



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:22 PM UTC

PDB ID : 3CCB / pdb_00003ccb
Title : Crystal Structure of Human DPP4 in complex with a benzimidazole derivative
Authors : Wallace, M.B.; Skene, R.J.
Deposited on : 2008-02-25
Resolution : 2.49 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)
Xtrriage (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

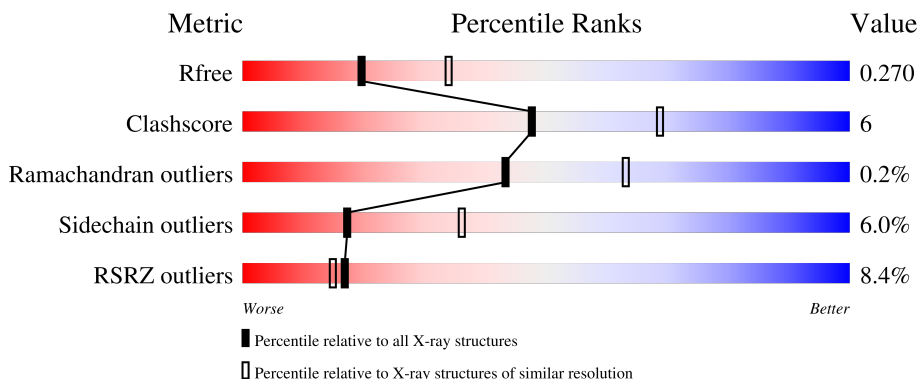
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	740	
1	B	740	
1	C	740	
1	D	740	
2	E	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 50% 50%
2	G	2	 100%
2	H	2	 50% 50%
2	I	2	 50% 50%

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
3	NAG	D	804	X	-	-	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 24805 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	724	5935	3812	977	1120	26	0	1	0
1	B	729	5965	3830	983	1126	26	0	0	0
1	C	724	5936	3813	977	1120	26	0	1	0
1	D	724	5929	3809	974	1120	26	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	expression tag	UNP P27487
A	28	ASP	-	expression tag	UNP P27487
A	29	PRO	-	expression tag	UNP P27487
A	30	GLY	-	expression tag	UNP P27487
A	31	GLY	-	expression tag	UNP P27487
A	32	SER	-	expression tag	UNP P27487
A	33	HIS	-	expression tag	UNP P27487
A	34	HIS	-	expression tag	UNP P27487
A	35	HIS	-	expression tag	UNP P27487
A	36	HIS	-	expression tag	UNP P27487
A	37	HIS	-	expression tag	UNP P27487
A	38	HIS	-	expression tag	UNP P27487
B	27	ALA	-	expression tag	UNP P27487
B	28	ASP	-	expression tag	UNP P27487
B	29	PRO	-	expression tag	UNP P27487
B	30	GLY	-	expression tag	UNP P27487
B	31	GLY	-	expression tag	UNP P27487
B	32	SER	-	expression tag	UNP P27487
B	33	HIS	-	expression tag	UNP P27487
B	34	HIS	-	expression tag	UNP P27487
B	35	HIS	-	expression tag	UNP P27487

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	expression tag	UNP P27487
B	37	HIS	-	expression tag	UNP P27487
B	38	HIS	-	expression tag	UNP P27487
C	27	ALA	-	expression tag	UNP P27487
C	28	ASP	-	expression tag	UNP P27487
C	29	PRO	-	expression tag	UNP P27487
C	30	GLY	-	expression tag	UNP P27487
C	31	GLY	-	expression tag	UNP P27487
C	32	SER	-	expression tag	UNP P27487
C	33	HIS	-	expression tag	UNP P27487
C	34	HIS	-	expression tag	UNP P27487
C	35	HIS	-	expression tag	UNP P27487
C	36	HIS	-	expression tag	UNP P27487
C	37	HIS	-	expression tag	UNP P27487
C	38	HIS	-	expression tag	UNP P27487
D	27	ALA	-	expression tag	UNP P27487
D	28	ASP	-	expression tag	UNP P27487
D	29	PRO	-	expression tag	UNP P27487
D	30	GLY	-	expression tag	UNP P27487
D	31	GLY	-	expression tag	UNP P27487
D	32	SER	-	expression tag	UNP P27487
D	33	HIS	-	expression tag	UNP P27487
D	34	HIS	-	expression tag	UNP P27487
D	35	HIS	-	expression tag	UNP P27487
D	36	HIS	-	expression tag	UNP P27487
D	37	HIS	-	expression tag	UNP P27487
D	38	HIS	-	expression tag	UNP P27487

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



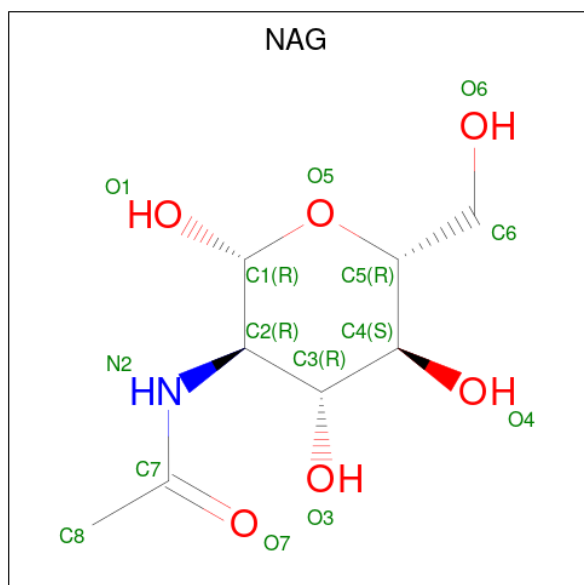
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
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			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



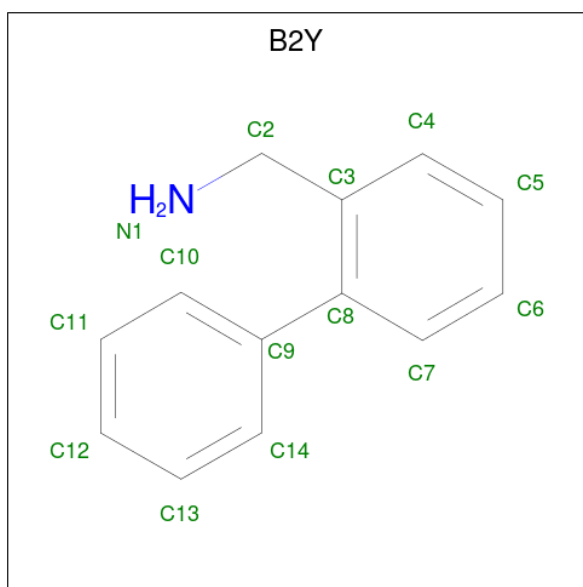
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is 1-biphenyl-2-ylmethanamine (CCD ID: B2Y) (formula: C₁₃H₁₃N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			14	13	1		
4	B	1	Total	C	N	0	0
			14	13	1		
4	C	1	Total	C	N	0	0
			14	13	1		
4	D	1	Total	C	N	0	0
			14	13	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total	O	0	0
			206	206		
5	B	191	Total	O	0	0
			191	191		

Continued on next page...

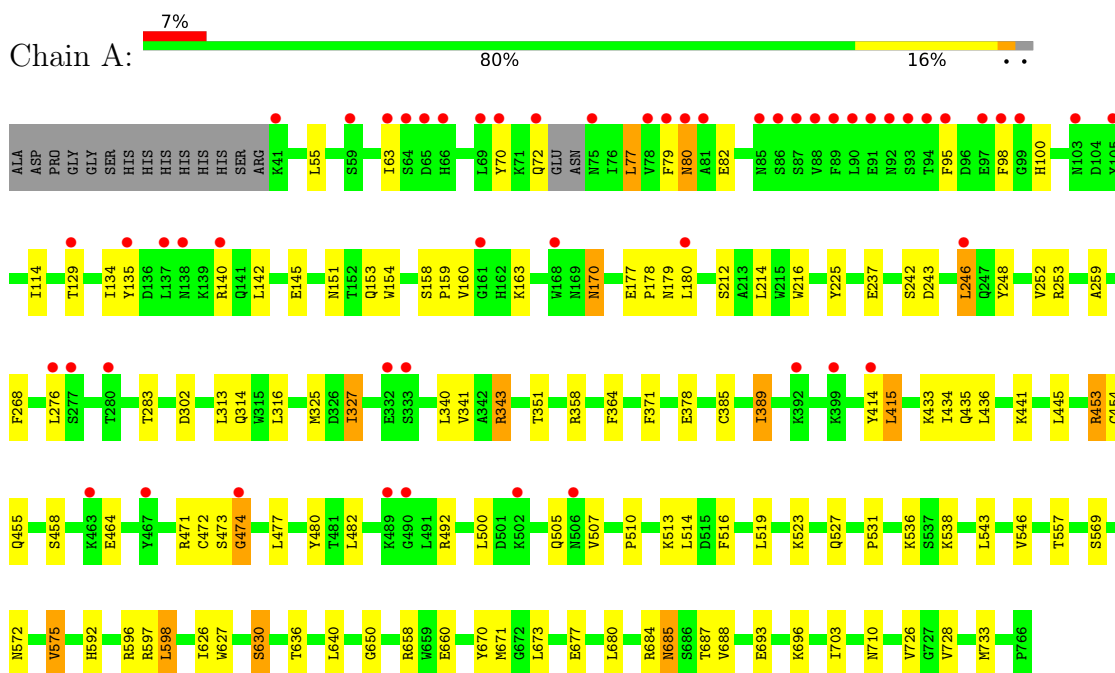
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	189	Total 189	O 189	0	0
5	D	90	Total 90	O 90	0	0

