WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 04:54 PM JST

PDB ID	:	5XN2
Title	:	HIV-1 reverse transcriptase Q151M:DNA:dGTP ternary complex
Authors	:	Yasutake, Y.; Tamura, N.; Hayashi, H.; Maeda, K.
Deposited on	:	2017-05-17
Resolution	:	2.38 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
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 ⓘ

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

The reported resolution of this entry is 2.38 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	Percentile Ranks	Value
Rfree		0.223
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		1.0%
RSRZ outliers		9.3%

Worse ← → Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
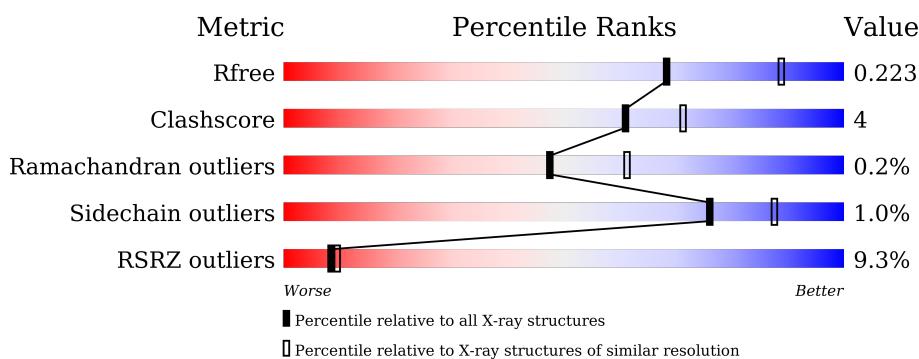
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	557	6% / 84% · 15% ··
1	C	557	11% / 88% · 11% ·
2	B	444	14% / 83% · 8% · 8%
2	D	444	6% / 83% · 9% 8%
3	E	38	61% · 26% · 5% 8%
3	F	38	3% / 58% · 37% · 5%
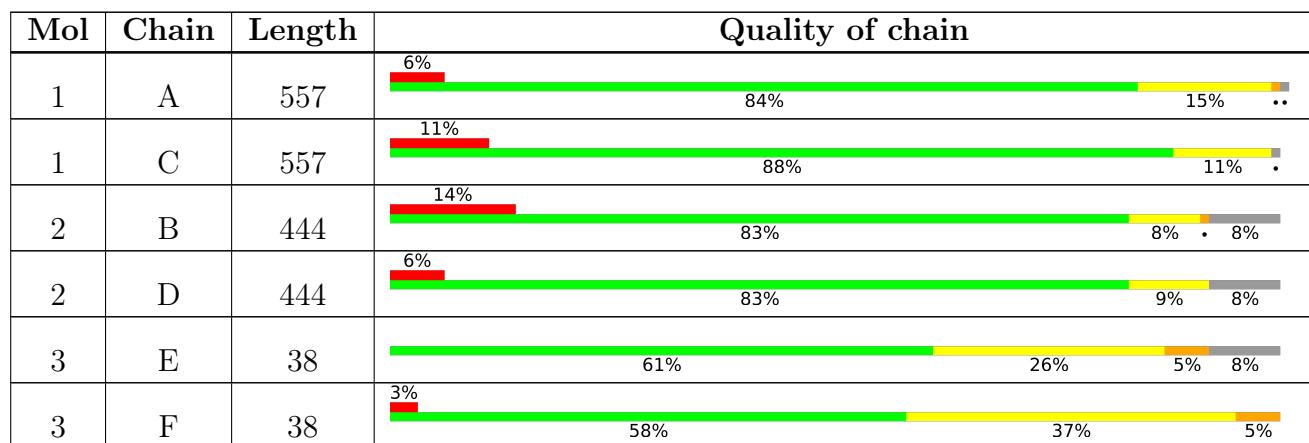
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Mol	Chain	Length	Quality of chain
4	G	2	100%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 17606 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 Pol protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total 4488	C 2903	N 748	O 829	S 8	0	1	0
1	C	551	Total 4483	C 2900	N 748	O 827	S 8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP D3XFN7
A	0	VAL	-	expression tag	UNP D3XFN7
A	151	MET	GLN	engineered mutation	UNP D3XFN7
A	162	SER	CYS	engineered mutation	UNP D3XFN7
A	280	SER	CYS	engineered mutation	UNP D3XFN7
C	-1	MET	-	expression tag	UNP D3XFN7
C	0	VAL	-	expression tag	UNP D3XFN7
C	151	MET	GLN	engineered mutation	UNP D3XFN7
C	162	SER	CYS	engineered mutation	UNP D3XFN7
C	280	SER	CYS	engineered mutation	UNP D3XFN7

