Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 02:01 PM EST

PDB ID	:	1CIW
Title	:	PEANUT LECTIN COMPLEXED WITH N-ACETYLLACTOSAMINE
Authors	:	Ravishankar, R.; Suguna, K.; Surolia, A.; Vijayan, M.
Deposited on	:	1999-04-06
Resolution	:	2.70 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 (i) 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 (i)) were used in the production of this report:

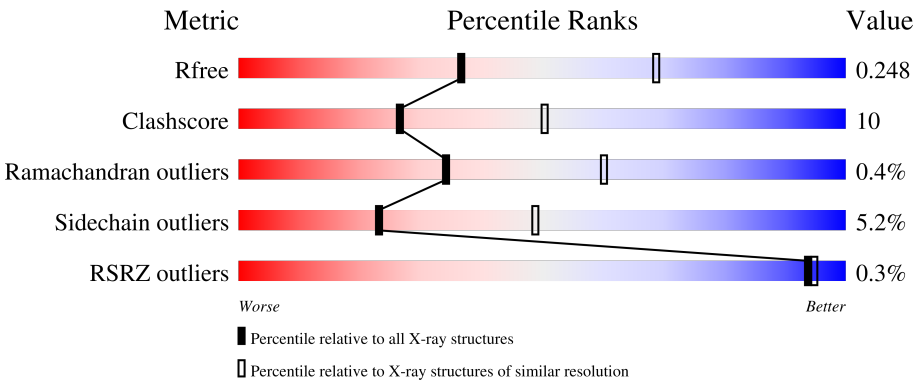
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	236	78% 18% • •
1	B	236	82% 13% • •
1	C	236	77% 19% • • •
1	D	236	78% 16% • • •
2	E	2	100%

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

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7511 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 PROTEIN (PEANUT LECTIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	1743	1102	287	352	2	0	0	0
1	B	232	1743	1102	287	352	2	0	0	0
1	C	232	1743	1102	287	352	2	0	0	0
1	D	232	1743	1102	287	352	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	2	26	14	1	11	0	0	0
2	F	2	26	14	1	11	0	0	0
2	G	2	26	14	1	11	0	0	0
2	H	2	26	14	1	11	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mn 1 1	0	0
4	B	1	Total Mn 1 1	0	0
4	C	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

- Molecule 5 is water.

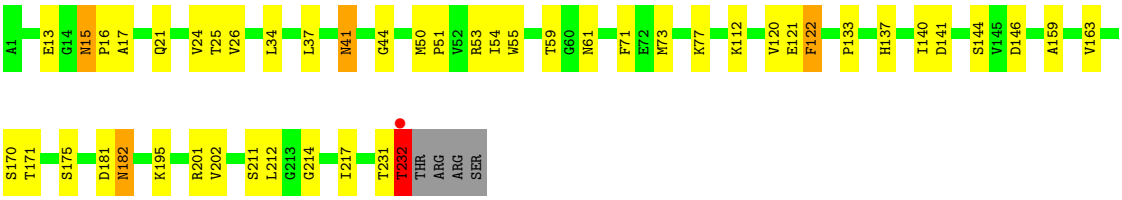
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	108	Total O 108 108	0	0
5	B	131	Total O 131 131	0	0
5	C	97	Total O 97 97	0	0
5	D	91	Total O 91 91	0	0

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.

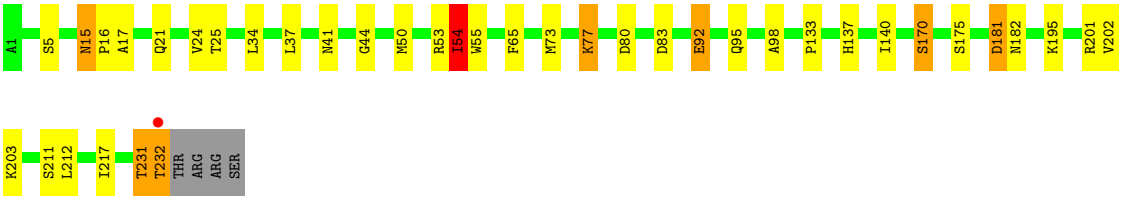
• Molecule 1: PROTEIN (PEANUT LECTIN)

Chain A:



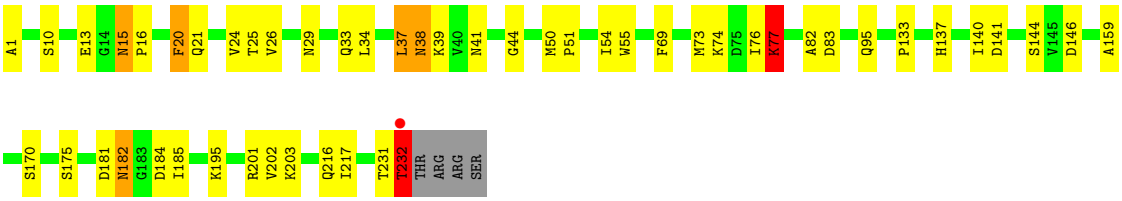
• Molecule 1: PROTEIN (PEANUT LECTIN)

Chain B:



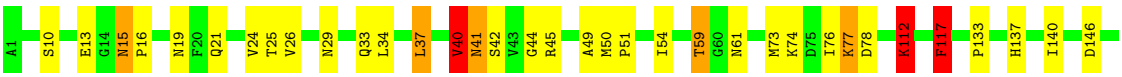
• Molecule 1: PROTEIN (PEANUT LECTIN)

Chain C:



• Molecule 1: PROTEIN (PEANUT LECTIN)

Chain D:



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

Chain E: 100%

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

Chain F: 50% 50%

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

Chain G: 100%

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

Chain H: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	129.38Å 126.92Å 76.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 9.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.0 (10.00-2.70) 81.0 (9.98-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.71Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.194 , 0.244 0.203 , 0.248	Depositor DCC
R_{free} test set	3362 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 72.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7511	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NDG, CA, MN, GAL

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	0.66	2/1779 (0.1%)	0.88	6/2426 (0.2%)
1	B	0.70	4/1779 (0.2%)	1.07	14/2426 (0.6%)
1	C	0.72	4/1779 (0.2%)	0.87	4/2426 (0.2%)
1	D	0.72	4/1779 (0.2%)	0.98	9/2426 (0.4%)
All	All	0.70	14/7116 (0.2%)	0.95	33/9704 (0.3%)

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	D	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	ILE	CB-CG2	-9.03	1.24	1.52
1	B	232	THR	CA-CB	-7.62	1.33	1.53
1	A	201	ARG	CZ-NH1	-6.96	1.24	1.33
1	A	232	THR	C-O	6.91	1.36	1.23
1	B	98	ALA	C-O	-6.68	1.10	1.23
1	C	201	ARG	CZ-NH1	-6.43	1.24	1.33
1	C	69	PHE	CG-CD2	-6.37	1.29	1.38
1	B	92	GLU	CD-OE1	-6.36	1.18	1.25
1	C	38	ASN	CG-OD1	-6.32	1.10	1.24
1	D	200	GLU	CD-OE1	-6.28	1.18	1.25
1	C	69	PHE	CG-CD1	-6.28	1.29	1.38
1	D	201	ARG	CZ-NH1	-5.38	1.26	1.33
1	D	117	PHE	CG-CD2	-5.22	1.30	1.38
1	D	200	GLU	CD-OE2	-5.20	1.20	1.25

