Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:41 PM BST

PDB ID	:	1ORV
Title	:	Crystal Structure of Porcine Dipeptidyl Peptidase IV (CD26)
Authors	:	Engel, M.; Hoffmann, T.; Wagner, L.; Wermann, M.; Heiser, U.; Kiefersauer, R.; Huber, R.; Bode, W.; Demuth, H.U.; Brandstetter, H.
Deposited on	:	2003-03-16
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

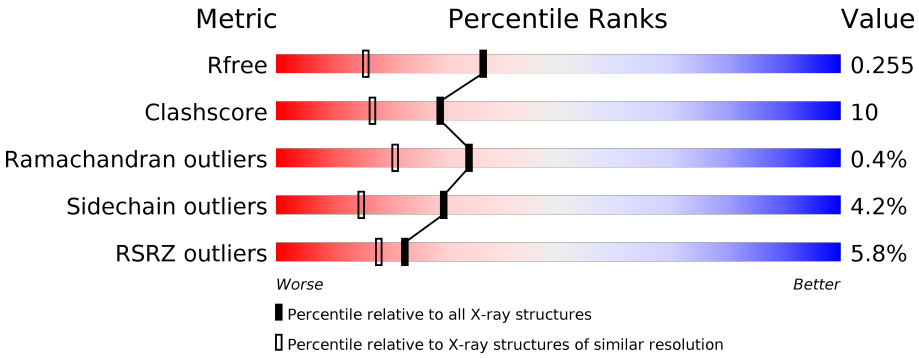
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	728	8% 79% 20%
1	B	728	4% 80% 20%
1	C	728	6% 78% 19%
1	D	728	6% 77% 21%
2	E	2	50% 50%
2	F	2	100%

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Mol	Chain	Length	Quality of chain
2	H	2	100%
2	I	2	50% 50%
2	K	2	100%
2	L	2	50% 50%
2	M	2	50% 50%
3	G	3	67% 33%
3	J	3	33% 33% 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	K	2	-	-	-	X
4	NAG	A	767(A)	-	-	-	X
4	NAG	D	767(A)	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25836 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 dipeptidyl peptidase IV.

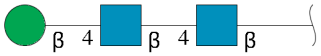
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	80	0	0
			5966	3825	986	1132	23			
1	B	728	Total	C	N	O	S	42	0	0
			5966	3825	986	1132	23			
1	C	728	Total	C	N	O	S	83	0	0
			5966	3825	986	1132	23			
1	D	728	Total	C	N	O	S	36	0	0
			5966	3825	986	1132	23			

- 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	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

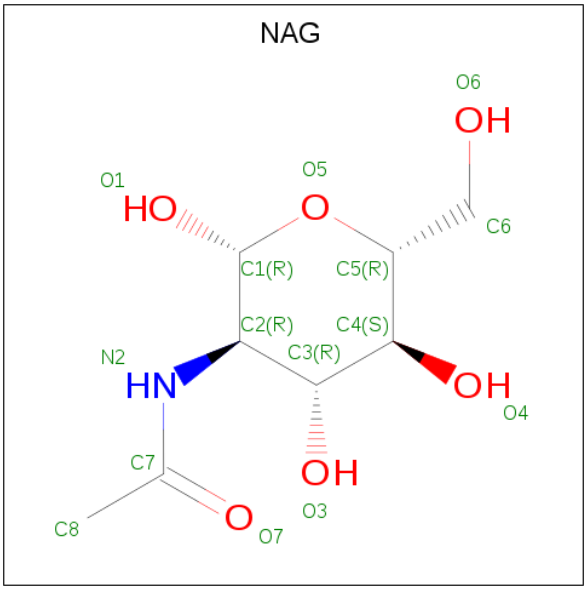
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	G	3	Total C N O 39 22 2 15	0	0	0
3	J	3	Total C N O 39 22 2 15	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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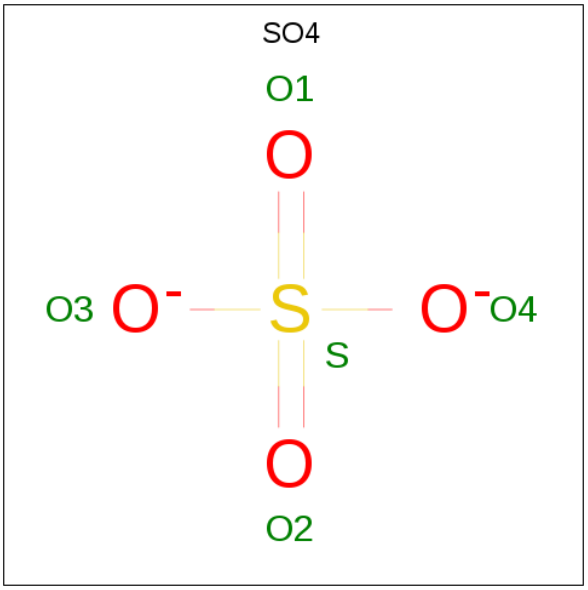
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0

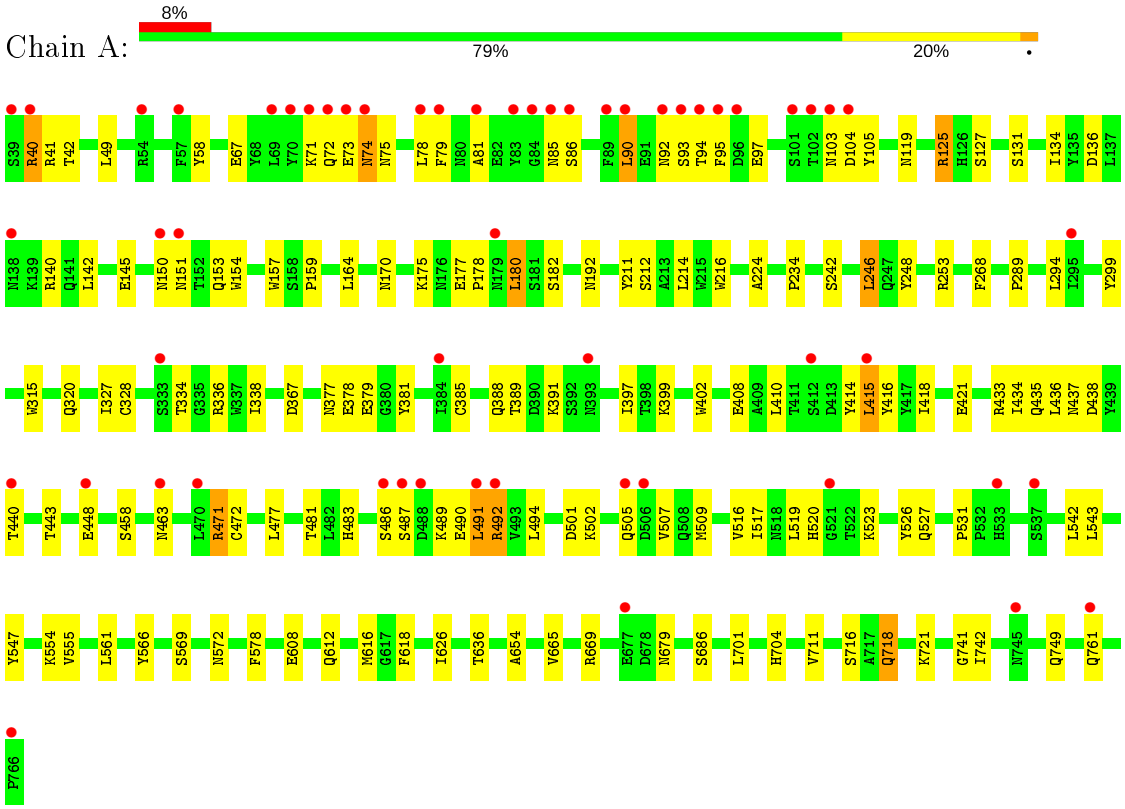
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	334	Total O 334 334	0	0
6	B	431	Total O 431 431	0	0
6	C	378	Total O 378 378	0	0
6	D	325	Total O 325 325	0	0

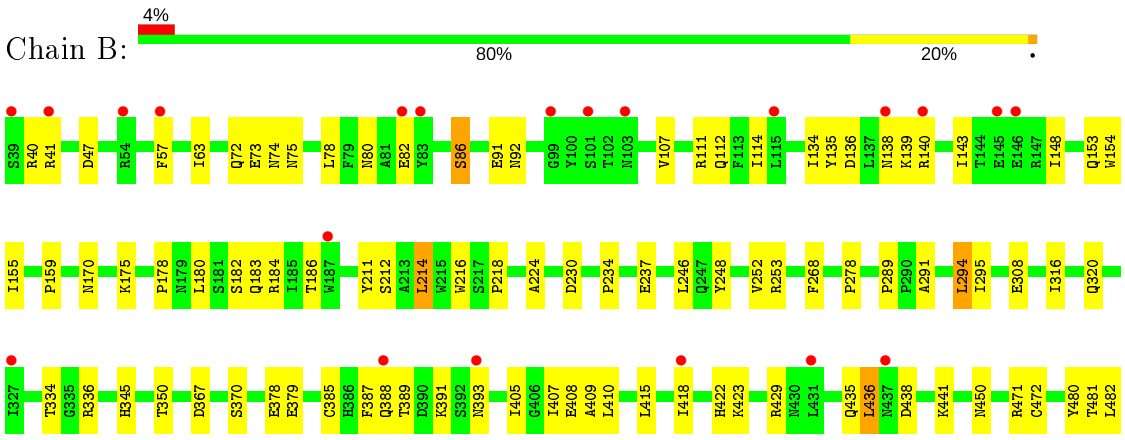
3 Residue-property plots (i)

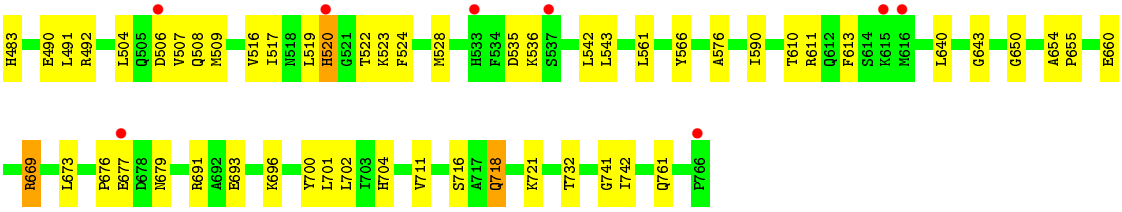
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: dipeptidyl peptidase IV



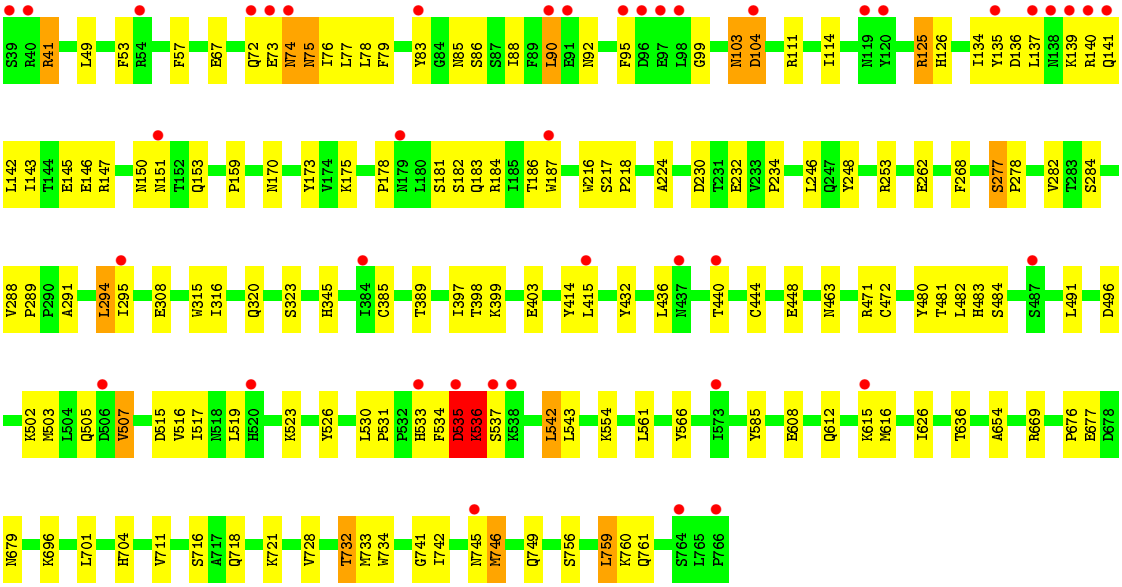
- Molecule 1: dipeptidyl peptidase IV





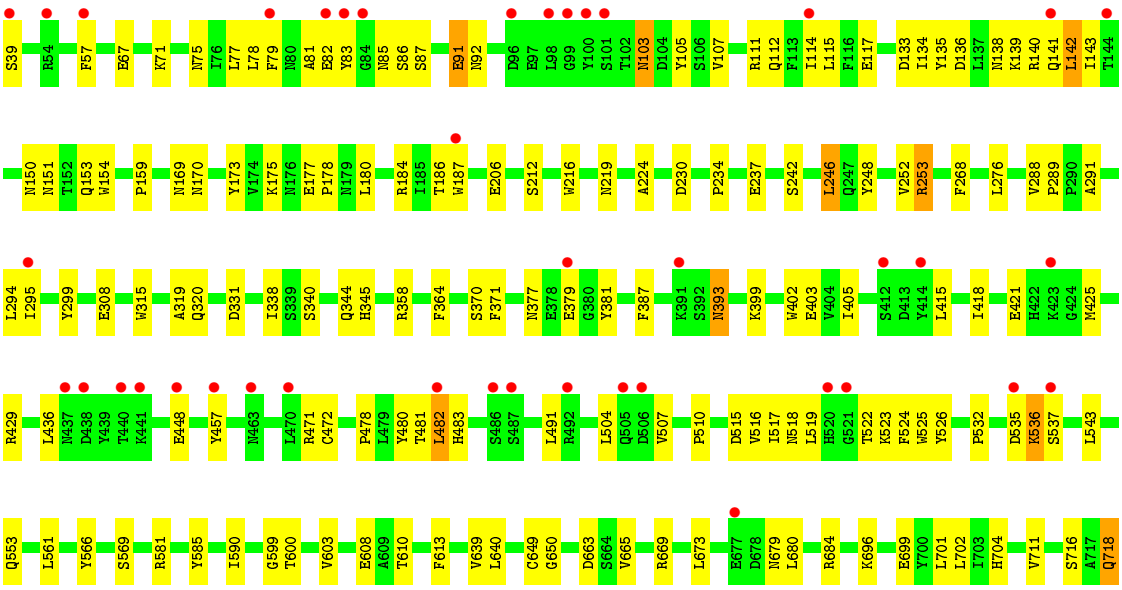
• Molecule 1: dipeptidyl peptidase IV

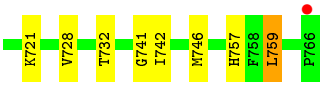
Chain C:



• Molecule 1: dipeptidyl peptidase IV

Chain D:



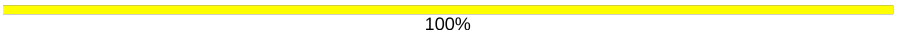


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

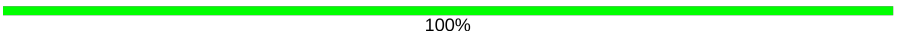
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain H:

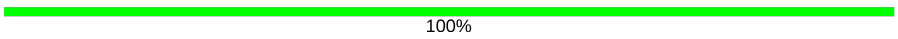


• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

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

Chain K:



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

Chain L:

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

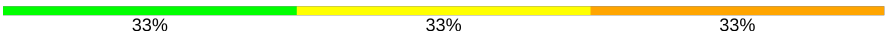
Chain M:

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

Chain G:

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

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	62.00Å 118.18Å 133.59Å 112.76° 94.93° 91.14°	Depositor
Resolution (Å)	19.25 – 1.80 19.25 – 1.78	Depositor EDS
% Data completeness (in resolution range)	96.2 (19.25-1.80) 96.1 (19.25-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 1.78Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.252 0.222 , 0.255	Depositor DCC
R_{free} test set	15446 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 53.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25836	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BMA, NAG, SO4

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	0.47	0/6141	0.71	1/8353 (0.0%)
1	B	0.51	0/6141	0.73	2/8353 (0.0%)
1	C	0.49	0/6141	0.73	3/8353 (0.0%)
1	D	0.44	0/6141	0.69	1/8353 (0.0%)
All	All	0.48	0/24564	0.71	7/33412 (0.0%)

