



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:02 AM UTC

PDB ID : 2JBK / pdb_00002jbk
Title : membrane-bound glutamate carboxypeptidase II (GCPII) in complex with quisqualic acid (quisqualate, alpha-amino-3,5-dioxo-1,2,4-oxadiazolidine-2-panoic acid)
Authors : Mesters, J.R.; Henning, K.; Hilgenfeld, R.
Deposited on : 2006-12-07
Resolution : 2.99 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

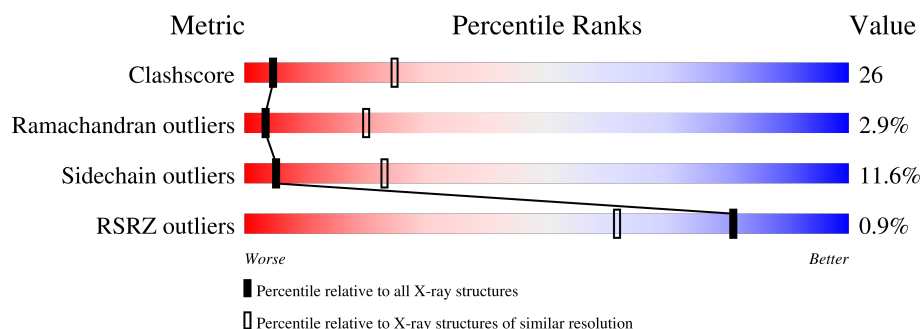
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	707	 48% 39% 9% . .
2	B	2	 100%
2	C	2	 50% 50%
2	D	2	 100%
3	E	4	 75% 25%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5532 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 GLUTAMATE CARBOXYPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5318	3430	881	990	17			

- 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	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
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 an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(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
3	E	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

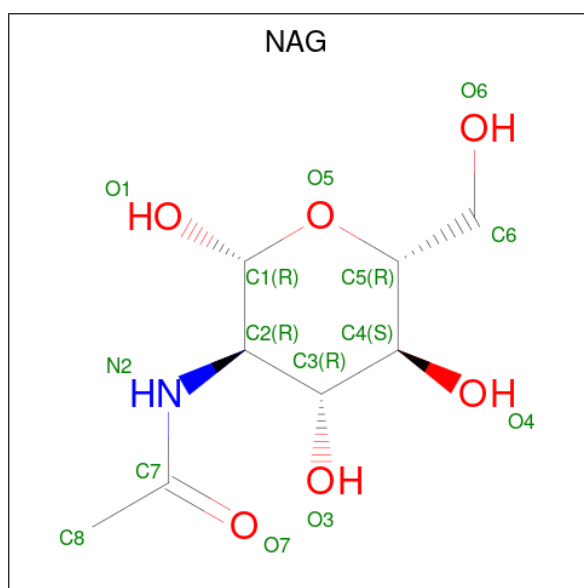
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

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

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

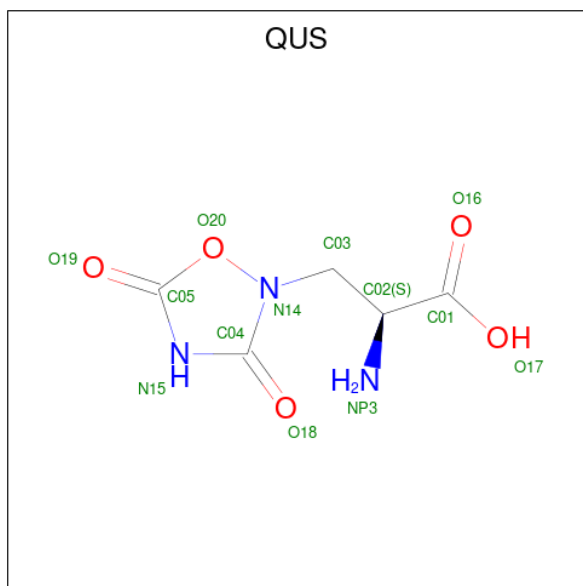
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 8 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC

ACID (CCD ID: QUS) (formula: $C_5H_7N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			13	5	3	5		

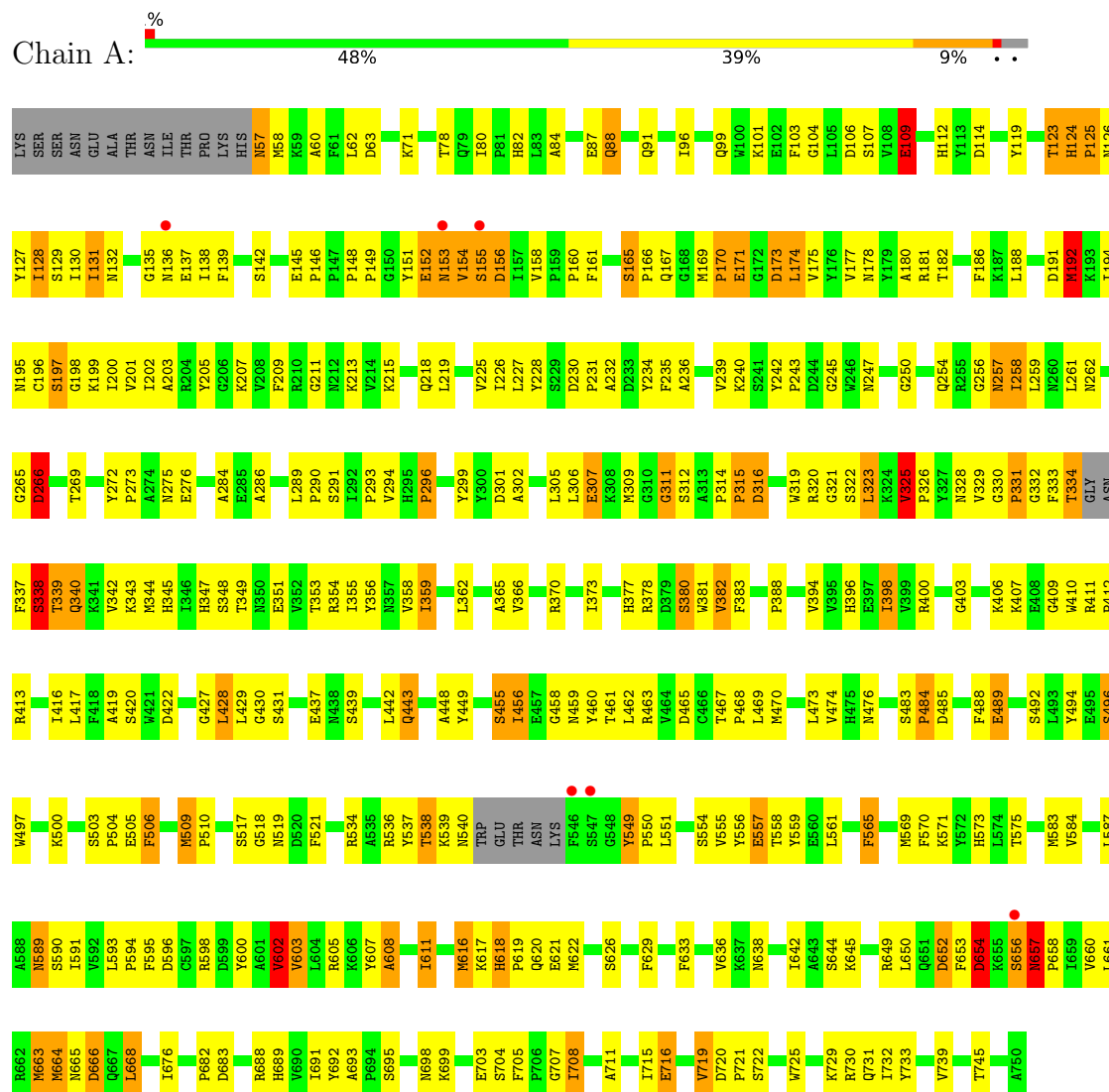
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	21	Total	O	0	0
			21	21		

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: GLUTAMATE CARBOXYPEPTIDASE 2



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

Chain B: 

MAG1
MAG2

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

Chain C:  50% 50%

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

- Molecule 3: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  75% 25%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	103.14Å 130.76Å 159.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.99 100.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.2 (100.00-2.99) 93.2 (100.00-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.210 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5532	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: CL, MAN, CA, ZN, NAG, BMA, QUS

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	1.38	14/5468 (0.3%)	1.47	67/7431 (0.9%)

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	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	ASP	CA-C	-6.41	1.46	1.53
1	A	668	LEU	C-O	-5.63	1.17	1.24
1	A	657	ASN	CA-C	5.58	1.59	1.52
1	A	320	ARG	CA-C	5.57	1.59	1.52
1	A	492	SER	N-CA	5.42	1.53	1.45
1	A	201	VAL	CA-CB	-5.39	1.47	1.54
1	A	170	PRO	C-O	5.39	1.30	1.23
1	A	84	ALA	CA-CB	-5.38	1.44	1.53
1	A	170	PRO	CA-C	5.30	1.58	1.52
1	A	296	PRO	CA-C	5.30	1.59	1.52
1	A	152	GLU	N-CA	5.22	1.52	1.46
1	A	654	ASP	C-O	5.16	1.30	1.24
1	A	359	ILE	C-O	-5.08	1.18	1.24
1	A	739	VAL	CA-CB	-5.06	1.47	1.54