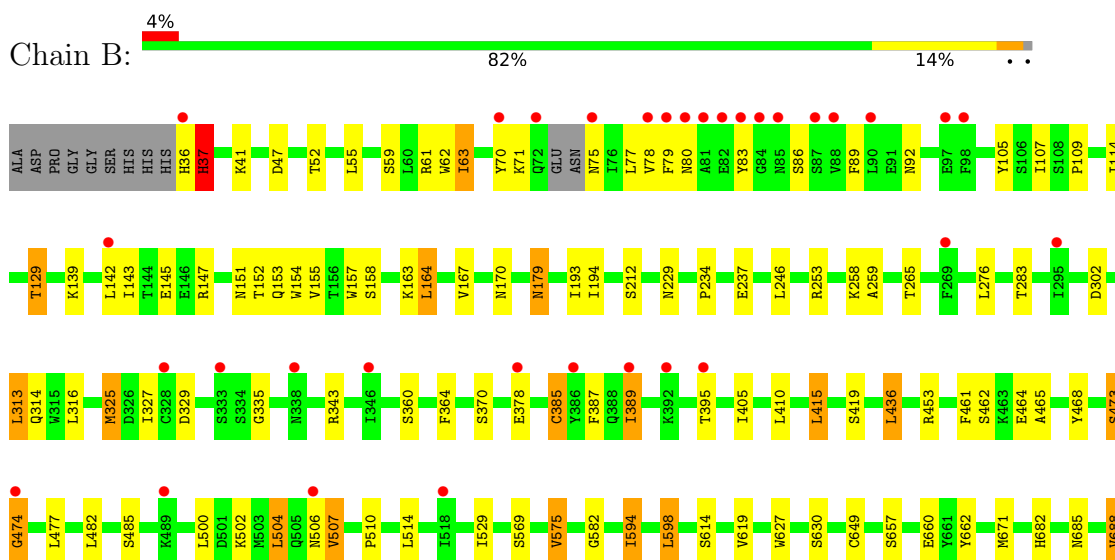
3 Residue-property plots i

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 4

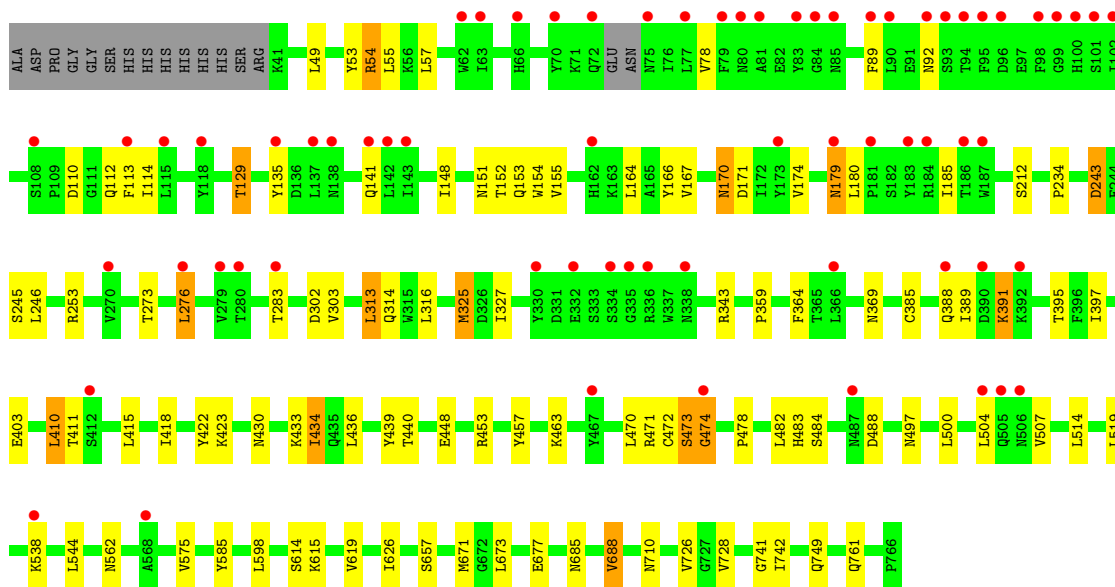
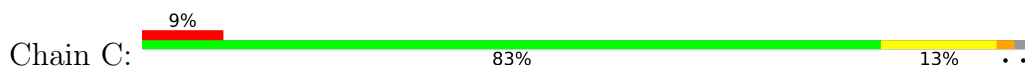


- Molecule 1: Dipeptidyl peptidase 4

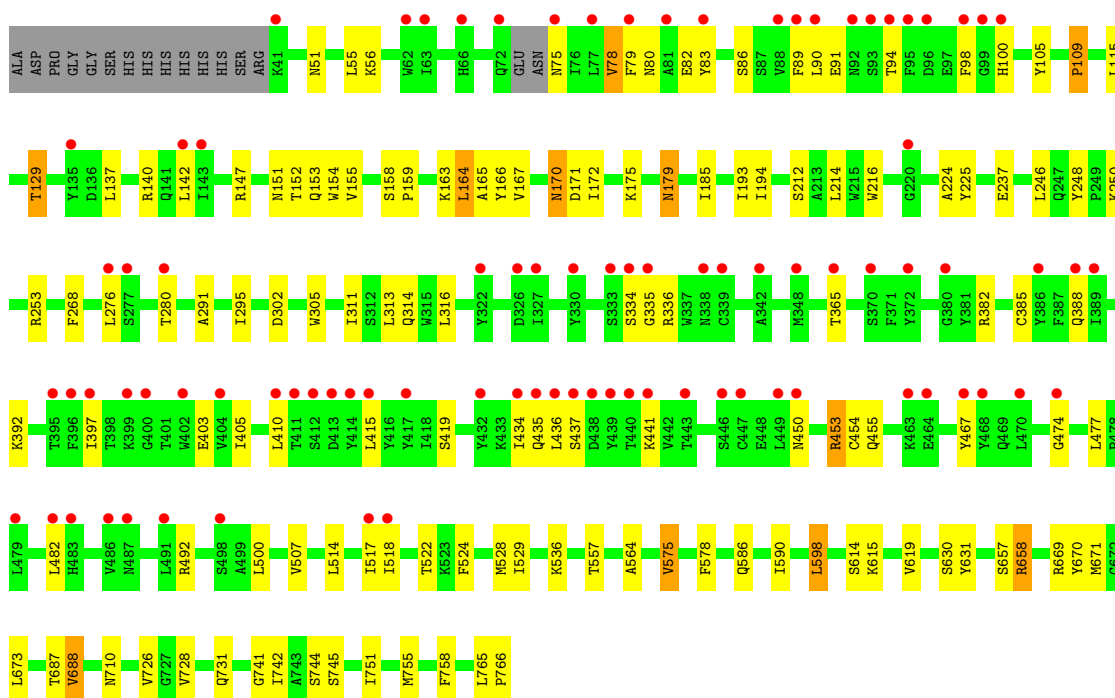
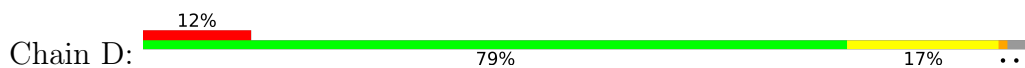




● Molecule 1: Dipeptidyl peptidase 4



● Molecule 1: Dipeptidyl peptidase 4



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

Chain E:  50% 50%

MAG1
MAG2

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

Chain F:  50% 50%

MAG1
MAG2

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

Chain G:  100%

MAG1
MAG2

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

Chain H:  50% 50%

MAG1
MAG2

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

Chain I:  50% 50%

MAG1
MAG2

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	122.09Å 123.01Å 144.65Å 90.00° 114.84° 90.00°	Depositor
Resolution (Å)	32.80 – 2.49 32.80 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.80-2.49) 98.5 (32.80-2.49)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 2.48Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.244 0.234 , 0.270	Depositor DCC
R_{free} test set	6730 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtrriage
Anisotropy	0.049	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24805	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, B2Y

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	0.52	0/6111	0.80	1/8311 (0.0%)
1	B	0.51	0/6138	0.82	2/8348 (0.0%)
1	C	0.51	0/6111	0.82	3/8311 (0.0%)
1	D	0.49	0/6100	0.80	3/8296 (0.0%)
All	All	0.51	0/24460	0.81	9/33266 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	94	THR	N-CA-C	-6.82	104.99	113.38
1	D	630	SER	CB-CA-C	-6.06	108.99	117.23
1	B	630	SER	CB-CA-C	-5.96	109.12	117.23
1	D	335	GLY	N-CA-C	-5.95	107.18	114.92
1	B	335	GLY	N-CA-C	-5.77	107.28	115.30
1	C	391	LYS	N-CA-C	5.36	118.44	110.14
1	A	630	SER	CB-CA-C	-5.30	110.02	117.23
1	C	141	GLN	N-CA-C	5.10	117.16	109.41
1	C	473	SER	N-CA-C	-5.01	106.86	113.17

There are no chirality outliers.

There are no planarity outliers.

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	5935	0	5657	74	0
1	B	5965	0	5672	66	0
1	C	5936	0	5660	66	0
1	D	5929	0	5651	64	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	56	0	52	0	0
3	B	56	0	52	1	0
3	C	28	0	26	0	0
3	D	28	0	26	1	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	206	0	0	2	0
5	B	191	0	0	0	0
5	C	189	0	0	1	0
5	D	90	0	0	0	0
All	All	24805	0	22973	262	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 6.