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	201	ARG	NE-CZ-NH2	13.84	127.22	120.30
1	D	200	GLU	OE1-CD-OE2	-12.08	108.81	123.30
1	B	181	ASP	CB-CG-OD2	11.84	128.96	118.30
1	B	201	ARG	NE-CZ-NH1	-11.44	114.58	120.30
1	D	201	ARG	NE-CZ-NH2	11.02	125.81	120.30
1	D	201	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	B	232	THR	CA-C-O	-9.64	99.86	120.10
1	B	232	THR	N-CA-C	9.14	135.68	111.00
1	B	232	THR	CA-CB-CG2	-8.73	100.18	112.40
1	D	112	LYS	CD-CE-NZ	-8.36	92.48	111.70
1	B	92	GLU	OE1-CD-OE2	-7.90	113.82	123.30
1	D	77	LYS	CD-CE-NZ	-7.63	94.15	111.70
1	A	77	LYS	CD-CE-NZ	-7.48	94.49	111.70
1	B	54	ILE	CA-CB-CG1	7.15	124.58	111.00
1	C	77	LYS	CB-CG-CD	7.05	129.93	111.60
1	C	201	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	B	53	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	B	92	GLU	CG-CD-OE2	5.90	130.09	118.30
1	A	112	LYS	CD-CE-NZ	-5.88	98.17	111.70
1	A	201	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	A	232	THR	CA-CB-CG2	-5.62	104.53	112.40
1	B	181	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	B	232	THR	CB-CA-C	-5.59	96.51	111.60
1	B	77	LYS	CD-CE-NZ	-5.58	98.86	111.70
1	D	182	ASN	N-CA-CB	-5.52	100.66	110.60
1	C	146	ASP	N-CA-C	-5.44	96.32	111.00
1	D	146	ASP	N-CA-C	-5.33	96.62	111.00
1	B	231	THR	C-N-CA	5.25	134.82	121.70
1	C	232	THR	N-CA-C	5.22	125.09	111.00
1	A	53	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	146	ASP	N-CA-C	-5.07	97.31	111.00
1	D	59	THR	N-CA-C	-5.03	97.43	111.00
1	D	200	GLU	CG-CD-OE2	5.02	128.34	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	40	VAL	Mainchain