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	B	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	103	ASN	N-CA-C	7.01	129.93	111.00
1	C	104	ASP	N-CA-C	-6.74	92.79	111.00
1	B	669	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	D	319	ALA	N-CA-C	-5.55	96.03	111.00
1	A	214	LEU	CA-CB-CG	5.21	127.28	115.30
1	B	214	LEU	CA-CB-CG	5.11	127.04	115.30
1	C	542	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	TYR	Sidechain
1	B	700	TYR	Sidechain

5.2 Too-close contacts (i)

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	5966	0	5663	102	0
1	B	5966	0	5663	105	0
1	C	5966	0	5662	125	0
1	D	5966	0	5662	129	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
3	G	39	0	34	1	0
3	J	39	0	34	1	0
4	A	56	0	52	2	0
4	B	56	0	52	2	0
4	C	70	0	65	1	0
4	D	28	0	26	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	334	0	0	5	0
6	B	431	0	0	11	0
6	C	378	0	0	8	0
6	D	325	0	0	10	0
All	All	25836	0	23088	449	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 (449) 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:C:516:VAL:HG11	1:C:523:LYS:HB2	1.40	1.01
1:C:535:ASP:C	1:C:536:LYS:HD3	1.83	0.97
1:C:536:LYS:HG2	1:C:537:SER:H	1.31	0.95
1:A:492:ARG:HH21	1:A:492:ARG:HB3	1.36	0.87
1:C:746:MET:CE	1:C:746:MET:H	1.89	0.86
1:D:75:ASN:ND2	1:D:92:ASN:H	1.78	0.81
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.78	0.81
1:D:746:MET:HE3	6:D:1816:HOH:O	1.81	0.80
1:B:378:GLU:H	1:B:378:GLU:CD	1.83	0.80
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.80	0.79
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.81	0.78
1:B:407:ILE:HG23	1:B:415:LEU:HD21	1.64	0.78
1:C:253:ARG:HH21	1:D:253:ARG:HH22	1.33	0.77
1:B:693:GLU:OE1	1:B:696:LYS:HE3	1.84	0.77
1:D:680:LEU:HD11	1:D:684:ARG:HE	1.49	0.77
1:D:291:ALA:O	1:D:295:ILE:HG13	1.85	0.77
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.83	0.76
1:C:516:VAL:CG1	1:C:523:LYS:HB2	2.15	0.75
1:B:75:ASN:ND2	1:B:92:ASN:H	1.85	0.75
1:A:492:ARG:NH2	1:A:492:ARG:HB3	2.02	0.74
1:A:75:ASN:HD22	1:A:92:ASN:ND2	1.85	0.73
1:B:490:GLU:O	1:B:492:ARG:N	2.21	0.73
1:D:184:ARG:HD3	1:D:186:THR:O	1.89	0.72
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.72	0.72
1:B:516:VAL:HG13	1:B:524:PHE:O	1.90	0.72
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.87	0.72
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.89	0.71
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.88	0.71
1:B:111:ARG:HD2	6:B:1806:HOH:O	1.89	0.71
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.71	0.71
1:C:746:MET:H	1:C:746:MET:HE3	1.54	0.71
1:C:184:ARG:HD3	1:C:186:THR:O	1.90	0.71
1:C:139:LYS:HD3	1:C:141:GLN:NE2	2.06	0.71
1:A:388:GLN:HB2	1:A:391:LYS:HB2	1.72	0.70
1:A:507:VAL:HG13	1:A:509:MET:HG2	1.73	0.70
1:C:519:LEU:HD22	1:C:608:GLU:OE1	1.92	0.70
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.88	0.69
1:C:733:MET:HA	1:D:732:THR:CG2	2.23	0.69
1:D:536:LYS:O	1:D:537:SER:HB2	1.91	0.69
1:D:704:HIS:HD2	1:D:716:SER:OG	1.77	0.68
1:D:83:TYR:HB3	1:D:85:ASN:OD1	1.93	0.68
1:C:75:ASN:HD22	1:C:92:ASN:HB2	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:HB3	1:A:92:ASN:N	2.08	0.68
1:C:440:THR:HG21	6:C:1719:HOH:O	1.95	0.67
1:C:734:TRP:CZ3	1:D:732:THR:OG1	2.48	0.66
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.16	0.66
1:D:87:SER:HB3	4:D:767(A):NAG:O6	1.95	0.66
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.79	0.66
1:B:490:GLU:O	1:B:490:GLU:HG2	1.95	0.66
1:B:704:HIS:HD2	1:B:716:SER:OG	1.78	0.66
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.79	0.65
1:B:691:ARG:HG3	1:B:691:ARG:HH11	1.62	0.64
1:C:90:LEU:HD13	1:C:90:LEU:O	1.98	0.64
1:D:288:VAL:CG1	1:D:289:PRO:HD2	2.28	0.64
1:A:418:ILE:HD12	6:A:1739:HOH:O	1.98	0.63
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.80	0.63
1:C:704:HIS:HD2	1:C:716:SER:OG	1.80	0.63
1:A:433:ARG:NH1	1:A:443:THR:HG21	2.14	0.63
1:C:612:GLN:O	1:C:615:LYS:HG2	1.98	0.63
1:C:536:LYS:HG2	1:C:537:SER:N	2.10	0.62
1:D:516:VAL:HG11	1:D:523:LYS:HB2	1.80	0.62
1:A:408:GLU:HG2	6:A:1624:HOH:O	1.98	0.62
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.97	0.62
1:A:93:SER:C	1:A:95:PHE:H	2.03	0.61
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.83	0.61
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.82	0.61
1:B:516:VAL:HG11	1:B:523:LYS:HB2	1.82	0.61
1:D:153:GLN:HE22	1:D:170:ASN:HD22	1.45	0.61
1:B:516:VAL:HG12	1:B:517:ILE:N	2.16	0.61
1:B:134:ILE:HG21	1:B:178:PRO:HB3	1.80	0.61
1:A:153:GLN:HE22	1:A:170:ASN:HD22	1.47	0.60
1:C:218:PRO:HD2	1:C:308:GLU:OE2	2.01	0.60
1:A:458:SER:OG	1:A:471:ARG:HD3	2.02	0.60
1:B:175:LYS:HZ1	1:B:178:PRO:HA	1.67	0.60
1:C:718:GLN:HE22	1:C:721:LYS:NZ	1.99	0.60
1:C:733:MET:HA	1:D:732:THR:HG22	1.84	0.60
1:D:111:ARG:HD2	6:D:1812:HOH:O	2.00	0.60
1:D:482:LEU:HD22	1:D:491:LEU:HD12	1.84	0.60
1:D:377:ASN:HB3	1:D:379:GLU:H	1.66	0.59
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.32	0.59
6:C:1685:HOH:O	1:D:746:MET:HE1	2.02	0.59
1:B:218:PRO:HD2	1:B:308:GLU:OE2	2.02	0.59
1:B:75:ASN:HD22	1:B:92:ASN:H	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.37	0.59
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.38	0.59
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.84	0.59
1:A:516:VAL:HG11	1:A:523:LYS:HB2	1.85	0.58
1:C:291:ALA:O	1:C:295:ILE:HG13	2.03	0.58
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.84	0.58
1:D:504:LEU:HA	1:D:507:VAL:HG12	1.85	0.58
1:D:746:MET:CE	6:D:1816:HOH:O	2.46	0.58
1:B:522:THR:HG21	1:B:590:ILE:HD11	1.85	0.58
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.24	0.58
1:C:414:TYR:HA	1:C:436:LEU:HD13	1.85	0.58
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.03	0.58
1:B:334:THR:OG1	1:B:336:ARG:HG2	2.04	0.58
1:B:418:ILE:HD12	6:B:1782:HOH:O	2.04	0.58
1:C:536:LYS:N	1:C:536:LYS:HD3	2.19	0.57
1:C:502:LYS:O	1:C:505:GLN:HG2	2.05	0.57
1:A:519:LEU:HD22	1:A:608:GLU:OE2	2.03	0.57
1:A:502:LYS:O	1:A:505:GLN:HG2	2.05	0.57
1:C:536:LYS:CG	1:C:537:SER:H	2.06	0.57
1:D:718:GLN:HE22	1:D:721:LYS:NZ	2.02	0.56
1:A:58:TYR:CD2	1:A:494:LEU:HB3	2.40	0.56
1:B:80:ASN:OD1	1:B:82:GLU:HB2	2.05	0.56
1:B:408:GLU:HG2	6:B:1696:HOH:O	2.05	0.56
1:A:704:HIS:HD2	1:A:716:SER:OG	1.88	0.56
1:B:704:HIS:HE1	1:B:711:VAL:O	1.89	0.56
1:D:522:THR:HB	1:D:524:PHE:CE1	2.41	0.56
1:B:175:LYS:HZ2	1:B:175:LYS:HB3	1.71	0.56
1:A:481:THR:OG1	1:A:483:HIS:CE1	2.58	0.55
1:A:72:GLN:HG2	1:A:73:GLU:HG3	1.87	0.55
1:B:291:ALA:O	1:B:295:ILE:HG23	2.07	0.55
1:C:74:ASN:HB2	1:C:92:ASN:ND2	2.22	0.55
1:A:41:ARG:HB2	6:A:1780:HOH:O	2.05	0.55
1:C:320:GLN:OE1	1:C:669:ARG:HD3	2.06	0.55
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.41	0.55
1:B:175:LYS:NZ	1:B:178:PRO:HA	2.21	0.55
1:B:57:PHE:HA	1:B:480:TYR:CE1	2.42	0.55
1:C:288:VAL:HG13	1:C:289:PRO:HD2	1.89	0.55
1:A:92:ASN:C	1:A:94:THR:H	2.09	0.55
1:C:676:PRO:HG2	1:C:677:GLU:OE2	2.07	0.55
1:A:377:ASN:HB2	1:A:381:TYR:O	2.07	0.55
1:A:93:SER:C	1:A:95:PHE:N	2.58	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:THR:HG22	4:B:773(A):NAG:H81	1.89	0.55
1:C:483:HIS:HA	1:C:491:LEU:HD23	1.89	0.55
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.37	0.55
1:D:134:ILE:HG21	1:D:178:PRO:HB3	1.89	0.54
1:B:507:VAL:HG13	1:B:509:MET:HG2	1.90	0.54
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.89	0.54
1:B:388:GLN:HB3	1:B:391:LYS:HB2	1.89	0.54
1:A:75:ASN:HD22	1:A:92:ASN:HD22	1.55	0.54
1:B:516:VAL:HG11	1:B:523:LYS:HD2	1.89	0.54
1:D:77:LEU:HB2	1:D:79:PHE:HE2	1.73	0.54
1:D:393:ASN:H	1:D:393:ASN:HD22	1.53	0.54
1:A:492:ARG:HH21	1:A:492:ARG:CB	2.15	0.54
1:C:535:ASP:CA	1:C:536:LYS:HD3	2.38	0.54
1:D:518:ASN:O	1:D:519:LEU:HD23	2.08	0.53
1:B:153:GLN:HE22	1:B:170:ASN:HD22	1.56	0.53
1:A:75:ASN:ND2	1:A:92:ASN:ND2	2.56	0.53
1:A:75:ASN:ND2	1:A:92:ASN:HD22	2.07	0.53
1:A:299:TYR:CZ	1:A:665:VAL:HG22	2.44	0.53
1:B:409:ALA:O	1:B:415:LEU:HD22	2.09	0.53
1:B:415:LEU:C	1:B:415:LEU:HD13	2.29	0.53
1:A:334:THR:OG1	1:A:336:ARG:HG3	2.09	0.53
1:A:489:LYS:HG3	1:A:491:LEU:H	1.74	0.53
1:A:74:ASN:O	1:A:95:PHE:HE2	1.92	0.53
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.06	0.53
1:A:289:PRO:HB3	1:A:315:TRP:CD2	2.44	0.52
1:D:532:PRO:HD3	1:D:569:SER:HA	1.91	0.52
1:B:148:ILE:HD13	1:B:155:ILE:CD1	2.39	0.52
1:B:490:GLU:CG	1:B:490:GLU:O	2.56	0.52
1:D:429:ARG:NH2	6:D:1663:HOH:O	2.42	0.52
1:D:553:GLN:NE2	6:D:1663:HOH:O	2.42	0.52
1:D:67:GLU:HB3	1:D:78:LEU:HD11	1.90	0.52
1:C:111:ARG:HD2	6:C:1865:HOH:O	2.09	0.52
1:B:669:ARG:HD2	6:B:1838:HOH:O	2.08	0.52
1:C:704:HIS:HE1	1:C:711:VAL:O	1.93	0.52
1:C:496:ASP:HB2	6:C:1655:HOH:O	2.08	0.52
1:D:288:VAL:HG12	1:D:289:PRO:HD2	1.92	0.52
1:B:41:ARG:NH1	1:B:47:ASP:OD1	2.43	0.51
1:C:153:GLN:HE22	1:C:170:ASN:HD22	1.54	0.51
1:C:484:SER:HB2	1:C:491:LEU:HD21	1.91	0.51
1:D:418:ILE:HD12	6:D:1706:HOH:O	2.10	0.51
1:A:49:LEU:HD22	1:A:749:GLN:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.46	0.51
1:D:482:LEU:HD23	1:D:483:HIS:N	2.26	0.51
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.92	0.51
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.92	0.51
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.31	0.51
1:C:484:SER:CB	1:C:491:LEU:HD21	2.40	0.51
1:A:71:LYS:HE3	1:A:105:TYR:CD2	2.45	0.51
1:D:288:VAL:HG13	1:D:289:PRO:HD2	1.92	0.51
1:A:415:LEU:C	1:A:415:LEU:HD13	2.31	0.51
1:D:289:PRO:HB3	1:D:315:TRP:CD2	2.46	0.51
1:D:331:ASP:HB2	1:D:338:ILE:HD12	1.93	0.51
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.46	0.51
1:D:472:CYS:O	1:D:478:PRO:HA	2.11	0.50
1:D:75:ASN:HD22	1:D:92:ASN:H	1.57	0.50
1:B:112:GLN:HB3	1:B:138:ASN:HD21	1.76	0.50
1:D:504:LEU:HA	1:D:507:VAL:CG1	2.41	0.50
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.93	0.50
1:A:438:ASP:OD1	1:A:440:THR:HB	2.11	0.50
1:A:94:THR:O	1:A:94:THR:HG22	2.11	0.50
1:C:142:LEU:C	1:C:142:LEU:HD23	2.32	0.50
1:A:131:SER:OG	1:A:150:ASN:ND2	2.45	0.50
1:B:422:HIS:CD2	1:B:423:LYS:HD3	2.46	0.50
1:B:73:GLU:OE2	1:B:73:GLU:HA	2.10	0.50
1:D:139:LYS:O	1:D:141:GLN:HG3	2.11	0.50
1:D:393:ASN:H	1:D:393:ASN:ND2	2.09	0.50
1:D:680:LEU:HD11	1:D:684:ARG:NE	2.23	0.50
1:B:175:LYS:NZ	1:B:175:LYS:HB3	2.27	0.50
1:A:103:ASN:O	1:A:104:ASP:HB2	2.12	0.49
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.49
1:D:103:ASN:OD1	1:D:117:GLU:OE2	2.29	0.49
1:D:177:GLU:HB2	1:D:180:LEU:HD23	1.93	0.49
1:B:471:ARG:NH2	6:B:1757:HOH:O	2.44	0.49
1:A:414:TYR:HA	1:A:436:LEU:HD13	1.95	0.49
1:B:370:SER:HB2	1:B:387:PHE:O	2.12	0.49
1:B:214:LEU:HD12	6:B:1630:HOH:O	2.12	0.49
1:B:407:ILE:CG2	1:B:415:LEU:HD21	2.37	0.49
1:C:72:GLN:O	1:C:74:ASN:N	2.46	0.49
1:D:133:ASP:HB3	1:D:142:LEU:HD21	1.94	0.49
1:A:327:ILE:HD13	1:A:389:THR:HG23	1.95	0.49
1:D:718:GLN:HE21	1:D:718:GLN:HA	1.78	0.49
1:B:183:GLN:HE22	1:B:278:PRO:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:LYS:HG2	1:C:616:MET:N	2.28	0.48
1:C:746:MET:H	1:C:746:MET:HE2	1.74	0.48
1:B:63:ILE:HD11	1:B:78:LEU:CD1	2.43	0.48
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.96	0.48
1:D:718:GLN:HE22	1:D:721:LYS:HZ1	1.61	0.48
1:C:253:ARG:NH2	1:D:253:ARG:NH2	2.62	0.48
1:C:463:ASN:N	1:C:463:ASN:HD22	2.12	0.48
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.48	0.48
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.49	0.48