All (262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.28	1.12
1:C:343:ARG:HD2	1:C:389:ILE:HG22	1.42	0.98
1:C:153:GLN:HE22	1:C:170:ASN:H	1.14	0.93
1:A:153:GLN:HE22	1:A:170:ASN:H	1.18	0.90
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.14	0.90
1:C:54:ARG:HG2	1:C:54:ARG:HH21	1.39	0.88
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.71	0.88
1:A:325:MET:HE3	1:A:327:ILE:CD1	2.03	0.87
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.71	0.87
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.58	0.85
1:D:153:GLN:HE22	1:D:170:ASN:H	1.22	0.84
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.88	0.83
1:B:343:ARG:HD3	1:B:389:ILE:HG23	1.59	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:GLN:HE22	1:B:170:ASN:H	1.27	0.82
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.64	0.79
1:A:325:MET:CE	1:A:327:ILE:HD11	2.11	0.75
1:C:434:ILE:HD11	1:C:439:TYR:HB2	1.67	0.74
1:A:129:THR:HG23	1:A:151:ASN:HA	1.70	0.73
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.73	0.70
1:D:179:ASN:H	1:D:179:ASN:HD22	1.42	0.67
1:A:129:THR:CG2	1:A:151:ASN:HA	2.25	0.67
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.79	0.64
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.92	0.64
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.32	0.64
1:B:36:HIS:O	1:B:37:HIS:HB2	1.98	0.63
1:B:614:SER:HA	1:B:619:VAL:HB	1.79	0.63
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.28	0.63
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.80	0.62
1:C:343:ARG:HD2	1:C:389:ILE:CG2	2.23	0.62
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.82	0.62
1:C:153:GLN:NE2	1:C:170:ASN:H	1.94	0.62
1:D:147:ARG:HE	3:D:801:NAG:H83	1.66	0.61
1:A:135:TYR:HD1	1:A:142:LEU:HD13	1.65	0.61
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.83	0.61
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.36	0.60
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.83	0.60
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.92	0.60
1:D:564:ALA:HB1	1:D:575:VAL:HG11	1.84	0.60
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.84	0.60
1:D:155:VAL:HG12	1:D:166:TYR:HB3	1.85	0.59
1:C:314:GLN:HG2	1:C:325:MET:HB2	1.85	0.59
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.85	0.59
1:B:711:VAL:CG2	4:B:800:B2Y:H11	2.32	0.58
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.84	0.58
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.86	0.58
1:B:529:ILE:HB	1:B:575:VAL:HG13	1.84	0.58
1:C:472:CYS:O	1:C:478:PRO:HA	2.04	0.57
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.67	0.57
1:D:522:THR:HB	1:D:524:PHE:CE2	2.40	0.57
1:D:382:ARG:H	1:D:403:GLU:HG2	1.69	0.57
1:D:415:LEU:HB2	1:D:436:LEU:HD11	1.86	0.57
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.86	0.56
1:D:529:ILE:HB	1:D:575:VAL:HG13	1.87	0.56
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:THR:HG21	1:C:155:VAL:HG13	1.88	0.55
1:B:582:GLY:HA2	1:B:594:ILE:HD12	1.88	0.55
1:C:369:ASN:C	1:C:389:ILE:HG12	2.32	0.55
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.71	0.55
1:D:78:VAL:HG22	1:D:89:PHE:HB2	1.88	0.55
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.89	0.55
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.42	0.54
1:C:153:GLN:HE22	1:C:170:ASN:N	1.95	0.54
1:B:343:ARG:HD3	1:B:389:ILE:CG2	2.32	0.54
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.89	0.54
1:B:89:PHE:HE1	1:B:107:ILE:HD12	1.73	0.54
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.91	0.54
1:D:614:SER:HA	1:D:619:VAL:HB	1.89	0.53
1:A:340:LEU:HD22	1:A:343:ARG:HH11	1.74	0.53
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.89	0.53
1:C:174:VAL:HG23	1:C:185:ILE:CD1	2.39	0.53
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.90	0.52
1:A:135:TYR:HE2	1:A:140:ARG:HG2	1.74	0.52
1:C:179:ASN:C	1:C:179:ASN:HD22	2.18	0.52
1:C:170:ASN:N	1:C:170:ASN:HD22	2.08	0.52
1:A:170:ASN:N	1:A:170:ASN:HD22	2.08	0.51
1:C:53:TYR:HB3	1:C:500:LEU:HD11	1.92	0.51
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.40	0.51
1:D:657:SER:HA	1:D:688:VAL:HG13	1.91	0.51
1:B:179:ASN:H	1:B:179:ASN:HD22	1.57	0.51
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.93	0.51
1:B:147:ARG:HE	3:B:802:NAG:H83	1.75	0.51
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.46	0.51
1:D:453:ARG:NH2	1:D:477:LEU:O	2.43	0.51
1:A:710:ASN:HD22	1:A:710:ASN:C	2.20	0.50
1:C:369:ASN:O	1:C:389:ILE:HG12	2.11	0.50
1:C:273:THR:HA	1:C:276:LEU:HD22	1.93	0.50
1:C:153:GLN:NE2	1:C:167:VAL:HG12	2.27	0.50
1:A:325:MET:HE1	1:A:371:PHE:CE2	2.47	0.50
1:C:741:GLY:O	1:C:742:ILE:C	2.55	0.50
1:D:435:GLN:HE21	1:D:437:SER:HG	1.60	0.50
1:D:598:LEU:HG	1:D:631:TYR:OH	2.12	0.49
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.93	0.49
1:D:334:SER:HB2	1:D:336:ARG:H	1.77	0.49
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.94	0.49
1:B:158:SER:HB3	1:B:163:LYS:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ARG:HG2	1:C:54:ARG:NH2	2.16	0.49
1:B:79:PHE:HA	1:B:86:SER:HB3	1.94	0.49
1:D:710:ASN:C	1:D:710:ASN:HD22	2.19	0.49
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.43	0.49
1:A:153:GLN:NE2	1:A:170:ASN:H	1.99	0.49
1:B:47:ASP:HA	1:B:52:THR:OG1	2.12	0.49
1:B:80:ASN:HD22	1:B:83:TYR:H	1.59	0.49
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.13	0.49
1:D:82:GLU:HG2	1:D:467:TYR:OH	2.13	0.49
1:B:378:GLU:CD	1:B:378:GLU:H	2.21	0.48
1:C:110:ASP:OD2	1:C:112:GLN:HG2	2.13	0.48
1:C:129:THR:HG23	1:C:151:ASN:HA	1.93	0.48
1:C:327:ILE:HD13	1:C:389:ILE:HG23	1.95	0.48
1:D:75:ASN:OD1	1:D:91:GLU:HG3	2.12	0.48
1:C:473:SER:O	1:C:474:GLY:O	2.32	0.48
1:B:598:LEU:HB2	1:B:671:MET:SD	2.54	0.48
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.48	0.48
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.95	0.48
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.46	0.48
1:A:435:GLN:OE1	1:A:441:LYS:HE2	2.14	0.48
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.96	0.47
1:B:473:SER:O	1:B:474:GLY:O	2.32	0.47
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.13	0.47
1:D:751:ILE:HG12	1:D:755:MET:HE2	1.96	0.47
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.48	0.47
1:B:71:LYS:HA	1:B:75:ASN:O	2.14	0.47
1:A:153:GLN:HE22	1:A:170:ASN:N	2.00	0.47
1:B:109:PRO:HG2	1:B:158:SER:O	2.14	0.47
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.96	0.47
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.96	0.47
1:D:305:TRP:CE2	1:D:311:ILE:HD12	2.49	0.47
2:G:1:NAG:H62	2:G:2:NAG:N2	2.30	0.47
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.96	0.47
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.80	0.47
1:D:80:ASN:HD22	1:D:83:TYR:HB2	1.80	0.47
1:B:465:ALA:O	1:B:485:SER:OG	2.25	0.47
1:C:303:VAL:HG22	1:C:313:LEU:HD12	1.97	0.47
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.49	0.46
1:D:586:GLN:HB3	1:D:590:ILE:HD12	1.97	0.46
1:D:158:SER:OG	1:D:163:LYS:HB2	2.15	0.46
1:A:378:GLU:CD	1:A:378:GLU:H	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ASN:N	1:D:170:ASN:HD22	2.14	0.46
1:A:685:ASN:ND2	5:A:866:HOH:O	2.48	0.46
1:A:693:GLU:OE1	1:A:696:LYS:NZ	2.43	0.46
1:B:314:GLN:HG2	1:B:325:MET:HB2	1.97	0.46
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.98	0.46
1:C:55:LEU:HD23	1:C:500:LEU:HD22	1.98	0.46
1:C:657:SER:HA	1:C:688:VAL:HG13	1.98	0.46
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.98	0.46
1:D:193:ILE:HG22	1:D:194:ILE:HG12	1.98	0.46
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.31	0.45
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.80	0.45
1:D:405:ILE:HG12	1:D:419:SER:HA	1.98	0.45
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.98	0.45
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.98	0.45
1:D:214:LEU:HD23	1:D:225:TYR:HB3	1.98	0.45
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.52	0.45
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.97	0.45
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.47	0.45
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.82	0.45
1:B:129:THR:HG23	1:B:151:ASN:HA	1.97	0.45
1:C:410:LEU:HD22	1:C:411:THR:O	2.16	0.45
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.52	0.45
1:B:153:GLN:NE2	1:B:170:ASN:H	2.06	0.45
1:D:129:THR:HG23	1:D:151:ASN:HA	1.98	0.45
1:D:731:GLN:HG3	1:D:758:PHE:HE1	1.82	0.44
1:A:135:TYR:CE2	1:A:140:ARG:HA	2.52	0.44
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.99	0.44
1:B:62:TRP:CG	1:B:462:SER:HA	2.53	0.44
1:B:75:ASN:ND2	1:B:92:ASN:HD22	2.15	0.44
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.33	0.44
1:C:614:SER:HA	1:C:619:VAL:HB	2.00	0.44
1:A:98:PHE:CD1	1:A:100:HIS:HB2	2.52	0.44
1:B:152:THR:HG21	1:B:155:VAL:HG22	1.98	0.44
1:B:193:ILE:HG22	1:B:194:ILE:HG12	2.00	0.44
1:D:455:GLN:HE21	1:D:557:THR:HG21	1.82	0.44
1:B:75:ASN:HD21	1:B:92:ASN:HD22	1.66	0.43
1:D:517:ILE:HD11	1:D:578:PHE:CE1	2.53	0.43
1:C:78:VAL:HG23	1:C:89:PHE:HB2	2.00	0.43
1:C:422:TYR:CE1	1:C:423:LYS:HE3	2.54	0.43
1:B:405:ILE:HG12	1:B:419:SER:HA	2.00	0.43
1:C:243:ASP:C	1:C:245:SER:N	2.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:ILE:HD12	1:D:434:ILE:HD13	2.01	0.43
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.43
1:C:544:LEU:HD23	1:C:626:ILE:HD12	2.00	0.43
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.53	0.43
1:C:710:ASN:C	1:C:710:ASN:HD22	2.26	0.43
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.54	0.43
1:A:473:SER:O	1:A:474:GLY:O	2.36	0.43
1:D:291:ALA:O	1:D:295:ILE:HG23	2.18	0.43
1:A:596:ARG:HA	1:A:670:TYR:O	2.19	0.43
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.54	0.43
1:D:165:ALA:HB2	1:D:216:TRP:CZ2	2.54	0.43
1:D:268:PHE:CD2	1:D:313:LEU:HD21	2.54	0.43
1:A:453:ARG:HG3	1:A:454:CYS:SG	2.58	0.43
1:C:112:GLN:HG3	1:C:113:PHE:CD2	2.53	0.43
1:C:148:ILE:HD11	1:C:164:LEU:HD21	2.01	0.43
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.49	0.42
1:D:268:PHE:CE2	1:D:313:LEU:HD11	2.54	0.42
1:A:72:GLN:HB2	1:A:77:LEU:HD21	2.01	0.42
1:A:80:ASN:HD22	1:A:82:GLU:H	1.66	0.42
1:B:415:LEU:HB2	1:B:436:LEU:HD11	2.02	0.42
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.54	0.42
1:A:433:LYS:HE2	1:A:445:LEU:HD21	2.01	0.42
1:C:54:ARG:HH21	1:C:54:ARG:CG	2.19	0.42
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.50	0.42
1:C:418:ILE:HA	1:C:430:ASN:O	2.19	0.42
1:A:129:THR:HG22	5:A:1002:HOH:O	2.18	0.42
1:C:155:VAL:HG12	1:C:166:TYR:HB3	2.01	0.42
1:D:450:ASN:O	1:D:454:CYS:HB2	2.20	0.42
1:A:596:ARG:N	1:A:670:TYR:O	2.47	0.42
1:C:179:ASN:HD22	1:C:180:LEU:N	2.17	0.42
1:D:435:GLN:OE1	1:D:441:LYS:HD3	2.19	0.42
1:D:741:GLY:O	1:D:742:ILE:C	2.62	0.42
1:D:765:LEU:HA	1:D:766:PRO:HD3	1.91	0.42
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.41
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.01	0.41
1:B:70:TYR:CG	1:B:71:LYS:N	2.88	0.41
1:B:258:LYS:O	1:B:259:ALA:C	2.62	0.41
1:B:313:LEU:O	1:B:325:MET:HA	2.19	0.41
1:C:167:VAL:HA	1:C:171:ASP:O	2.20	0.41
1:D:744:SER:O	1:D:745:SER:C	2.63	0.41
1:C:302:ASP:HB3	1:C:314:GLN:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:LYS:O	1:A:527:GLN:HA	2.20	0.41
1:B:506:ASN:HB2	1:C:440:THR:CG2	2.49	0.41
1:C:397:ILE:HD12	1:C:434:ILE:HD13	2.03	0.41
1:D:79:PHE:CD2	1:D:86:SER:HB3	2.54	0.41
1:D:98:PHE:CD1	1:D:100:HIS:HB2	2.55	0.41
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.55	0.41
1:A:458:SER:OG	1:A:471:ARG:HB3	2.21	0.41
1:A:703:ILE:HA	1:A:733:MET:O	2.21	0.41
1:B:662:TYR:HE1	1:B:710:ASN:HD22	1.69	0.41
1:B:710:ASN:HD22	1:B:710:ASN:C	2.27	0.41
1:C:457:TYR:HA	1:C:471:ARG:O	2.20	0.41
1:D:237:GLU:HG2	1:D:253:ARG:HG2	2.02	0.41
1:D:598:LEU:HB2	1:D:671:MET:SD	2.60	0.41
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.56	0.41
1:D:105:TYR:HA	1:D:115:LEU:O	2.20	0.41
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.56	0.41
1:A:135:TYR:CE2	1:A:140:ARG:HG2	2.55	0.41
1:C:478:PRO:HB2	1:C:497:ASN:ND2	2.36	0.41
1:D:55:LEU:HD23	1:D:500:LEU:HD22	2.02	0.41
1:D:598:LEU:HD22	1:D:671:MET:HG2	2.02	0.41
1:B:657:SER:HA	1:B:688:VAL:HG13	2.02	0.41
1:C:49:LEU:HD22	1:C:749:GLN:HA	2.03	0.41
1:A:242:SER:OG	1:A:243:ASP:N	2.53	0.41
1:D:167:VAL:HA	1:D:171:ASP:O	2.21	0.41
1:A:154:TRP:CD2	1:A:212:SER:HB3	2.56	0.41
1:A:177:GLU:HB2	1:A:180:LEU:HG	2.02	0.41
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.77	0.41
1:A:598:LEU:HB2	1:A:671:MET:SD	2.60	0.41
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.51	0.41
1:B:598:LEU:O	1:B:682:HIS:NE2	2.52	0.41
1:C:562:ASN:HB2	5:C:841:HOH:O	2.20	0.41
1:A:543:LEU:O	1:A:575:VAL:HA	2.22	0.41
1:B:582:GLY:CA	1:B:594:ILE:HD12	2.50	0.40
1:C:484:SER:O	1:C:488:ASP:HA	2.20	0.40
1:D:55:LEU:HD23	1:D:500:LEU:CD2	2.51	0.40
1:A:158:SER:OG	1:A:163:LYS:HB2	2.22	0.40
1:A:237:GLU:HA	1:A:252:VAL:O	2.21	0.40
1:A:546:VAL:HG12	1:A:627:TRP:O	2.21	0.40
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.02	0.40
1:D:164:LEU:HB3	1:D:175:LYS:HB2	2.03	0.40
1:A:414:TYR:CE2	1:A:433:LYS:HD3	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ILE:HD12	1:B:63:ILE:HA	1.81	0.40
1:B:741:GLY:O	1:B:742:ILE:C	2.64	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	721/740 (97%)	684 (95%)	36 (5%)	1 (0%)	48 68
1	B	725/740 (98%)	698 (96%)	25 (3%)	2 (0%)	36 55
1	C	721/740 (97%)	688 (95%)	31 (4%)	2 (0%)	36 55
1	D	720/740 (97%)	684 (95%)	34 (5%)	2 (0%)	36 55
All	All	2887/2960 (98%)	2754 (95%)	126 (4%)	7 (0%)	43 63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	474	GLY
1	A	474	GLY
1	B	37	HIS
1	B	474	GLY
1	D	474	GLY
1	C	92	ASN
1	D	109	PRO