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	1743	0	1699	46	0
1	B	1743	0	1699	31	0
1	C	1743	0	1699	38	0
1	D	1743	0	1699	37	0
2	E	26	0	21	7	0
2	F	26	0	21	2	0
2	G	26	0	21	0	0
2	H	26	0	21	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	108	0	0	1	0
5	B	131	0	0	5	0
5	C	97	0	0	6	0
5	D	91	0	0	4	0
All	All	7511	0	6880	144	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 (144) 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)
2:H:1:NDG:C1	2:H:1:NDG:C2	1.77	1.56
2:E:1:NDG:C1	2:E:1:NDG:C2	1.77	1.54
1:C:77:LYS:HB2	1:C:77:LYS:NZ	1.69	1.06
2:H:1:NDG:C2	2:H:1:NDG:O1	2.02	1.06
1:A:212:LEU:HD22	2:E:1:NDG:H8C1	1.46	0.95
1:C:77:LYS:HB2	1:C:77:LYS:HZ2	1.35	0.88
2:E:1:NDG:C2	2:E:1:NDG:O1	2.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PHE:CZ	1:A:122:PHE:HD2	1.96	0.84
1:C:29:ASN:HA	1:D:217:ILE:HD13	1.58	0.83
1:C:77:LYS:HB2	1:C:77:LYS:HZ3	1.41	0.80
1:D:40:VAL:HG12	1:D:41:ASN:H	1.46	0.79
1:A:121:GLU:C	1:A:122:PHE:HD1	1.88	0.76
1:D:112:LYS:HZ3	1:D:112:LYS:CB	1.88	0.76
1:C:231:THR:O	1:C:232:THR:HG22	1.88	0.74
1:C:181:ASP:HB3	5:C:490:HOH:O	1.88	0.73
1:A:120:VAL:HG12	1:A:122:PHE:HE1	1.54	0.72
1:A:71:PHE:CZ	1:A:122:PHE:CD2	2.78	0.71
1:A:50:MET:CE	1:B:17:ALA:HB2	2.20	0.71
1:C:217:ILE:HD13	1:D:29:ASN:HA	1.72	0.71
1:D:40:VAL:O	1:D:42:SER:N	2.24	0.70
1:C:10:SER:HB3	1:D:74:LYS:HE2	1.73	0.70
1:B:54:ILE:HD12	1:B:202:VAL:HG21	1.72	0.70
2:H:1:NDG:O1	2:H:1:NDG:N2	2.23	0.70
1:A:15:ASN:HD22	1:A:16:PRO:HD2	1.56	0.70
1:D:231:THR:C	1:D:232:THR:HG22	2.14	0.68
1:B:15:ASN:HD22	1:B:16:PRO:HD2	1.59	0.67
1:A:122:PHE:HD1	1:A:122:PHE:N	1.94	0.64
2:H:1:NDG:C1	2:H:1:NDG:H2	2.14	0.64
1:B:212:LEU:HD13	2:F:1:NDG:H8C1	1.78	0.64
1:C:231:THR:C	1:C:232:THR:HG22	2.16	0.64
1:A:17:ALA:HA	1:B:50:MET:HE2	1.79	0.64
1:D:231:THR:O	1:D:232:THR:HG22	1.97	0.64
1:A:231:THR:C	1:A:232:THR:HG22	2.18	0.64
1:C:74:LYS:HE2	1:D:10:SER:HB3	1.81	0.63
1:D:25:THR:HG22	1:D:33:GLN:HB3	1.81	0.62
1:A:54:ILE:HD13	1:A:202:VAL:HG21	1.82	0.62
1:A:71:PHE:HZ	1:A:122:PHE:HD2	1.48	0.60
1:D:117:PHE:C	1:D:117:PHE:CD1	2.76	0.59
1:A:71:PHE:CE2	1:A:122:PHE:CD2	2.91	0.59
1:C:77:LYS:HZ3	1:C:77:LYS:CB	2.09	0.58
1:A:122:PHE:N	1:A:122:PHE:CD1	2.68	0.58
1:A:71:PHE:HE2	1:A:122:PHE:CE2	2.22	0.58
1:C:25:THR:HG22	1:C:33:GLN:HB3	1.86	0.57
1:A:71:PHE:CE2	1:A:122:PHE:CE2	2.93	0.57
1:A:41:ASN:HD22	1:A:211:SER:HA	1.70	0.57
1:D:182:ASN:HB2	5:D:442:HOH:O	2.03	0.57
1:A:17:ALA:CA	1:B:50:MET:HE2	2.35	0.56
1:B:41:ASN:HD22	1:B:211:SER:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ALA:CB	1:B:50:MET:HE2	2.36	0.55
1:D:40:VAL:HG12	1:D:41:ASN:N	2.17	0.55
2:E:1:NDG:O1	2:E:1:NDG:N2	2.39	0.55
1:D:117:PHE:C	1:D:117:PHE:HD1	2.10	0.55
1:A:50:MET:HE3	1:B:17:ALA:HB2	1.89	0.55
1:B:34:LEU:O	1:B:44:GLY:HA3	2.05	0.55
1:D:34:LEU:O	1:D:44:GLY:HA3	2.07	0.55
1:B:231:THR:C	1:B:232:THR:HG22	2.27	0.54
1:A:120:VAL:HG12	1:A:122:PHE:CE1	2.40	0.54
1:A:34:LEU:O	1:A:44:GLY:HA3	2.07	0.54
2:E:1:NDG:C1	2:E:1:NDG:H2	2.16	0.53
1:A:122:PHE:HE2	1:A:163:VAL:HG21	1.74	0.53
1:C:54:ILE:HD13	1:C:202:VAL:HG21	1.90	0.52
1:D:41:ASN:HD22	1:D:211:SER:HA	1.75	0.52
1:D:54:ILE:HD13	1:D:202:VAL:HG21	1.90	0.52
1:A:17:ALA:CB	1:B:50:MET:CE	2.88	0.51
1:A:13:GLU:HG3	1:A:26:VAL:HB	1.92	0.51
1:A:17:ALA:HB2	1:B:50:MET:CE	2.41	0.51
1:C:10:SER:HB3	1:D:74:LYS:CE	2.41	0.50
1:B:15:ASN:HD22	1:B:16:PRO:CD	2.24	0.50
1:C:133:PRO:HD2	1:C:137:HIS:CE1	2.47	0.50
1:D:59:THR:O	1:D:61:ASN:N	2.44	0.50
1:A:50:MET:HE1	1:B:17:ALA:HB2	1.93	0.49
1:A:17:ALA:HB2	1:B:50:MET:HE2	1.95	0.49
1:A:59:THR:O	1:A:61:ASN:N	2.45	0.49
1:C:34:LEU:O	1:C:44:GLY:HA3	2.12	0.49
1:D:25:THR:CG2	1:D:33:GLN:HB3	2.43	0.48
1:A:122:PHE:CE2	1:A:163:VAL:HG21	2.48	0.48
1:C:77:LYS:HZ2	1:C:77:LYS:CB	2.09	0.48
1:A:15:ASN:HD22	1:A:16:PRO:CD	2.23	0.48
1:D:133:PRO:HD2	1:D:137:HIS:CE1	2.48	0.48
1:B:95:GLN:NE2	5:B:434:HOH:O	2.46	0.48
2:E:1:NDG:C1	2:E:1:NDG:C3	2.72	0.48
1:D:15:ASN:HD22	1:D:16:PRO:HD2	1.80	0.47
1:D:24:VAL:HG21	1:D:45:ARG:O	2.15	0.47
1:D:201:ARG:HD2	5:D:473:HOH:O	2.15	0.47
1:B:212:LEU:HD22	2:F:1:NDG:H8C1	1.97	0.47
1:A:50:MET:HE1	1:B:17:ALA:CB	2.45	0.46
1:B:133:PRO:HD2	1:B:137:HIS:CE1	2.50	0.46
1:D:73:MET:HA	1:D:217:ILE:O	2.16	0.46
1:B:55:TRP:CD2	1:B:195:LYS:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:HB3	1:A:144:SER:O	2.15	0.46
1:C:141:ASP:HB3	1:C:144:SER:O	2.16	0.46
1:A:73:MET:HA	1:A:217:ILE:O	2.15	0.46
1:D:112:LYS:HZ2	1:D:112:LYS:HG3	1.35	0.46
1:A:133:PRO:HD2	1:A:137:HIS:CE1	2.50	0.45
1:C:20:PHE:HE2	1:C:26:VAL:CG2	2.30	0.45
1:C:20:PHE:N	1:C:20:PHE:CD1	2.84	0.45
1:C:203:LYS:HA	5:C:405:HOH:O	2.16	0.45
1:D:19:ASN:ND2	1:D:49:ALA:HA	2.31	0.45
1:D:21:GLN:O	1:D:24:VAL:HG23	2.17	0.45
1:A:50:MET:CE	1:B:17:ALA:CB	2.91	0.45
1:C:21:GLN:O	1:C:24:VAL:HG23	2.16	0.45
1:A:182:ASN:HD22	1:A:182:ASN:H	1.65	0.45
1:C:15:ASN:HD22	1:C:16:PRO:HD2	1.82	0.45
1:B:73:MET:HA	1:B:217:ILE:O	2.17	0.44
1:C:1:ALA:N	5:C:468:HOH:O	2.51	0.44
1:C:95:GLN:NE2	5:C:465:HOH:O	2.50	0.44
1:B:137:HIS:CE1	5:B:525:HOH:O	2.70	0.44
1:D:112:LYS:HZ3	1:D:112:LYS:HB2	1.78	0.44
1:B:83:ASP:HB3	5:B:531:HOH:O	2.17	0.43
1:B:203:LYS:HA	5:B:405:HOH:O	2.19	0.43
1:C:20:PHE:N	1:C:20:PHE:HD1	2.17	0.43
1:D:77:LYS:O	1:D:78:ASP:HB2	2.17	0.43
1:A:71:PHE:HE2	1:A:122:PHE:HE2	1.64	0.43
1:D:37:LEU:HG	1:D:76:ILE:HD13	2.01	0.43
1:A:121:GLU:C	1:A:122:PHE:CD1	2.79	0.43
1:A:171:THR:HG23	5:D:460:HOH:O	2.19	0.43
1:A:159:ALA:HB1	1:A:181:ASP:HB2	2.01	0.42
1:D:13:GLU:HG2	1:D:26:VAL:HB	2.01	0.42
1:C:182:ASN:HD21	1:C:184:ASP:HB2	1.84	0.42
1:A:50:MET:HA	1:A:51:PRO:HD3	1.90	0.42
1:B:137:HIS:HE1	5:B:525:HOH:O	2.02	0.42
1:C:37:LEU:HG	1:C:76:ILE:HD13	2.01	0.42
1:C:231:THR:O	1:C:232:THR:CG2	2.65	0.42
1:C:82:ALA:HB1	1:C:83:ASP:HA	2.02	0.42
1:C:159:ALA:HB1	1:C:181:ASP:HB2	2.01	0.42
1:B:65:PHE:HA	1:C:185:ILE:HD11	2.00	0.41
1:C:25:THR:CG2	1:C:33:GLN:HB3	2.49	0.41
1:A:55:TRP:CD2	1:A:195:LYS:HG3	2.55	0.41
1:C:73:MET:HA	1:C:217:ILE:O	2.20	0.41
1:B:21:GLN:O	1:B:24:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ILE:HG21	1:B:54:ILE:HD13	1.26	0.41
1:C:15:ASN:HA	1:C:16:PRO:HD2	1.91	0.41
1:D:231:THR:O	1:D:232:THR:CG2	2.68	0.41
1:C:55:TRP:CD2	1:C:195:LYS:HG3	2.56	0.41
1:D:216:GLN:NE2	5:D:477:HOH:O	2.53	0.41
1:C:50:MET:HA	1:C:51:PRO:HD3	1.93	0.41
1:A:21:GLN:O	1:A:24:VAL:HG23	2.21	0.41
1:A:50:MET:HB2	5:A:410:HOH:O	2.21	0.41
1:D:212:LEU:HD22	2:H:1:NDG:H8C1	2.02	0.40
1:A:214:GLY:HA3	2:E:2:GAL:H61	2.03	0.40
1:D:50:MET:HA	1:D:51:PRO:HD3	1.94	0.40
1:B:170:SER:HB2	5:C:461:HOH:O	2.21	0.40
1:D:153:TRP:CG	1:D:154:ASN:N	2.90	0.40
1:C:216:GLN:NE2	5:C:409:HOH:O	2.55	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	230/236 (98%)	219 (95%)	10 (4%)	1 (0%)	34	60
1	B	230/236 (98%)	223 (97%)	7 (3%)	0	100	100
1	C	230/236 (98%)	221 (96%)	8 (4%)	1 (0%)	34	60
1	D	230/236 (98%)	218 (95%)	10 (4%)	2 (1%)	17	40
All	All	920/944 (98%)	881 (96%)	35 (4%)	4 (0%)	34	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	40	VAL