1:C:288:VAL:HG11	1:C:294:LEU:HD11	1.96	0.48
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.49	0.48
1:A:92:ASN:O	1:A:94:THR:N	2.43	0.48
1:C:83:TYR:HB2	1:C:85:ASN:OD1	2.13	0.48
1:D:82:GLU:H	1:D:491:LEU:HD13	1.78	0.48
1:C:135:TYR:HD2	1:C:137:LEU:HD23	1.78	0.48
1:C:146:GLU:OE1	1:C:181:SER:HA	2.13	0.48
1:D:57:PHE:HA	1:D:480:TYR:CE1	2.49	0.48
1:A:547:TYR:HB2	1:A:554:LYS:HD3	1.96	0.47
1:D:340:SER:O	1:D:344:GLN:HG3	2.14	0.47
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.44	0.47
1:C:183:GLN:NE2	1:C:277:SER:C	2.68	0.47
1:D:173:TYR:CE2	1:D:184:ARG:HG3	2.49	0.47
1:D:600:THR:O	1:D:603:VAL:CG1	2.63	0.47
1:D:175:LYS:HE3	1:D:180:LEU:O	2.15	0.47
1:D:81:ALA:O	1:D:82:GLU:HB3	2.13	0.47
1:C:704:HIS:CD2	1:C:716:SER:OG	2.66	0.47
1:A:435:GLN:OE1	1:A:437:ASN:OD1	2.32	0.47
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.49	0.47
1:A:150:ASN:O	1:A:151:ASN:HB2	2.15	0.47
1:A:177:GLU:HB2	1:A:180:LEU:HB2	1.97	0.47
1:A:75:ASN:HB3	1:A:92:ASN:H	1.77	0.47
1:B:643:GLY:HA2	6:B:1631:HOH:O	2.14	0.47
1:B:438:ASP:OD2	1:B:441:LYS:HE3	2.15	0.46
1:B:184:ARG:HD3	1:B:186:THR:O	2.16	0.46
1:C:516:VAL:HG12	1:C:517:ILE:N	2.29	0.46
1:C:403:GLU:OE1	1:C:585:TYR:HA	2.15	0.46
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.80	0.46
1:B:482:LEU:O	1:B:490:GLU:O	2.32	0.46
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.51	0.46
1:B:435:GLN:OE1	1:B:441:LYS:HD2	2.16	0.46
1:D:75:ASN:HD22	1:D:91:GLU:HA	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.97	0.46
1:D:379:GLU:HG2	1:D:381:TYR:CD1	2.50	0.46
1:A:414:TYR:CA	1:A:436:LEU:HD13	2.45	0.46
1:A:477:LEU:HD12	1:A:501:ASP:HB2	1.98	0.46
1:A:517:ILE:HD11	1:A:578:PHE:CE1	2.50	0.46
1:D:177:GLU:CB	1:D:180:LEU:HD23	2.46	0.46
1:A:81:ALA:O	1:A:492:ARG:NH1	2.48	0.46
1:A:78:LEU:O	4:A:767(A):NAG:H81	2.15	0.46
1:C:345:HIS:HE1	1:C:389:THR:O	1.99	0.46
1:C:57:PHE:HA	1:C:480:TYR:CE1	2.51	0.46
1:D:140:ARG:HH11	1:D:140:ARG:HG2	1.80	0.46
1:D:543:LEU:HD22	1:D:759:LEU:HD11	1.98	0.46
1:B:516:VAL:CG1	1:B:517:ILE:N	2.79	0.46
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.51	0.46
1:B:86:SER:C	4:B:767(A):NAG:H81	2.36	0.46
1:C:49:LEU:HD22	1:C:749:GLN:HA	1.98	0.46
1:D:425:MET:HG2	1:D:525:TRP:CH2	2.51	0.46
1:D:345:HIS:HD2	6:D:1728:HOH:O	1.98	0.45
1:A:686:SER:HA	2:F:1:NAG:H82	1.98	0.45
1:B:528:MET:HG2	1:B:576:ALA:HB2	1.98	0.45
1:B:136:ASP:O	1:B:140:ARG:HA	2.16	0.45
1:B:741:GLY:O	1:B:742:ILE:C	2.54	0.45
1:C:142:LEU:HD23	1:C:143:ILE:O	2.16	0.45
1:D:77:LEU:HB2	1:D:79:PHE:CE2	2.50	0.45
1:B:660:GLU:CG	6:B:1520:HOH:O	2.64	0.45
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.52	0.45
1:D:600:THR:O	1:D:603:VAL:HG13	2.16	0.45
1:C:175:LYS:CG	1:C:182:SER:HB3	2.46	0.45
1:C:432:TYR:CE2	1:C:444:CYS:HB2	2.52	0.45
1:D:704:HIS:HE1	1:D:711:VAL:O	2.00	0.45
1:C:41:ARG:HH11	1:C:507:VAL:HG12	1.82	0.45
1:B:704:HIS:CD2	1:B:716:SER:OG	2.65	0.45
1:C:612:GLN:O	1:C:615:LYS:CG	2.64	0.45
1:B:73:GLU:HB3	3:G:1:NAG:H4	1.99	0.45
1:C:150:ASN:O	1:C:151:ASN:HB2	2.18	0.45
1:A:67:GLU:HB3	1:A:78:LEU:HD11	1.99	0.44
1:B:345:HIS:HE1	1:B:389:THR:O	2.00	0.44
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.99	0.44
1:C:414:TYR:CA	1:C:436:LEU:HD13	2.46	0.44
1:A:136:ASP:O	1:A:140:ARG:HA	2.17	0.44
1:C:554:LYS:HG2	6:C:1747:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.52	0.44
1:D:379:GLU:HG2	1:D:381:TYR:HD1	1.82	0.44
1:C:535:ASP:O	1:C:536:LYS:HB3	2.18	0.44
1:D:159:PRO:HD3	1:D:216:TRP:HB3	2.00	0.44
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.53	0.44
1:D:603:VAL:HG23	1:D:639:VAL:CG2	2.48	0.44
1:D:206:GLU:OE2	1:D:663:ASP:OD2	2.34	0.44
1:A:85:ASN:ND2	4:A:767(A):NAG:O7	2.51	0.44
1:B:175:LYS:HZ2	1:B:175:LYS:CB	2.31	0.44
1:C:125:ARG:HB3	6:C:1518:HOH:O	2.16	0.44
1:C:626:ILE:HG23	1:C:636:THR:HG23	1.98	0.44
1:D:184:ARG:HH11	1:D:187:TRP:HA	1.82	0.44
1:D:370:SER:HB2	1:D:387:PHE:O	2.18	0.44
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.18	0.44
1:D:415:LEU:C	1:D:415:LEU:HD23	2.38	0.44
1:A:79:PHE:CD1	1:A:86:SER:HB3	2.52	0.44
1:B:691:ARG:HH11	1:B:691:ARG:CG	2.27	0.44
1:C:77:LEU:CD2	1:C:88:ILE:HG12	2.48	0.44
1:C:92:ASN:O	1:C:95:PHE:HD2	2.01	0.44
1:A:718:GLN:HE22	1:A:721:LYS:NZ	2.15	0.44
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.47	0.44
1:C:733:MET:HA	1:D:732:THR:HG21	2.00	0.44
1:C:76:ILE:HD12	1:C:90:LEU:CD1	2.48	0.44
1:C:90:LEU:HD22	1:C:90:LEU:C	2.38	0.44
1:D:590:ILE:HG12	6:D:1722:HOH:O	2.18	0.44
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.47	0.43
1:C:515:ASP:HB3	1:C:526:TYR:CZ	2.53	0.43
1:B:72:GLN:HG2	1:B:73:GLU:HG2	1.99	0.43
1:C:517:ILE:HG23	1:C:526:TYR:CE2	2.53	0.43
1:C:543:LEU:HD22	1:C:759:LEU:HD11	1.99	0.43
1:D:741:GLY:O	1:D:742:ILE:C	2.57	0.43
1:B:393:ASN:H	1:B:393:ASN:HD22	1.66	0.43
1:B:673:LEU:HD12	1:B:673:LEU:N	2.33	0.43
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.83	0.43
1:C:67:GLU:HB3	1:C:78:LEU:HD11	2.01	0.43
1:A:92:ASN:O	1:A:93:SER:OG	2.30	0.43
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.82	0.43
1:C:114:ILE:HG22	1:C:135:TYR:HB3	2.01	0.43
1:C:316:ILE:HG22	1:C:323:SER:HB2	2.00	0.43
3:J:1:NAG:H62	3:J:2:NAG:HN2	1.83	0.43
1:A:125:ARG:HB3	6:A:1550:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ASN:ND2	6:A:1745:HOH:O	2.50	0.43
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.49	0.43
1:A:377:ASN:HB3	1:A:379:GLU:H	1.84	0.43
1:C:746:MET:HE1	6:C:1622:HOH:O	2.19	0.43
1:C:756:SER:O	1:C:760:LYS:HG3	2.19	0.43
1:D:516:VAL:CG1	1:D:517:ILE:N	2.82	0.43
1:A:397:ILE:HD12	1:A:434:ILE:HD13	2.01	0.43
1:A:517:ILE:HG23	1:A:526:TYR:CE2	2.54	0.43
1:A:612:GLN:HE21	1:A:612:GLN:HB3	1.66	0.43
1:C:463:ASN:N	1:C:463:ASN:ND2	2.67	0.43
1:A:516:VAL:HG12	1:A:517:ILE:N	2.32	0.43
1:B:175:LYS:CG	1:B:182:SER:HB3	2.48	0.43
1:B:73:GLU:O	1:B:74:ASN:HB2	2.19	0.43
1:C:183:GLN:HE22	1:C:278:PRO:N	2.17	0.43
1:C:741:GLY:O	1:C:742:ILE:C	2.56	0.43
1:A:127:SER:HB3	1:A:211:TYR:CG	2.54	0.42
1:A:378:GLU:CD	1:A:378:GLU:H	2.22	0.42
1:A:42:THR:HB	1:A:569:SER:OG	2.19	0.42
1:B:175:LYS:HG3	1:B:182:SER:HB3	2.00	0.42
1:C:125:ARG:HG2	1:C:126:HIS:NE2	2.34	0.42
1:C:745:ASN:HB2	1:C:746:MET:HE2	2.01	0.42
1:C:732:THR:HG22	1:D:732:THR:HG23	2.01	0.42
1:A:415:LEU:HD13	1:A:416:TYR:N	2.33	0.42
1:C:135:TYR:CD2	1:C:137:LEU:HD23	2.54	0.42
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.84	0.42
1:D:515:ASP:HB3	1:D:526:TYR:CE2	2.54	0.42
1:B:673:LEU:HD11	6:B:1720:HOH:O	2.18	0.42
1:C:53:PHE:CZ	1:C:507:VAL:HG11	2.55	0.42
1:C:75:ASN:ND2	1:C:92:ASN:HB2	2.29	0.42
1:B:143:ILE:N	1:B:143:ILE:HD12	2.34	0.42
1:C:289:PRO:HB3	1:C:315:TRP:CD2	2.54	0.42
1:C:612:GLN:HB3	1:C:612:GLN:HE21	1.65	0.42
1:C:615:LYS:CG	1:C:616:MET:N	2.82	0.42
1:D:377:ASN:HB2	1:D:381:TYR:H	1.84	0.42
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.80	0.42
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.00	0.42
1:B:378:GLU:N	1:B:378:GLU:CD	2.61	0.42
1:C:114:ILE:CG2	1:C:135:TYR:HB3	2.50	0.42
1:A:490:GLU:O	1:A:492:ARG:N	2.53	0.42
1:B:524:PHE:CE2	1:B:590:ILE:HD12	2.54	0.42
1:B:718:GLN:HE21	1:B:718:GLN:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:PRO:HG2	1:B:294:LEU:HG	2.01	0.42
1:D:112:GLN:HG2	1:D:138:ASN:HD21	1.84	0.42
1:D:610:THR:HA	1:D:613:PHE:CD2	2.55	0.42
1:D:299:TYR:CZ	1:D:665:VAL:HG22	2.55	0.42
1:B:316:ILE:HD11	1:B:320:GLN:HA	2.02	0.42
1:C:184:ARG:HH11	1:C:187:TRP:HA	1.84	0.42
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.54	0.42
1:B:134:ILE:O	1:B:143:ILE:HD13	2.20	0.42
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.55	0.42
1:D:457:TYR:HA	1:D:471:ARG:O	2.20	0.42
1:A:704:HIS:HE1	1:A:711:VAL:O	2.02	0.42
1:B:654:ALA:N	1:B:655:PRO:CD	2.82	0.42
1:C:533:HIS:O	1:C:534:PHE:C	2.57	0.42
1:C:73:GLU:CD	4:C:768(A):NAG:H61	2.40	0.42
1:D:107:VAL:HG12	1:D:114:ILE:HG13	2.01	0.42
1:D:114:ILE:HG22	1:D:135:TYR:HB3	2.01	0.42
1:A:502:LYS:HD2	1:A:505:GLN:OE1	2.20	0.41
1:A:626:ILE:HG23	1:A:636:THR:HG23	2.02	0.41
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.50	0.41
1:D:39:SER:N	6:D:1670:HOH:O	2.52	0.41
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.55	0.41
1:C:159:PRO:HG2	1:C:217:SER:O	2.19	0.41
1:D:288:VAL:HG12	1:D:289:PRO:CD	2.49	0.41
1:D:405:ILE:HG13	1:D:429:ARG:CD	2.50	0.41
1:D:482:LEU:HD23	1:D:483:HIS:H	1.85	0.41
1:D:603:VAL:HG23	1:D:639:VAL:HG22	2.01	0.41
1:C:696:LYS:HG3	1:C:728:VAL:HG22	2.02	0.41
1:D:134:ILE:CG2	1:D:143:ILE:HD12	2.51	0.41
1:D:150:ASN:O	1:D:151:ASN:HB2	2.21	0.41
1:D:237:GLU:HA	1:D:252:VAL:O	2.20	0.41
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.35	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.41
1:D:757:HIS:CE1	6:D:1744:HOH:O	2.73	0.41
1:A:92:ASN:C	1:A:94:THR:N	2.73	0.41
1:B:107:VAL:HG22	1:B:114:ILE:HD12	2.03	0.41
1:D:82:GLU:N	1:D:491:LEU:HD13	2.36	0.41
1:D:82:GLU:HA	1:D:491:LEU:HD13	2.03	0.41
1:B:140:ARG:NH1	1:B:140:ARG:HG2	2.35	0.41
1:B:507:VAL:HG22	1:B:508:GLN:N	2.36	0.41
1:B:519:LEU:HB3	1:B:520:HIS:CE1	2.56	0.41
1:A:328:CYS:HA	1:A:338:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:ASP:HB3	1:D:526:TYR:CZ	2.55	0.41
1:C:491:LEU:HD22	1:C:491:LEU:N	2.36	0.41
1:D:184:ARG:HD2	1:D:187:TRP:CD2	2.55	0.41
1:A:415:LEU:C	1:A:415:LEU:CD1	2.88	0.41
1:B:436:LEU:HD12	1:B:436:LEU:HA	1.87	0.41
1:C:483:HIS:CA	1:C:491:LEU:HD23	2.50	0.41
1:D:105:TYR:HA	1:D:115:LEU:O	2.21	0.41
1:D:140:ARG:HG2	1:D:140:ARG:NH1	2.36	0.41
1:D:169:ASN:O	1:D:170:ASN:HB2	2.21	0.41
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.03	0.41
1:A:157:TRP:CZ3	1:A:164:LEU:HG	2.56	0.41
1:A:527:GLN:HB3	1:A:555:VAL:HG13	2.02	0.41
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.56	0.41
1:C:232:GLU:HB3	1:C:262:GLU:HG2	2.03	0.41
1:C:530:LEU:HA	1:C:531:PRO:HD3	1.90	0.41
1:D:364:PHE:CD2	1:D:371:PHE:HB3	2.56	0.41
1:D:516:VAL:HG12	1:D:517:ILE:N	2.35	0.41
1:D:516:VAL:HG13	1:D:524:PHE:O	2.20	0.41
1:A:486:SER:OG	1:A:487:SER:N	2.54	0.41
1:A:616:MET:HB3	1:A:618:PHE:CE2	2.55	0.41
1:B:660:GLU:HG3	6:B:1520:HOH:O	2.21	0.41
1:C:134:ILE:HG21	1:C:178:PRO:HB3	2.03	0.41
1:B:610:THR:HA	1:B:613:PHE:CD2	2.56	0.40
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.55	0.40
1:B:418:ILE:HD11	6:B:1506:HOH:O	2.20	0.40
1:C:345:HIS:HD2	6:C:1610:HOH:O	2.05	0.40
1:C:415:LEU:HD23	1:C:415:LEU:C	2.41	0.40
1:B:504:LEU:HA	1:B:507:VAL:HG12	2.03	0.40
1:C:282:VAL:HG12	1:C:284:SER:OG	2.22	0.40
1:C:654:ALA:HA	1:C:704:HIS:CD2	2.56	0.40
1:D:599:GLY:O	1:D:603:VAL:HG11	2.20	0.40
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.56	0.40
1:D:219:ASN:HB2	1:D:308:GLU:CD	2.42	0.40
1:D:242:SER:HB3	1:D:246:LEU:HD12	2.02	0.40
1:B:405:ILE:HG13	1:B:429:ARG:HD3	2.04	0.40
1:C:41:ARG:NH1	1:C:507:VAL:HG12	2.36	0.40
1:C:76:ILE:HB	1:C:90:LEU:HD12	2.03	0.40
1:D:71:LYS:HA	1:D:75: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	726/728 (100%)	689 (95%)	34 (5%)	3 (0%)	34	21
1	B	726/728 (100%)	699 (96%)	25 (3%)	2 (0%)	41	27
1	C	726/728 (100%)	685 (94%)	35 (5%)	6 (1%)	19	7
1	D	726/728 (100%)	698 (96%)	28 (4%)	0	100	100
All	All	2904/2912 (100%)	2771 (95%)	122 (4%)	11 (0%)	34	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	B	491	LEU
1	C	103	ASN
1	C	104	ASP
1	C	535	ASP
1	C	536	LYS
1	A	491	LEU
1	B	40	ARG
1	A	97	GLU
1	C	74	ASN
1	C	99	GLY