- Molecule 2 is a protein called Pol protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	407	Total 3354	C 2183	N 558	O 607	S 6	0	0	0
2	D	407	Total 3354	C 2183	N 558	O 607	S 6	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	expression tag	UNP D3XFN7
B	-14	ALA	-	expression tag	UNP D3XFN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP D3XFN7
B	-12	HIS	-	expression tag	UNP D3XFN7
B	-11	HIS	-	expression tag	UNP D3XFN7
B	-10	HIS	-	expression tag	UNP D3XFN7
B	-9	HIS	-	expression tag	UNP D3XFN7
B	-8	HIS	-	expression tag	UNP D3XFN7
B	-7	ALA	-	expression tag	UNP D3XFN7
B	-6	LEU	-	expression tag	UNP D3XFN7
B	-5	GLU	-	expression tag	UNP D3XFN7
B	-4	VAL	-	expression tag	UNP D3XFN7
B	-3	LEU	-	expression tag	UNP D3XFN7
B	-2	PHE	-	expression tag	UNP D3XFN7
B	-1	GLN	-	expression tag	UNP D3XFN7
B	0	GLY	-	expression tag	UNP D3XFN7
B	162	SER	CYS	engineered mutation	UNP D3XFN7
B	280	SER	CYS	engineered mutation	UNP D3XFN7
D	-15	MET	-	expression tag	UNP D3XFN7
D	-14	ALA	-	expression tag	UNP D3XFN7
D	-13	HIS	-	expression tag	UNP D3XFN7
D	-12	HIS	-	expression tag	UNP D3XFN7
D	-11	HIS	-	expression tag	UNP D3XFN7
D	-10	HIS	-	expression tag	UNP D3XFN7
D	-9	HIS	-	expression tag	UNP D3XFN7
D	-8	HIS	-	expression tag	UNP D3XFN7
D	-7	ALA	-	expression tag	UNP D3XFN7
D	-6	LEU	-	expression tag	UNP D3XFN7
D	-5	GLU	-	expression tag	UNP D3XFN7
D	-4	VAL	-	expression tag	UNP D3XFN7
D	-3	LEU	-	expression tag	UNP D3XFN7
D	-2	PHE	-	expression tag	UNP D3XFN7
D	-1	GLN	-	expression tag	UNP D3XFN7
D	0	GLY	-	expression tag	UNP D3XFN7
D	162	SER	CYS	engineered mutation	UNP D3XFN7
D	280	SER	CYS	engineered mutation	UNP D3XFN7

- Molecule 3 is DNA/RNA hybrid called 38-MER DNA aptamer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			718	339	128	216	35			
3	F	38	Total	C	N	O	P	0	0	0
			777	369	140	231	37			

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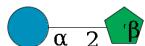

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	G	2	Total 23	C 12	O 11	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mg 1	0	0
5	C	1	Total 1	Mg 1	0	0