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Mol	Chain	Res	Type
1	D	41	ASN
1	C	41	ASN
1	A	41	ASN

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	197/201 (98%)	188 (95%)	9 (5%)	27	54
1	B	197/201 (98%)	184 (93%)	13 (7%)	16	38
1	C	197/201 (98%)	185 (94%)	12 (6%)	18	41
1	D	197/201 (98%)	190 (96%)	7 (4%)	35	64
All	All	788/804 (98%)	747 (95%)	41 (5%)	23	49

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	25	THR
1	A	37	LEU
1	A	122	PHE
1	A	140	ILE
1	A	170	SER
1	A	175	SER
1	A	182	ASN
1	A	232	THR
1	B	5	SER
1	B	15	ASN
1	B	25	THR
1	B	37	LEU
1	B	54	ILE
1	B	77	LYS
1	B	80	ASP
1	B	92	GLU
1	B	140	ILE

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Mol	Chain	Res	Type
1	B	170	SER
1	B	175	SER
1	B	181	ASP
1	B	182	ASN
1	C	13	GLU
1	C	15	ASN
1	C	20	PHE
1	C	37	LEU
1	C	38	ASN
1	C	39	LYS
1	C	77	LYS
1	C	140	ILE
1	C	170	SER
1	C	175	SER
1	C	182	ASN
1	C	232	THR
1	D	15	ASN
1	D	37	LEU
1	D	112	LYS
1	D	117	PHE
1	D	140	ILE
1	D	170	SER
1	D	232	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	19	ASN
1	A	31	ASN
1	A	33	GLN
1	A	41	ASN
1	A	61	ASN
1	A	95	GLN
1	A	182	ASN
1	A	216	GLN
1	B	9	ASN
1	B	15	ASN
1	B	19	ASN
1	B	31	ASN
1	B	33	GLN
1	B	41	ASN

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Mol	Chain	Res	Type
1	B	61	ASN
1	B	95	GLN
1	B	182	ASN
1	B	216	GLN
1	C	15	ASN
1	C	19	ASN
1	C	33	GLN
1	C	41	ASN
1	C	61	ASN
1	C	95	GLN
1	C	182	ASN
1	C	216	GLN
1	D	15	ASN
1	D	19	ASN
1	D	33	GLN
1	D	41	ASN
1	D	61	ASN
1	D	95	GLN
1	D	182	ASN
1	D	216	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)

8 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	NDG	E	1	2	15,15,15	6.36	5 (33%)	21,21,21	3.89	10 (47%)
2	GAL	E	2	2	11,11,12	0.92	0	15,15,17	1.57	3 (20%)
2	NDG	F	1	2	15,15,15	5.96	6 (40%)	21,21,21	3.83	12 (57%)
2	GAL	F	2	2	11,11,12	1.08	1 (9%)	15,15,17	1.72	4 (26%)
2	NDG	G	1	2	15,15,15	3.99	6 (40%)	21,21,21	4.49	16 (76%)
2	GAL	G	2	2	11,11,12	0.83	0	15,15,17	1.16	1 (6%)
2	NDG	H	1	2	15,15,15	6.40	6 (40%)	21,21,21	4.81	12 (57%)
2	GAL	H	2	2	11,11,12	0.82	0	15,15,17	1.22	2 (13%)

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	NDG	E	1	2	-	3/6/26/26	0/1/1/1
2	GAL	E	2	2	-	0/2/19/22	0/1/1/1
2	NDG	F	1	2	-	2/6/26/26	0/1/1/1
2	GAL	F	2	2	-	0/2/19/22	0/1/1/1
2	NDG	G	1	2	-	0/6/26/26	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	NDG	H	1	2	-	0/6/26/26	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	NDG	C1-C2	20.61	1.77	1.52
2	E	1	NDG	C1-C2	20.28	1.77	1.52
2	F	1	NDG	C1-C2	17.93	1.74	1.52
2	G	1	NDG	C1-C2	10.06	1.65	1.52
2	F	1	NDG	C2-N2	9.64	1.61	1.45
2	E	1	NDG	C3-C2	-7.74	1.38	1.53
2	H	1	NDG	C2-N2	7.63	1.58	1.45
2	H	1	NDG	O1-C1	7.34	1.63	1.39
2	G	1	NDG	O5-C1	6.97	1.60	1.42
2	E	1	NDG	O5-C1	6.94	1.60	1.42
2	F	1	NDG	O5-C1	6.54	1.59	1.42
2	E	1	NDG	C2-N2	6.50	1.56	1.45
2	G	1	NDG	O1-C1	6.29	1.59	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NDG	C3-C2	-6.19	1.41	1.53
2	H	1	NDG	C3-C2	-5.99	1.41	1.53
2	E	1	NDG	O1-C1	5.85	1.58	1.39
2	H	1	NDG	O5-C1	5.54	1.56	1.42
2	G	1	NDG	C2-N2	5.30	1.54	1.45
2	F	1	NDG	O1-C1	5.00	1.55	1.39
2	G	1	NDG	C8-C7	3.09	1.57	1.50
2	F	2	GAL	C2-C3	-2.55	1.48	1.52
2	F	1	NDG	O3-C3	2.48	1.48	1.43
2	G	1	NDG	O5-C5	-2.04	1.39	1.44
2	H	1	NDG	O7-C7	2.00	1.27	1.23