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	652/652 (100%)	623 (96%)	29 (4%)	28 14
1	B	652/652 (100%)	625 (96%)	27 (4%)	30 16
1	C	652/652 (100%)	624 (96%)	28 (4%)	29 14
1	D	652/652 (100%)	626 (96%)	26 (4%)	31 16
All	All	2608/2608 (100%)	2498 (96%)	110 (4%)	30 15

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	74	ASN
1	A	90	LEU
1	A	119	ASN
1	A	125	ARG
1	A	142	LEU
1	A	145	GLU
1	A	180	LEU
1	A	192	ASN
1	A	246	LEU
1	A	294	LEU
1	A	367	ASP
1	A	385	CYS
1	A	399	LYS
1	A	415	LEU
1	A	448	GLU
1	A	463	ASN
1	A	471	ARG
1	A	472	CYS
1	A	492	ARG
1	A	520	HIS
1	A	542	LEU
1	A	543	LEU
1	A	561	LEU
1	A	566	TYR
1	A	679	ASN
1	A	701	LEU
1	A	718	GLN
1	A	761	GLN
1	B	86	SER
1	B	91	GLU
1	B	180	LEU
1	B	230	ASP

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Mol	Chain	Res	Type
1	B	246	LEU
1	B	294	LEU
1	B	367	ASP
1	B	379	GLU
1	B	385	CYS
1	B	436	LEU
1	B	450	ASN
1	B	472	CYS
1	B	506	ASP
1	B	520	HIS
1	B	535	ASP
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU
1	B	561	LEU
1	B	566	TYR
1	B	611	ARG
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	718	GLN
1	B	732	THR
1	B	761	GLN
1	C	41	ARG
1	C	75	ASN
1	C	90	LEU
1	C	125	ARG
1	C	145	GLU
1	C	147	ARG
1	C	230	ASP
1	C	246	LEU
1	C	277	SER
1	C	294	LEU
1	C	385	CYS
1	C	399	LYS
1	C	448	GLU
1	C	472	CYS
1	C	482	LEU
1	C	503	MET
1	C	507	VAL
1	C	535	ASP
1	C	536	LYS

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Mol	Chain	Res	Type
1	C	542	LEU
1	C	561	LEU
1	C	566	TYR
1	C	679	ASN
1	C	701	LEU
1	C	732	THR
1	C	746	MET
1	C	759	LEU
1	C	761	GLN
1	D	91	GLU
1	D	103	ASN
1	D	142	LEU
1	D	230	ASP
1	D	246	LEU
1	D	253	ARG
1	D	276	LEU
1	D	294	LEU
1	D	358	ARG
1	D	393	ASN
1	D	399	LYS
1	D	436	LEU
1	D	448	GLU
1	D	482	LEU
1	D	535	ASP
1	D	536	LYS
1	D	561	LEU
1	D	566	TYR
1	D	581	ARG
1	D	608	GLU
1	D	673	LEU
1	D	679	ASN
1	D	701	LEU
1	D	702	LEU
1	D	718	GLN
1	D	759	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	74	ASN
1	A	75	ASN

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Mol	Chain	Res	Type
1	A	123	GLN
1	A	141	GLN
1	A	150	ASN
1	A	169	ASN
1	A	170	ASN
1	A	176	ASN
1	A	183	GLN
1	A	192	ASN
1	A	247	GLN
1	A	345	HIS
1	A	377	ASN
1	A	435	GLN
1	A	463	ASN
1	A	483	HIS
1	A	572	ASN
1	A	586	GLN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	745	ASN
1	B	61	GLN
1	B	72	GLN
1	B	75	ASN
1	B	138	ASN
1	B	169	ASN
1	B	170	ASN
1	B	176	ASN
1	B	183	GLN
1	B	192	ASN
1	B	247	GLN
1	B	345	HIS
1	B	369	ASN
1	B	393	ASN
1	B	430	ASN
1	B	435	GLN
1	B	463	ASN
1	B	483	HIS
1	B	505	GLN
1	B	533	HIS
1	B	586	GLN

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Mol	Chain	Res	Type
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	731	GLN
1	B	761	GLN
1	C	72	GLN
1	C	75	ASN
1	C	119	ASN
1	C	138	ASN
1	C	141	GLN
1	C	169	ASN
1	C	170	ASN
1	C	176	ASN
1	C	183	GLN
1	C	192	ASN
1	C	247	GLN
1	C	345	HIS
1	C	369	ASN
1	C	393	ASN
1	C	435	GLN
1	C	463	ASN
1	C	483	HIS
1	C	505	GLN
1	C	586	GLN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	745	ASN
1	C	757	HIS
1	C	761	GLN
1	D	61	GLN
1	D	72	GLN
1	D	75	ASN
1	D	103	ASN
1	D	138	ASN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN

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Mol	Chain	Res	Type
1	D	176	ASN
1	D	183	GLN
1	D	192	ASN
1	D	247	GLN
1	D	393	ASN
1	D	463	ASN
1	D	483	HIS
1	D	505	GLN
1	D	586	GLN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	745	ASN

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

20 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	E	1	1,2	14,14,15	0.73	0	17,19,21	0.59	0
2	NAG	E	2	2	14,14,15	0.52	0	17,19,21	0.68	1 (5%)
2	NAG	F	1	1,2	14,14,15	0.70	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	F	2	2	14,14,15	0.52	0	17,19,21	0.69	1 (5%)
3	NAG	G	1	1,3	14,14,15	0.52	0	17,19,21	0.69	0
3	NAG	G	2	3	14,14,15	0.61	0	17,19,21	0.66	0
3	BMA	G	3	3	11,11,12	0.45	0	15,15,17	0.65	0
2	NAG	H	1	1,2	14,14,15	0.48	0	17,19,21	0.70	0
2	NAG	H	2	2	14,14,15	0.52	0	17,19,21	0.79	0
2	NAG	I	1	1,2	14,14,15	0.72	0	17,19,21	0.73	0
2	NAG	I	2	2	14,14,15	0.60	0	17,19,21	0.76	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.59	0	17,19,21	0.79	1 (5%)
3	NAG	J	2	3	14,14,15	0.44	0	17,19,21	0.68	0
3	BMA	J	3	3	11,11,12	0.64	0	15,15,17	0.60	0
2	NAG	K	1	1,2	14,14,15	0.64	0	17,19,21	0.52	0
2	NAG	K	2	2	14,14,15	0.49	0	17,19,21	0.63	0
2	NAG	L	1	1,2	14,14,15	0.72	0	17,19,21	0.79	0
2	NAG	L	2	2	14,14,15	0.60	0	17,19,21	0.68	1 (5%)
2	NAG	M	1	1,2	14,14,15	0.71	0	17,19,21	0.60	0
2	NAG	M	2	2	14,14,15	0.56	0	17,19,21	1.04	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
3	NAG	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	0/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	BMA	J	3	3	-	1/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	L	2	2	-	2/6/23/26	0/1/1/1
2	NAG	M	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	M	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	2	NAG	C1-C2-N2	2.44	114.66	110.49
2	I	2	NAG	C2-N2-C7	-2.32	119.59	122.90
2	M	2	NAG	O5-C1-C2	-2.10	107.97	111.29
2	F	2	NAG	C2-N2-C7	-2.08	119.94	122.90
3	J	1	NAG	C2-N2-C7	-2.07	119.95	122.90
2	E	2	NAG	C2-N2-C7	-2.05	119.98	122.90
2	L	2	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	M	2	NAG	C1-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
2	L	1	NAG	C8-C7-N2-C2
2	L	1	NAG	O7-C7-N2-C2
2	K	2	NAG	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
2	K	2	NAG	C8-C7-N2-C2
2	K	2	NAG	O7-C7-N2-C2
2	K	2	NAG	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	M	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6
2	M	2	NAG	O7-C7-N2-C2
3	J	1	NAG	C8-C7-N2-C2
3	G	1	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O7-C7-N2-C2
3	G	1	NAG	O5-C5-C6-O6
3	J	3	BMA	C4-C5-C6-O6
2	L	2	NAG	C8-C7-N2-C2
2	L	1	NAG	C4-C5-C6-O6
2	L	2	NAG	O7-C7-N2-C2

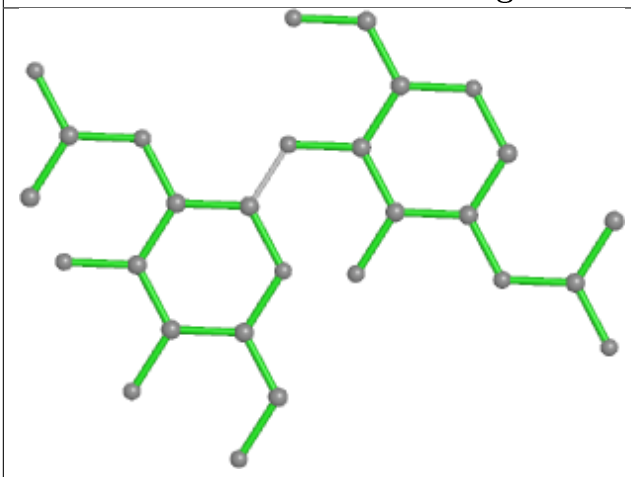
There are no ring outliers.

4 monomers are involved in 3 short contacts:

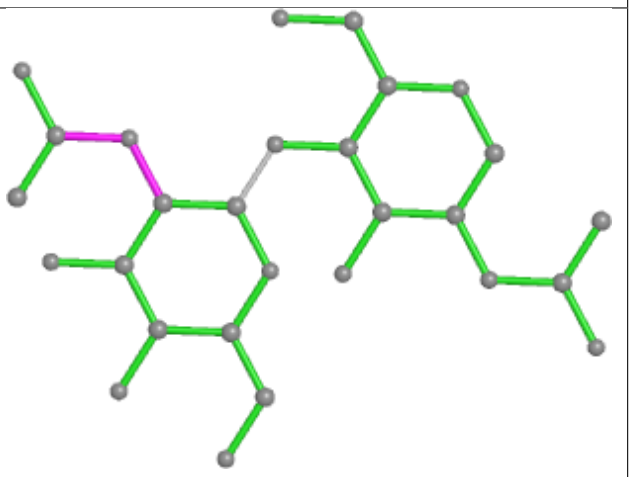
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	1	0
3	J	1	NAG	1	0
2	F	1	NAG	1	0
3	G	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