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	HIS	CA-C-N	15.32	138.99	119.84
1	A	124	HIS	C-N-CA	15.32	138.99	119.84
1	A	156	ASP	N-CA-C	10.33	124.76	107.20
1	A	266	ASP	CA-C-N	9.09	128.84	119.56
1	A	266	ASP	C-N-CA	9.09	128.84	119.56
1	A	593	LEU	CA-C-N	9.02	131.12	119.84
1	A	593	LEU	C-N-CA	9.02	131.12	119.84
1	A	732	ILE	CB-CA-C	-8.53	100.62	112.14
1	A	365	ALA	N-CA-C	-8.42	102.94	113.55
1	A	194	ILE	N-CA-C	-8.26	98.92	109.58
1	A	719	VAL	CB-CA-C	-8.06	101.56	111.88
1	A	312	SER	N-CA-C	7.82	120.03	110.41
1	A	314	PRO	N-CA-C	-7.39	101.69	110.70
1	A	165	SER	CA-C-N	-7.25	112.31	119.78
1	A	165	SER	C-N-CA	-7.25	112.31	119.78
1	A	136	ASN	N-CA-C	-7.23	99.33	110.10
1	A	652	ASP	N-CA-C	7.12	125.97	110.80
1	A	315	PRO	N-CA-C	-6.97	105.83	114.20
1	A	565	PHE	N-CA-C	6.89	121.93	112.90
1	A	745	THR	N-CA-C	-6.74	104.88	113.23
1	A	78	THR	CB-CA-C	-6.48	101.08	111.18
1	A	608	ALA	N-CA-C	-6.40	104.38	111.36
1	A	428	LEU	N-CA-C	-6.38	105.44	113.23
1	A	705	PHE	O-C-N	6.26	124.41	121.53
1	A	398	ILE	N-CA-C	6.26	116.93	110.36
1	A	711	ALA	N-CA-C	-6.18	103.86	112.45
1	A	492	SER	N-CA-C	6.14	118.63	110.53
1	A	611	ILE	N-CA-C	-5.93	103.67	111.09
1	A	322	SER	CA-C-N	-5.91	112.97	121.42
1	A	322	SER	C-N-CA	-5.91	112.97	121.42
1	A	693	ALA	CA-C-N	5.91	125.92	119.90
1	A	693	ALA	C-N-CA	5.91	125.92	119.90
1	A	156	ASP	CA-C-N	5.85	129.99	121.80
1	A	156	ASP	C-N-CA	5.85	129.99	121.80
1	A	307	GLU	N-CA-C	5.82	118.37	111.33
1	A	99	GLN	N-CA-C	-5.74	105.77	112.89
1	A	665	ASN	N-CA-C	-5.71	105.04	112.23
1	A	109	GLU	N-CA-C	5.63	119.24	110.17
1	A	693	ALA	N-CA-C	-5.62	101.67	108.14
1	A	497	TRP	N-CA-C	-5.62	105.24	111.36
1	A	458	GLY	N-CA-C	-5.56	104.34	110.96
1	A	319	TRP	N-CA-C	5.48	119.67	113.15
1	A	338	SER	N-CA-C	5.45	122.42	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	ASP	N-CA-C	-5.43	105.27	111.14
1	A	708	ILE	CB-CA-C	-5.43	105.10	111.94
1	A	131	ILE	N-CA-C	5.41	115.78	107.77
1	A	309	MET	N-CA-C	5.41	116.94	109.15
1	A	262	ASN	CB-CA-C	-5.36	103.04	111.51
1	A	652	ASP	CB-CA-C	-5.30	99.88	110.42
1	A	549	TYR	CA-C-N	-5.28	113.48	118.97
1	A	549	TYR	C-N-CA	-5.28	113.48	118.97
1	A	88	GLN	N-CA-C	-5.20	105.61	111.28
1	A	351	GLU	N-CA-C	5.19	116.83	108.32
1	A	431	SER	N-CA-C	5.19	116.93	111.28
1	A	173	ASP	CA-C-N	-5.17	113.61	121.31
1	A	173	ASP	C-N-CA	-5.17	113.61	121.31
1	A	443	GLN	N-CA-C	5.14	119.27	112.89
1	A	284	ALA	N-CA-C	5.14	118.33	111.75
1	A	359	ILE	N-CA-C	5.09	115.19	107.75
1	A	325	VAL	CB-CA-C	-5.08	102.11	111.36
1	A	146	PRO	CA-C-N	5.07	123.36	119.66
1	A	146	PRO	C-N-CA	5.07	123.36	119.66
1	A	123	THR	CA-C-N	-5.06	117.67	122.37
1	A	123	THR	C-N-CA	-5.06	117.67	122.37
1	A	104	GLY	N-CA-C	5.05	123.34	115.72
1	A	719	VAL	CA-C-N	-5.02	116.07	123.30
1	A	719	VAL	C-N-CA	-5.02	116.07	123.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	GLU	Peptide
1	A	338	SER	Peptide
1	A	506	PHE	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	5318	0	5004	271	1
2	B	28	0	25	0	0
2	C	28	0	25	5	0
2	D	28	0	25	2	0
3	E	50	0	43	0	1
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
7	A	42	0	39	4	0
8	A	13	0	6	2	0
9	A	21	0	0	13	0
All	All	5532	0	5167	273	1

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 26.