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	NDG	O1-C1-C2	-17.48	72.90	109.22
2	G	1	NDG	O1-C1-C2	-15.20	77.63	109.22
2	E	1	NDG	O1-C1-C2	-12.39	83.46	109.22
2	F	1	NDG	O1-C1-C2	-11.47	85.38	109.22
2	G	1	NDG	C1-C2-C3	7.74	121.10	110.54
2	H	1	NDG	C1-C2-C3	6.88	119.93	110.54
2	F	1	NDG	C1-C2-C3	6.26	119.09	110.54
2	E	1	NDG	C1-C2-C3	6.20	119.00	110.54
2	E	1	NDG	O1-C1-O5	-5.82	92.92	110.38
2	H	1	NDG	O1-C1-O5	-5.54	93.76	110.38
2	F	1	NDG	O1-C1-O5	-5.53	93.79	110.38
2	E	1	NDG	C1-O5-C5	4.82	122.76	113.66
2	G	1	NDG	O1-C1-O5	-4.65	96.43	110.38
2	H	1	NDG	C1-O5-C5	4.58	122.30	113.66
2	G	1	NDG	C1-O5-C5	4.40	121.97	113.66
2	F	1	NDG	C3-C2-N2	-4.36	102.38	110.62
2	F	2	GAL	C1-O5-C5	4.30	118.01	112.19
2	E	1	NDG	O7-C7-C8	-4.15	114.34	122.06
2	F	1	NDG	C1-O5-C5	4.07	121.34	113.66
2	H	1	NDG	C8-C7-N2	3.98	122.84	116.10
2	E	1	NDG	C8-C7-N2	3.76	122.46	116.10
2	G	1	NDG	O5-C5-C6	-3.72	97.17	106.44
2	F	1	NDG	O5-C5-C6	-3.63	97.40	106.44
2	G	1	NDG	C1-C2-N2	3.54	114.83	110.73
2	H	1	NDG	O5-C5-C6	-3.35	98.12	106.44
2	H	1	NDG	O3-C3-C4	3.22	117.80	110.35
2	H	2	GAL	C1-O5-C5	3.06	116.34	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2	GAL	O2-C2-C3	-3.01	104.12	110.14
2	F	1	NDG	C2-N2-C7	-2.89	116.14	123.18
2	E	1	NDG	O5-C5-C6	-2.86	99.31	106.44
2	H	1	NDG	O5-C5-C4	2.85	114.87	109.69
2	H	1	NDG	O4-C4-C3	2.85	116.93	110.35
2	G	1	NDG	O3-C3-C4	2.83	116.90	110.35
2	F	1	NDG	O7-C7-C8	-2.82	116.82	122.06
2	G	1	NDG	O3-C3-C2	2.77	115.25	109.66
2	F	1	NDG	C1-C2-N2	2.75	113.91	110.73
2	G	1	NDG	O7-C7-N2	-2.69	117.00	121.95
2	E	2	GAL	C1-O5-C5	2.67	115.81	112.19
2	H	1	NDG	C3-C4-C5	2.61	114.90	110.24
2	G	2	GAL	C1-O5-C5	2.60	115.72	112.19
2	F	1	NDG	O4-C4-C3	2.56	116.28	110.35
2	H	1	NDG	O7-C7-N2	-2.56	117.24	121.95
2	G	1	NDG	O4-C4-C3	2.55	116.23	110.35
2	F	1	NDG	C8-C7-N2	2.50	120.32	116.10
2	G	1	NDG	O5-C5-C4	2.48	114.19	109.69
2	H	2	GAL	C3-C4-C5	-2.44	105.89	110.24
2	E	2	GAL	C3-C4-C5	-2.42	105.93	110.24
2	F	2	GAL	C1-C2-C3	2.33	112.53	109.67
2	G	1	NDG	C3-C4-C5	2.29	114.33	110.24
2	G	1	NDG	O5-C1-C2	2.29	111.82	109.52
2	H	1	NDG	O7-C7-C8	-2.25	117.88	122.06
2	E	1	NDG	C3-C4-C5	2.24	114.24	110.24
2	E	2	GAL	C1-C2-C3	2.20	112.37	109.67
2	E	1	NDG	C3-C2-N2	-2.17	106.52	110.62
2	G	1	NDG	C4-C3-C2	-2.13	107.22	110.34
2	F	1	NDG	C3-C4-C5	2.13	114.04	110.24
2	G	1	NDG	C3-C2-N2	-2.11	106.63	110.62
2	F	2	GAL	O4-C4-C3	2.10	115.20	110.35
2	E	1	NDG	O4-C4-C3	2.03	115.04	110.35
2	G	1	NDG	C6-C5-C4	2.02	117.73	113.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NDG	C3-C2-N2-C7
2	F	1	NDG	C1-C2-N2-C7
2	E	1	NDG	O7-C7-N2-C2
2	E	1	NDG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
2	E	1	NDG	C3-C2-N2-C7

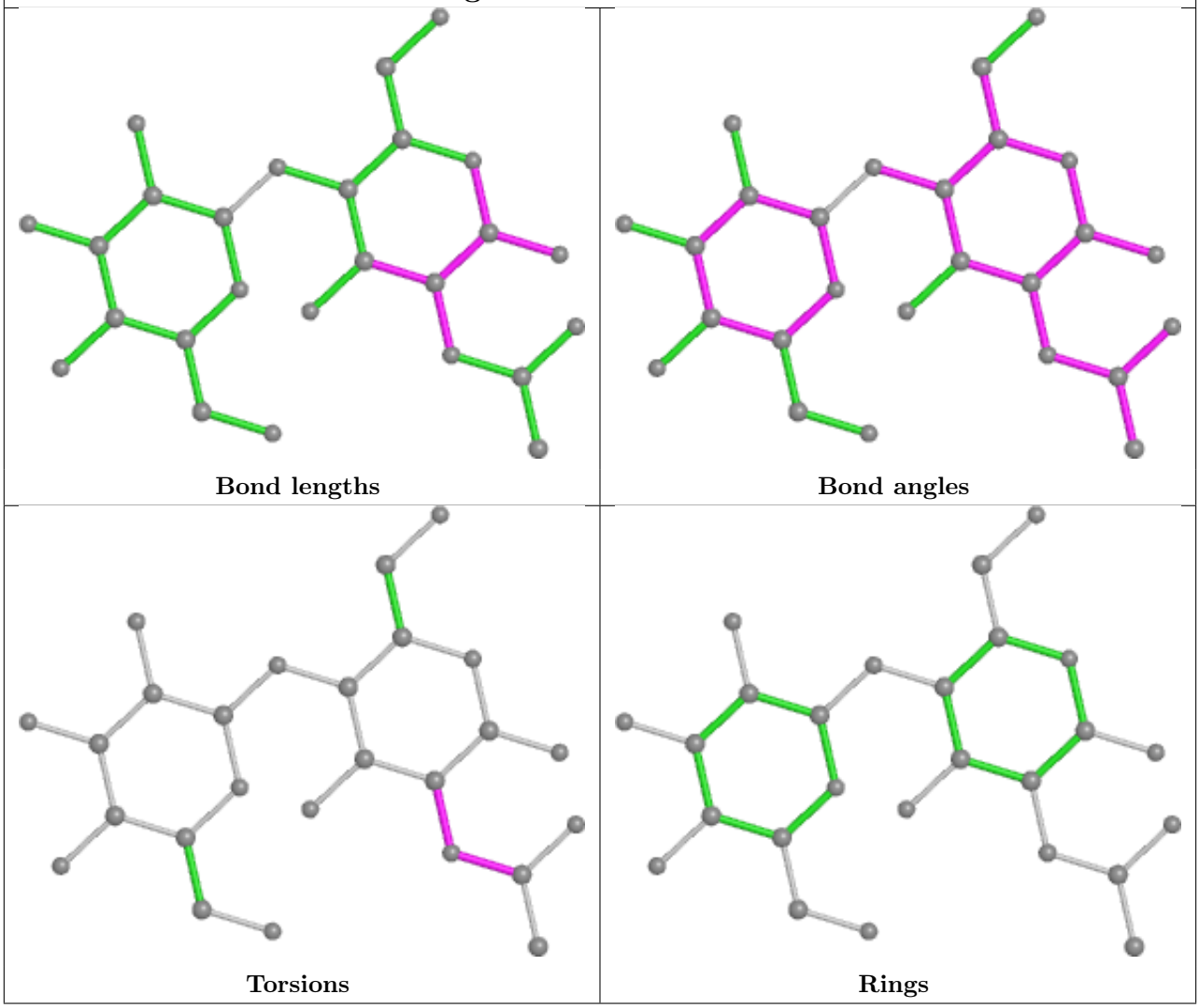
There are no ring outliers.