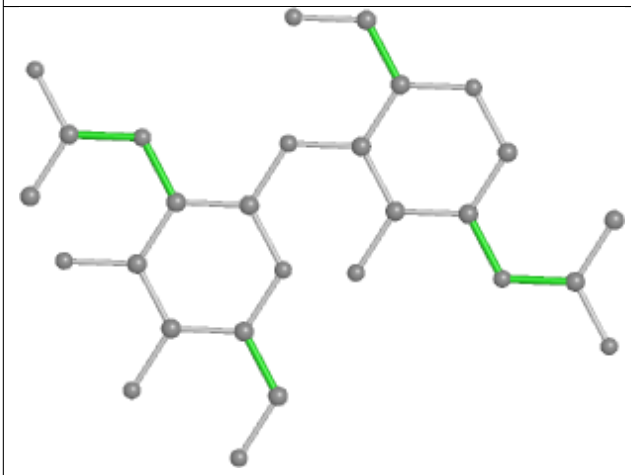
Oligosaccharide Chain E



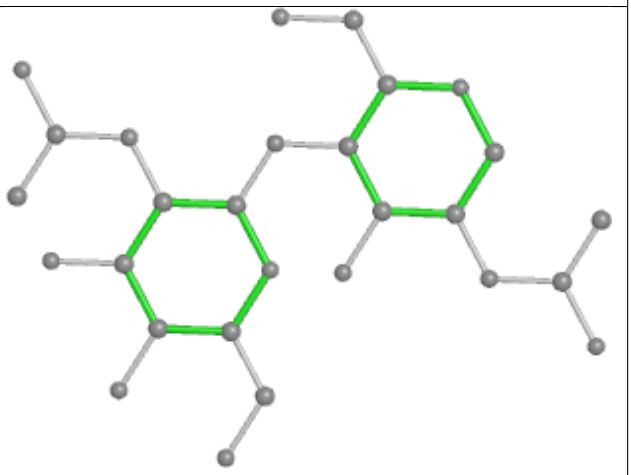
Bond lengths



Bond angles

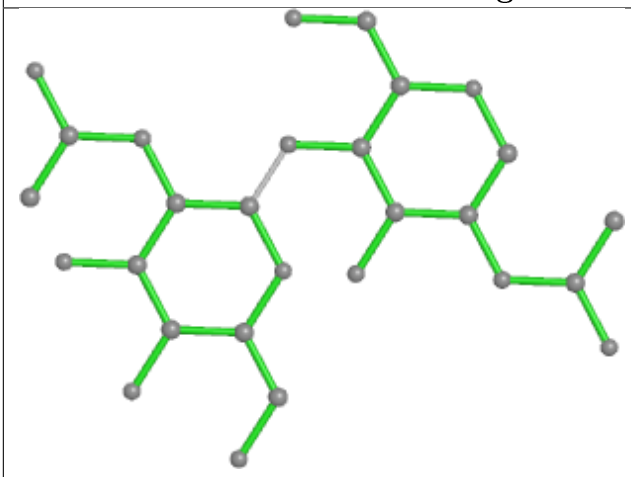


Torsions

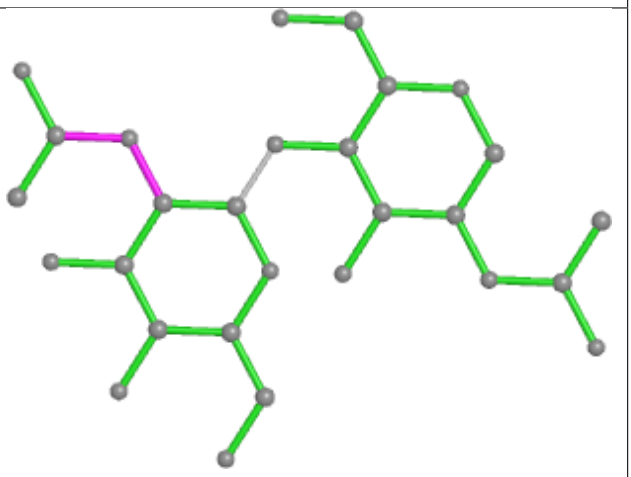


Rings

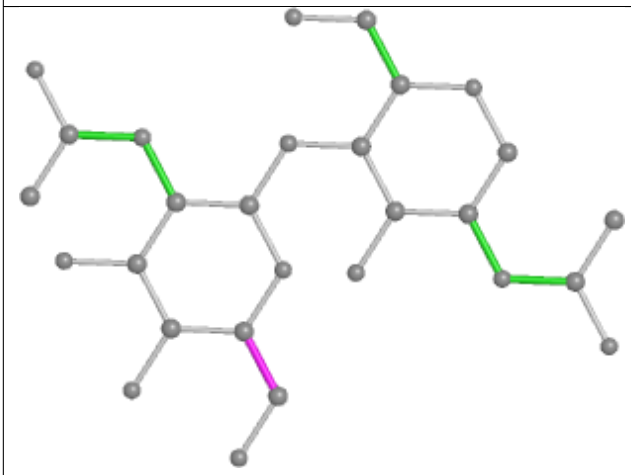
Oligosaccharide Chain F



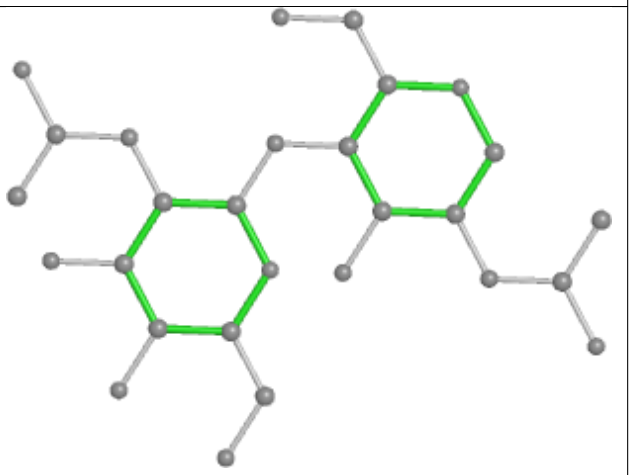
Bond lengths



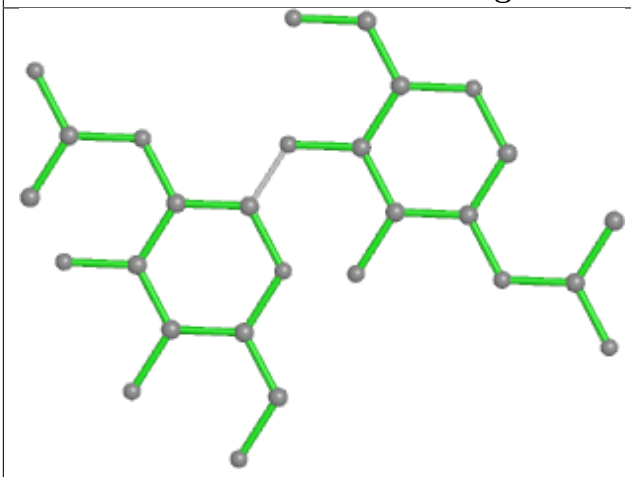
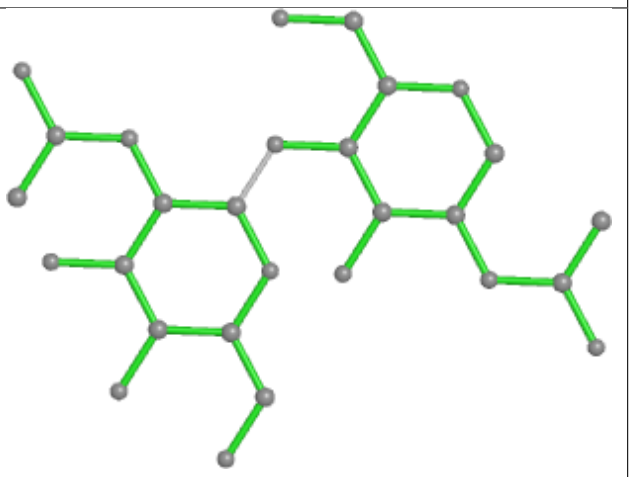
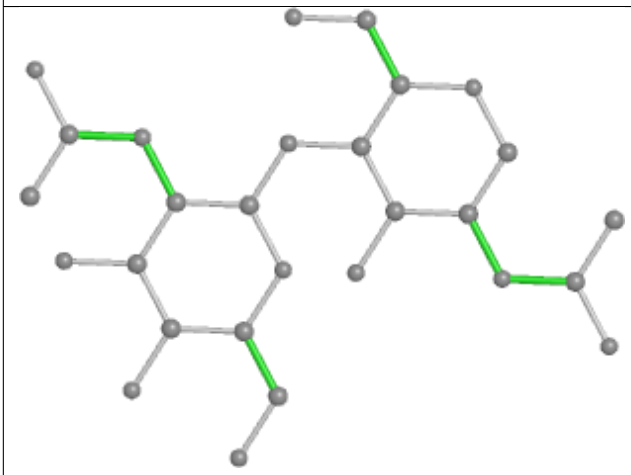
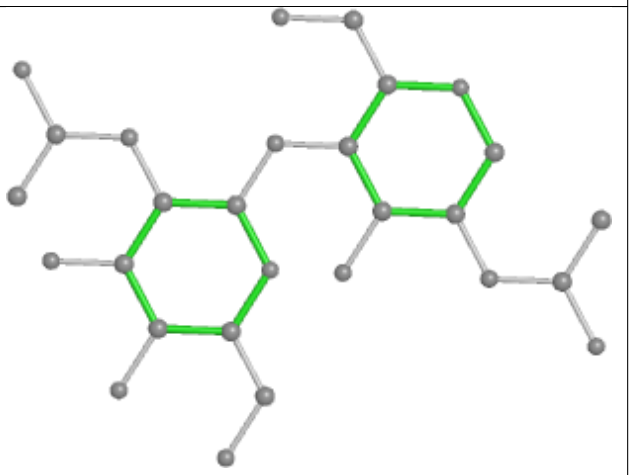
Bond angles



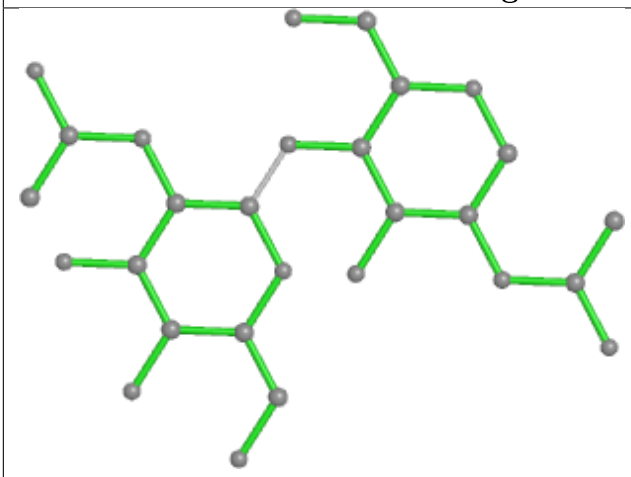
Torsions



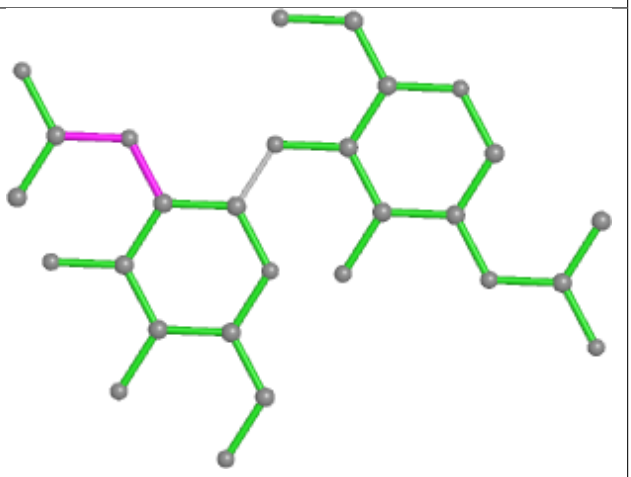
Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