All (273) 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)
9:A:2019:HOH:O	2:C:1:NAG:H3	1.46	1.12
1:A:337:PHE:HB3	1:A:340:GLN:NE2	1.70	1.07
1:A:337:PHE:C	1:A:339:THR:HB	1.80	1.06
1:A:657:ASN:HD21	1:A:660:VAL:HG23	1.18	1.06
1:A:657:ASN:ND2	1:A:660:VAL:CG2	2.19	1.04
1:A:620:GLN:HA	1:A:620:GLN:NE2	1.71	1.02
1:A:337:PHE:HB3	1:A:340:GLN:HE21	0.85	1.01
1:A:315:PRO:O	1:A:316:ASP:HB3	1.56	1.00
1:A:337:PHE:CB	1:A:340:GLN:HE21	1.74	0.99
1:A:509:MET:HA	1:A:509:MET:CE	1.92	0.99
1:A:620:GLN:HA	1:A:620:GLN:HE21	1.27	0.97
1:A:657:ASN:ND2	1:A:660:VAL:HG23	1.79	0.97
1:A:509:MET:HE2	1:A:510:PRO:HD2	1.46	0.96
1:A:257:ASN:ND2	8:A:1764:QUS:O18	2.01	0.92
1:A:509:MET:HA	1:A:509:MET:HE2	1.52	0.92
1:A:197:SER:O	1:A:199:LYS:HD2	1.71	0.91
1:A:494:TYR:OH	1:A:509:MET:CE	2.19	0.91
1:A:638:ASN:O	1:A:642:ILE:HG13	1.71	0.90
1:A:456:ILE:HD13	1:A:573:HIS:CE1	2.07	0.90
1:A:138:ILE:O	2:C:1:NAG:C8	2.21	0.89
1:A:175:VAL:CG2	1:A:331:PRO:HB3	2.05	0.86
1:A:138:ILE:O	2:C:1:NAG:H83	1.74	0.86
1:A:645:LYS:O	1:A:649:ARG:HG3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:HG21	7:A:1753:NAG:H81	1.61	0.82
1:A:180:ALA:HB3	1:A:213:LYS:HB3	1.62	0.82
1:A:494:TYR:OH	1:A:509:MET:HE1	1.80	0.81
1:A:657:ASN:HD21	1:A:660:VAL:CG2	1.81	0.81
1:A:109:GLU:OE2	1:A:109:GLU:HA	1.81	0.80
1:A:618:HIS:HB3	1:A:621:GLU:OE1	1.81	0.80
1:A:654:ASP:OD1	1:A:656:SER:CB	2.30	0.79
1:A:370:ARG:NH2	1:A:666:ASP:OD1	2.17	0.78
1:A:654:ASP:OD1	1:A:656:SER:HB2	1.85	0.77
1:A:339:THR:HA	9:A:2006:HOH:O	1.85	0.76
1:A:337:PHE:HA	9:A:2005:HOH:O	1.86	0.75
1:A:337:PHE:N	9:A:2005:HOH:O	2.19	0.75
1:A:509:MET:HA	1:A:509:MET:HE3	1.68	0.74
1:A:325:VAL:HB	1:A:326:PRO:CD	2.18	0.73
1:A:456:ILE:CD1	1:A:573:HIS:CE1	2.71	0.72
1:A:175:VAL:HG22	1:A:331:PRO:HB3	1.70	0.72
1:A:334:THR:HG23	1:A:334:THR:O	1.90	0.72
1:A:439:SER:O	1:A:443:GLN:HG2	1.89	0.72
1:A:460:TYR:CE1	1:A:500:LYS:HE2	2.24	0.72
1:A:337:PHE:O	1:A:339:THR:HB	1.89	0.71
1:A:716:GLU:CD	1:A:716:GLU:H	1.97	0.71
1:A:422:ASP:O	1:A:430:GLY:HA3	1.90	0.70
1:A:235:PHE:HA	1:A:247:ASN:OD1	1.91	0.70
1:A:205:TYR:CE1	1:A:254:GLN:HB3	2.26	0.70
1:A:602:VAL:HG12	1:A:603:VAL:N	2.06	0.69
1:A:616:MET:O	1:A:619:PRO:HD3	1.93	0.68
1:A:166:PRO:HD3	1:A:290:PRO:HG2	1.74	0.68
1:A:657:ASN:ND2	1:A:660:VAL:HG21	2.05	0.68
1:A:138:ILE:O	2:C:1:NAG:H82	1.93	0.68
1:A:228:TYR:CE1	1:A:230:ASP:HB2	2.29	0.68
1:A:456:ILE:CD1	1:A:573:HIS:HE1	2.05	0.67
1:A:171:GLU:HA	1:A:342:VAL:O	1.95	0.67
1:A:334:THR:O	1:A:334:THR:CG2	2.43	0.66
1:A:719:VAL:O	1:A:721:PRO:HD3	1.96	0.66
1:A:494:TYR:OH	1:A:509:MET:HE3	1.94	0.65
1:A:173:ASP:O	1:A:174:LEU:C	2.39	0.65
1:A:366:VAL:HB	1:A:413:ARG:HG2	1.77	0.65
1:A:169:MET:HE3	1:A:347:HIS:NE2	2.11	0.65
1:A:180:ALA:CB	1:A:213:LYS:HB3	2.26	0.65
1:A:461:THR:HG23	1:A:462:LEU:O	1.96	0.65
1:A:509:MET:CE	1:A:509:MET:CA	2.72	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:CA	9:A:2005:HOH:O	2.40	0.64
1:A:509:MET:HE2	1:A:509:MET:CA	2.27	0.64
1:A:551:LEU:HD12	1:A:561:LEU:HD22	1.79	0.64
1:A:259:LEU:HD13	1:A:261:LEU:HD21	1.80	0.64
1:A:315:PRO:O	1:A:316:ASP:CB	2.34	0.63
1:A:556:TYR:O	1:A:558:THR:HG23	1.97	0.63
1:A:377:HIS:CE1	1:A:388:PRO:HB3	2.32	0.63
1:A:337:PHE:CD2	1:A:340:GLN:NE2	2.67	0.63
1:A:538:THR:HG23	1:A:539:LYS:O	1.99	0.62
1:A:155:SER:O	1:A:156:ASP:CG	2.42	0.62
1:A:448:ALA:HB3	1:A:587:LEU:HD13	1.80	0.62
1:A:137:GLU:OE2	2:C:1:NAG:H5	1.99	0.62
1:A:232:ALA:HB2	1:A:321:GLY:HA2	1.82	0.62
1:A:460:TYR:CD1	1:A:500:LYS:HE2	2.34	0.62
1:A:337:PHE:O	1:A:340:GLN:N	2.23	0.62
1:A:225:VAL:HB	1:A:294:VAL:HG22	1.82	0.61
1:A:459:ASN:OD1	7:A:1757:NAG:H2	1.99	0.61
1:A:707:GLY:O	1:A:731:GLN:HG3	1.99	0.61
1:A:177:VAL:CG2	1:A:203:ALA:HB2	2.29	0.61
1:A:339:THR:HG23	9:A:2006:HOH:O	2.00	0.61
1:A:394:VAL:O	1:A:398:ILE:HG13	2.00	0.61
1:A:195:ASN:OD1	1:A:197:SER:HB3	2.00	0.61
1:A:225:VAL:O	1:A:344:MET:HE1	2.01	0.61
1:A:620:GLN:HE21	1:A:620:GLN:CA	2.06	0.60
1:A:358:VAL:O	1:A:419:ALA:HA	2.01	0.60
1:A:325:VAL:HB	1:A:326:PRO:HD2	1.84	0.60
1:A:476:ASN:HD22	2:D:1:NAG:H83	1.66	0.60
1:A:195:ASN:ND2	7:A:1756:NAG:C7	2.65	0.60
1:A:192:MET:HE1	1:A:329:VAL:HG21	1.83	0.59
1:A:484:PRO:HD2	1:A:485:ASP:OD1	2.02	0.59
1:A:460:TYR:CD2	1:A:540:ASN:HA	2.38	0.59
1:A:174:LEU:HD13	1:A:342:VAL:HG21	1.85	0.58
1:A:232:ALA:HB2	1:A:321:GLY:CA	2.33	0.58
1:A:657:ASN:HD22	1:A:660:VAL:CG2	2.14	0.57
1:A:88:GLN:N	1:A:88:GLN:OE1	2.37	0.57
1:A:165:SER:OG	1:A:293:PRO:HA	2.05	0.57
1:A:470:MET:HE2	1:A:587:LEU:HD11	1.85	0.57
1:A:127:TYR:HE1	1:A:129:SER:OG	1.88	0.57
1:A:338:SER:N	1:A:339:THR:HB	2.16	0.57
1:A:703:GLU:HG3	1:A:704:SER:N	2.19	0.57
1:A:175:VAL:HG23	1:A:331:PRO:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:HG21	7:A:1753:NAG:C8	2.32	0.57
1:A:689:HIS:CE1	1:A:691:ILE:HB	2.40	0.57
1:A:169:MET:HE3	1:A:347:HIS:CE1	2.40	0.56
1:A:381:TRP:CH2	9:A:2003:HOH:O	2.52	0.56
1:A:509:MET:CE	1:A:510:PRO:HD2	2.27	0.56
1:A:382:VAL:HB	9:A:2008:HOH:O	2.06	0.56
1:A:412:PRO:HA	1:A:589:ASN:OD1	2.05	0.56
1:A:657:ASN:ND2	1:A:660:VAL:CB	2.68	0.56
1:A:656:SER:O	1:A:658:PRO:HD3	2.05	0.56
1:A:153:ASN:O	1:A:154:VAL:C	2.49	0.55
1:A:258:ILE:HD12	1:A:290:PRO:HG3	1.86	0.55
1:A:483:SER:HB2	1:A:496:SER:OG	2.07	0.55
1:A:650:LEU:HD13	1:A:664:MET:HE2	1.89	0.55
1:A:82:HIS:HB2	1:A:380:SER:OG	2.06	0.55
1:A:699:LYS:HE2	8:A:1764:QUS:O19	2.07	0.55
1:A:619:PRO:HA	1:A:622:MET:HB2	1.89	0.55
1:A:103:PHE:O	1:A:403:GLY:HA3	2.07	0.54
1:A:494:TYR:HH	1:A:509:MET:HE3	1.71	0.54
1:A:129:SER:HA	1:A:139:PHE:O	2.07	0.54
1:A:618:HIS:N	1:A:618:HIS:CD2	2.75	0.54
1:A:484:PRO:HG3	1:A:575:THR:OG1	2.07	0.54
1:A:109:GLU:OE2	1:A:109:GLU:CA	2.53	0.53
1:A:181:ARG:HH11	1:A:207:LYS:HG2	1.74	0.53
1:A:460:TYR:HD2	1:A:540:ASN:HA	1.72	0.53
2:D:1:NAG:H61	2:D:2:NAG:C1	2.37	0.53
1:A:236:ALA:N	1:A:247:ASN:OD1	2.41	0.53
1:A:621:GLU:O	1:A:622:MET:C	2.52	0.53
1:A:301:ASP:O	1:A:302:ALA:C	2.52	0.53
1:A:311:GLY:HA3	1:A:330:GLY:O	2.08	0.52
1:A:334:THR:HG22	1:A:337:PHE:HD1	1.73	0.52
1:A:338:SER:HB3	1:A:339:THR:OG1	2.09	0.52
1:A:191:ASP:OD1	1:A:191:ASP:N	2.41	0.51
1:A:373:ILE:HG12	1:A:417:LEU:HB2	1.92	0.51
1:A:688:ARG:HD3	9:A:2016:HOH:O	2.10	0.51
1:A:382:VAL:HG12	1:A:383:PHE:N	2.25	0.51
1:A:71:LYS:HE2	1:A:570:PHE:CE2	2.46	0.51
1:A:103:PHE:HB3	1:A:400:ARG:HA	1.93	0.51
1:A:225:VAL:O	1:A:294:VAL:HA	2.11	0.51
1:A:239:VAL:HB	1:A:247:ASN:ND2	2.26	0.51
1:A:608:ALA:O	1:A:611:ILE:HG22	2.11	0.51
1:A:242:TYR:CG	1:A:243:PRO:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:HG3	1:A:570:PHE:CZ	2.46	0.50
1:A:137:GLU:HB2	9:A:2019:HOH:O	2.11	0.50
1:A:231:PRO:HD2	1:A:323:LEU:HD13	1.93	0.50
1:A:695:SER:HB3	1:A:698:ASN:O	2.11	0.50
1:A:330:GLY:HA2	1:A:331:PRO:O	2.11	0.50
1:A:455:SER:O	1:A:536:ARG:HB2	2.12	0.50
1:A:534:ARG:HB2	9:A:2011:HOH:O	2.12	0.50
1:A:148:PRO:HG2	1:A:151:TYR:CD2	2.47	0.49
1:A:302:ALA:O	1:A:305:LEU:N	2.41	0.49
1:A:629:PHE:O	1:A:633:PHE:HD2	1.96	0.49
1:A:488:PHE:O	1:A:489:GLU:C	2.54	0.49
1:A:130:ILE:HG22	1:A:131:ILE:N	2.28	0.49
1:A:653:PHE:O	1:A:653:PHE:CD1	2.65	0.49
1:A:720:ASP:C	1:A:720:ASP:OD1	2.55	0.49
1:A:128:ILE:CD1	1:A:226:ILE:HG12	2.43	0.49
1:A:325:VAL:CB	1:A:326:PRO:CD	2.87	0.49
1:A:551:LEU:HD12	1:A:561:LEU:CD2	2.42	0.49
1:A:654:ASP:C	1:A:656:SER:N	2.71	0.49
1:A:657:ASN:HD22	1:A:660:VAL:HG21	1.74	0.48
1:A:413:ARG:HG3	1:A:413:ARG:HH11	1.79	0.48
1:A:114:ASP:OD1	1:A:354:ARG:HB2	2.13	0.48
1:A:273:PRO:HG3	1:A:437:GLU:HA	1.96	0.48
1:A:356:TYR:O	1:A:378:ARG:NH2	2.30	0.48
1:A:682:PRO:O	1:A:683:ASP:HB2	2.12	0.48
1:A:175:VAL:HG22	1:A:331:PRO:CB	2.41	0.48
1:A:333:PHE:HD1	1:A:340:GLN:O	1.96	0.48
1:A:142:SER:N	1:A:301:ASP:OD2	2.40	0.47
1:A:657:ASN:ND2	1:A:660:VAL:HB	2.29	0.47
1:A:240:LYS:O	1:A:245:GLY:HA3	2.14	0.47
1:A:602:VAL:CG1	1:A:603:VAL:N	2.77	0.47
1:A:620:GLN:NE2	1:A:620:GLN:CA	2.53	0.47
1:A:209:PHE:CE2	1:A:211:GLY:HA3	2.49	0.47
1:A:456:ILE:HD11	1:A:573:HIS:HE1	1.79	0.47
1:A:463:ARG:HD3	1:A:536:ARG:CZ	2.44	0.47
1:A:621:GLU:CD	1:A:621:GLU:H	2.21	0.47
1:A:87:GLU:CD	1:A:91:GLN:CD	2.83	0.47
1:A:652:ASP:N	1:A:652:ASP:OD2	2.48	0.47
1:A:127:TYR:CD1	1:A:127:TYR:C	2.93	0.47
1:A:337:PHE:HD2	1:A:340:GLN:NE2	2.13	0.47
1:A:330:GLY:CA	1:A:331:PRO:O	2.63	0.47
1:A:407:LYS:C	1:A:409:GLY:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PRO:HG2	1:A:323:LEU:CD1	2.45	0.46
1:A:353:THR:HG22	1:A:354:ARG:N	2.30	0.46
1:A:449:TYR:CE2	1:A:521:PHE:HA	2.50	0.46
1:A:654:ASP:C	1:A:656:SER:H	2.24	0.46
1:A:112:HIS:HA	1:A:355:ILE:O	2.15	0.46
1:A:250:GLY:CA	1:A:299:TYR:CE2	2.98	0.46
1:A:406:LYS:HA	1:A:410:TRP:O	2.16	0.45
1:A:583:MET:O	1:A:584:VAL:C	2.57	0.45
1:A:126:ASN:HA	1:A:345:HIS:O	2.16	0.45
1:A:57:ASN:ND2	1:A:60:ALA:H	2.14	0.45
1:A:518:GLY:O	1:A:519:ASN:HB2	2.16	0.45
1:A:616:MET:CE	1:A:619:PRO:HB3	2.47	0.45
1:A:616:MET:C	1:A:618:HIS:N	2.75	0.45
1:A:650:LEU:CD1	1:A:664:MET:HE2	2.47	0.45
1:A:653:PHE:CD1	1:A:653:PHE:C	2.94	0.45
1:A:191:ASP:O	1:A:192:MET:C	2.60	0.45
1:A:715:ILE:HD13	1:A:725:TRP:CE2	2.52	0.45
1:A:729:LYS:O	1:A:730:ARG:C	2.58	0.45
1:A:188:LEU:HD23	1:A:196:CYS:SG	2.57	0.45
1:A:469:LEU:O	1:A:595:PHE:HA	2.17	0.45
1:A:265:GLY:O	1:A:266:ASP:C	2.60	0.45
1:A:551:LEU:O	1:A:557:GLU:HG3	2.17	0.45
1:A:234:TYR:HD2	1:A:550:PRO:HA	1.82	0.44
1:A:106:ASP:OD1	1:A:411:ARG:NH2	2.45	0.44
1:A:658:PRO:O	1:A:661:LEU:HB3	2.17	0.44
1:A:333:PHE:O	1:A:334:THR:C	2.61	0.44
1:A:559:TYR:CD2	1:A:559:TYR:C	2.95	0.44
1:A:119:TYR:O	1:A:348:SER:HB3	2.17	0.44
1:A:132:ASN:C	1:A:132:ASN:OD1	2.60	0.44
1:A:145:GLU:OE1	1:A:555:VAL:HB	2.18	0.44
1:A:382:VAL:HG11	1:A:555:VAL:HG23	1.99	0.44
1:A:467:THR:O	1:A:468:PRO:C	2.60	0.44
1:A:561:LEU:HD12	1:A:565:PHE:HD2	1.82	0.44
1:A:170:PRO:O	1:A:343:LYS:HA	2.17	0.43
1:A:195:ASN:OD1	1:A:195:ASN:C	2.61	0.43
1:A:231:PRO:HD3	1:A:299:TYR:CD1	2.53	0.43
1:A:167:GLN:HG2	1:A:347:HIS:HA	2.00	0.43
1:A:239:VAL:HB	1:A:247:ASN:HD21	1.82	0.43
1:A:611:ILE:HD11	1:A:708:ILE:HG22	1.99	0.43
1:A:663:MET:O	1:A:663:MET:HG3	2.16	0.43
1:A:132:ASN:HB3	1:A:138:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASP:HA	1:A:429:LEU:HD22	2.00	0.43
1:A:344:MET:C	1:A:345:HIS:CD2	2.97	0.43
1:A:275:ASN:OD1	1:A:275:ASN:C	2.61	0.43
1:A:186:PHE:HD1	1:A:186:PHE:HA	1.70	0.43
1:A:333:PHE:CD1	1:A:340:GLN:O	2.72	0.43
1:A:80:ILE:HD12	1:A:88:GLN:HG2	2.01	0.42
1:A:521:PHE:CD1	1:A:521:PHE:C	2.97	0.42
1:A:131:ILE:HB	1:A:135:GLY:HA2	2.00	0.42
1:A:362:LEU:HD23	1:A:416:ILE:HD12	2.00	0.42
1:A:62:LEU:O	1:A:63:ASP:C	2.63	0.42
1:A:307:GLU:HA	1:A:325:VAL:HG12	2.02	0.42
1:A:517:SER:OG	1:A:518:GLY:N	2.53	0.42
1:A:603:VAL:HG23	1:A:607:TYR:CE2	2.53	0.42
1:A:407:LYS:C	1:A:409:GLY:N	2.76	0.42
1:A:339:THR:CA	9:A:2006:HOH:O	2.56	0.42
1:A:181:ARG:HE	1:A:181:ARG:HB2	1.39	0.41
1:A:256:GLY:HA2	9:A:2021:HOH:O	2.19	0.41
1:A:160:PRO:O	1:A:161:PHE:HB3	2.20	0.41
1:A:427:GLY:O	1:A:428:LEU:HB2	2.19	0.41
1:A:504:PRO:O	1:A:506:PHE:N	2.53	0.41
1:A:689:HIS:HB3	1:A:692:TYR:O	2.21	0.41
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.76	0.41
1:A:166:PRO:HG3	1:A:291:SER:C	2.46	0.41
1:A:272:TYR:CD2	1:A:272:TYR:N	2.89	0.41
1:A:549:TYR:O	1:A:550:PRO:C	2.63	0.41
1:A:215:LYS:HE2	1:A:219:LEU:HD11	2.01	0.41
1:A:538:THR:HG23	1:A:539:LYS:N	2.36	0.41
1:A:596:ASP:C	1:A:598:ARG:N	2.79	0.41
1:A:691:ILE:O	1:A:704:SER:HA	2.21	0.41
1:A:149:PRO:HG2	1:A:243:PRO:HG3	2.02	0.41
1:A:227:LEU:O	1:A:296:PRO:HA	2.20	0.41
1:A:334:THR:CG2	1:A:337:PHE:HD1	2.34	0.41
1:A:382:VAL:HG12	1:A:383:PHE:CD2	2.56	0.41
1:A:485:ASP:OD1	1:A:485:ASP:N	2.54	0.41
1:A:124:HIS:N	1:A:125:PRO:CD	2.82	0.40
1:A:266:ASP:OD2	1:A:269:THR:OG1	2.39	0.40
1:A:556:TYR:C	1:A:558:THR:HG23	2.46	0.40
1:A:676:ILE:HG23	1:A:688:ARG:HB2	2.02	0.40
1:A:155:SER:O	1:A:156:ASP:CB	2.69	0.40
1:A:286:ALA:HB3	1:A:289:LEU:HG	2.03	0.40
1:A:378:ARG:HB2	1:A:420:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PHE:CD2	1:A:400:ARG:HB2	2.57	0.40
1:A:326:PRO:HB2	1:A:328:ASN:CG	2.46	0.40
1:A:145:GLU:OE2	1:A:554:SER:HB2	2.20	0.40
1:A:250:GLY:HA2	1:A:299:TYR:CE2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:OE2	3:E:3:BMA:O2[2_565]	2.19	0.01