- Molecule 6 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
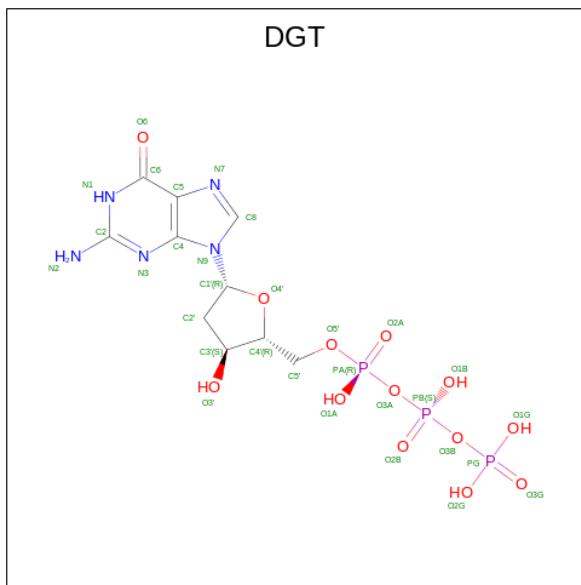
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
6	C	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
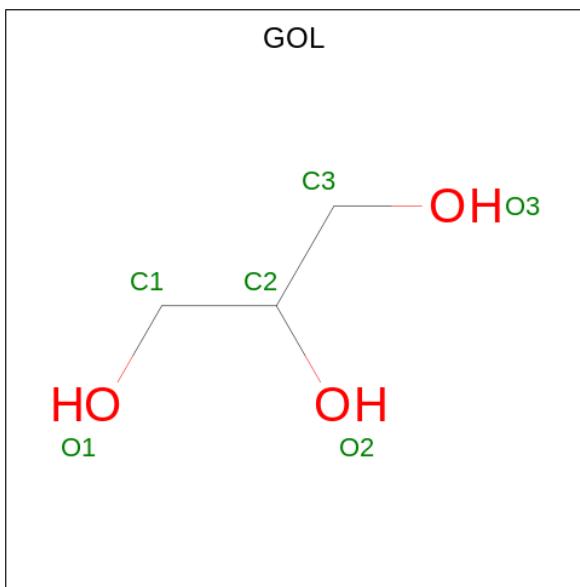
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0
7	D	1	Total 6	C 3	O 3	0	0

• Molecule 8 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	103	Total 103	O 103	0	0
8	B	31	Total 31	O 31	0	0
8	E	36	Total 36	O 36	0	0
8	C	70	Total 70	O 70	0	0
8	D	58	Total 58	O 58	0	0
8	F	23	Total 23	O 23	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: Pol protein
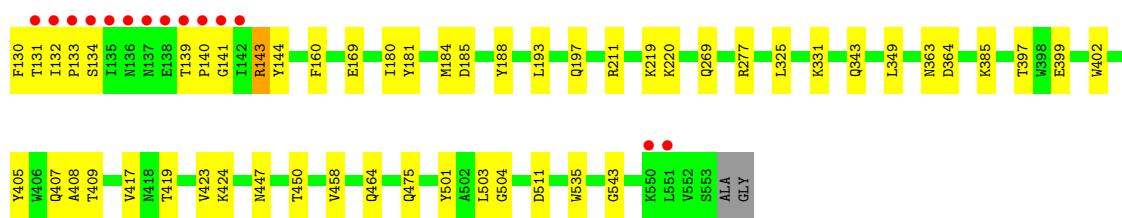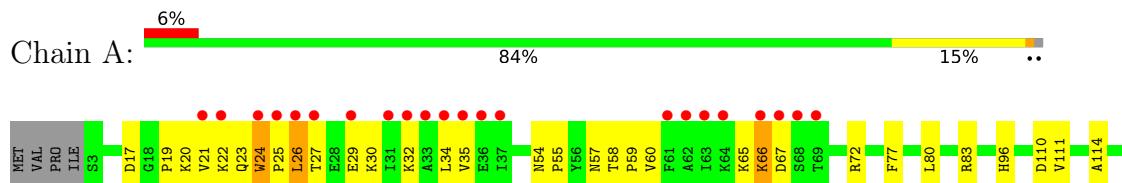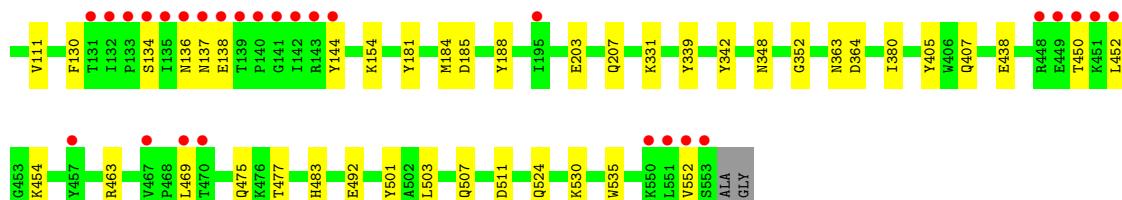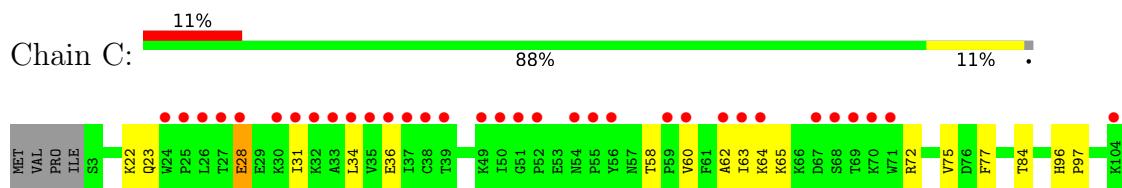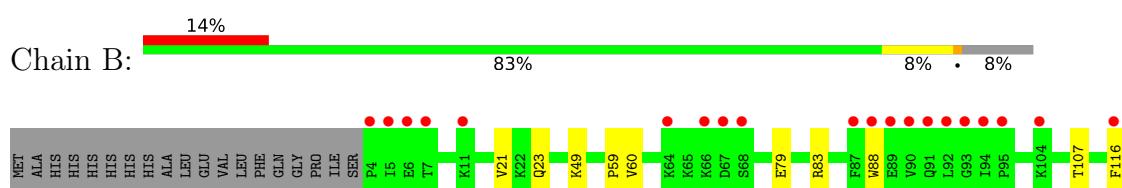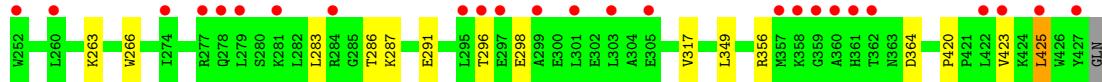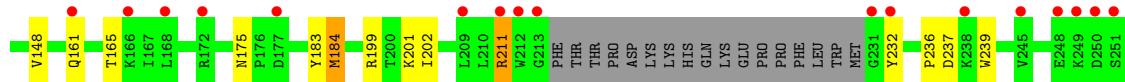
Chain A:

• Molecule 1: Pol protein

Chain C:

• Molecule 2: Pol protein

Chain B:

• Molecule 2: Pol protein

Chain D:

• Molecule 3: 38-MER DNA aptamer

Chain E:

• Molecule 3: 38-MER DNA aptamer

Chain F:
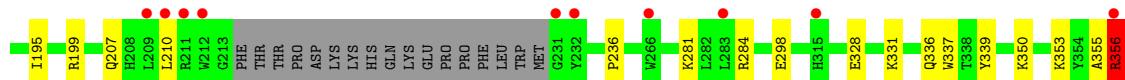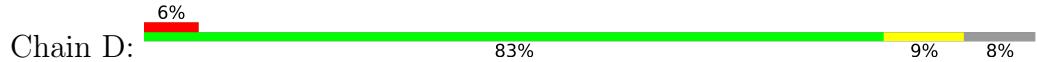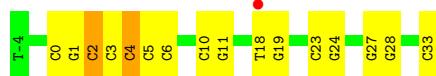
• Molecule 4: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	285.69Å 285.69Å 96.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.90 – 2.38 48.90 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.90-2.38) 99.8 (48.90-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.39Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.189 , 0.223 0.189 , 0.223	Depositor DCC
R_{free} test set	5960 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17606	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG, DGT, OMC, GOL, FRU, GLC