4 monomers are involved in 14 short contacts:

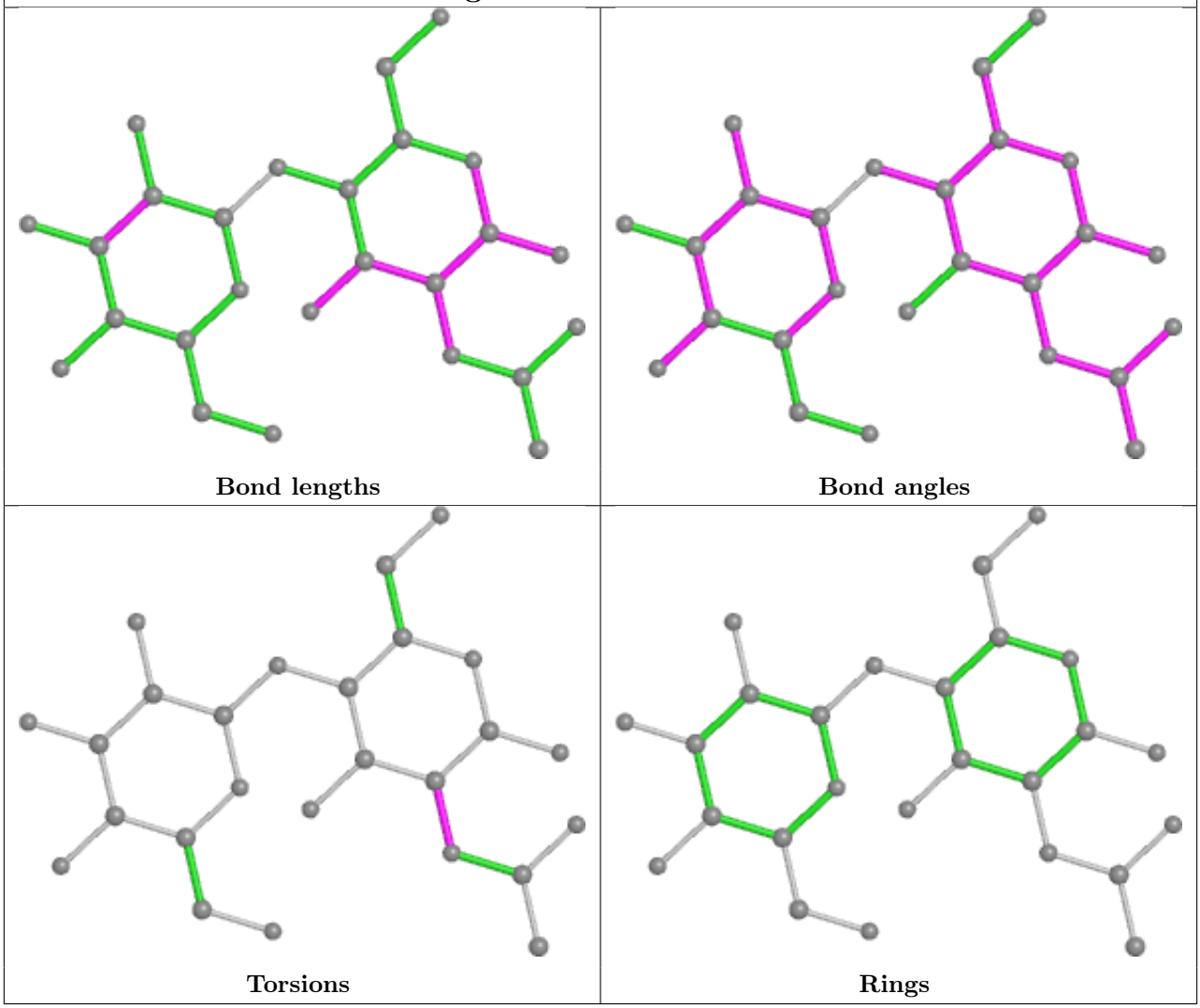
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NDG	2	0
2	E	1	NDG	6	0
2	H	1	NDG	5	0
2	E	2	GAL	1	0