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	681/707 (96%)	587 (86%)	74 (11%)	20 (3%)	3 20

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	154	VAL
1	A	338	SER
1	A	505	GLU
1	A	192	MET
1	A	332	GLY
1	A	339	THR
1	A	602	VAL
1	A	178	ASN
1	A	617	LYS
1	A	125	PRO
1	A	382	VAL

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Mol	Chain	Res	Type
1	A	557	GLU
1	A	594	PRO
1	A	316	ASP
1	A	484	PRO
1	A	657	ASN
1	A	311	GLY
1	A	198	GLY
1	A	331	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	536/603 (89%)	474 (88%)	62 (12%)	5 23

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	58	MET
1	A	96	ILE
1	A	101	LYS
1	A	107	SER
1	A	109	GLU
1	A	123	THR
1	A	128	ILE
1	A	155	SER
1	A	158	VAL
1	A	171	GLU
1	A	174	LEU
1	A	182	THR
1	A	192	MET
1	A	197	SER
1	A	200	ILE
1	A	202	ILE
1	A	218	GLN

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Mol	Chain	Res	Type
1	A	257	ASN
1	A	258	ILE
1	A	266	ASP
1	A	306	LEU
1	A	323	LEU
1	A	325	VAL
1	A	334	THR
1	A	340	GLN
1	A	359	ILE
1	A	380	SER
1	A	396	HIS
1	A	455	SER
1	A	456	ILE
1	A	465	ASP
1	A	473	LEU
1	A	474	VAL
1	A	489	GLU
1	A	496	SER
1	A	503	SER
1	A	509	MET
1	A	537	TYR
1	A	538	THR
1	A	569	MET
1	A	571	LYS
1	A	589	ASN
1	A	590	SER
1	A	591	ILE
1	A	600	TYR
1	A	602	VAL
1	A	603	VAL
1	A	605	ARG
1	A	616	MET
1	A	618	HIS
1	A	626	SER
1	A	636	VAL
1	A	644	SER
1	A	654	ASP
1	A	656	SER
1	A	663	MET
1	A	664	MET
1	A	668	LEU
1	A	716	GLU