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	0.27	0/4608	0.46	0/6257
1	C	0.25	0/4600	0.44	0/6246
2	B	0.24	0/3449	0.44	1/4684 (0.0%)
2	D	0.25	0/3449	0.44	0/4684
3	E	0.48	0/756	0.93	1/1165 (0.1%)
3	F	0.46	0/823	0.90	0/1269
All	All	0.28	0/17685	0.51	2/24305 (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	A	0	1
2	D	0	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	31	DG	O4'-C4'-C3'	-5.51	102.29	104.50
2	B	425	LEU	CA-CB-CG	5.12	127.08	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	24	TRP	Peptide
2	D	355	ALA	Peptide
2	D	356	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4488	0	4536	61	1
1	C	4483	0	4532	32	0
2	B	3354	0	3387	22	0
2	D	3354	0	3387	24	1
3	E	718	0	397	9	0
3	F	777	0	432	12	0
4	G	23	0	21	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	31	0	11	1	0
6	C	31	0	12	1	0
7	A	6	0	8	1	0
7	B	6	0	8	0	0
7	D	12	0	16	1	0
8	A	103	0	0	0	0
8	B	31	0	0	0	0
8	C	70	0	0	0	0
8	D	58	0	0	1	0
8	E	36	0	0	0	0
8	F	23	0	0	0	0
All	All	17606	0	16747	152	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (152) 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:26:LEU:HG	1:A:133:PRO:HG2	1.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:GLN:HE22	2:B:60:VAL:H	1.24	0.83
2:D:336:GLN:NE2	2:D:356:ARG:HH21	1.90	0.70
1:A:26:LEU:CG	1:A:133:PRO:HG2	2.20	0.69
2:D:336:GLN:HE21	2:D:356:ARG:NH2	1.92	0.67
1:C:136:ASN:O	1:C:138:GLU:N	2.27	0.67
3:F:1:DG:H2'	3:F:2:OMC:C6	2.30	0.66
3:F:3:DC:H2'	3:F:4:OMC:C6	2.31	0.66
1:A:21:VAL:HG12	1:A:22:LYS:H	1.61	0.66
2:B:287:LYS:NZ	2:B:291:GLU:OE2	2.30	0.64
3:E:1:DG:H2'	3:E:2:OMC:C6	2.32	0.64
3:E:3:DC:H2'	3:E:4:OMC:C6	2.32	0.63
1:A:54:ASN:O	1:A:143:ARG:NH2	2.32	0.62
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.35	0.60
2:D:207:GLN:HA	2:D:210:LEU:HB2	1.84	0.60
2:B:296:THR:HG22	2:B:298:GLU:H	1.68	0.58
1:A:21:VAL:HG12	1:A:22:LYS:N	2.19	0.58
1:A:27:THR:HB	1:A:30:LYS:HG3	1.85	0.58
1:C:450:THR:HG23	1:C:452:LEU:H	1.68	0.58
3:E:3:DC:H2'	3:E:4:OMC:H6	1.69	0.58
1:C:22:LYS:HD3	1:C:23:GLN:N	2.19	0.57
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.85	0.57
1:A:27:THR:HG22	1:A:29:GLU:H	1.70	0.57
3:F:3:DC:H2'	3:F:4:OMC:H6	1.69	0.57
2:D:90:VAL:HG21	2:D:158:ALA:HA	1.87	0.56
2:D:336:GLN:NE2	2:D:356:ARG:NH2	2.52	0.56
1:C:28:GLU:O	1:C:31:ILE:HG22	2.06	0.56
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.88	0.56
3:F:27:DG:H2'	3:F:28:DG:C8	2.40	0.56
1:A:25:PRO:HG2	1:A:30:LYS:HD2	1.88	0.55
1:A:325:LEU:HD12	1:A:385:LYS:HE2	1.88	0.55
2:D:336:GLN:HE21	2:D:356:ARG:HH21	1.48	0.54
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.87	0.54
2:D:163:SER:O	2:D:167:ILE:HG12	2.07	0.54
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.72	0.54
1:A:67:ASP:OD2	1:A:219:LYS:NZ	2.40	0.54
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.90	0.54
1:A:23:GLN:HG3	1:A:24:TRP:H	1.72	0.54
1:A:34:LEU:HD13	1:A:132:ILE:HG12	1.90	0.54
3:F:18:DT:H4'	3:F:19:DG:C8	2.43	0.54
1:A:134:SER:HB2	1:A:141:GLY:HA2	1.89	0.53