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	650/662 (98%)	609 (94%)	41 (6%)	16	34
1	B	652/662 (98%)	608 (93%)	44 (7%)	15	31
1	C	650/662 (98%)	615 (95%)	35 (5%)	20	41
1	D	649/662 (98%)	612 (94%)	37 (6%)	18	39
All	All	2601/2648 (98%)	2444 (94%)	157 (6%)	17	36

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	77	LEU
1	A	80	ASN
1	A	95	PHE
1	A	145	GLU
1	A	160	VAL
1	A	170	ASN
1	A	179	ASN
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	327	ILE
1	A	341	VAL
1	A	343	ARG
1	A	358[A]	ARG
1	A	358[B]	ARG
1	A	385	CYS
1	A	389	ILE
1	A	415	LEU
1	A	436	LEU
1	A	453	ARG
1	A	464	GLU
1	A	472	CYS
1	A	477	LEU
1	A	482	LEU
1	A	492	ARG
1	A	505	GLN
1	A	507	VAL
1	A	514	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	519	LEU
1	A	536	LYS
1	A	538	LYS
1	A	575	VAL
1	A	597	ARG
1	A	598	LEU
1	A	630	SER
1	A	673	LEU
1	A	677	GLU
1	A	685	ASN
1	A	688	VAL
1	B	37	HIS
1	B	41	LYS
1	B	59	SER
1	B	61	ARG
1	B	63	ILE
1	B	77	LEU
1	B	129	THR
1	B	139	LYS
1	B	142	LEU
1	B	143	ILE
1	B	145	GLU
1	B	164	LEU
1	B	179	ASN
1	B	246	LEU
1	B	276	LEU
1	B	283	THR
1	B	313	LEU
1	B	316	LEU
1	B	325	MET
1	B	360	SER
1	B	370	SER
1	B	385	CYS
1	B	389	ILE
1	B	395	THR
1	B	410	LEU
1	B	415	LEU
1	B	436	LEU
1	B	453	ARG
1	B	464	GLU
1	B	473	SER
1	B	477	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	482	LEU
1	B	502	LYS
1	B	504	LEU
1	B	507	VAL
1	B	514	LEU
1	B	575	VAL
1	B	594	ILE
1	B	598	LEU
1	B	627	TRP
1	B	660	GLU
1	B	685	ASN
1	B	688	VAL
1	B	710	ASN
1	C	54	ARG
1	C	57	LEU
1	C	129	THR
1	C	170	ASN
1	C	179	ASN
1	C	243	ASP
1	C	246	LEU
1	C	276	LEU
1	C	283	THR
1	C	313	LEU
1	C	316	LEU
1	C	325	MET
1	C	385	CYS
1	C	395	THR
1	C	410	LEU
1	C	415	LEU
1	C	433	LYS
1	C	434	ILE
1	C	436	LEU
1	C	448	GLU
1	C	453	ARG
1	C	463	LYS
1	C	482	LEU
1	C	504	LEU
1	C	507	VAL
1	C	514	LEU
1	C	519	LEU
1	C	538	LYS
1	C	575	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	615	LYS
1	C	673	LEU
1	C	677	GLU
1	C	685	ASN
1	C	688	VAL
1	C	761	GLN
1	D	51	ASN
1	D	56	LYS
1	D	78	VAL
1	D	90	LEU
1	D	109	PRO
1	D	129	THR
1	D	137	LEU
1	D	140	ARG
1	D	142	LEU
1	D	152	THR
1	D	164	LEU
1	D	170	ASN
1	D	179	ASN
1	D	246	LEU
1	D	250	LYS
1	D	276	LEU
1	D	280	THR
1	D	316	LEU
1	D	365	THR
1	D	385	CYS
1	D	388	GLN
1	D	392	LYS
1	D	410	LEU
1	D	453	ARG
1	D	482	LEU
1	D	492	ARG
1	D	507	VAL
1	D	514	LEU
1	D	518	ILE
1	D	528	MET
1	D	536	LYS
1	D	575	VAL
1	D	598	LEU
1	D	615	LYS
1	D	658	ARG
1	D	673	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	688	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	72	GLN
1	A	80	ASN
1	A	100	HIS
1	A	153	GLN
1	A	170	ASN
1	A	179	ASN
1	A	344	GLN
1	A	345	HIS
1	A	430	ASN
1	A	455	GLN
1	A	572	ASN
1	A	592	HIS
1	A	595	ASN
1	A	710	ASN
1	A	757	HIS
1	B	75	ASN
1	B	80	ASN
1	B	92	ASN
1	B	123	GLN
1	B	138	ASN
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	179	ASN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	572	ASN
1	B	592	HIS
1	B	606	GLN
1	B	710	ASN
1	B	731	GLN
1	C	51	ASN
1	C	80	ASN
1	C	100	HIS
1	C	138	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	153	GLN
1	C	170	ASN
1	C	179	ASN
1	C	227	GLN
1	C	344	GLN
1	C	435	GLN
1	C	455	GLN
1	C	586	GLN
1	C	694	ASN
1	C	710	ASN
1	C	731	GLN
1	D	80	ASN
1	D	138	ASN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	179	ASN
1	D	344	GLN
1	D	388	GLN
1	D	450	ASN
1	D	455	GLN
1	D	572	ASN
1	D	592	HIS
1	D	606	GLN
1	D	621	ASN
1	D	697	GLN
1	D	710	ASN
1	D	731	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	E	1	1,2	14,14,15	0.60	0	17,19,21	0.87	1 (5%)
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	1.04	0
2	NAG	F	1	1,2	14,14,15	0.55	0	17,19,21	1.45	3 (17%)
2	NAG	F	2	2	14,14,15	0.57	0	17,19,21	0.77	0
2	NAG	G	1	1,2	14,14,15	0.63	0	17,19,21	0.93	0
2	NAG	G	2	2	14,14,15	0.53	0	17,19,21	0.93	0
2	NAG	H	1	1,2	14,14,15	0.64	0	17,19,21	0.98	0
2	NAG	H	2	2	14,14,15	0.62	0	17,19,21	1.26	2 (11%)
2	NAG	I	1	1,2	14,14,15	0.45	0	17,19,21	1.02	1 (5%)
2	NAG	I	2	2	14,14,15	0.61	0	17,19,21	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	NAG	F	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	4/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	4/6/23/26	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(°)	Ideal(°)
2	H	2	NAG	C4-C3-C2	3.87	116.68	111.02
2	F	1	NAG	C1-O5-C5	2.94	116.13	112.19
2	F	1	NAG	O5-C1-C2	-2.66	107.17	111.29
2	I	1	NAG	C1-O5-C5	2.54	115.59	112.19
2	F	1	NAG	C2-N2-C7	-2.35	119.76	122.90
2	E	1	NAG	O5-C1-C2	-2.22	107.85	111.29
2	H	2	NAG	C3-C4-C5	2.15	114.13	110.23

There are no chirality outliers.