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

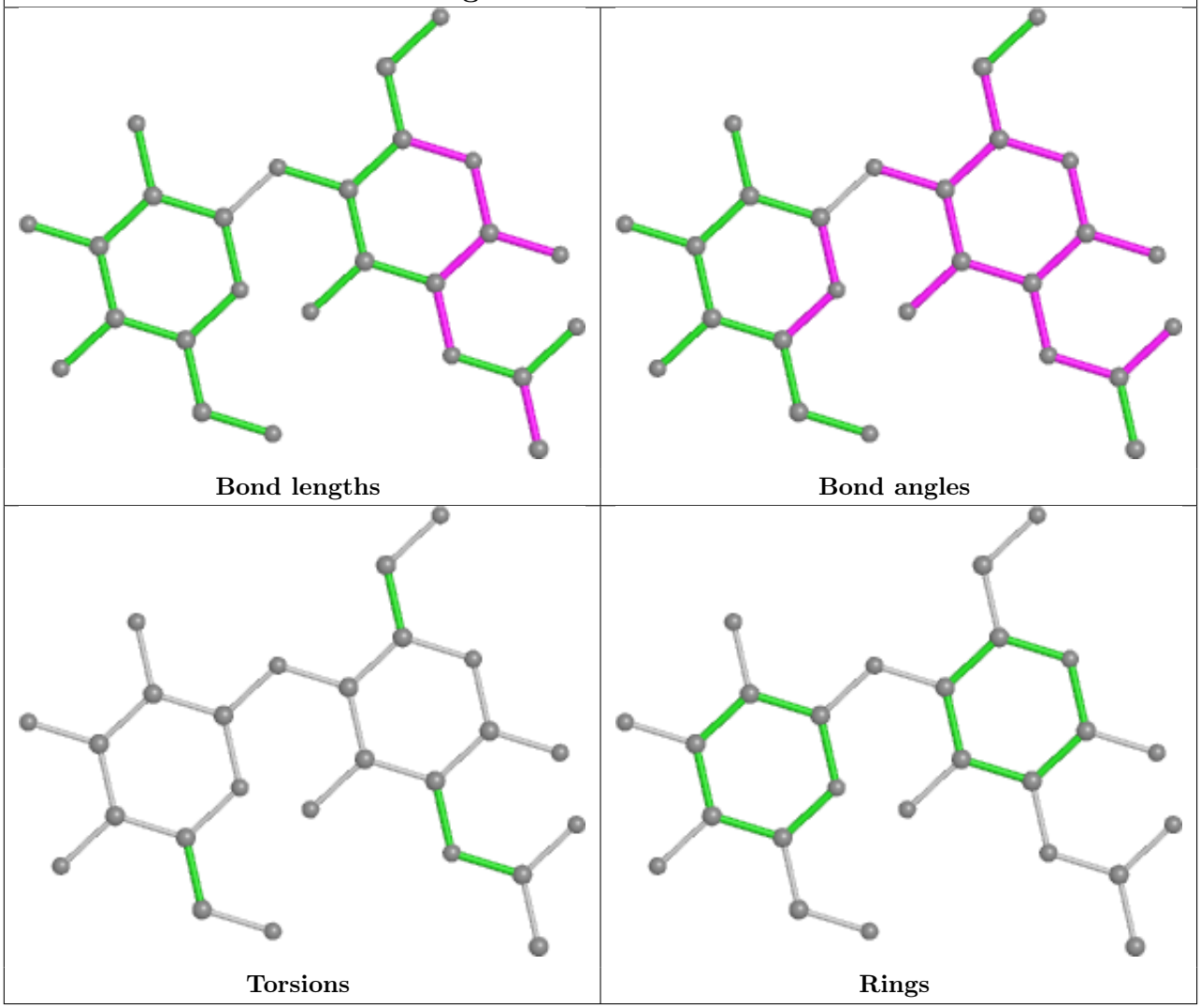
Oligosaccharide Chain E



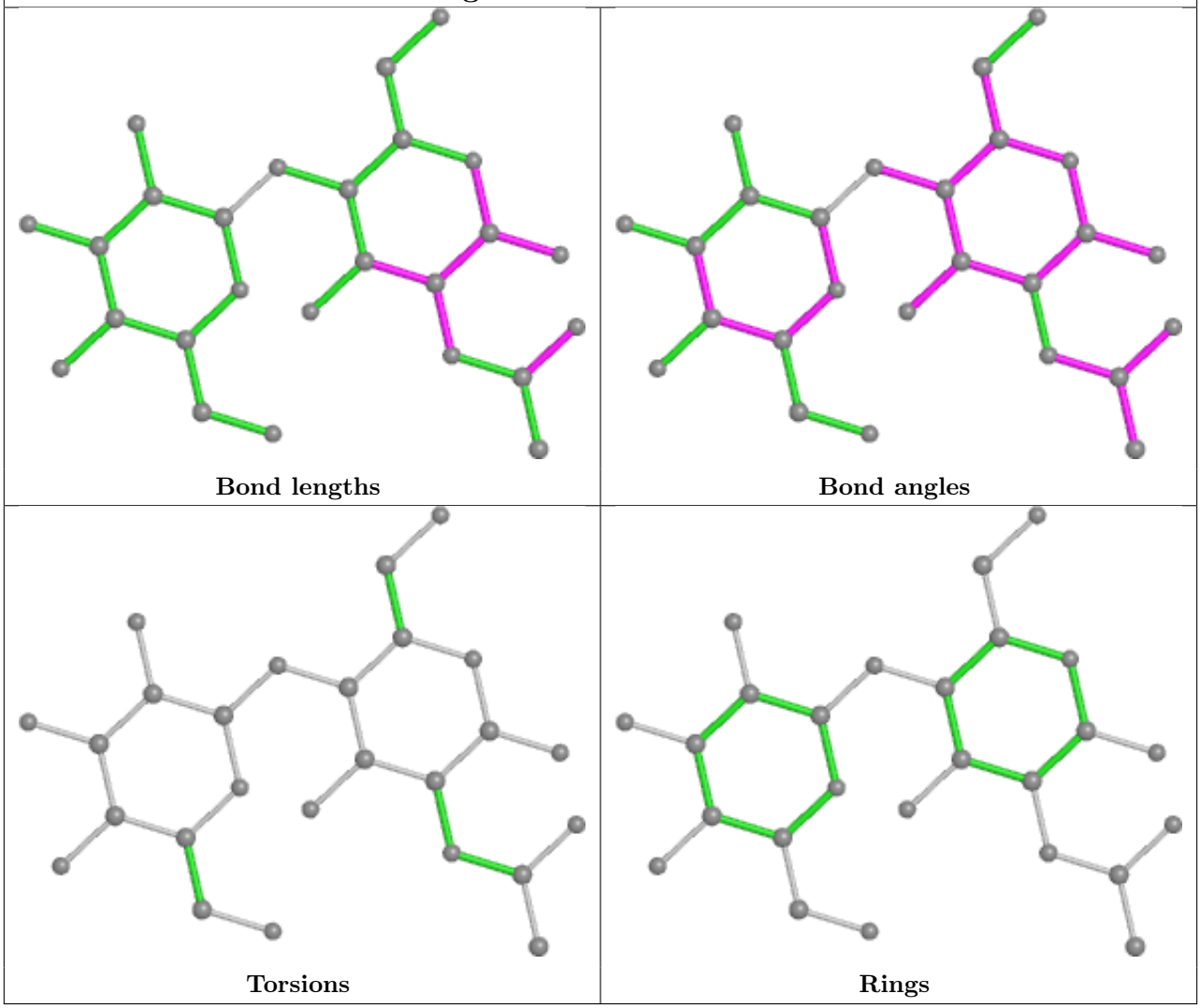
Oligosaccharide Chain F



Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	232/236 (98%)	-0.84	1 (0%)	92	93	7, 21, 51, 141	0
1	B	232/236 (98%)	-0.77	1 (0%)	92	93	4, 21, 50, 165	0
1	C	232/236 (98%)	-0.70	1 (0%)	92	93	7, 24, 63, 169	0
1	D	232/236 (98%)	-0.75	0	100	100	6, 23, 62, 142	0
All	All	928/944 (98%)	-0.76	3 (0%)	94	95	4, 22, 60, 169	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	232	THR	4.7
1	B	232	THR	3.7
1	A	232	THR	2.3

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	NDG	G	1	15/15	0.56	0.37	187,188,188,188	0
2	NDG	F	1	15/15	0.69	0.34	105,105,106,106	0
2	NDG	E	1	15/15	0.75	0.31	132,133,133,133	0
2	NDG	H	1	15/15	0.75	0.31	137,137,138,138	0