1:A:23:GLN:HG3	1:A:24:TRP:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:27:DG:H2'	3:F:28:DG:H8	1.74	0.52
2:B:266:TRP:NE1	2:B:425:LEU:HD21	2.25	0.52
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.91	0.52
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.92	0.52
1:C:63:ILE:HG22	1:C:64:LYS:H	1.74	0.52
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.91	0.52
1:A:26:LEU:HG	1:A:133:PRO:CG	2.26	0.52
1:A:32:LYS:HA	1:A:35:VAL:HG22	1.91	0.52
1:C:454:LYS:HB2	1:C:552:VAL:HG13	1.91	0.51
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.93	0.51
1:C:84:THR:HB	1:C:154:LYS:HE2	1.91	0.51
3:E:27:DG:H2'	3:E:28:DG:C8	2.46	0.51
1:C:203:GLU:O	1:C:207:GLN:HG2	2.11	0.51
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.93	0.51
1:A:24:TRP:HD1	1:A:25:PRO:CD	2.23	0.51
2:B:107:THR:HA	2:B:232:TYR:O	2.10	0.51
1:A:96:HIS:HE2	1:A:269:GLN:HE21	1.56	0.50
2:B:263:LYS:HB2	2:B:423:VAL:HG11	1.94	0.50
1:A:169:GLU:OE2	2:B:49:LYS:NZ	2.45	0.50
2:B:116:PHE:HA	2:B:148:VAL:HG11	1.92	0.50
1:A:23:GLN:HE22	1:A:60:VAL:H	1.60	0.50
1:A:504:GLY:HA2	2:B:420:PRO:HG3	1.94	0.49
1:A:21:VAL:CG1	1:A:22:LYS:H	2.25	0.49
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.94	0.49
3:F:10:DC:H2"	3:F:11:DG:C8	2.48	0.49
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.48	0.49
1:A:24:TRP:C	1:A:24:TRP:CD1	2.86	0.48
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.47	0.48
1:C:503:LEU:HD23	2:D:422:LEU:HD21	1.94	0.48
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.49	0.48
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.96	0.48
1:A:26:LEU:CD1	1:A:133:PRO:HG2	2.43	0.48
1:A:543:GLY:HA2	2:B:283:LEU:O	2.14	0.47
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.49	0.47
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.49	0.47
6:A:602:DGT:N2	3:E:0:DC:O2	2.36	0.47
1:C:60:VAL:HG22	1:C:75:VAL:HG22	1.96	0.47
1:C:483:HIS:ND1	1:C:524:GLN:OE1	2.48	0.47
1:C:65:LYS:HE2	1:C:72:ARG:HB2	1.96	0.47
2:D:350:LYS:NZ	2:D:378:GLU:OE2	2.41	0.47
1:A:110[A]:ASP:HB2	1:A:220:LYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HG3	1:A:72:ARG:HB2	1.97	0.46
1:A:193:LEU:HB3	1:A:197:GLN:HG3	1.98	0.46
1:C:438:GLU:OE1	1:C:463:ARG:NH2	2.48	0.46
2:D:195:ILE:O	2:D:199:ARG:HG3	2.16	0.46
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.98	0.46
1:A:24:TRP:HD1	1:A:25:PRO:HD2	1.80	0.46
1:A:17:ASP:O	1:A:83:ARG:HD3	2.17	0.45
2:B:211:ARG:O	2:B:211:ARG:NH2	2.49	0.45
3:E:27:DG:H2'	3:E:28:DG:H8	1.79	0.45
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.97	0.45
1:A:409:THR:HB	7:A:603:GOL:H11	1.99	0.45
2:D:25:PRO:HA	7:D:501:GOL:H31	1.99	0.45
1:A:34:LEU:HB3	1:A:132:ILE:HD13	1.97	0.45
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.51	0.45
1:A:22:LYS:O	1:A:59:PRO:HG3	2.17	0.45
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.52	0.45
1:C:380:ILE:HD12	2:D:27:THR:HG22	1.99	0.44
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.99	0.44
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.52	0.44
1:C:469:LEU:HD12	1:C:477:THR:HG22	2.00	0.44