All (22) torsion outliers are listed below:

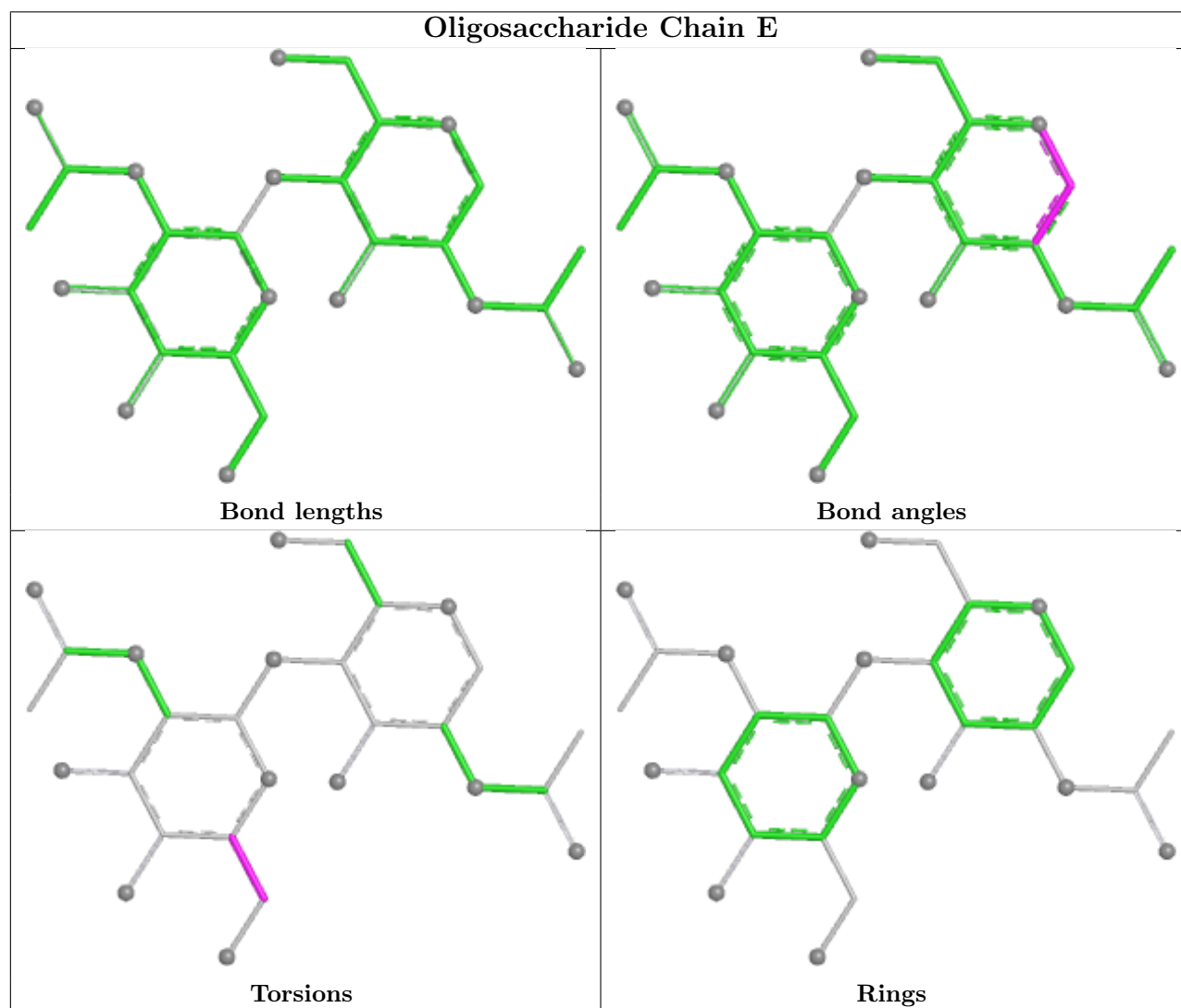
Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C8-C7-N2-C2
2	I	2	NAG	O7-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	G	1	NAG	C8-C7-N2-C2
2	G	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	G	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C8-C7-N2-C2
2	F	1	NAG	O5-C5-C6-O6
2	H	2	NAG	O7-C7-N2-C2
2	I	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6

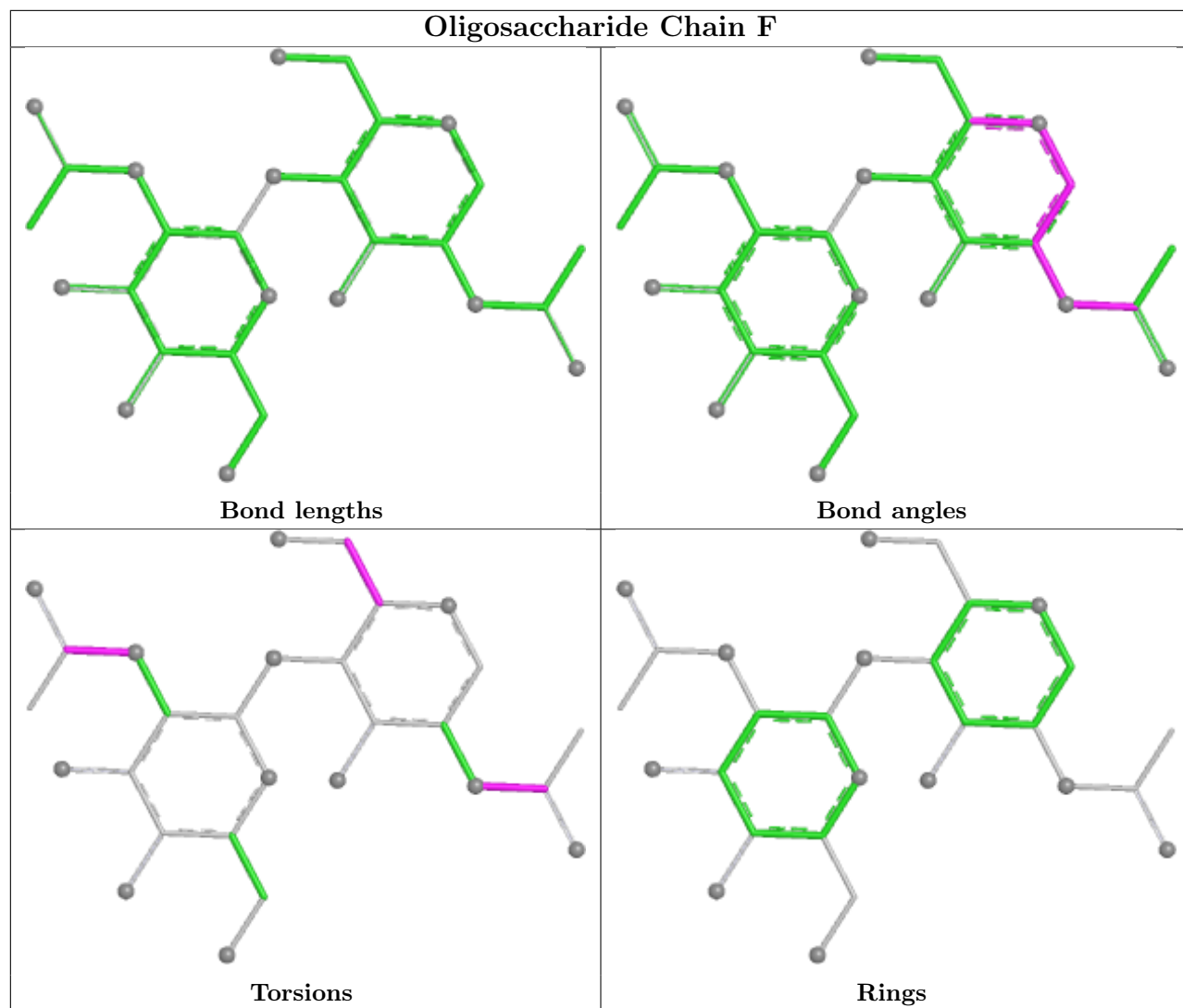
There are no ring outliers.

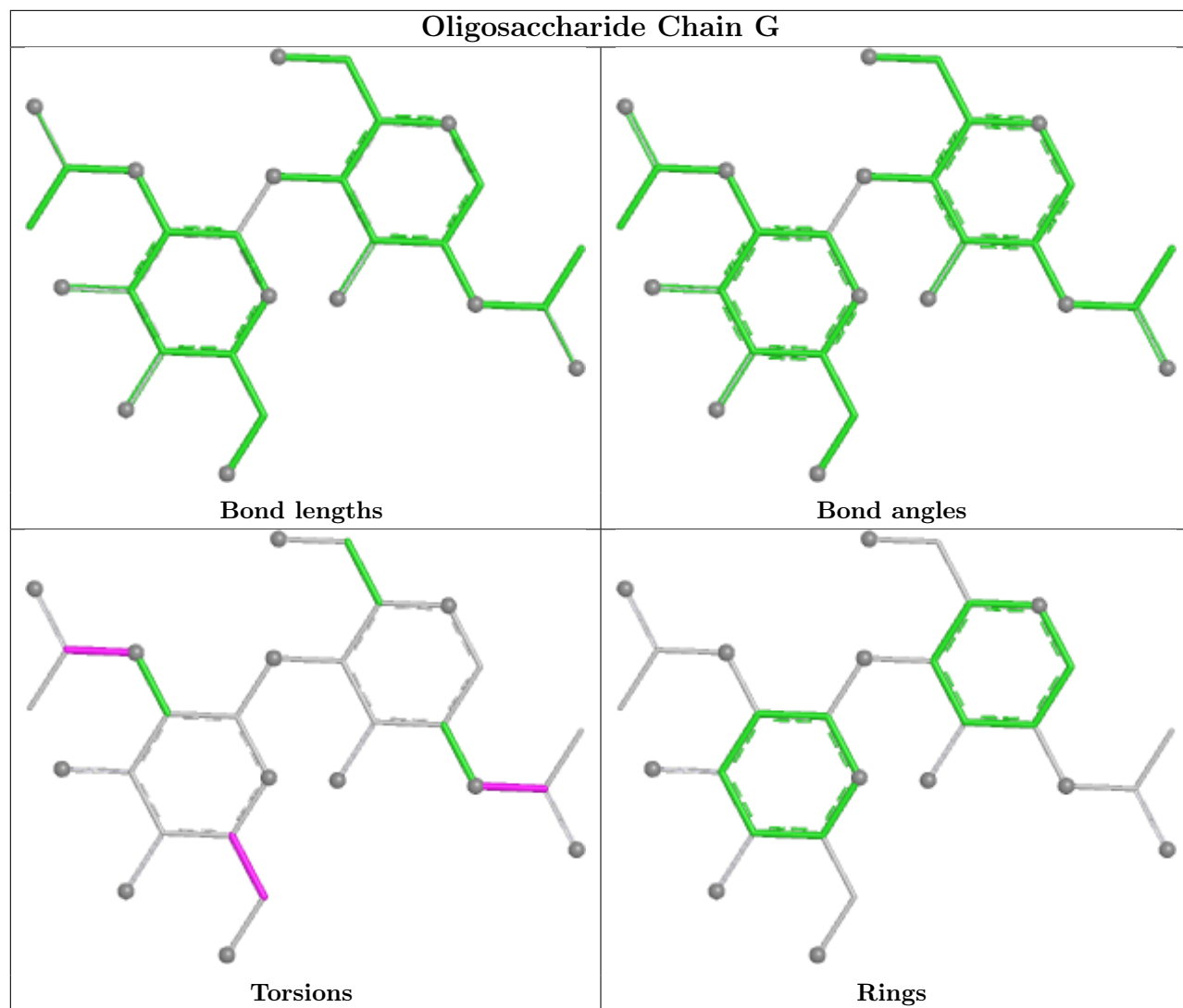
2 monomers are involved in 1 short contact:

