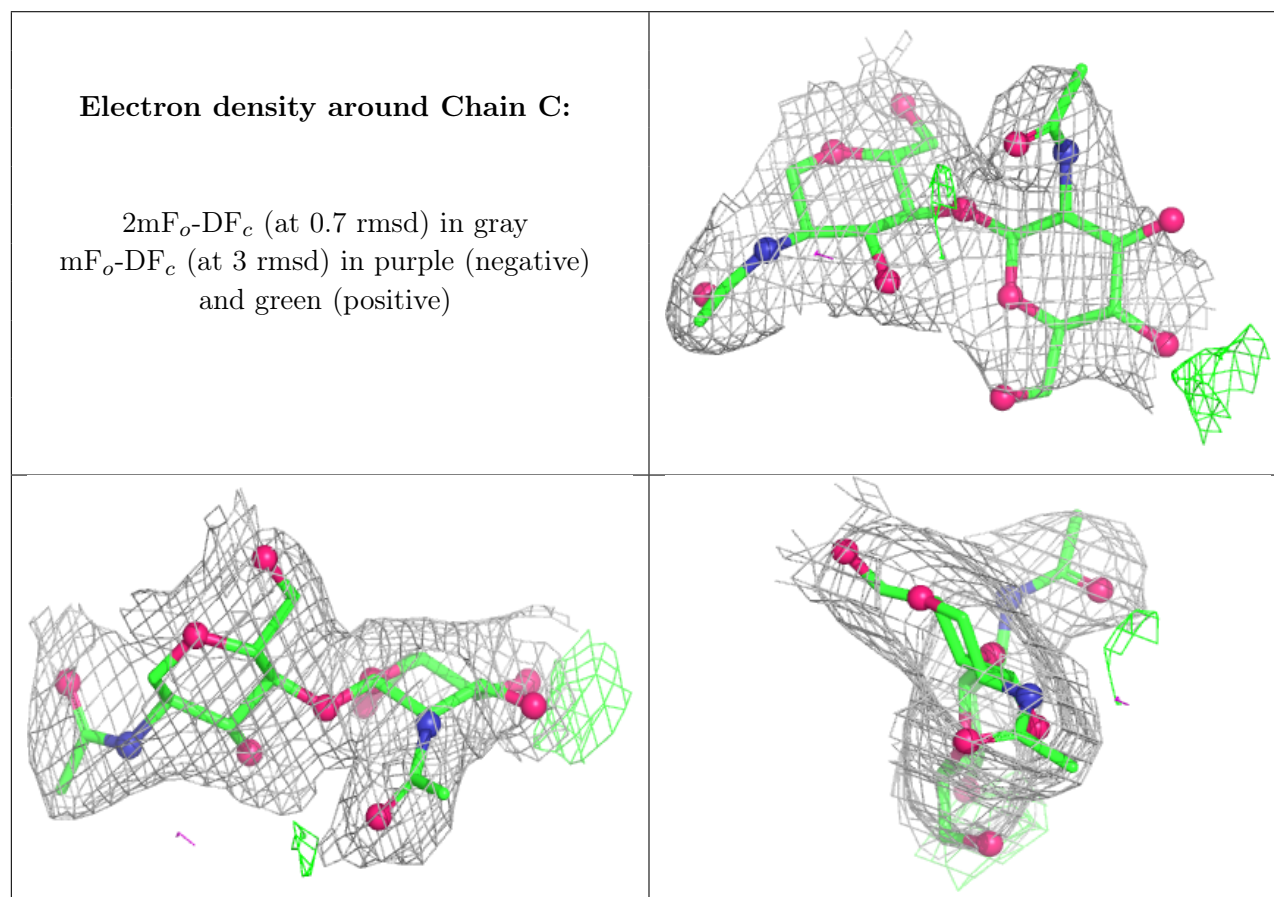
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TPQ	B	471	14/15	0.93	0.11	21,26,31,32	0
1	TPQ	A	471	14/15	0.95	0.11	21,25,30,32	0

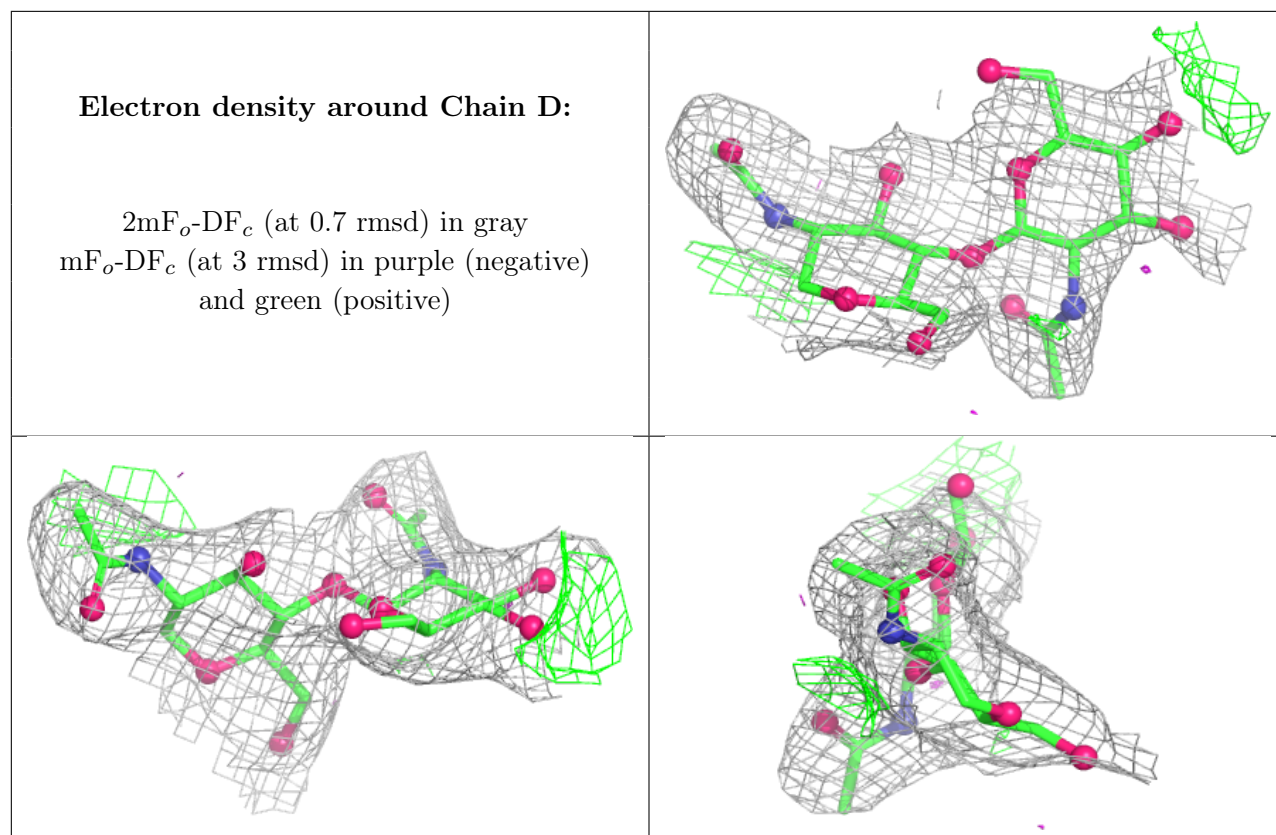
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
2	NAG	D	2	14/15	0.84	0.13	43,47,50,52	0
2	NAG	C	2	14/15	0.86	0.13	42,45,51,53	0
2	NAG	C	1	14/15	0.92	0.09	31,33,38,40	0
2	NAG	D	1	14/15	0.93	0.09	30,34,37,42	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, 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
3	NAG	A	2781	14/15	0.86	0.13	49,51,52,53	0
3	NAG	B	2781	14/15	0.86	0.12	47,51,53,53	0
5	CA	A	802	1/1	0.93	0.07	24,24,24,24	0
5	CA	B	802	1/1	0.96	0.04	23,23,23,23	0
5	CA	A	803	1/1	0.98	0.05	37,37,37,37	0
5	CA	B	803	1/1	0.98	0.07	37,37,37,37	0
4	CU	B	801	1/1	0.99	0.02	22,22,22,22	0
4	CU	A	801	1/1	1.00	0.01	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.