6:C:602:DGT:N2	3:F:0:DC:O2	2.33	0.44
1:A:57:ASN:OD1	1:A:131:THR:N	2.46	0.44
1:A:447:ASN:HB3	1:A:450:THR:HB	2.00	0.44
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.52	0.44
1:A:417:VAL:HG22	1:A:419:THR:HG23	2.00	0.44
3:E:10:DC:H2"	3:E:11:DG:C8	2.53	0.44
3:F:23:DC:H2"	3:F:24:DG:C8	2.53	0.44
3:E:13:DT:H2"	3:E:14:DG:C8	2.53	0.43
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.53	0.43
2:D:105:SER:O	2:D:190:GLY:HA2	2.18	0.43
1:A:66:LYS:HD3	1:A:66:LYS:HA	1.82	0.43
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.99	0.43
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.16	0.43
2:D:328:GLU:O	2:D:339:TYR:HA	2.18	0.43
2:D:298:GLU:OE2	2:D:298:GLU:N	2.34	0.43
2:D:361:HIS:HB2	8:D:640:HOH:O	2.18	0.43
1:C:181:TYR:HB2	1:C:188:TYR:HB3	2.01	0.43
1:C:184:MET:HG3	3:F:33:DC:H1'	2.00	0.43
3:F:5:DC:H2'	3:F:6:DC:C6	2.54	0.43
2:D:79:GLU:HG3	2:D:83:ARG:HE	1.84	0.43
1:C:450:THR:HG23	1:C:452:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:336:GLN:HE21	2:D:356:ARG:HD2	1.84	0.42
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.02	0.42
2:B:317:VAL:HG12	2:B:349:LEU:HD23	2.01	0.42
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.18	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.54	0.42
3:E:1:DG:H2'	3:E:2:OMC:H6	1.84	0.41
2:B:161:GLN:O	2:B:165:THR:HG23	2.19	0.41
2:D:61:PHE:CZ	2:D:74:LEU:HD23	2.55	0.41
2:B:201:LYS:HD3	2:B:201:LYS:HA	1.79	0.41
1:C:331:LYS:NZ	1:C:364:ASP:OD2	2.41	0.41
3:F:1:DG:H2'	3:F:2:OMC:H6	1.79	0.41
1:A:397:THR:HG21	1:A:424:LYS:HA	2.03	0.41
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.55	0.41
1:C:503:LEU:HG	1:C:507:GLN:HG3	2.02	0.41
1:C:492:GLU:HG2	1:C:530:LYS:HB2	2.02	0.41
1:C:342:TYR:HB3	1:C:348:ASN:HA	2.02	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.20	0.41
2:D:101:LYS:O	2:D:236:PRO:HB2	2.21	0.41
2:D:353:LYS:HE3	2:D:353:LYS:HB2	1.83	0.41
2:D:281:LYS:HG2	2:D:284:ARG:HH21	1.85	0.41
1:A:30:LYS:O	1:A:34:LEU:HG	2.21	0.40
1:A:458:VAL:HG22	1:A:464:GLN:HG2	2.02	0.40
1:C:58:THR:HG21	1:C:77:PHE:CD1	2.55	0.40
1:A:24:TRP:CD1	1:A:25:PRO:CD	3.04	0.40
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.56	0.40
1:A:180:ILE:HA	1:A:188:TYR:O	2.21	0.40
2:D:331:LYS:HB2	2:D:337:TRP:CZ3	2.55	0.40
1:C:96:HIS:CG	1:C:97:PRO:HD2	2.56	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:OG1	2:D:207:GLN:NE2[8_755]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/557 (99%)	535 (97%)	15 (3%)	0	100	100
1	C	549/557 (99%)	530 (96%)	17 (3%)	2 (0%)	34	46
2	B	403/444 (91%)	394 (98%)	9 (2%)	0	100	100
2	D	403/444 (91%)	389 (96%)	12 (3%)	2 (0%)	29	39
All	All	1905/2002 (95%)	1848 (97%)	53 (3%)	4 (0%)	47	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	ASN
2	D	359	GLY
1	C	134	SER
2	D	424	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	491/494 (99%)	485 (99%)	6 (1%)	71	84
1	C	490/494 (99%)	488 (100%)	2 (0%)	91	96
2	B	366/400 (92%)	361 (99%)	5 (1%)	67	81
2	D	366/400 (92%)	362 (99%)	4 (1%)	73	86
All	All	1713/1788 (96%)	1696 (99%)	17 (1%)	76	87