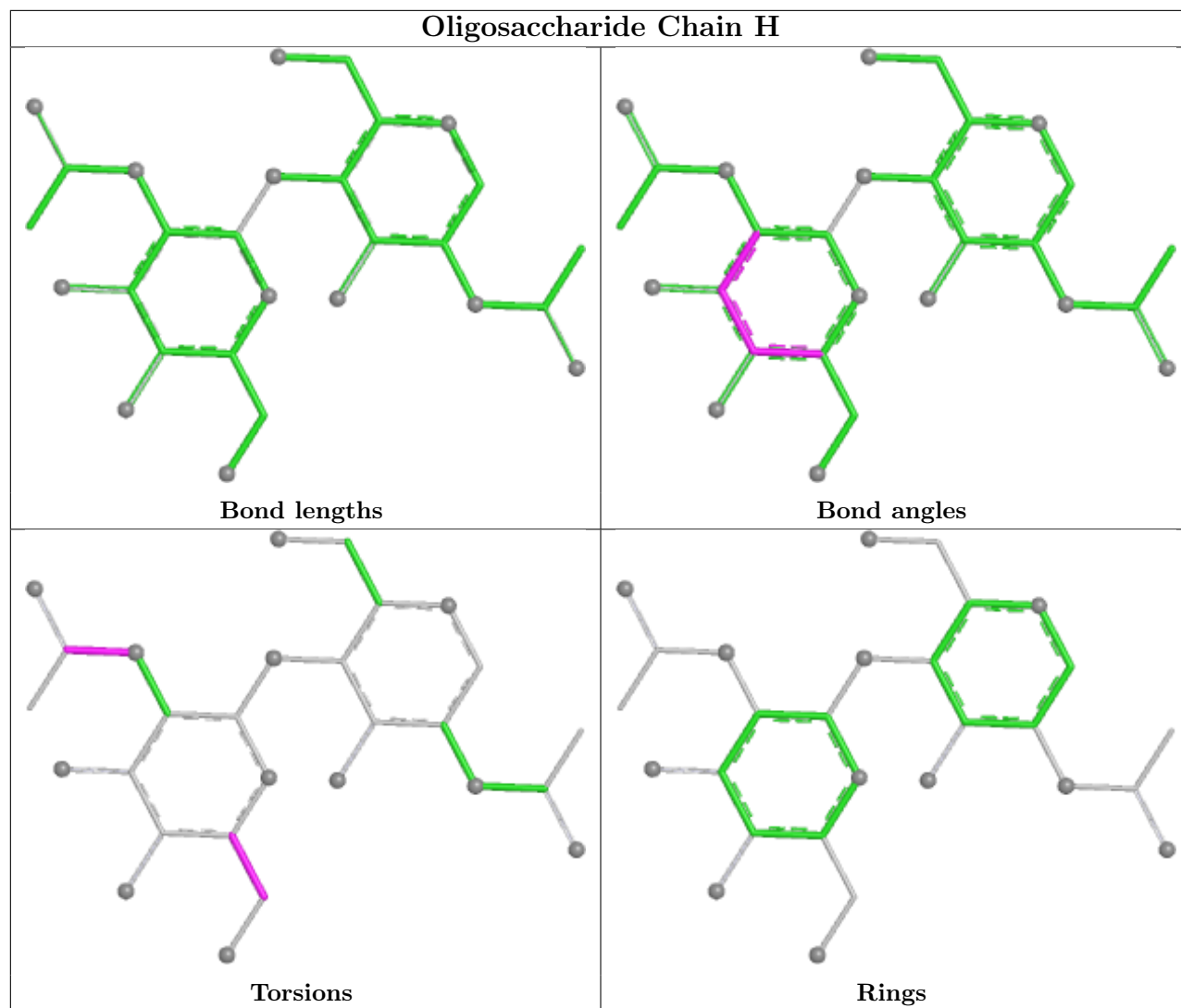
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1	NAG	1	0
2	G	2	NAG	1	0

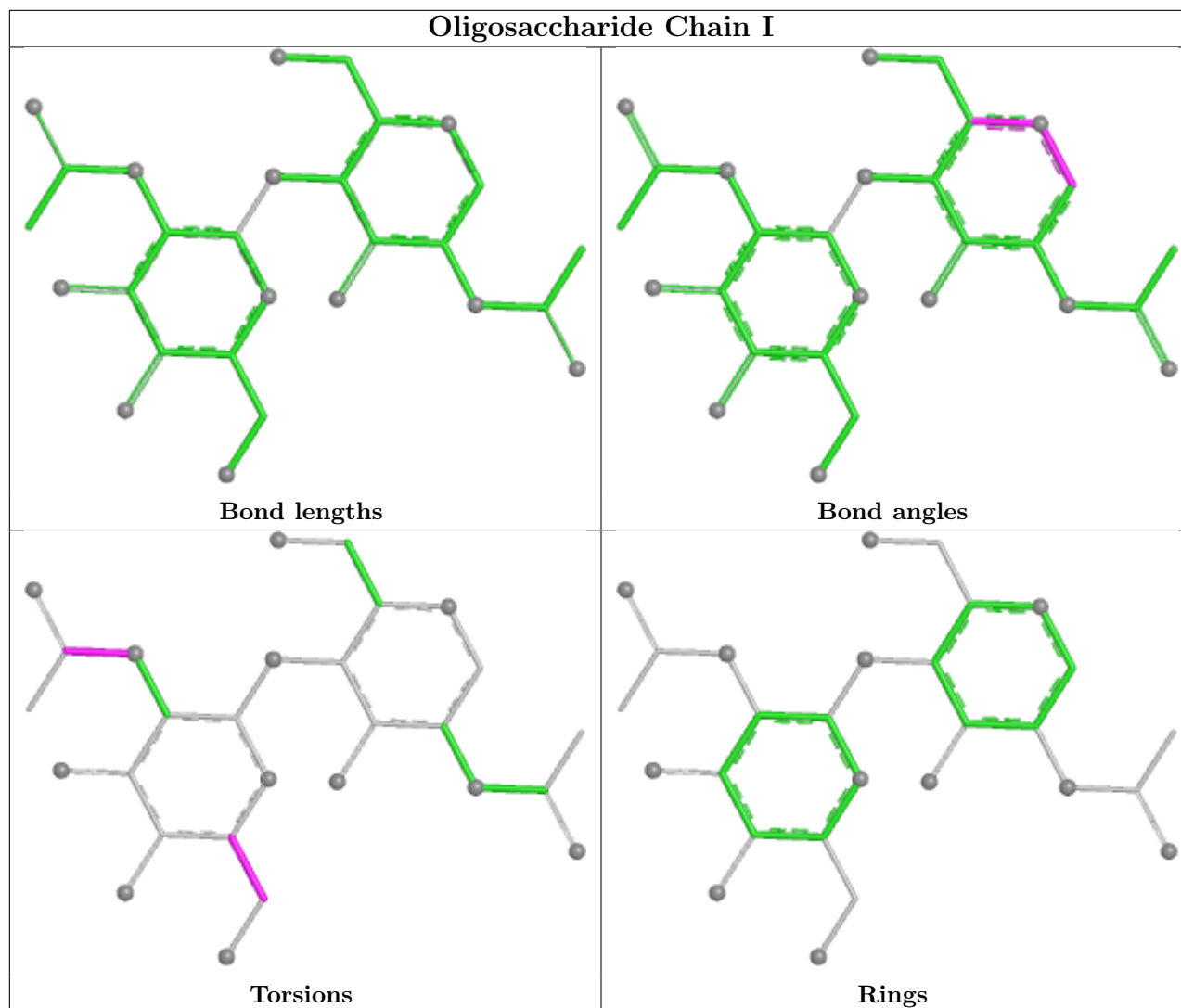
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
3	NAG	D	801	1	14,14,15	0.60	0	17,19,21	1.06	1 (5%)
3	NAG	C	801	1	14,14,15	0.50	0	17,19,21	1.40	1 (5%)
3	NAG	D	804	1	14,14,15	0.79	1 (7%)	17,19,21	1.61	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	B2Y	A	800	-	15,15,15	0.46	0	19,19,19	0.80	0
3	NAG	A	803	1	14,14,15	0.59	0	17,19,21	0.99	1 (5%)
3	NAG	B	802	1	14,14,15	0.53	0	17,19,21	1.17	1 (5%)
3	NAG	B	803	1	14,14,15	0.63	0	17,19,21	1.21	1 (5%)
3	NAG	B	806	1	14,14,15	0.56	0	17,19,21	1.64	1 (5%)
3	NAG	C	802	1	14,14,15	0.64	0	17,19,21	1.32	1 (5%)
3	NAG	A	808	1	14,14,15	0.57	0	17,19,21	1.41	1 (5%)
4	B2Y	B	800	-	15,15,15	0.46	0	19,19,19	0.59	0
3	NAG	B	801	1	14,14,15	0.78	1 (7%)	17,19,21	1.39	2 (11%)
3	NAG	A	801	1	14,14,15	0.59	0	17,19,21	1.44	1 (5%)
4	B2Y	D	800	-	15,15,15	0.42	0	19,19,19	0.66	0
4	B2Y	C	800	-	15,15,15	0.44	0	19,19,19	0.77	0
3	NAG	A	802	1	14,14,15	0.58	0	17,19,21	1.41	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	801	1	-	0/6/23/26	0/1/1/1
3	NAG	C	801	1	-	0/6/23/26	0/1/1/1
3	NAG	D	804	1	1/1/5/7	5/6/23/26	0/1/1/1
4	B2Y	A	800	-	-	1/6/6/6	0/2/2/2
3	NAG	A	803	1	-	2/6/23/26	0/1/1/1
3	NAG	B	802	1	-	1/6/23/26	0/1/1/1
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NAG	B	806	1	-	4/6/23/26	0/1/1/1
3	NAG	C	802	1	-	2/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1
4	B2Y	B	800	-	-	0/6/6/6	0/2/2/2
3	NAG	A	801	1	-	2/6/23/26	0/1/1/1
3	NAG	B	801	1	-	3/6/23/26	0/1/1/1
4	B2Y	D	800	-	-	0/6/6/6	0/2/2/2
4	B2Y	C	800	-	-	1/6/6/6	0/2/2/2
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	804	NAG	C1-C2	2.53	1.55	1.52
3	B	801	NAG	C1-C2	2.18	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	806	NAG	C1-O5-C5	5.75	119.89	112.19
3	A	802	NAG	C1-O5-C5	5.49	119.54	112.19
3	A	801	NAG	C1-O5-C5	4.90	118.75	112.19
3	A	808	NAG	C1-O5-C5	4.70	118.49	112.19
3	C	801	NAG	C1-O5-C5	4.48	118.19	112.19
3	B	803	NAG	C1-O5-C5	4.04	117.60	112.19
3	B	802	NAG	C1-O5-C5	4.04	117.60	112.19
3	D	804	NAG	C1-O5-C5	3.89	117.40	112.19
3	C	802	NAG	C4-C3-C2	3.80	116.59	111.02
3	B	801	NAG	C4-C3-C2	3.27	115.81	111.02
3	D	801	NAG	C1-O5-C5	2.66	115.75	112.19
3	D	804	NAG	O5-C1-C2	2.66	115.41	111.29
3	A	803	NAG	C4-C3-C2	2.66	114.91	111.02
3	B	801	NAG	O5-C5-C6	2.39	112.32	107.66
3	D	804	NAG	C3-C4-C5	-2.32	106.03	110.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	D	804	NAG	C1

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	NAG	C8-C7-N2-C2
3	A	803	NAG	O7-C7-N2-C2
3	B	801	NAG	C8-C7-N2-C2
3	B	801	NAG	O7-C7-N2-C2
3	B	806	NAG	C8-C7-N2-C2
3	B	806	NAG	O7-C7-N2-C2
3	C	802	NAG	C8-C7-N2-C2
3	C	802	NAG	O7-C7-N2-C2
3	D	804	NAG	C8-C7-N2-C2
3	D	804	NAG	O7-C7-N2-C2
3	B	806	NAG	O5-C5-C6-O6
3	B	806	NAG	C4-C5-C6-O6
3	D	804	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	D	804	NAG	C3-C2-N2-C7
3	D	804	NAG	C4-C5-C6-O6
3	B	802	NAG	C4-C5-C6-O6
3	B	801	NAG	C3-C2-N2-C7
4	A	800	B2Y	N1-C2-C3-C8
4	C	800	B2Y	N1-C2-C3-C8