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Mol	Chain	Res	Type
1	A	722	SER
1	A	733	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	95	GLN
1	A	303	GLN
1	A	340	GLN
1	A	345	HIS
1	A	443	GLN
1	A	475	HIS
1	A	618	HIS
1	A	620	GLN
1	A	657	ASN
1	A	697	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

10 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	B	1	2,1	14,14,15	1.03	1 (7%)	17,19,21	1.90	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	2	2	14,14,15	0.97	1 (7%)	17,19,21	2.82	7 (41%)
2	NAG	C	1	2,1	14,14,15	1.55	3 (21%)	17,19,21	2.95	9 (52%)
2	NAG	C	2	2	14,14,15	1.12	1 (7%)	17,19,21	3.01	7 (41%)
2	NAG	D	1	2,1	14,14,15	0.88	0	17,19,21	2.82	7 (41%)
2	NAG	D	2	2	14,14,15	0.77	0	17,19,21	3.36	7 (41%)
3	NAG	E	1	3,1	14,14,15	0.59	0	17,19,21	2.37	5 (29%)
3	NAG	E	2	3	14,14,15	1.31	3 (21%)	17,19,21	3.65	7 (41%)
3	BMA	E	3	3	11,11,12	1.04	1 (9%)	15,15,17	1.39	2 (13%)
3	MAN	E	4	3	11,11,12	0.86	0	15,15,17	2.48	8 (53%)

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	B	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	4/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	4/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	NAG	C1-C2	3.85	1.57	1.52
3	E	2	NAG	C8-C7	2.66	1.56	1.50
2	C	1	NAG	O7-C7	2.55	1.29	1.23
2	B	1	NAG	O7-C7	2.49	1.28	1.23
3	E	2	NAG	O5-C1	-2.37	1.39	1.43
2	C	1	NAG	C2-N2	2.36	1.50	1.46
3	E	2	NAG	O5-C5	-2.30	1.39	1.43
2	C	2	NAG	C1-C2	2.27	1.55	1.52
2	B	2	NAG	O5-C5	2.16	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	BMA	C2-C3	2.00	1.55	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C2-N2-C7	-11.51	107.48	122.90
3	E	2	NAG	C2-N2-C7	-10.43	108.92	122.90
2	D	1	NAG	C2-N2-C7	-7.92	112.29	122.90
2	C	1	NAG	C2-N2-C7	-7.10	113.38	122.90
2	C	2	NAG	C2-N2-C7	-6.92	113.62	122.90
3	E	2	NAG	C1-O5-C5	-6.82	103.04	112.19
2	B	2	NAG	C1-O5-C5	6.75	121.23	112.19
2	B	2	NAG	O3-C3-C2	-6.20	96.53	109.40
3	E	2	NAG	C3-C4-C5	-5.82	99.69	110.23
3	E	1	NAG	C2-N2-C7	5.58	130.38	122.90
2	C	2	NAG	O3-C3-C2	-5.29	98.41	109.40
3	E	4	MAN	C1-O5-C5	-5.12	105.32	112.19
2	C	1	NAG	C1-O5-C5	-4.77	105.79	112.19
2	C	2	NAG	O5-C5-C4	-4.61	99.60	110.83
2	C	1	NAG	C1-C2-N2	4.44	117.43	110.43
2	B	2	NAG	O5-C5-C4	4.43	121.59	110.83
2	D	2	NAG	O4-C4-C5	4.31	119.94	109.32
2	C	2	NAG	C1-C2-N2	3.91	116.59	110.43
2	D	1	NAG	O5-C5-C6	-3.87	100.14	107.66
2	B	1	NAG	O4-C4-C3	-3.85	101.30	110.38
2	D	1	NAG	O3-C3-C2	-3.79	101.53	109.40
2	C	1	NAG	O5-C5-C6	3.77	115.00	107.66
3	E	4	MAN	O5-C5-C4	-3.72	101.78	110.83
3	E	1	NAG	C6-C5-C4	-3.67	104.02	113.02
3	E	3	BMA	O4-C4-C5	3.61	118.20	109.32
2	B	1	NAG	C1-O5-C5	3.54	116.93	112.19
3	E	2	NAG	O5-C1-C2	-3.41	106.01	111.29
3	E	1	NAG	O7-C7-C8	-3.35	116.09	122.05
2	C	1	NAG	C3-C4-C5	3.34	116.29	110.23
3	E	4	MAN	O5-C5-C6	3.16	113.81	107.66
2	C	1	NAG	O7-C7-C8	-3.15	116.44	122.05
2	D	1	NAG	O3-C3-C4	-3.15	102.94	110.38
2	C	2	NAG	C8-C7-N2	3.15	121.34	116.12
3	E	4	MAN	C3-C4-C5	-3.15	104.52	110.23
3	E	1	NAG	O4-C4-C3	3.14	117.78	110.38
2	B	1	NAG	O5-C5-C6	3.09	113.67	107.66
3	E	1	NAG	O7-C7-N2	3.07	127.40	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	O5-C1-C2	3.03	115.98	111.29
2	C	2	NAG	O7-C7-C8	-3.03	116.66	122.05
3	E	4	MAN	O4-C4-C3	-2.93	103.47	110.38
2	D	1	NAG	O4-C4-C5	2.82	116.26	109.32
2	C	1	NAG	C8-C7-N2	2.80	120.77	116.12
3	E	4	MAN	C6-C5-C4	2.78	119.85	113.02
2	D	1	NAG	O6-C6-C5	-2.78	101.87	111.33
2	B	1	NAG	C4-C3-C2	-2.68	107.09	111.02
2	D	2	NAG	O6-C6-C5	-2.62	102.43	111.33
2	B	1	NAG	C3-C4-C5	-2.60	105.52	110.23
3	E	2	NAG	O4-C4-C3	2.59	116.49	110.38
2	B	2	NAG	C6-C5-C4	-2.56	106.73	113.02
3	E	4	MAN	O2-C2-C1	2.56	115.08	109.22
3	E	3	BMA	C1-C2-C3	2.44	113.20	109.64
2	D	2	NAG	C1-C2-N2	-2.44	106.59	110.43
2	B	2	NAG	C8-C7-N2	2.41	120.11	116.12
2	C	2	NAG	O4-C4-C5	2.39	115.21	109.32
2	C	1	NAG	C4-C3-C2	2.35	114.46	111.02
3	E	4	MAN	C2-C3-C4	2.19	114.72	110.86
2	B	2	NAG	O4-C4-C5	2.18	114.68	109.32
3	E	2	NAG	O5-C5-C6	-2.16	103.47	107.66
2	C	1	NAG	O4-C4-C3	-2.09	105.46	110.38
2	B	1	NAG	C8-C7-N2	-2.08	112.68	116.12
2	D	2	NAG	C3-C4-C5	-2.07	106.48	110.23
2	D	2	NAG	O7-C7-N2	-2.06	118.34	121.98
2	B	2	NAG	O7-C7-N2	-2.04	118.38	121.98
2	D	1	NAG	O5-C1-C2	-2.02	108.17	111.29
3	E	2	NAG	C6-C5-C4	2.00	117.93	113.02

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

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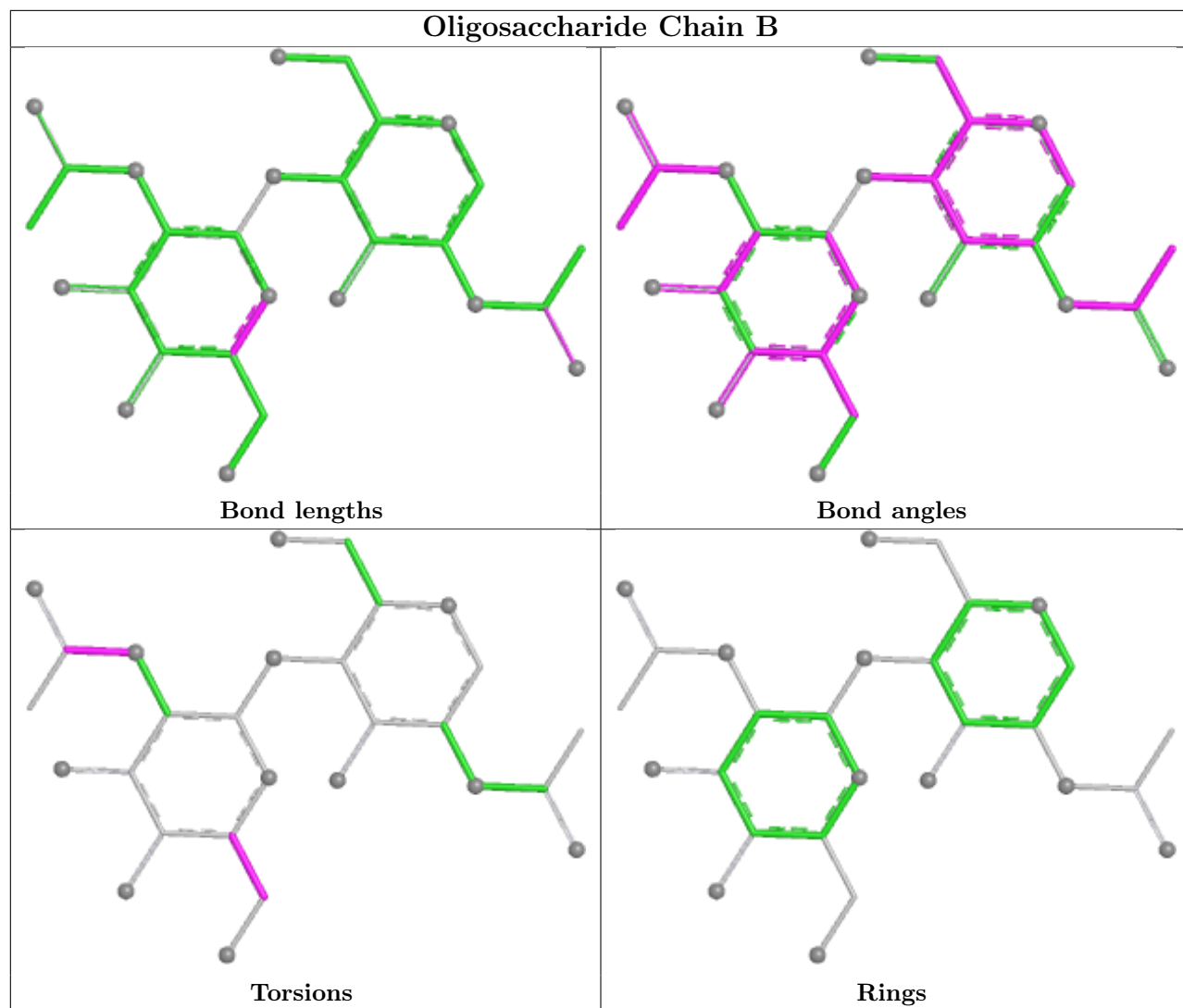
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	D	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
2	C	1	NAG	O7-C7-N2-C2