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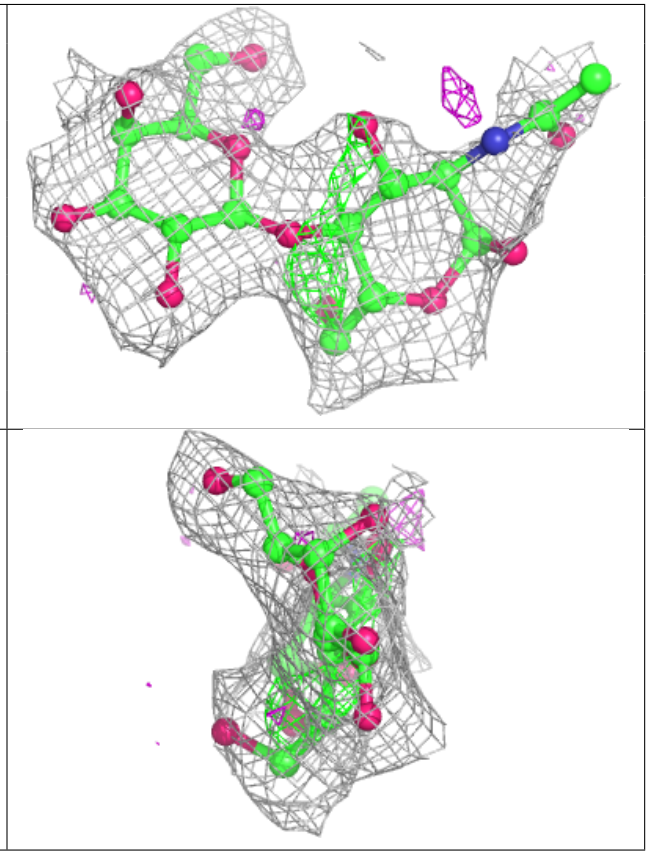
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GAL	G	2	11/12	0.91	0.19	46,47,47,47	0
2	GAL	H	2	11/12	0.91	0.18	32,33,33,33	0
2	GAL	F	2	11/12	0.92	0.17	33,33,33,33	0
2	GAL	E	2	11/12	0.96	0.12	23,24,24,24	0

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.

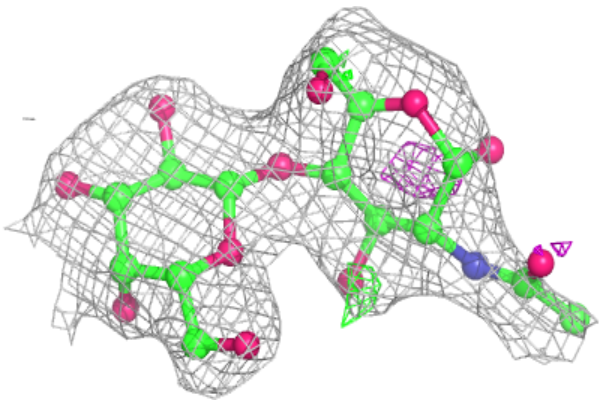
Electron density around Chain E:

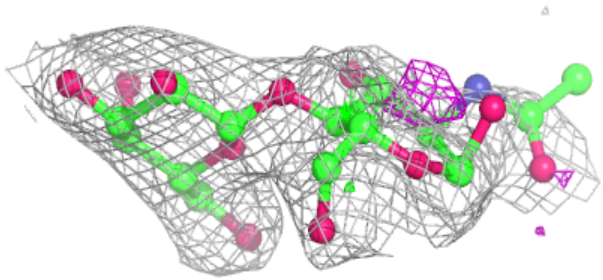
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

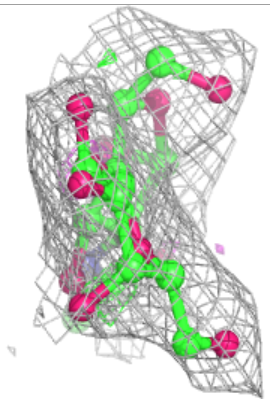


Electron density around Chain F:

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

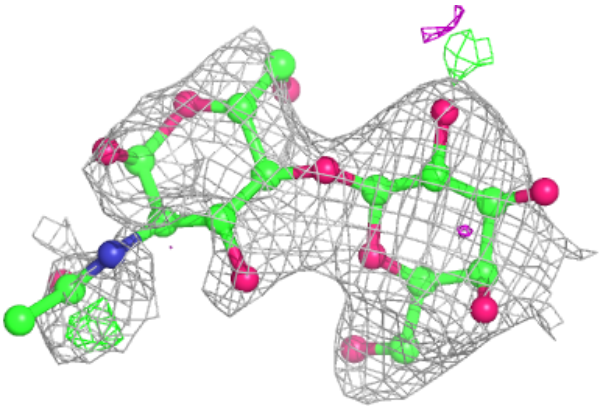


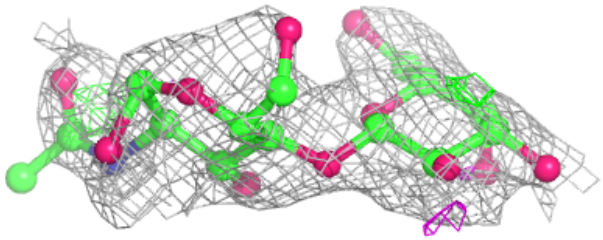


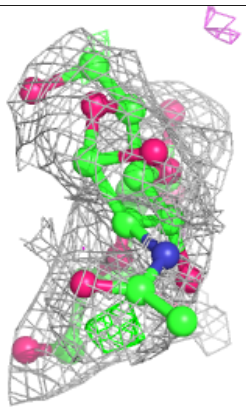


Electron density around Chain G:

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

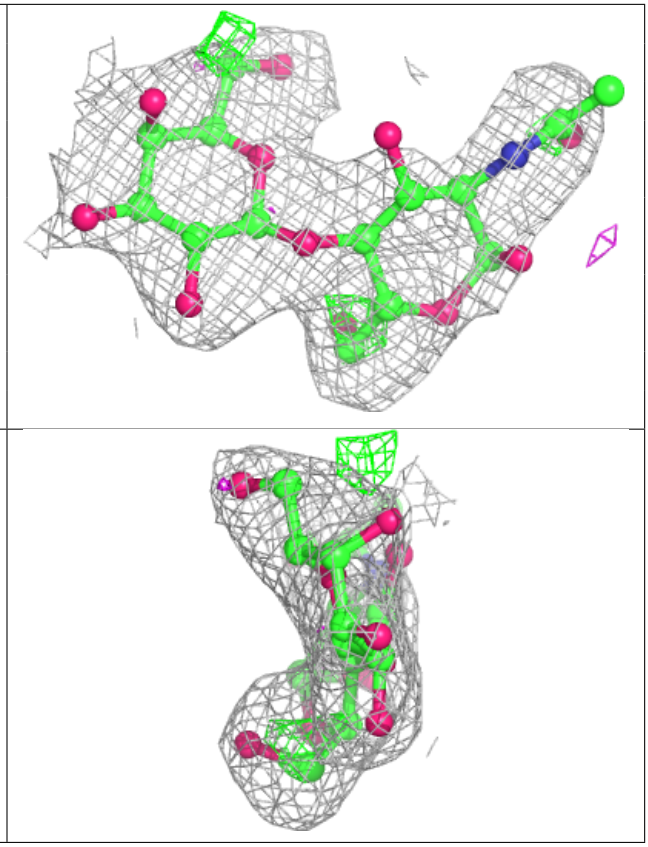






Electron density around Chain H:

$2mF_o$-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
4	MN	A	238	1/1	0.91	0.06	40,40,40,40	0
3	CA	D	237	1/1	0.95	0.07	20,20,20,20	0
4	MN	D	238	1/1	0.97	0.06	36,36,36,36	0
3	CA	C	237	1/1	0.98	0.09	21,21,21,21	0
3	CA	A	237	1/1	0.99	0.05	17,17,17,17	0
4	MN	B	238	1/1	0.99	0.03	41,41,41,41	0
4	MN	C	238	1/1	0.99	0.06	44,44,44,44	0
3	CA	B	237	1/1	0.99	0.05	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.