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	NAG	1	0
3	B	802	NAG	1	0
4	B	800	B2Y	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	724/740 (97%)	0.74	54 (7%) 20 18	31, 48, 68, 104	1 (0%)
1	B	729/740 (98%)	0.61	33 (4%) 38 33	36, 47, 67, 83	0
1	C	724/740 (97%)	0.81	67 (9%) 14 12	28, 48, 69, 101	1 (0%)
1	D	724/740 (97%)	0.94	89 (12%) 8 7	36, 51, 69, 107	0
All	All	2901/2960 (98%)	0.78	243 (8%) 17 15	28, 48, 68, 107	2 (0%)

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	TYR	6.3
1	C	474	GLY	5.4
1	A	135	TYR	5.3
1	C	95	PHE	5.2
1	A	81	ALA	5.1
1	A	88	VAL	5.0
1	D	95	PHE	4.9
1	C	141	GLN	4.7
1	D	94	THR	4.7
1	A	332	GLU	4.6
1	D	92	ASN	4.5
1	B	72	GLN	4.5
1	B	81	ALA	4.4
1	D	386	TYR	4.3
1	B	83	TYR	4.2
1	C	98	PHE	4.2
1	A	474	GLY	4.1
1	C	187	TRP	4.1
1	D	93	SER	4.1
1	A	94	THR	4.1
1	A	95	PHE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	78	VAL	4.1
1	D	83	TYR	4.0
1	D	339	CYS	4.0
1	A	98	PHE	3.9
1	D	98	PHE	3.9
1	D	487	ASN	3.9
1	D	88	VAL	3.9
1	A	506	ASN	3.9
1	C	94	THR	3.7
1	C	279	VAL	3.7
1	D	135	TYR	3.7
1	C	186	THR	3.6
1	D	335	GLY	3.6
1	A	140	ARG	3.6
1	A	138	ASN	3.6
1	A	90	LEU	3.6
1	A	86	SER	3.5
1	C	137	LEU	3.5
1	D	468	TYR	3.5
1	D	389	ILE	3.5
1	C	99	GLY	3.4
1	D	322	TYR	3.4
1	D	432	TYR	3.4
1	C	93	SER	3.4
1	D	388	GLN	3.3
1	A	69	LEU	3.3
1	D	395	THR	3.3
1	A	489	LYS	3.3
1	B	70	TYR	3.3
1	D	486	VAL	3.3
1	C	142	LEU	3.3
1	A	80	ASN	3.2
1	C	568	ALA	3.2
1	D	342	ALA	3.2
1	A	92	ASN	3.2
1	B	75	ASN	3.2
1	C	390	ASP	3.2
1	A	72	GLN	3.1
1	C	113	PHE	3.1
1	D	66	HIS	3.1
1	C	79	PHE	3.1
1	B	90	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	414	TYR	3.1
1	D	334	SER	3.1
1	C	330	TYR	3.0
1	D	447	CYS	3.0
1	B	88	VAL	3.0
1	C	392	LYS	3.0
1	D	370	SER	3.0
1	C	92	ASN	3.0
1	B	389	ILE	2.9
1	A	93	SER	2.9
1	D	400	GLY	2.9
1	D	327	ILE	2.9
1	B	79	PHE	2.9
1	B	474	GLY	2.9
1	D	99	GLY	2.8
1	C	332	GLU	2.8
1	A	467	TYR	2.8
1	D	518	ILE	2.8
1	D	412	SER	2.8
1	A	79	PHE	2.8
1	D	441	LYS	2.8
1	C	102	ILE	2.7
1	D	62	TRP	2.7
1	D	467	TYR	2.7
1	B	82	GLU	2.7
1	D	338	ASN	2.7
1	C	101	SER	2.7
1	C	72	GLN	2.7
1	C	75	ASN	2.7
1	C	70	TYR	2.7
1	C	83	TYR	2.7
1	D	81	ALA	2.7
1	C	100	HIS	2.7
1	A	277	SER	2.7
1	A	502	LYS	2.6
1	A	91	GLU	2.6
1	C	388	GLN	2.6
1	D	411	THR	2.6
1	C	143	ILE	2.6
1	B	142	LEU	2.6
1	D	75	ASN	2.6
1	D	415	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	491	LEU	2.6
1	C	89	PHE	2.6
1	D	89	PHE	2.6
1	D	396	PHE	2.6
1	A	333	SER	2.6
1	C	81	ALA	2.6
1	C	467	TYR	2.6
1	C	270	VAL	2.6
1	D	498	SER	2.6
1	B	378	GLU	2.5
1	C	504	LEU	2.5
1	B	338	ASN	2.5
1	C	66	HIS	2.5
1	D	483	HIS	2.5
1	A	392	LYS	2.5
1	D	372	TYR	2.5
1	C	84	GLY	2.5
1	B	328	CYS	2.5
1	A	99	GLY	2.5
1	A	161	GLY	2.5
1	D	380	GLY	2.5
1	D	90	LEU	2.5
1	C	85	ASN	2.5
1	D	365	THR	2.5
1	A	490	GLY	2.4
1	A	180	LEU	2.4
1	D	276	LEU	2.4
1	A	64	SER	2.4
1	D	463	LYS	2.4
1	A	70	TYR	2.4
1	B	36	HIS	2.4
1	A	75	ASN	2.4
1	B	78	VAL	2.4
1	A	59	SER	2.4
1	C	63	ILE	2.4
1	C	183	TYR	2.4
1	C	487	ASN	2.4
1	D	402	TRP	2.4
1	B	295	ILE	2.4
1	A	276	LEU	2.4
1	C	505	GLN	2.4
1	D	417	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	103	ASN	2.4
1	A	129	THR	2.3
1	C	335	GLY	2.3
1	D	474	GLY	2.3
1	B	346	ILE	2.3
1	D	77	LEU	2.3
1	D	397	ILE	2.3
1	D	438	ASP	2.3
1	D	450	ASN	2.3
1	A	87	SER	2.3
1	B	84	GLY	2.3
1	A	137	LEU	2.3
1	C	366	LEU	2.3
1	D	410	LEU	2.3
1	A	463	LYS	2.3
1	B	269	PHE	2.3
1	C	138	ASN	2.3
1	D	435	GLN	2.3
1	D	143	ILE	2.3
1	D	436	LEU	2.3
1	C	96	ASP	2.3
1	A	414	TYR	2.3
1	A	280	THR	2.3
1	B	97	GLU	2.3
1	B	85	ASN	2.2
1	C	173	TYR	2.3
1	D	330	TYR	2.3
1	C	283	THR	2.2
1	D	280	THR	2.2
1	D	443	THR	2.2
1	D	399	LYS	2.2
1	D	482	LEU	2.2
1	C	62	TRP	2.2
1	D	96	ASP	2.2
1	D	326	ASP	2.2
1	C	338	ASN	2.2
1	C	506	ASN	2.2
1	A	246	LEU	2.2
1	D	348	MET	2.2
1	D	470	LEU	2.2
1	D	479	LEU	2.2
1	D	63	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	277	SER	2.2
1	D	464	GLU	2.2
1	C	181	PRO	2.2
1	D	404	VAL	2.2
1	B	489	LYS	2.2
1	D	100	HIS	2.2
1	C	280	THR	2.2
1	D	220	GLY	2.2
1	B	518	ILE	2.2
1	D	434	ILE	2.2
1	B	87	SER	2.2
1	D	413	ASP	2.2
1	D	41	LYS	2.2
1	B	80	ASN	2.2
1	C	276	LEU	2.2
1	C	334	SER	2.2
1	C	412	SER	2.2
1	A	97	GLU	2.2
1	C	184	ARG	2.2
1	B	392	LYS	2.2
1	C	179	ASN	2.1
1	C	77	LEU	2.1
1	C	90	LEU	2.1
1	D	439	TYR	2.1
1	D	517	ILE	2.1
1	C	538	LYS	2.1
1	A	66	HIS	2.1
1	D	72	GLN	2.1
1	C	80	ASN	2.1
1	A	41	LYS	2.1
1	A	89	PHE	2.1
1	A	168	TRP	2.1
1	A	85	ASN	2.1
1	B	506	ASN	2.1
1	A	63	ILE	2.1
1	A	105	TYR	2.1
1	C	108	SER	2.1
1	D	437	SER	2.1
1	D	79	PHE	2.1
1	D	142	LEU	2.1
1	D	449	LEU	2.1
1	D	446	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	162	HIS	2.1
1	B	98	PHE	2.0
1	C	336	ARG	2.0
1	C	115	LEU	2.0
1	A	399	LYS	2.0
1	D	440	THR	2.0
1	B	386	TYR	2.0
1	C	118	TYR	2.0
1	D	333	SER	2.0
1	B	395	THR	2.0
1	A	65	ASP	2.0
1	B	333	SER	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](#)

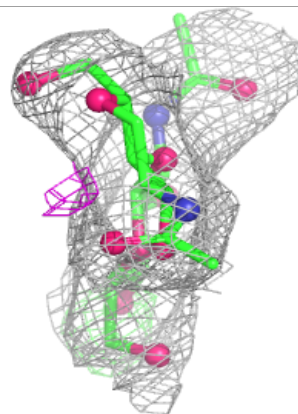
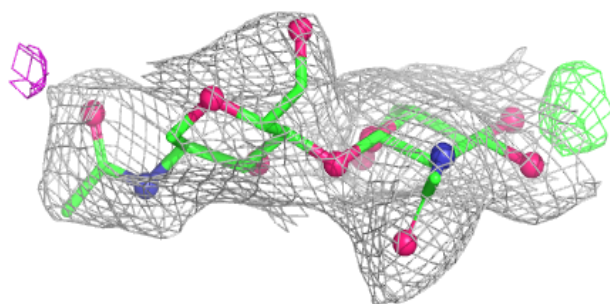
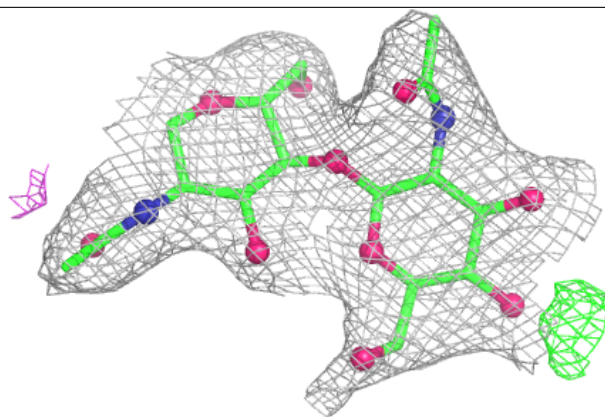
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	F	1	14/15	0.65	0.15	73,76,79,80	0
2	NAG	F	2	14/15	0.72	0.16	83,84,85,85	0
2	NAG	H	2	14/15	0.77	0.14	73,76,78,78	0
2	NAG	I	2	14/15	0.79	0.15	67,68,72,72	0
2	NAG	G	2	14/15	0.80	0.15	80,82,83,83	0
2	NAG	E	2	14/15	0.84	0.10	68,70,71,71	0
2	NAG	I	1	14/15	0.86	0.13	55,58,61,63	0
2	NAG	G	1	14/15	0.86	0.13	67,69,73,77	0
2	NAG	H	1	14/15	0.89	0.11	63,65,68,72	0
2	NAG	E	1	14/15	0.92	0.10	58,60,62,66	0