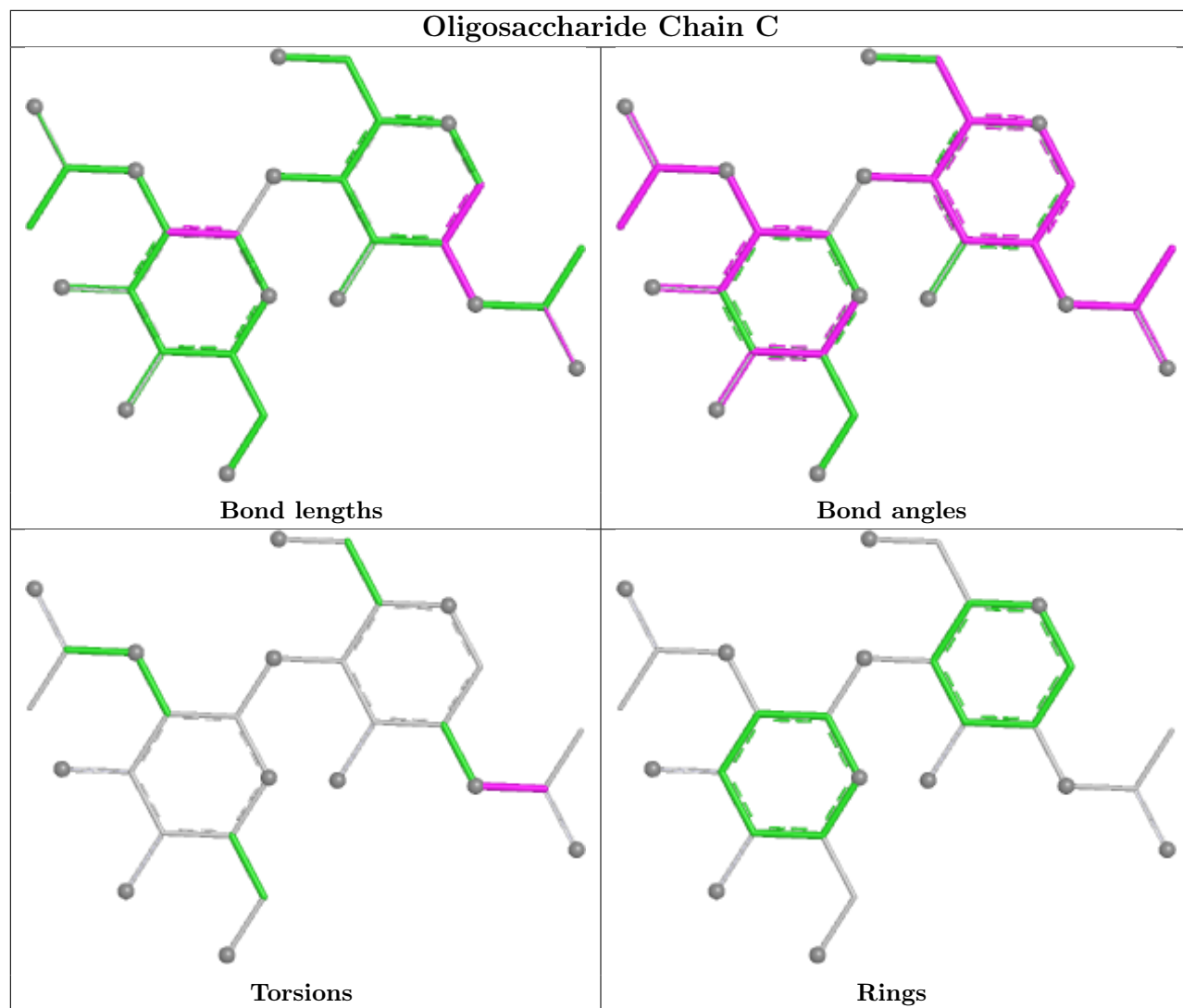
There are no ring outliers.

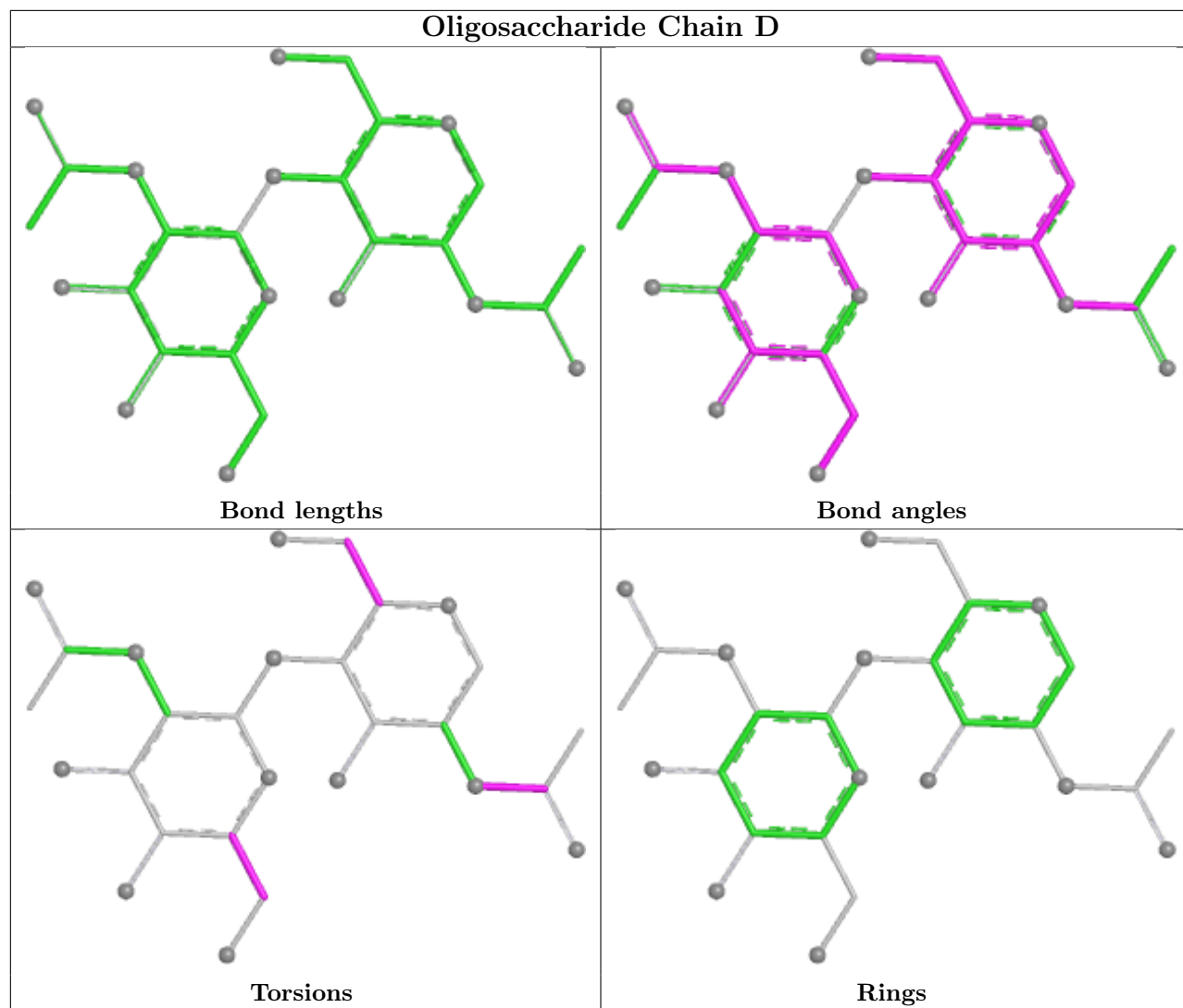
4 monomers are involved in 8 short contacts:

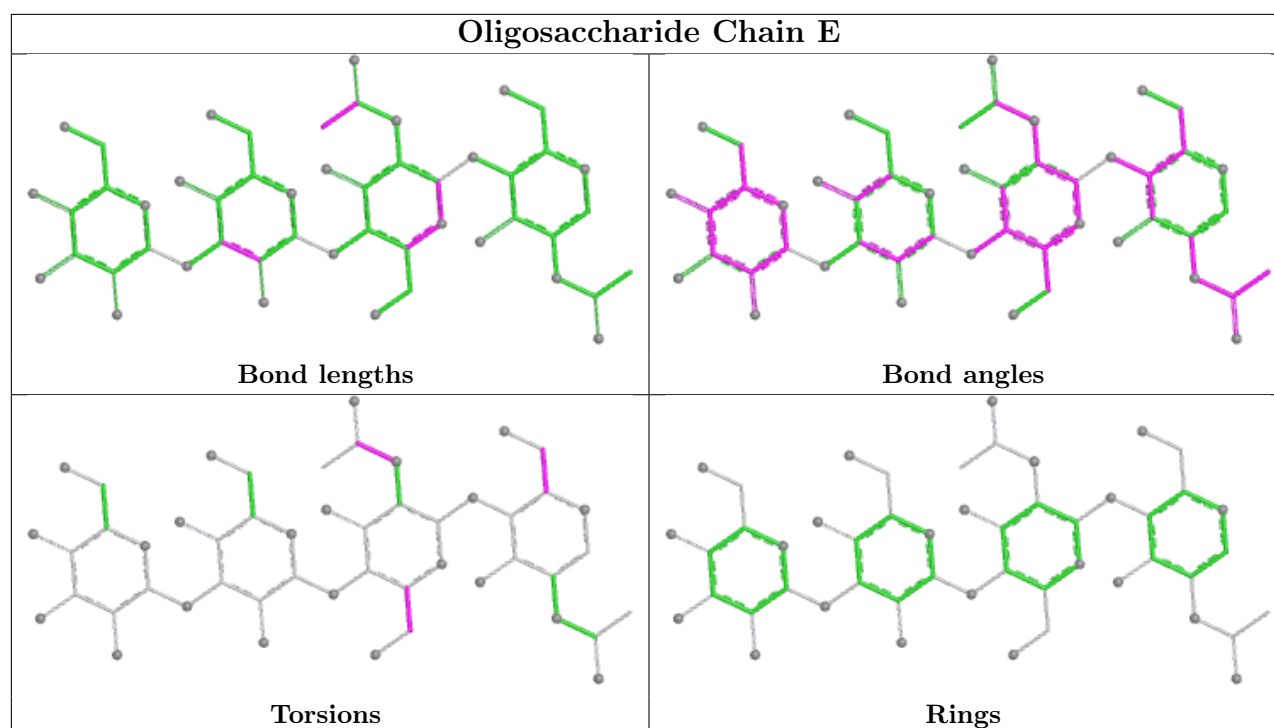
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3	BMA	0	1
2	D	2	NAG	1	0
2	D	1	NAG	2	0
2	C	1	NAG	5	0

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
7	NAG	A	1757	1	14,14,15	1.09	1 (7%)	17,19,21	2.68	7 (41%)
7	NAG	A	1753	1	14,14,15	1.37	3 (21%)	17,19,21	3.01	7 (41%)
7	NAG	A	1756	1	14,14,15	1.90	6 (42%)	17,19,21	2.63	8 (47%)
8	QUS	A	1764	-	9,13,13	1.69	2 (22%)	10,18,18	1.84	4 (40%)

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
7	NAG	A	1757	1	-	5/6/23/26	0/1/1/1
7	NAG	A	1753	1	-	4/6/23/26	0/1/1/1
7	NAG	A	1756	1	-	5/6/23/26	0/1/1/1
8	QUS	A	1764	-	-	1/6/8/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1764	QUS	C04-N15	-3.51	1.32	1.38
7	A	1756	NAG	O5-C5	3.14	1.49	1.43
7	A	1756	NAG	O5-C1	2.92	1.48	1.43
7	A	1756	NAG	C8-C7	2.63	1.56	1.50
7	A	1757	NAG	O5-C1	2.60	1.48	1.43
7	A	1753	NAG	O5-C5	2.48	1.48	1.43
7	A	1756	NAG	O7-C7	2.48	1.28	1.23
8	A	1764	QUS	O18-C04	-2.37	1.18	1.23
7	A	1753	NAG	O5-C1	2.26	1.47	1.43
7	A	1753	NAG	C6-C5	2.17	1.59	1.51
7	A	1756	NAG	C4-C3	2.03	1.57	1.52
7	A	1756	NAG	C1-C2	2.01	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1757	NAG	C4-C3-C2	-6.26	101.85	111.02
7	A	1756	NAG	C1-O5-C5	6.25	120.56	112.19
7	A	1753	NAG	O5-C5-C6	5.80	118.94	107.66
7	A	1757	NAG	C1-O5-C5	5.60	119.69	112.19
7	A	1753	NAG	C3-C4-C5	-5.43	100.38	110.23
7	A	1753	NAG	C1-O5-C5	5.09	119.01	112.19
7	A	1753	NAG	C4-C3-C2	-4.94	103.78	111.02
7	A	1756	NAG	O5-C5-C6	4.07	115.58	107.66
7	A	1753	NAG	C2-N2-C7	-3.85	117.74	122.90
7	A	1757	NAG	C2-N2-C7	-3.64	118.02	122.90
7	A	1756	NAG	O4-C4-C3	3.56	118.77	110.38
8	A	1764	QUS	O18-C04-N14	-3.45	121.85	126.37
7	A	1756	NAG	C1-C2-N2	3.29	115.61	110.43
7	A	1756	NAG	C6-C5-C4	-3.15	105.28	113.02
7	A	1753	NAG	O4-C4-C5	3.02	116.76	109.32
7	A	1757	NAG	O7-C7-N2	2.96	127.21	121.98
7	A	1756	NAG	O5-C1-C2	-2.90	106.80	111.29
7	A	1757	NAG	O5-C5-C6	2.86	113.24	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1764	QUS	N15-C04-N14	2.50	108.50	106.10
7	A	1757	NAG	C8-C7-N2	-2.38	112.17	116.12
7	A	1756	NAG	C2-N2-C7	2.33	126.03	122.90
7	A	1757	NAG	O5-C1-C2	2.28	114.83	111.29
7	A	1756	NAG	C3-C4-C5	2.14	114.12	110.23
8	A	1764	QUS	O20-N14-C03	2.06	117.92	113.83
7	A	1753	NAG	O6-C6-C5	2.04	118.29	111.33
8	A	1764	QUS	O20-C05-N15	2.04	107.98	106.14

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1753	NAG	C8-C7-N2-C2
7	A	1753	NAG	O7-C7-N2-C2
7	A	1756	NAG	C1-C2-N2-C7
7	A	1756	NAG	C8-C7-N2-C2
7	A	1756	NAG	O7-C7-N2-C2
8	A	1764	QUS	C01-C02-C03-N14
7	A	1753	NAG	O5-C5-C6-O6
7	A	1756	NAG	O5-C5-C6-O6
7	A	1757	NAG	C4-C5-C6-O6
7	A	1756	NAG	C4-C5-C6-O6
7	A	1757	NAG	O5-C5-C6-O6
7	A	1753	NAG	C4-C5-C6-O6
7	A	1757	NAG	C8-C7-N2-C2
7	A	1757	NAG	O7-C7-N2-C2
7	A	1757	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1757	NAG	1	0
7	A	1753	NAG	2	0
7	A	1756	NAG	1	0
8	A	1764	QUS	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 [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	687/707 (97%)	0.12	6 (0%) 81 61	35, 35, 35, 35	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	SER	3.4
1	A	656	SER	2.9
1	A	136	ASN	2.5
1	A	153	ASN	2.4
1	A	155	SER	2.2
1	A	546	PHE	2.2

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

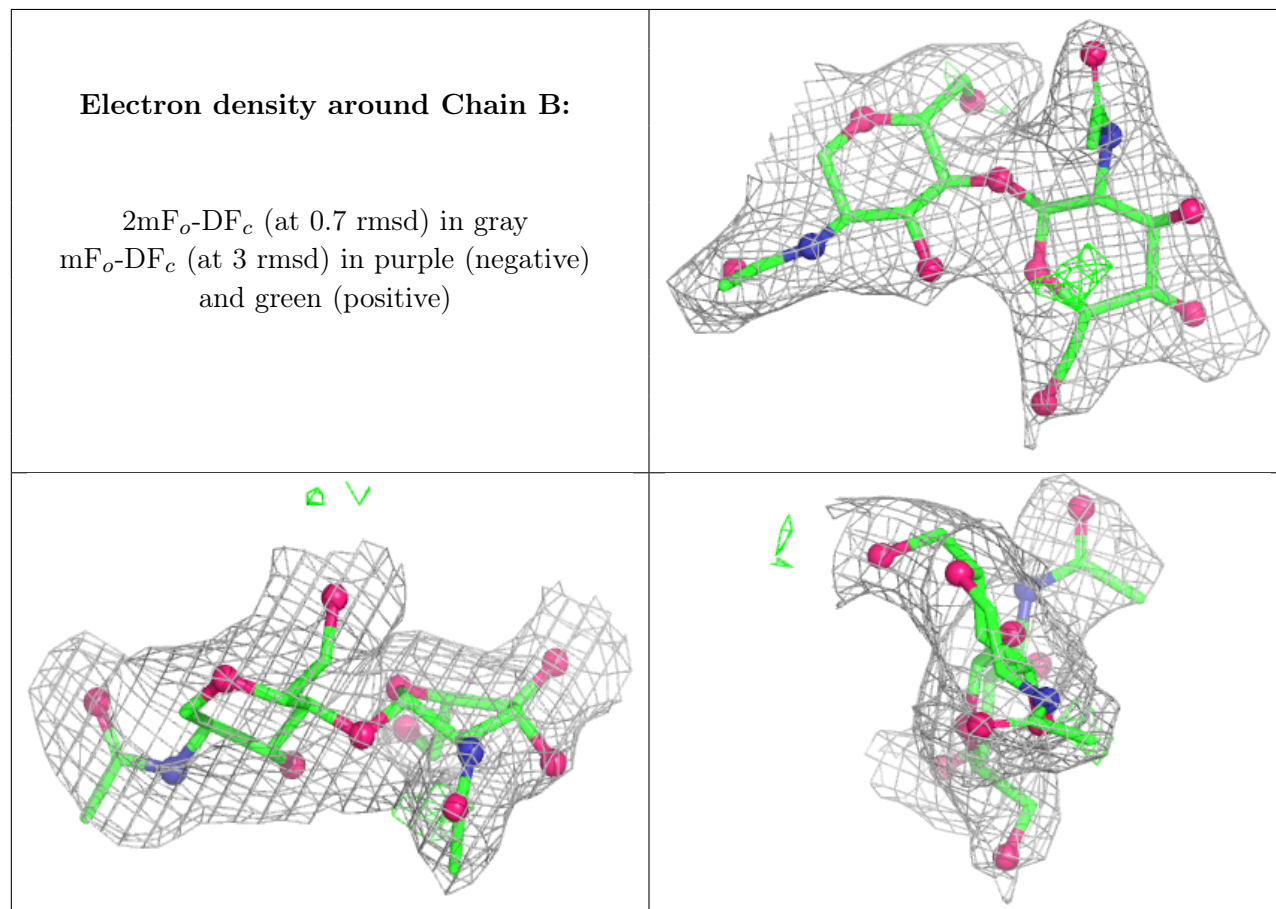
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	C	2	14/15	0.81	0.12	35,35,35,35	0
3	NAG	E	2	14/15	0.85	0.13	35,35,35,35	0
2	NAG	B	2	14/15	0.86	0.13	35,35,35,35	0
2	NAG	D	2	14/15	0.88	0.10	35,35,35,35	0
2	NAG	C	1	14/15	0.90	0.10	35,35,35,35	0
3	MAN	E	4	11/12	0.90	0.09	35,35,35,35	0