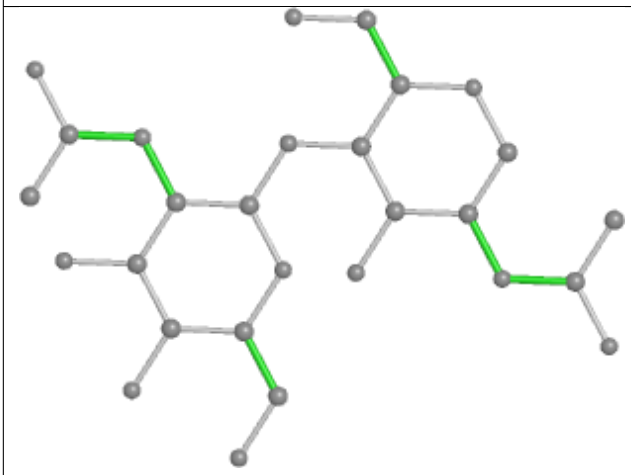
Oligosaccharide Chain I



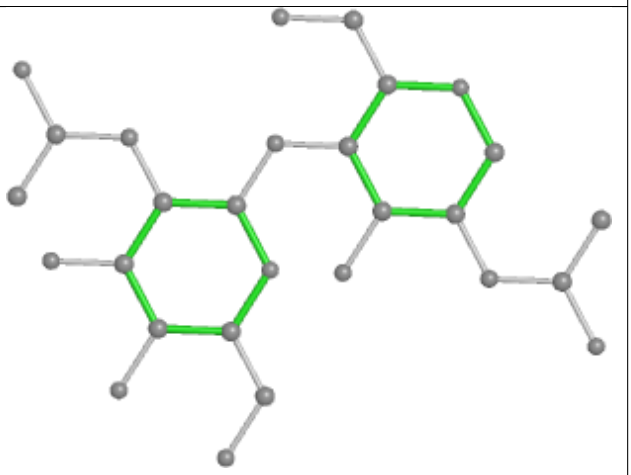
Bond lengths



Bond angles

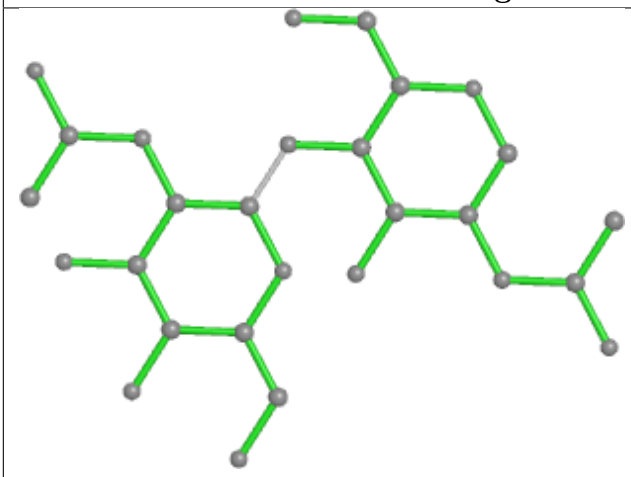


Torsions

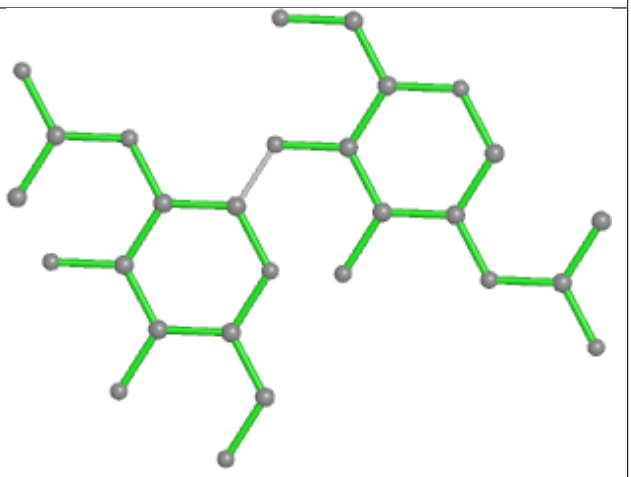


Rings

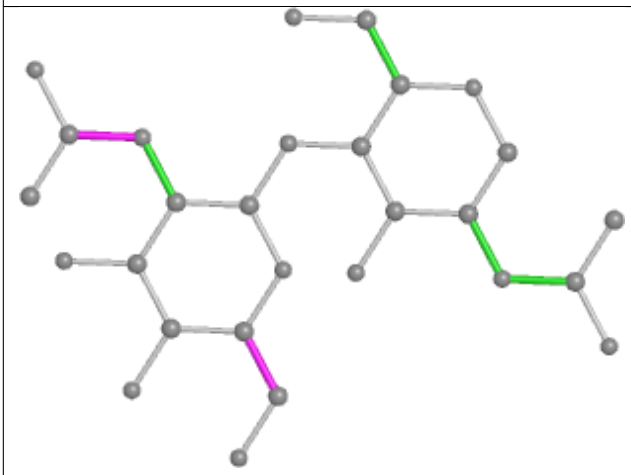
Oligosaccharide Chain K



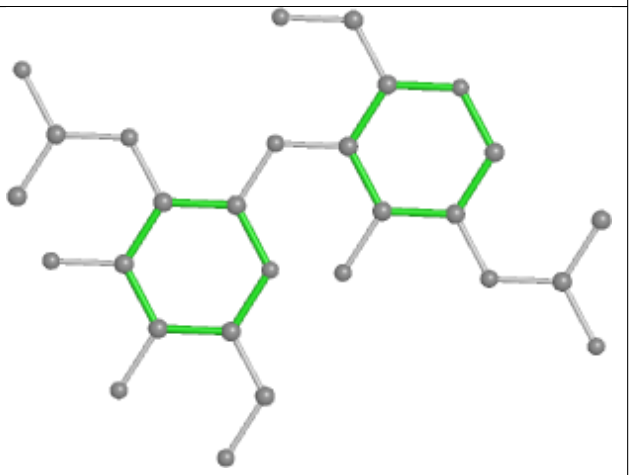
Bond lengths



Bond angles

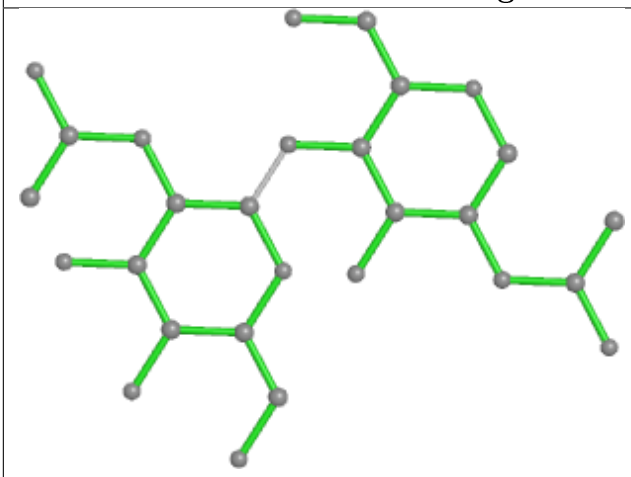


Torsions

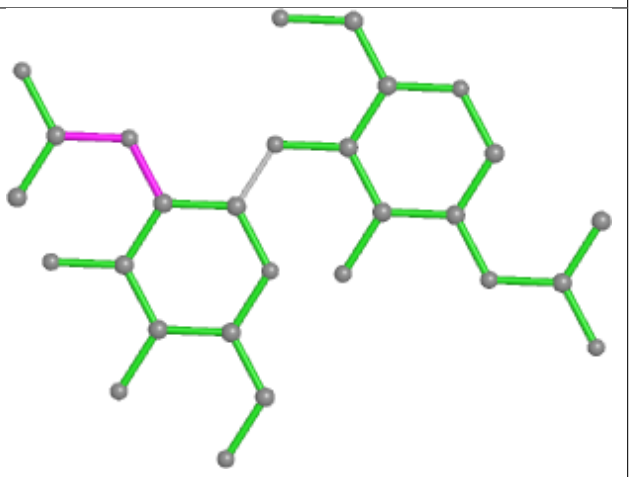


Rings

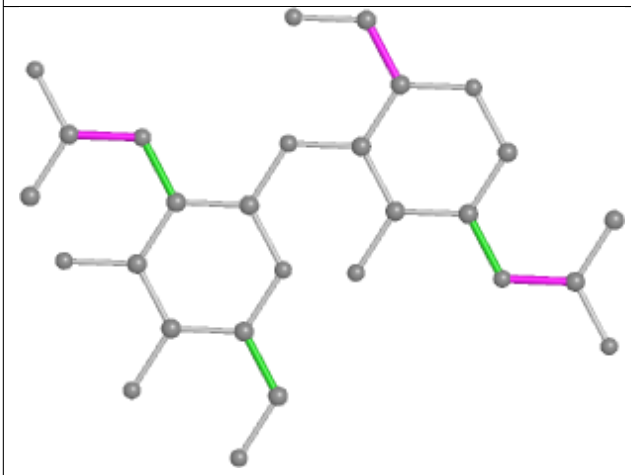
Oligosaccharide Chain L



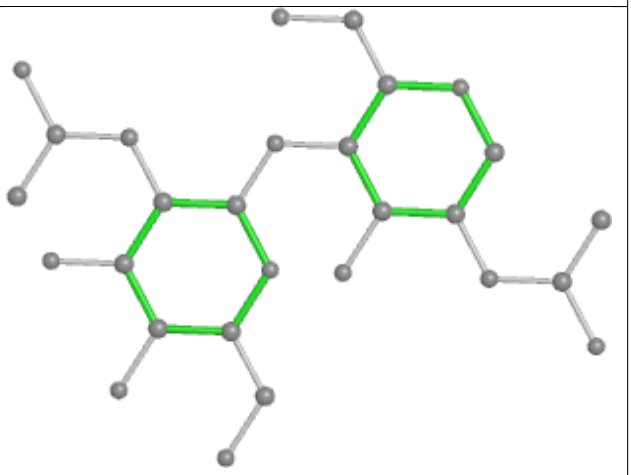
Bond lengths



Bond angles

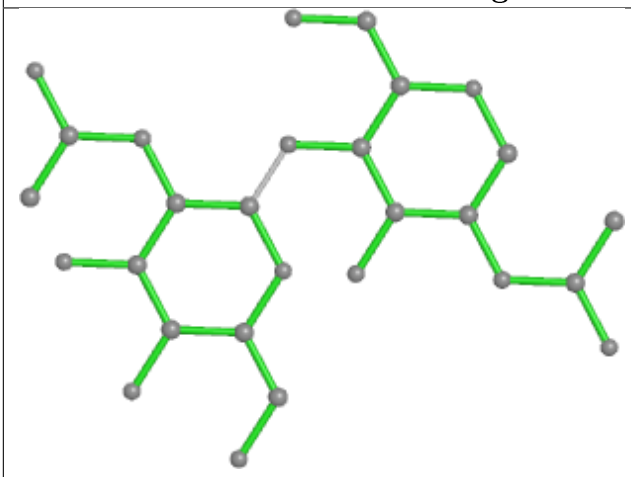


Torsions

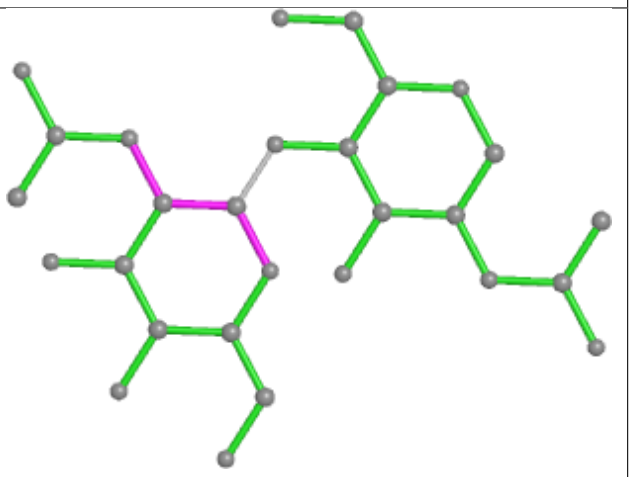


Rings

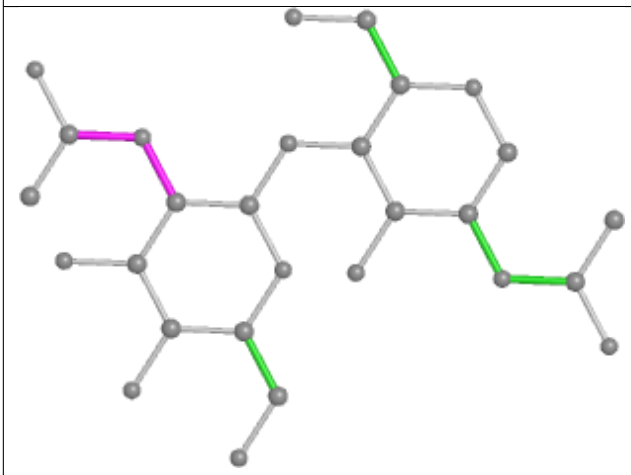
Oligosaccharide Chain M



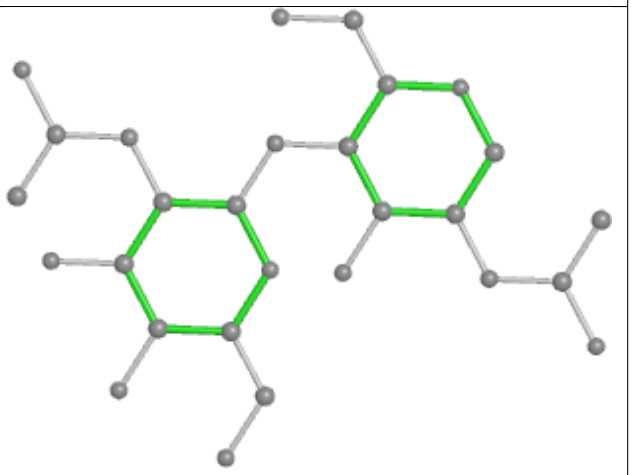
Bond lengths



Bond angles

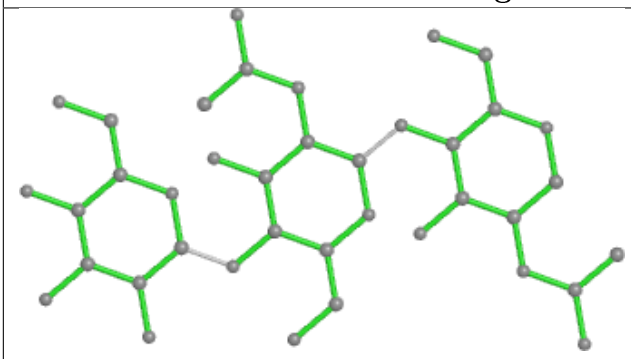


Torsions

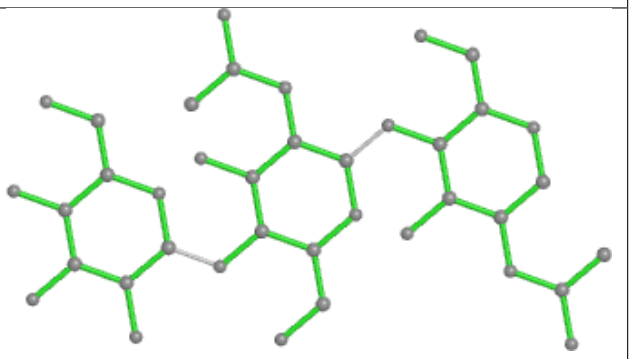


Rings

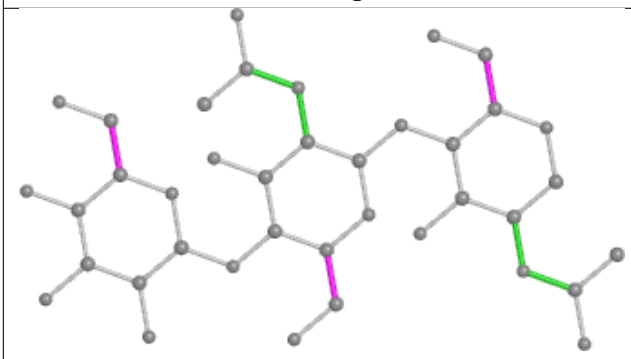
Oligosaccharide Chain G



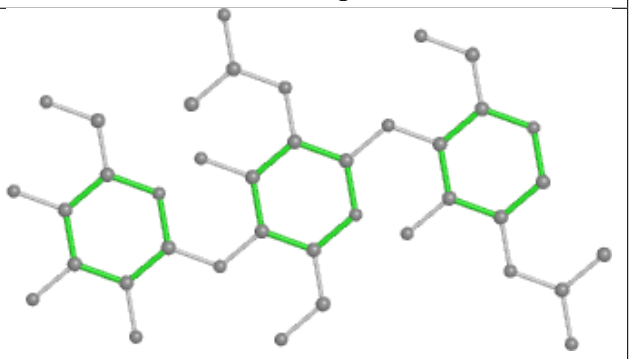
Bond lengths



Bond angles

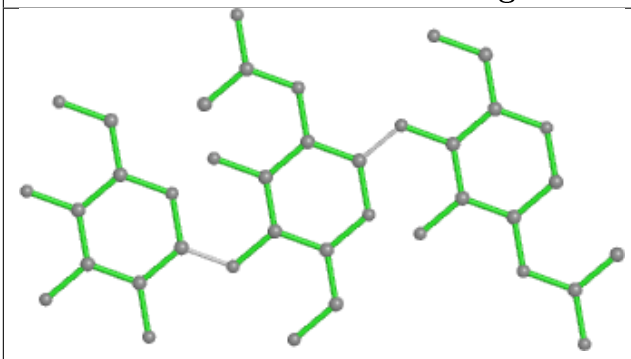


Torsions

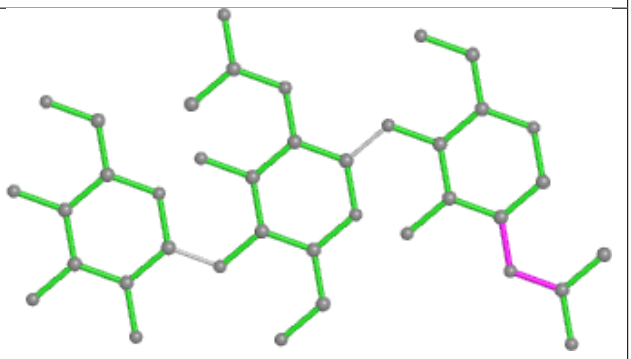


Rings

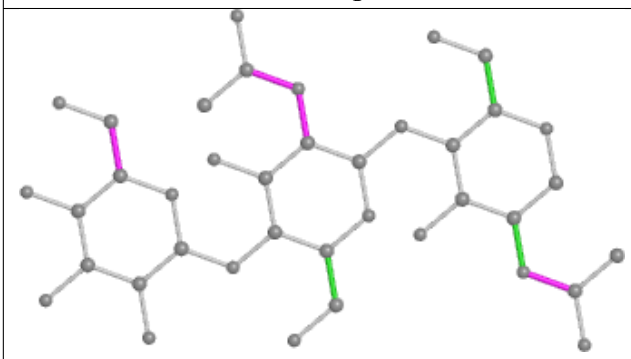
Oligosaccharide Chain J



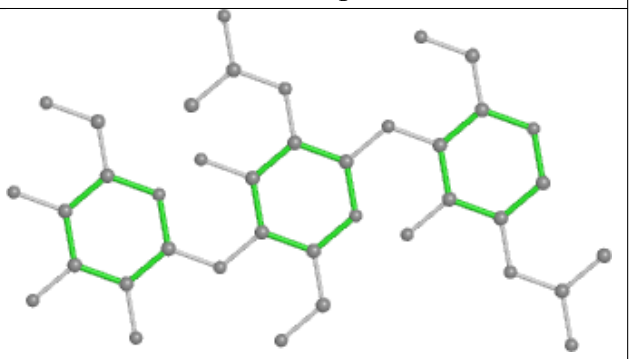
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

19 ligands 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	$\#\|Z\| > 2$
4	NAG	C	769(A)	1	14,14,15	0.53	0	17,19,21	0.77	1 (5%)
4	NAG	A	772(A)	1	14,14,15	0.56	0	17,19,21	0.77	0
4	NAG	C	768(A)	1	14,14,15	0.54	0	17,19,21	0.71	1 (5%)
5	SO4	B	1501	-	4,4,4	0.28	0	6,6,6	0.63	0
4	NAG	A	771(A)	1	14,14,15	0.48	0	17,19,21	0.72	1 (5%)
5	SO4	D	1503	-	4,4,4	0.29	0	6,6,6	0.72	0
4	NAG	B	771(A)	1	14,14,15	0.69	0	17,19,21	0.58	0
4	NAG	C	771(A)	1	14,14,15	0.50	0	17,19,21	0.89	0
4	NAG	B	772(A)	1	14,14,15	0.63	0	17,19,21	0.85	0
4	NAG	B	773(A)	1	14,14,15	0.53	0	17,19,21	0.76	1 (5%)
4	NAG	C	770(A)	1	14,14,15	0.62	0	17,19,21	0.62	0
4	NAG	D	767(A)	1	14,14,15	0.61	0	17,19,21	0.80	1 (5%)
4	NAG	D	773(A)	1	14,14,15	0.62	0	17,19,21	0.67	0
4	NAG	A	768(A)	1	14,14,15	0.56	0	17,19,21	0.70	0
4	NAG	C	767(A)	1	14,14,15	0.46	0	17,19,21	0.70	0
5	SO4	A	1500	-	4,4,4	0.54	0	6,6,6	0.70	0
4	NAG	A	767(A)	1	14,14,15	0.63	0	17,19,21	0.63	0
4	NAG	B	767(A)	1	14,14,15	0.50	0	17,19,21	0.76	1 (5%)
5	SO4	C	1502	-	4,4,4	0.42	0	6,6,6	0.54	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
4	NAG	C	769(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	A	772(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	C	768(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	A	771(A)	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	773(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	B	771(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	C	771(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	B	772(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	C	770(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	D	767(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	D	773(A)	1	-	4/6/23/26	0/1/1/1
4	NAG	A	768(A)	1	-	2/6/23/26	0/1/1/1
4	NAG	C	767(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	A	767(A)	1	-	0/6/23/26	0/1/1/1
4	NAG	B	767(A)	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	773(A)	NAG	C2-N2-C7	-2.44	119.43	122.90
4	D	767(A)	NAG	C2-N2-C7	-2.27	119.67	122.90
4	C	769(A)	NAG	C2-N2-C7	-2.13	119.86	122.90
4	A	771(A)	NAG	C2-N2-C7	-2.09	119.93	122.90
4	B	767(A)	NAG	C2-N2-C7	-2.09	119.93	122.90
4	C	768(A)	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	768(A)	NAG	C8-C7-N2-C2
4	C	768(A)	NAG	O7-C7-N2-C2
4	A	771(A)	NAG	C8-C7-N2-C2
4	A	771(A)	NAG	O7-C7-N2-C2
4	C	771(A)	NAG	C8-C7-N2-C2
4	C	771(A)	NAG	O7-C7-N2-C2
4	D	773(A)	NAG	C8-C7-N2-C2
4	D	773(A)	NAG	O7-C7-N2-C2
4	A	768(A)	NAG	C8-C7-N2-C2
4	A	768(A)	NAG	O7-C7-N2-C2
4	B	772(A)	NAG	C8-C7-N2-C2
4	D	773(A)	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	772(A)	NAG	O7-C7-N2-C2
4	C	770(A)	NAG	C8-C7-N2-C2
4	D	773(A)	NAG	C4-C5-C6-O6
4	C	770(A)	NAG	O7-C7-N2-C2
4	A	772(A)	NAG	C4-C5-C6-O6
4	B	773(A)	NAG	C4-C5-C6-O6
4	A	772(A)	NAG	O5-C5-C6-O6
4	B	773(A)	NAG	O5-C5-C6-O6
4	A	771(A)	NAG	O5-C5-C6-O6
4	D	767(A)	NAG	C8-C7-N2-C2
4	D	767(A)	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	768(A)	NAG	1	0
4	B	773(A)	NAG	1	0
4	D	767(A)	NAG	1	0
4	A	767(A)	NAG	2	0
4	B	767(A)	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	724/728 (99%)	0.23	56 (7%)	13	10	19, 33, 63, 90	13 (1%)
1	B	728/728 (100%)	0.02	29 (3%)	38	32	18, 30, 52, 71	12 (1%)
1	C	723/728 (99%)	0.14	42 (5%)	23	18	19, 31, 56, 97	12 (1%)
1	D	728/728 (100%)	0.22	42 (5%)	23	18	20, 36, 63, 87	10 (1%)
All	All	2903/2912 (99%)	0.15	169 (5%)	23	18	18, 33, 59, 97	47 (1%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	LEU	12.8
1	A	101	SER	12.7
1	C	97	GLU	9.9
1	D	83	TYR	8.3
1	C	95	PHE	7.7
1	C	39	SER	7.7
1	B	39	SER	7.5
1	D	99	GLY	7.1
1	A	96	ASP	6.8
1	C	537	SER	6.8
1	A	83	TYR	6.4
1	A	766	PRO	6.4
1	D	295	ILE	6.1
1	B	83	TYR	5.9
1	A	103	ASN	5.7
1	C	766	PRO	5.6
1	A	102	THR	5.3
1	D	82	GLU	5.2
1	C	141	GLN	5.1
1	C	73	GLU	5.0
1	C	120	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	766	PRO	5.0
1	C	138	ASN	4.9
1	A	93	SER	4.9
1	A	94	THR	4.9
1	D	521	GLY	4.6
1	D	537	SER	4.6
1	B	99	GLY	4.5
1	A	85	ASN	4.5
1	C	96	ASP	4.5
1	D	487	SER	4.5
1	B	54	ARG	4.3
1	B	537	SER	4.3
1	C	295	ILE	4.2
1	D	470	LEU	4.0
1	A	57	PHE	3.9
1	C	104	ASP	3.9
1	C	40	ARG	3.9
1	A	505	GLN	3.8
1	B	82	GLU	3.7
1	C	535	ASP	3.7
1	A	72	GLN	3.7
1	D	84	GLY	3.7
1	A	138	ASN	3.6
1	B	101	SER	3.5
1	D	57	PHE	3.5
1	C	139	LYS	3.5
1	D	39	SER	3.5
1	D	100	TYR	3.5
1	A	521	GLY	3.5
1	A	39	SER	3.4
1	A	677	GLU	3.3
1	B	506	ASP	3.3
1	A	179	ASN	3.3
1	A	150	ASN	3.3
1	B	57	PHE	3.2
1	D	79	PHE	3.2
1	C	520	HIS	3.2
1	C	187	TRP	3.2
1	A	81	ALA	3.1
1	A	86	SER	3.1
1	B	138	ASN	3.1
1	C	74	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	141	GLN	3.1
1	D	677	GLU	3.0
1	D	187	TRP	3.0
1	D	505	GLN	3.0
1	A	470	LEU	3.0
1	D	54	ARG	3.0
1	D	98	LEU	3.0
1	D	379	GLU	3.0
1	D	492	ARG	3.0
1	A	71	LYS	2.9
1	A	74	ASN	2.9
1	D	144	THR	2.9
1	D	440	THR	2.9
1	A	440	THR	2.8
1	B	533	HIS	2.8
1	A	73	GLU	2.8
1	A	104	ASP	2.8
1	C	140	ARG	2.8
1	A	393	ASN	2.8
1	D	486	SER	2.7
1	C	83	TYR	2.7
1	D	412	SER	2.7
1	D	391	LYS	2.7
1	B	393	ASN	2.7
1	A	84	GLY	2.6
1	D	437	ASN	2.6
1	A	463	ASN	2.6
1	B	615	LYS	2.6
1	C	90	LEU	2.6
1	A	95	PHE	2.6
1	A	506	ASP	2.6
1	D	438	ASP	2.6
1	A	412	SER	2.6
1	C	54	ARG	2.6
1	C	91	GLU	2.6
1	D	96	ASP	2.5
1	D	520	HIS	2.5
1	A	487	SER	2.5
1	D	101	SER	2.5
1	C	179	ASN	2.5
1	D	414	TYR	2.5
1	A	69	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	41	ARG	2.5
1	A	79	PHE	2.5
1	B	115	LEU	2.5
1	A	745	ASN	2.5
1	B	103	ASN	2.5
1	C	573	ILE	2.4
1	A	78	LEU	2.4
1	A	491	LEU	2.4
1	D	766	PRO	2.4
1	C	135	TYR	2.4
1	B	437	ASN	2.4
1	D	423	LYS	2.4
1	A	384	ILE	2.4
1	B	145	GLU	2.3
1	C	745	ASN	2.3
1	C	119	ASN	2.3
1	D	535	ASP	2.3
1	C	137	LEU	2.3
1	D	482	LEU	2.3
1	C	615	LYS	2.3
1	A	492	ARG	2.3
1	A	537	SER	2.3
1	B	520	HIS	2.3
1	A	486	SER	2.3
1	A	415	LEU	2.3
1	C	506	ASP	2.3
1	D	506	ASP	2.3
1	D	457	TYR	2.2
1	A	295	ILE	2.2
1	A	70	TYR	2.2
1	A	40	ARG	2.2
1	A	90	LEU	2.2
1	C	415	LEU	2.2
1	C	533	HIS	2.2
1	A	54	ARG	2.2
1	B	418	ILE	2.1
1	D	114	ILE	2.1
1	C	440	THR	2.1
1	A	92	ASN	2.1
1	C	437	ASN	2.1
1	A	488	ASP	2.1
1	C	764	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	533	HIS	2.1
1	B	140	ARG	2.1
1	B	431	LEU	2.1
1	C	72	GLN	2.1
1	A	151	ASN	2.1
1	B	616	MET	2.1
1	D	448	GLU	2.1
1	C	151	ASN	2.1
1	D	463	ASN	2.1
1	A	761	GLN	2.1
1	B	187	TRP	2.1
1	B	388	GLN	2.1
1	B	327	ILE	2.1
1	B	146	GLU	2.0
1	B	677	GLU	2.0
1	A	333	SER	2.0
1	C	487	SER	2.0
1	A	89	PHE	2.0
1	C	384	ILE	2.0
1	C	538	LYS	2.0
1	D	441	LYS	2.0
1	A	448	GLU	2.0