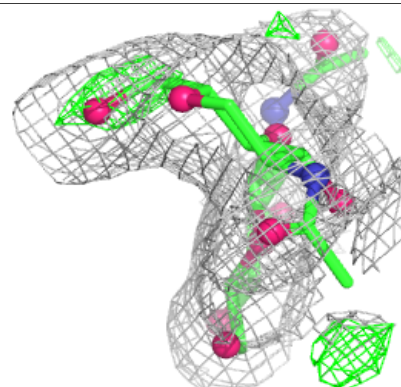
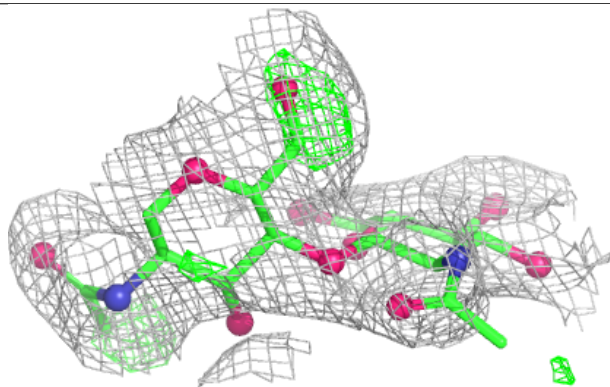
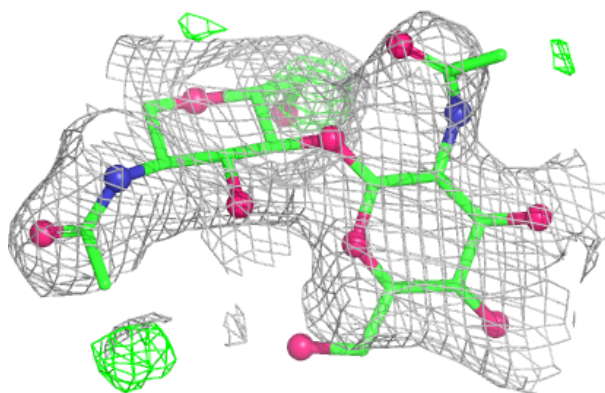
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

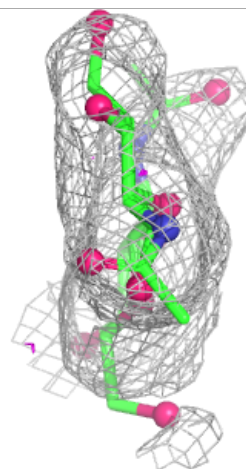
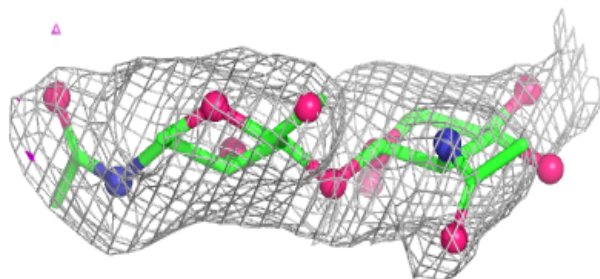
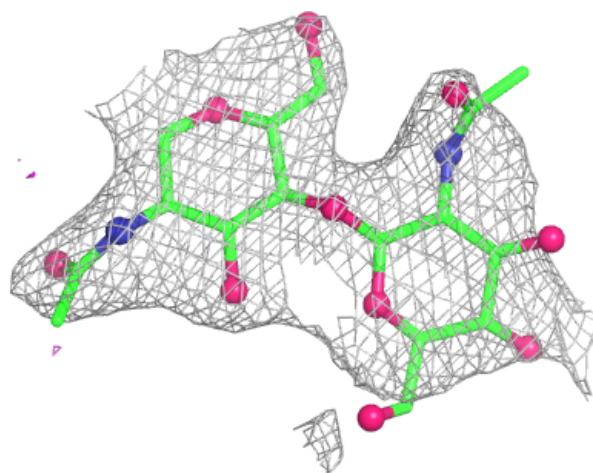
**Electron density around Chain F:**

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



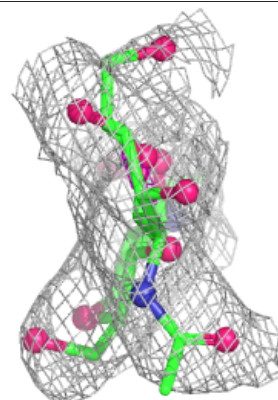
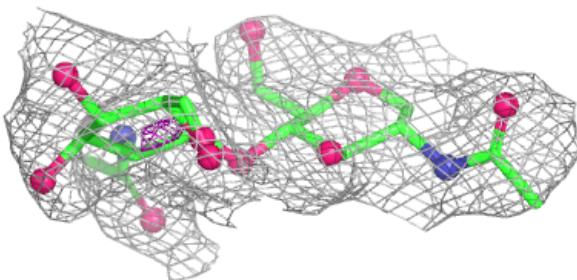
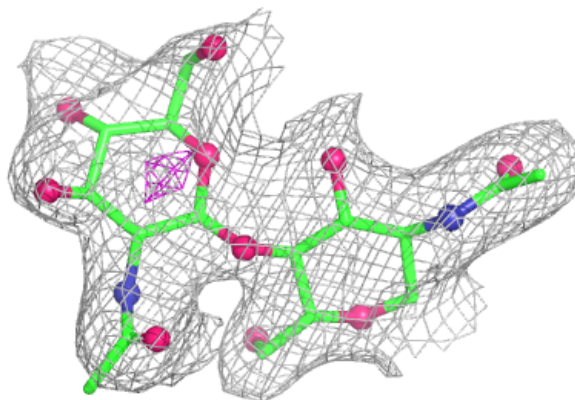
Electron density around Chain G:

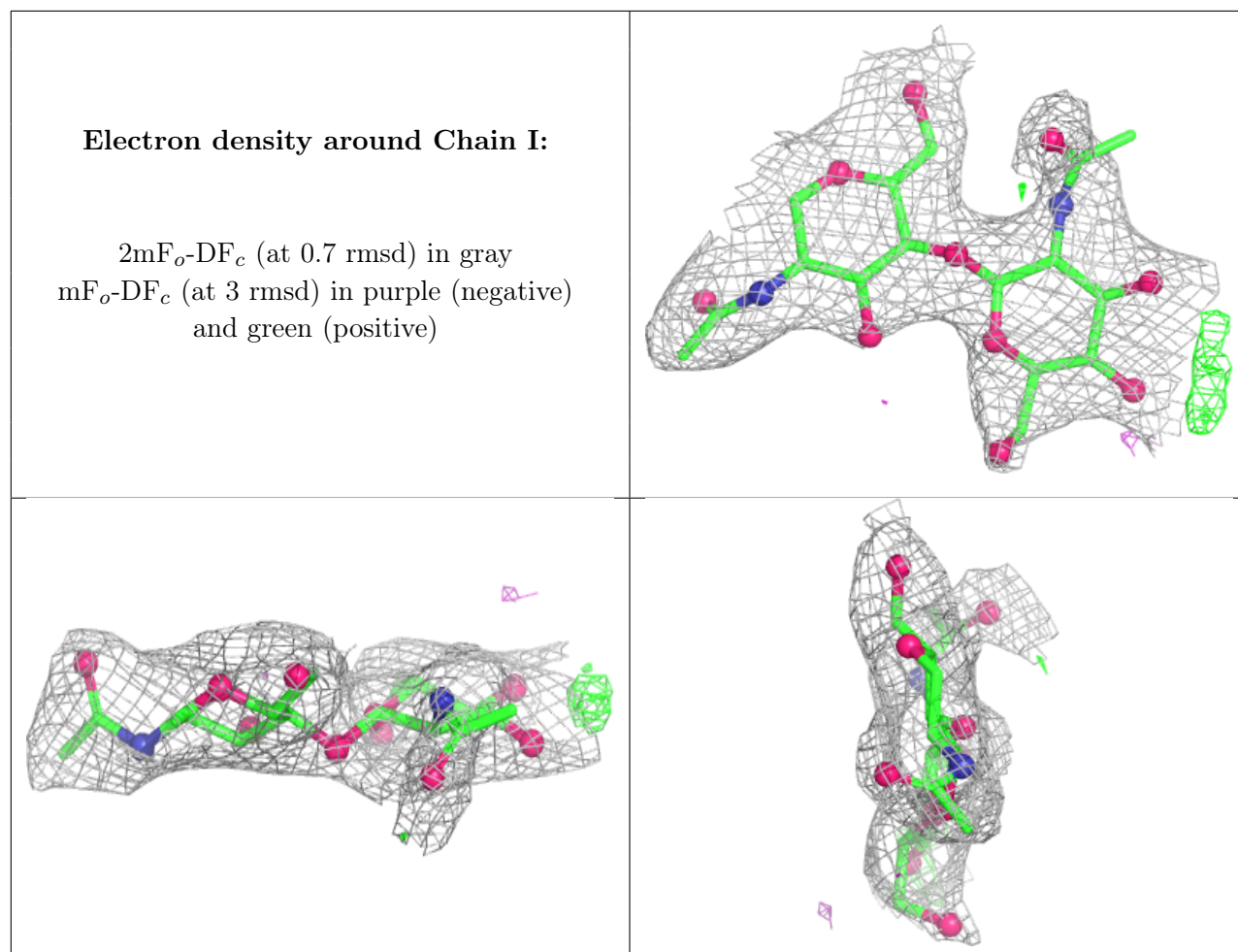
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

$2mF_o-DF_c$ (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
3	NAG	A	801	14/15	0.58	0.17	72,73,74,74	0
3	NAG	B	801	14/15	0.64	0.22	78,79,80,80	0
3	NAG	D	804	14/15	0.67	0.18	78,80,82,82	0
3	NAG	C	801	14/15	0.70	0.15	55,55,56,57	0
3	NAG	B	803	14/15	0.71	0.15	63,65,68,68	0
3	NAG	A	802	14/15	0.72	0.16	65,66,68,68	0
3	NAG	A	803	14/15	0.73	0.14	71,73,76,77	0
3	NAG	D	801	14/15	0.75	0.15	58,60,62,63	0
3	NAG	B	806	14/15	0.75	0.15	67,69,73,74	0
3	NAG	C	802	14/15	0.76	0.14	68,70,74,74	0
3	NAG	A	808	14/15	0.79	0.12	61,63,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	B	802	14/15	0.86	0.10	63,64,66,66	0
4	B2Y	C	800	14/14	0.89	0.16	50,54,55,55	0
4	B2Y	A	800	14/14	0.90	0.17	53,56,58,58	0
4	B2Y	B	800	14/14	0.91	0.19	60,62,63,64	0
4	B2Y	D	800	14/14	0.92	0.12	42,44,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.