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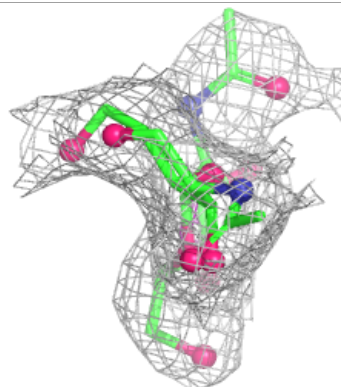
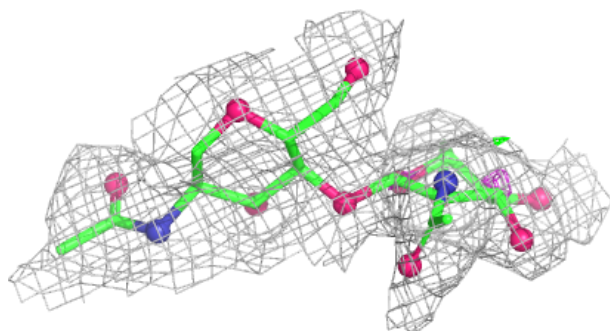
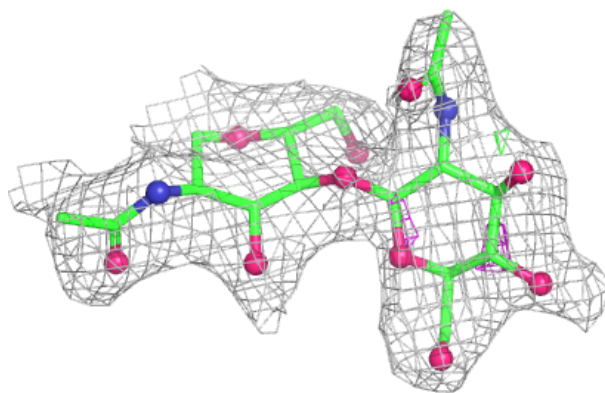
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	D	1	14/15	0.93	0.10	35,35,35,35	0
3	BMA	E	3	11/12	0.93	0.07	35,35,35,35	0
3	NAG	E	1	14/15	0.93	0.10	35,35,35,35	0
2	NAG	B	1	14/15	0.95	0.07	35,35,35,35	0

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.

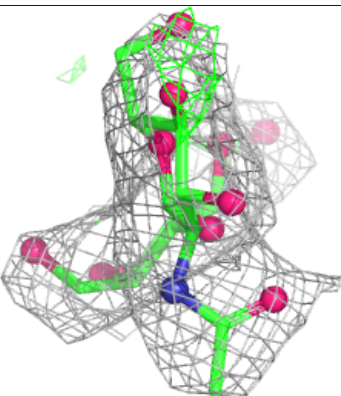
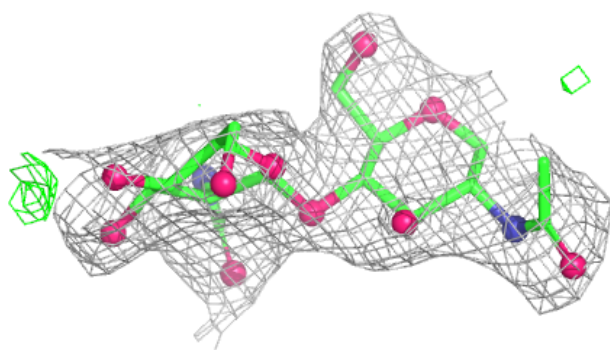
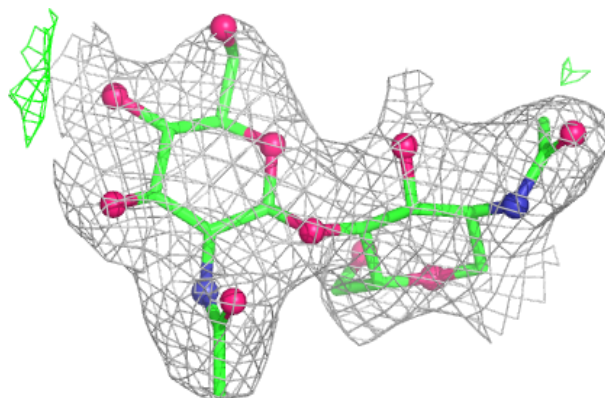


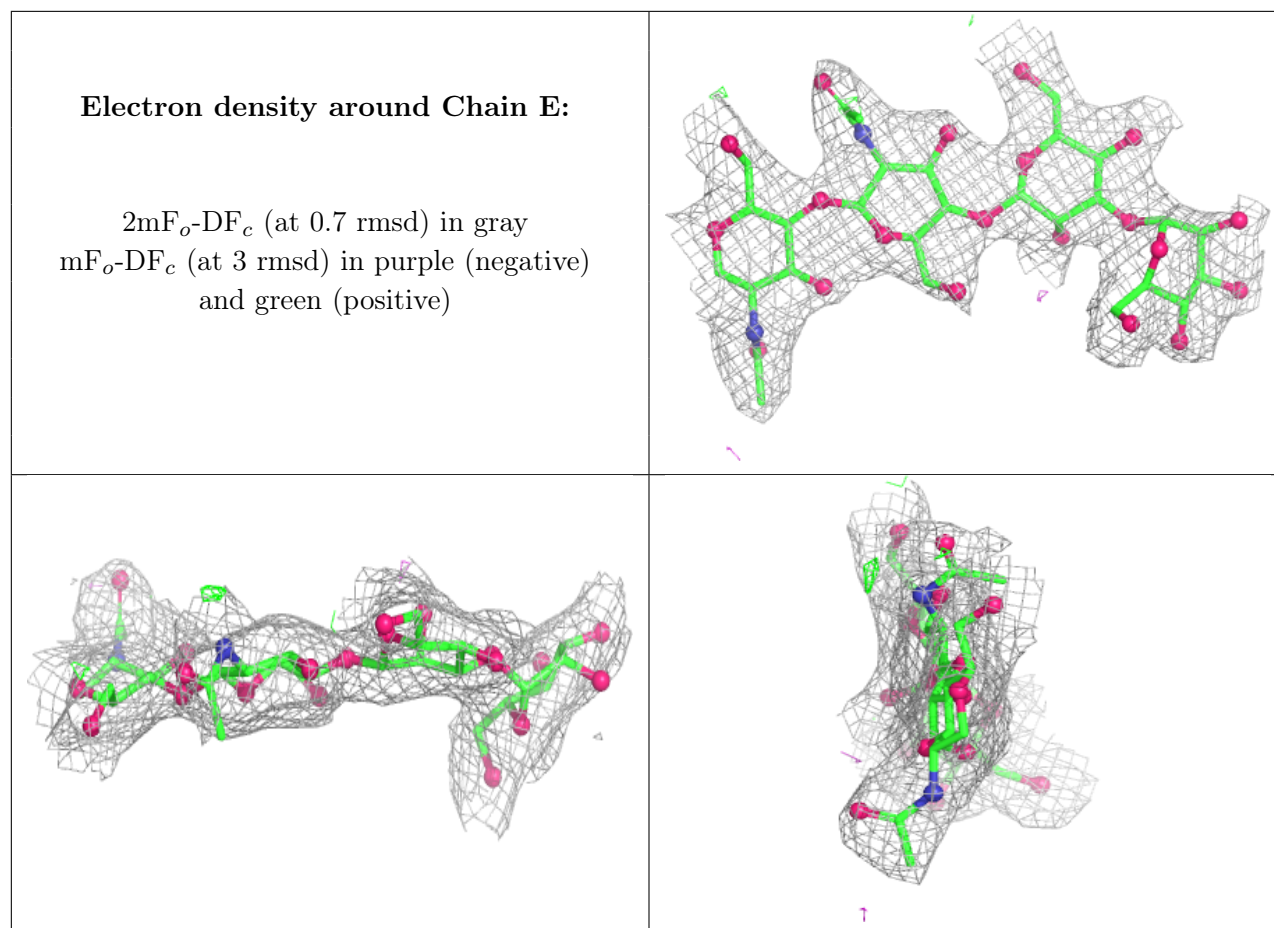
Electron density around Chain C:

$2mF_o-DF_c$ (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(Å ²)	Q<0.9
7	NAG	A	1756	14/15	0.70	0.16	35,35,35,35	0
7	NAG	A	1753	14/15	0.87	0.15	35,35,35,35	0
7	NAG	A	1757	14/15	0.90	0.13	35,35,35,35	0
6	CL	A	804	1/1	0.96	0.08	35,35,35,35	0
8	QUS	A	1764	13/13	0.96	0.10	35,35,35,35	0
4	ZN	A	801	1/1	0.98	0.06	35,35,35,35	0
5	CA	A	803	1/1	0.99	0.07	35,35,35,35	0
4	ZN	A	802	1/1	0.99	0.04	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.