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, 95^{th} 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	K	2	14/15	0.56	0.40	58,62,64,67	0
2	NAG	L	1	14/15	0.64	0.20	51,55,57,58	0
2	NAG	M	1	14/15	0.71	0.15	34,41,45,50	0
2	NAG	M	2	14/15	0.72	0.34	53,56,58,58	0
3	BMA	J	3	11/12	0.76	0.39	58,59,59,60	0
2	NAG	L	2	14/15	0.76	0.33	58,59,61,61	0

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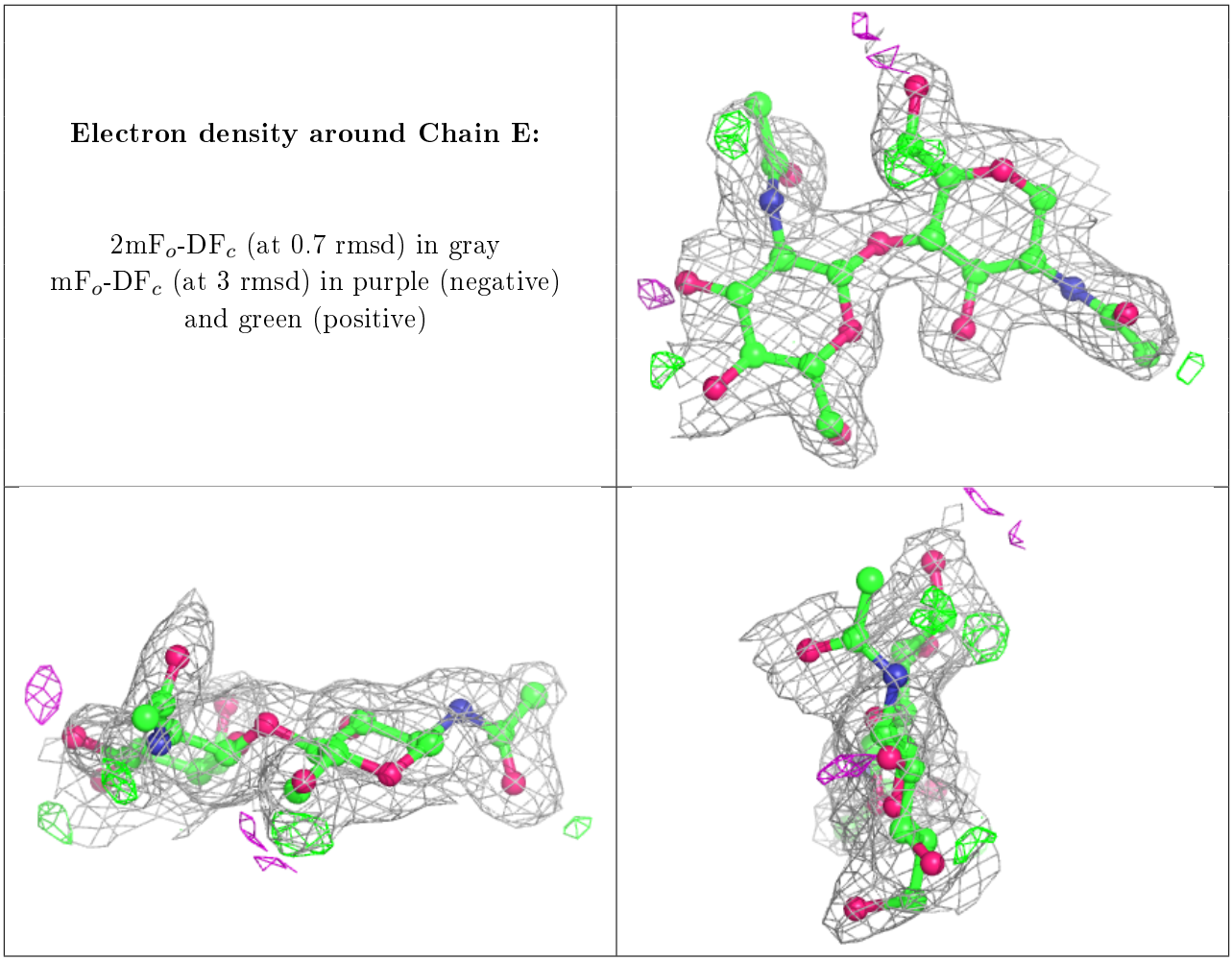
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	J	2	14/15	0.77	0.34	60,62,70,70	0
2	NAG	H	2	14/15	0.77	0.33	52,54,59,62	0
2	NAG	E	2	14/15	0.78	0.33	52,57,58,60	0
3	BMA	G	3	11/12	0.80	0.32	60,61,62,64	0
2	NAG	F	2	14/15	0.81	0.32	51,54,57,59	0
2	NAG	F	1	14/15	0.83	0.12	31,38,44,46	0
2	NAG	I	1	14/15	0.84	0.15	30,35,41,42	0
2	NAG	I	2	14/15	0.85	0.24	45,50,54,55	0
3	NAG	J	1	14/15	0.86	0.14	56,59,60,61	0
3	NAG	G	2	14/15	0.87	0.21	51,54,55,58	0
2	NAG	K	1	14/15	0.88	0.12	35,40,44,50	0
2	NAG	H	1	14/15	0.89	0.10	27,36,41,44	0
3	NAG	G	1	14/15	0.92	0.12	44,47,49,52	0
2	NAG	E	1	14/15	0.92	0.10	31,36,43,44	0

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

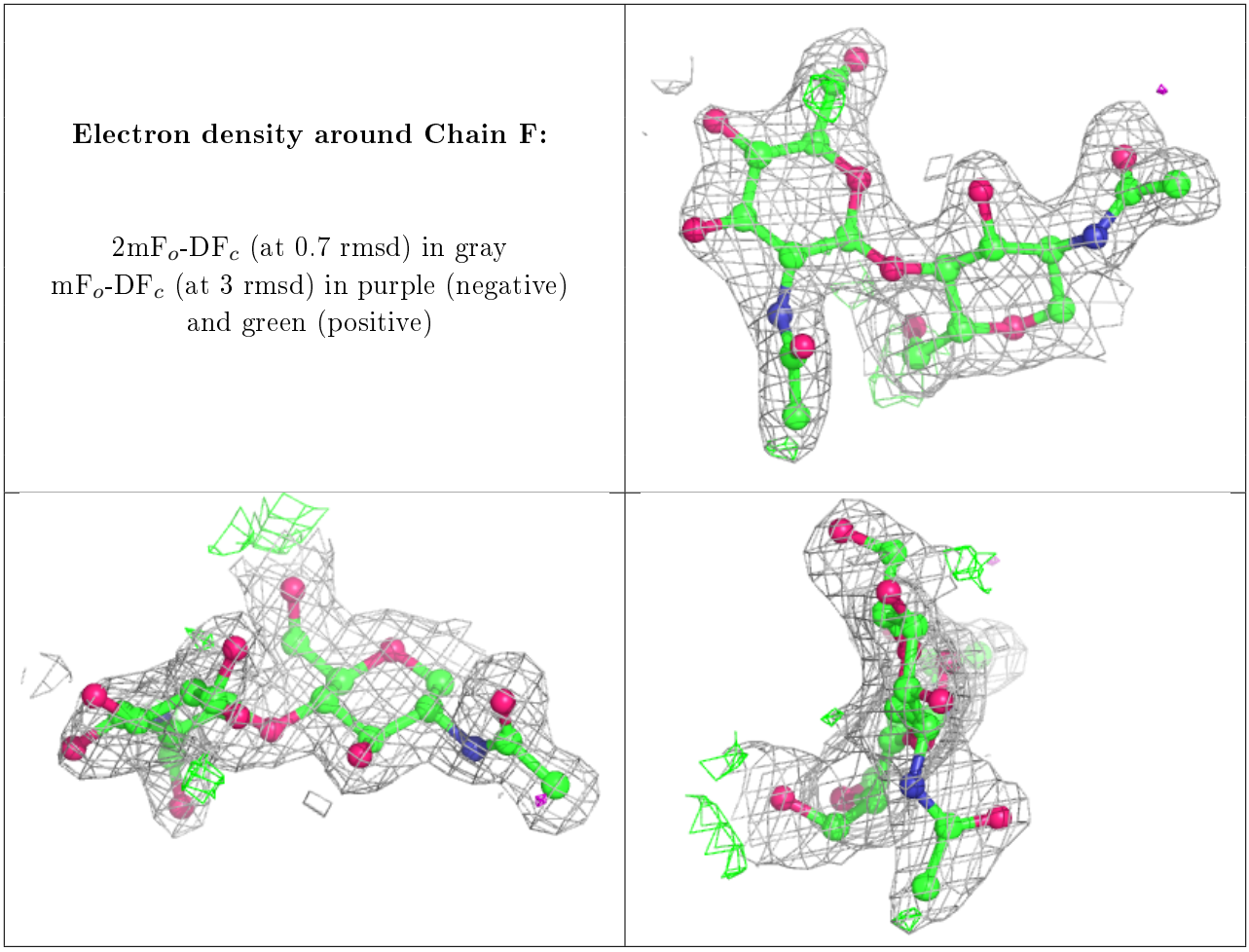
Electron density around Chain E:

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



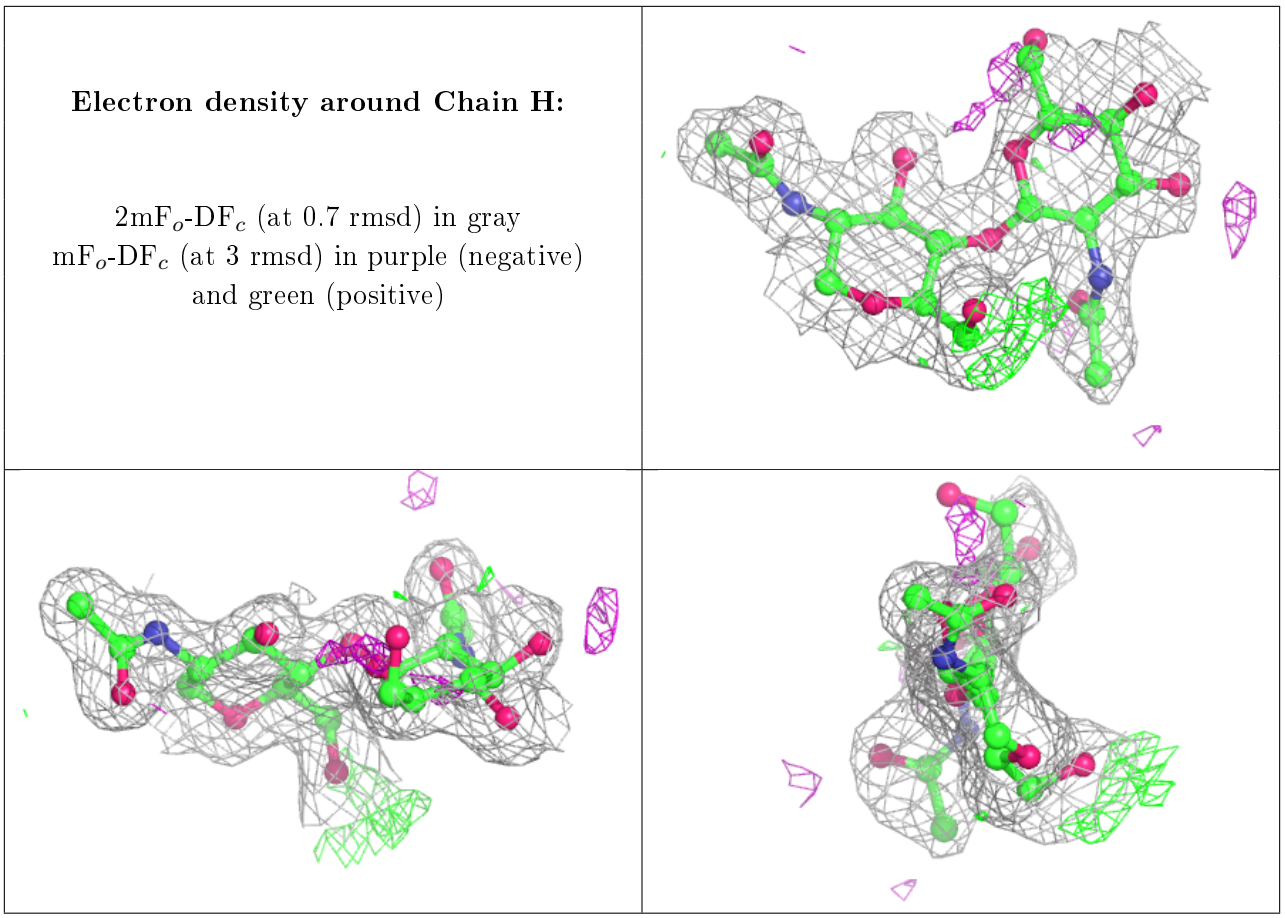
Electron density around Chain F:

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



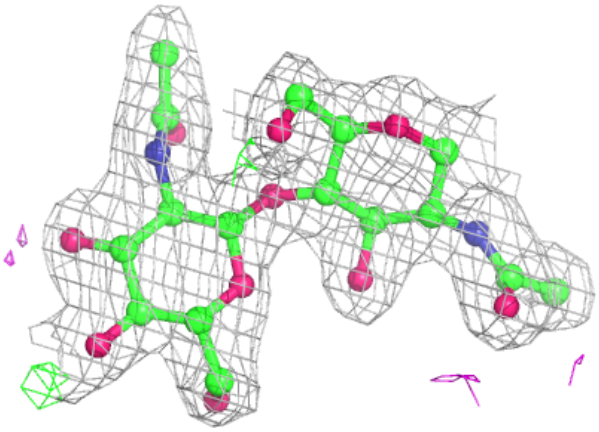
Electron density around Chain H:

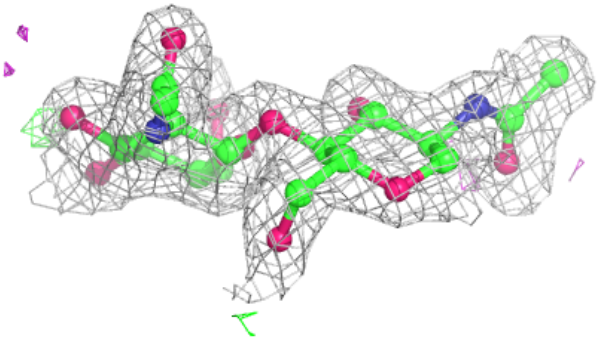
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

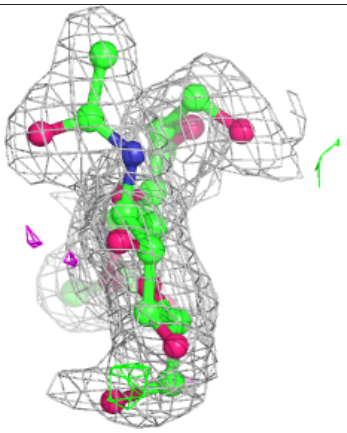


Electron density around Chain I:

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

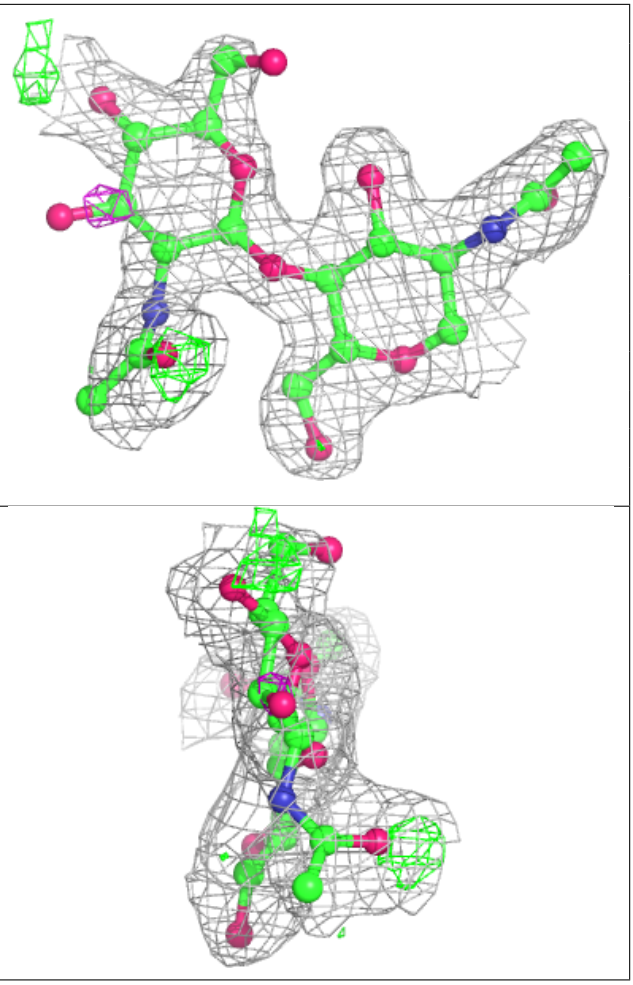






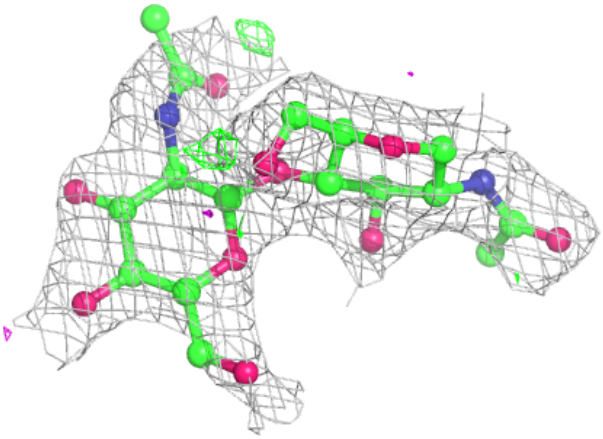
Electron density around Chain K:

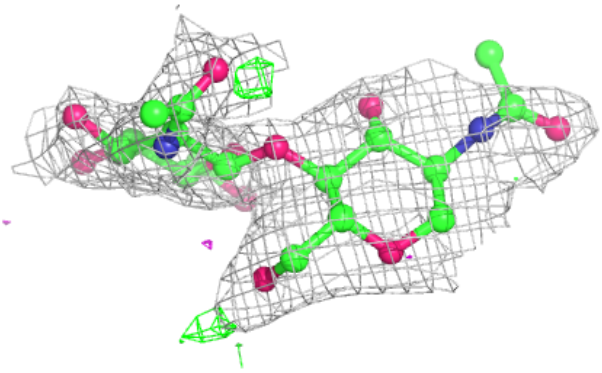
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

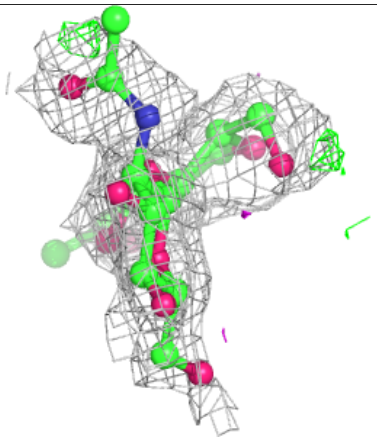


Electron density around Chain L:

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

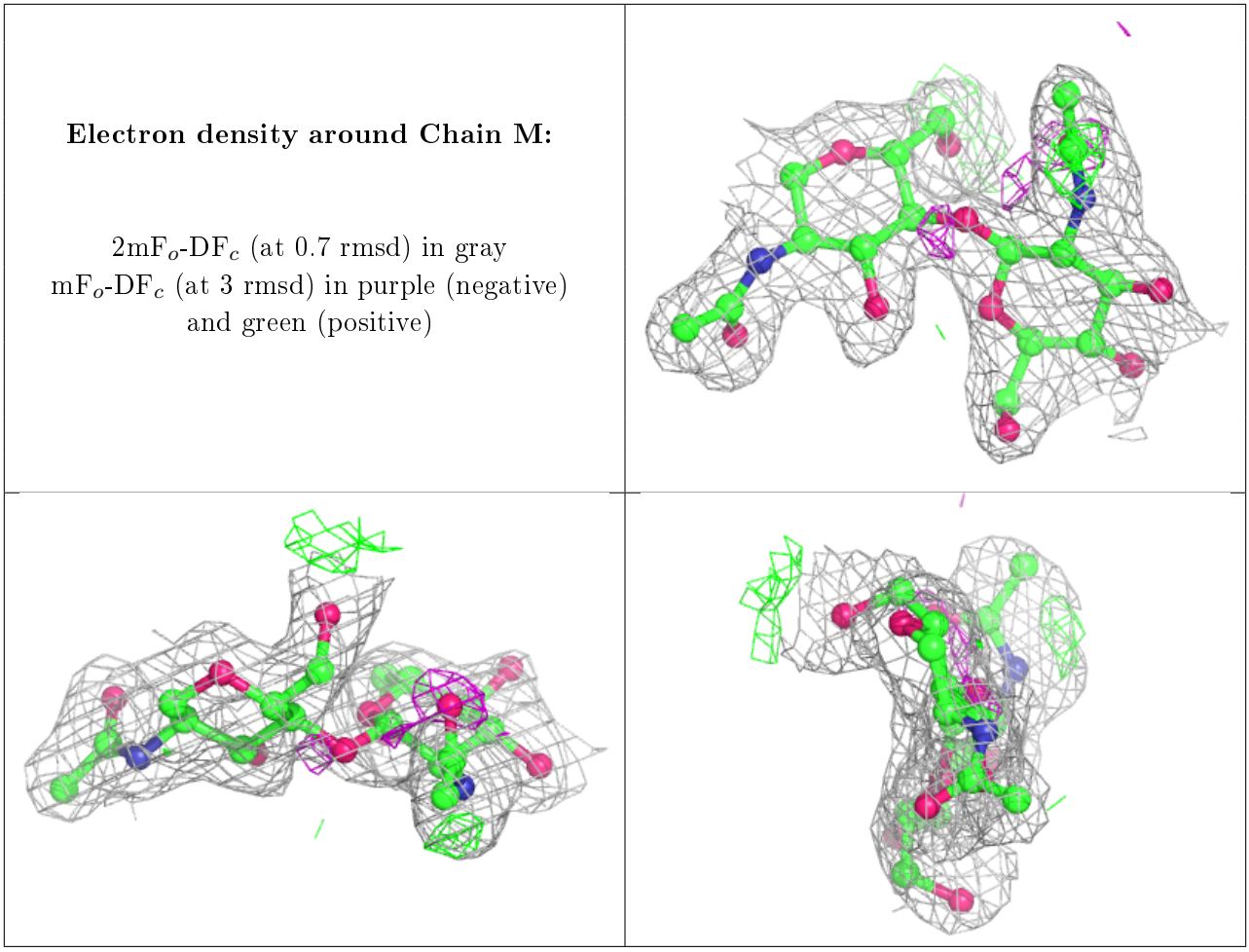






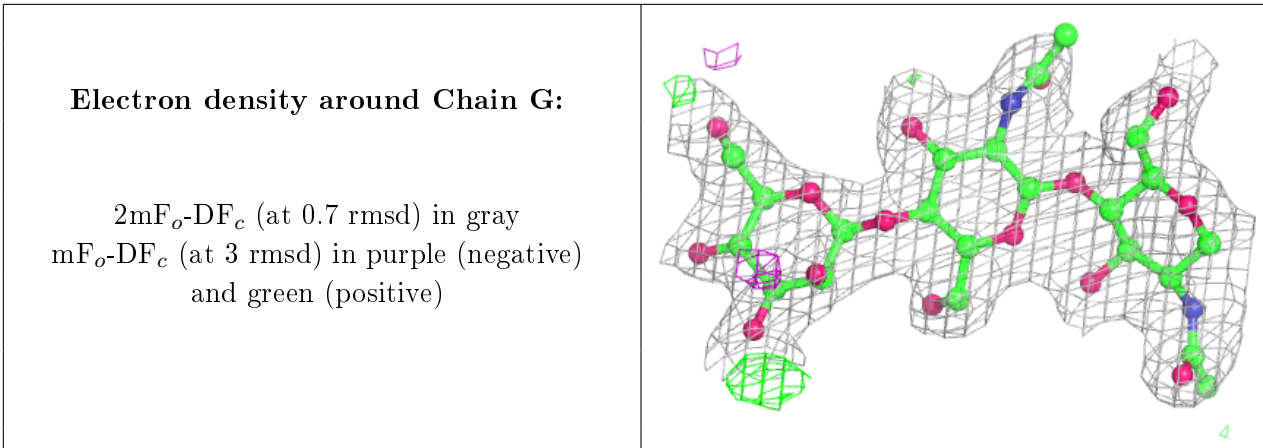
Electron density around Chain M:

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



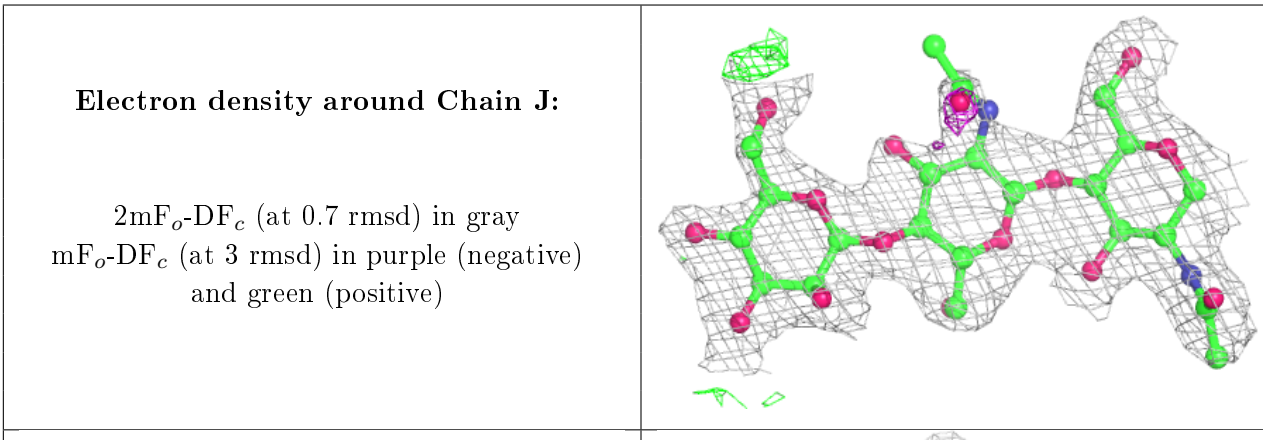
Electron density around Chain G:

$2mF_o$-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 J:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
4	NAG	D	767(A)	14/15	0.45	0.60	62,64,65,65	0
4	NAG	A	767(A)	14/15	0.58	0.43	70,73,73,74	0
4	NAG	D	773(A)	14/15	0.64	0.29	59,63,66,66	0
4	NAG	C	771(A)	14/15	0.65	0.21	47,52,56,56	0
4	NAG	C	768(A)	14/15	0.67	0.30	82,84,87,87	0
4	NAG	C	767(A)	14/15	0.70	0.21	60,62,64,66	0
4	NAG	C	770(A)	14/15	0.73	0.24	39,41,47,49	0
4	NAG	A	768(A)	14/15	0.76	0.18	78,78,79,79	0
4	NAG	A	771(A)	14/15	0.77	0.19	50,53,55,56	3
4	NAG	B	772(A)	14/15	0.78	0.24	45,47,50,51	0
4	NAG	B	767(A)	14/15	0.84	0.32	65,66,69,70	0
4	NAG	A	772(A)	14/15	0.85	0.13	44,48,54,54	0
4	NAG	B	773(A)	14/15	0.89	0.13	41,45,50,52	0
4	NAG	C	769(A)	14/15	0.89	0.13	31,36,40,43	0
4	NAG	B	771(A)	14/15	0.92	0.12	30,34,39,43	0
5	SO4	B	1501	5/5	0.98	0.10	28,29,30,33	0
5	SO4	D	1503	5/5	0.98	0.10	38,40,41,42	0
5	SO4	A	1500	5/5	0.99	0.11	33,34,35,37	0
5	SO4	C	1502	5/5	0.99	0.07	31,32,33,33	0

6.5 Other polymers

There are no such residues in this entry.