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All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	66	LYS
1	A	143	ARG
1	A	184	MET
1	A	211	ARG
1	A	277	ARG
2	B	88	TRP
2	B	184	MET
2	B	211	ARG
2	B	237	ASP
2	B	356	ARG
1	C	28	GLU
1	C	36	GLU
2	D	66	LYS
2	D	356	ARG
2	D	357	MET
2	D	418	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	221	HIS
1	A	269	GLN
1	A	464	GLN
2	B	23	GLN
2	B	96	HIS
2	B	137	ASN
2	B	151	GLN
2	B	174	GLN
2	B	175	ASN
2	B	334	GLN
1	C	102	GLN
1	C	174	GLN
1	C	175	ASN
1	C	221	HIS
1	C	265	ASN
1	C	332	GLN
1	C	428	GLN
2	D	182	GLN
2	D	255	ASN

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Mol	Chain	Res	Type
2	D	336	GLN
2	D	373	GLN
2	D	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	OMC	F	4	3	19,22,23	2.86	8 (42%)	26,31,34	0.75	0
3	OMC	E	4	3	19,22,23	2.85	8 (42%)	26,31,34	0.77	0
3	OMC	F	2	3	19,22,23	2.83	8 (42%)	26,31,34	0.72	0
3	OMC	E	2	3	19,22,23	2.85	8 (42%)	26,31,34	0.73	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
3	OMC	F	4	3	-	0/9/27/28	0/2/2/2
3	OMC	E	4	3	-	0/9/27/28	0/2/2/2
3	OMC	F	2	3	-	0/9/27/28	0/2/2/2
3	OMC	E	2	3	-	0/9/27/28	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	OMC	C2-N3	6.30	1.49	1.36
3	E	4	OMC	C2-N3	6.25	1.49	1.36
3	E	2	OMC	C2-N3	6.20	1.48	1.36
3	F	2	OMC	C2-N3	6.17	1.48	1.36
3	F	2	OMC	C6-C5	5.97	1.48	1.35
3	E	4	OMC	C6-C5	5.96	1.48	1.35
3	E	2	OMC	C6-C5	5.96	1.48	1.35
3	F	4	OMC	C6-C5	5.96	1.48	1.35
3	F	4	OMC	C4-N3	5.06	1.44	1.34
3	E	2	OMC	C4-N3	5.01	1.44	1.34
3	E	4	OMC	C4-N3	4.98	1.44	1.34
3	F	2	OMC	C4-N3	4.97	1.44	1.34
3	E	4	OMC	C2-N1	4.81	1.50	1.40
3	E	2	OMC	C2-N1	4.76	1.50	1.40
3	F	4	OMC	C2-N1	4.75	1.50	1.40
3	F	2	OMC	C2-N1	4.64	1.50	1.40
3	F	4	OMC	C4-N4	3.08	1.41	1.33
3	E	2	OMC	C4-N4	3.08	1.41	1.33
3	F	2	OMC	C4-N4	3.08	1.41	1.33
3	E	4	OMC	C4-N4	3.06	1.41	1.33
3	F	4	OMC	C6-N1	3.05	1.45	1.38
3	E	2	OMC	C6-N1	3.04	1.45	1.38
3	E	4	OMC	C6-N1	3.00	1.45	1.38
3	F	2	OMC	C6-N1	2.98	1.45	1.38
3	E	2	OMC	C5-C4	2.75	1.49	1.42
3	E	4	OMC	C5-C4	2.73	1.49	1.42
3	F	2	OMC	C5-C4	2.72	1.49	1.42
3	F	4	OMC	C5-C4	2.69	1.49	1.42
3	F	2	OMC	O2-C2	-2.17	1.19	1.23
3	E	2	OMC	O2-C2	-2.13	1.19	1.23
3	E	4	OMC	O2-C2	-2.12	1.19	1.23
3	F	4	OMC	O2-C2	-2.09	1.19	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	OMC	2	0
3	E	4	OMC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	OMC	2	0
3	E	2	OMC	2	0

5.5　Carbohydrates ⓘ

2 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	$\#|Z| > 2$
4	GLC	G	1	4	11,11,12	0.58	0	15,15,17	0.68	0
4	FRU	G	2	4	11,12,12	0.55	0	10,18,18	0.64	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	GLC	G	1	4	-	1/2/19/22	0/1/1/1
4	FRU	G	2	4	-	5/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	2	FRU	O1-C1-C2-O2
4	G	2	FRU	O1-C1-C2-O5
4	G	2	FRU	C4-C5-C6-O6
4	G	2	FRU	O1-C1-C2-C3
4	G	2	FRU	O5-C5-C6-O6
4	G	1	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings
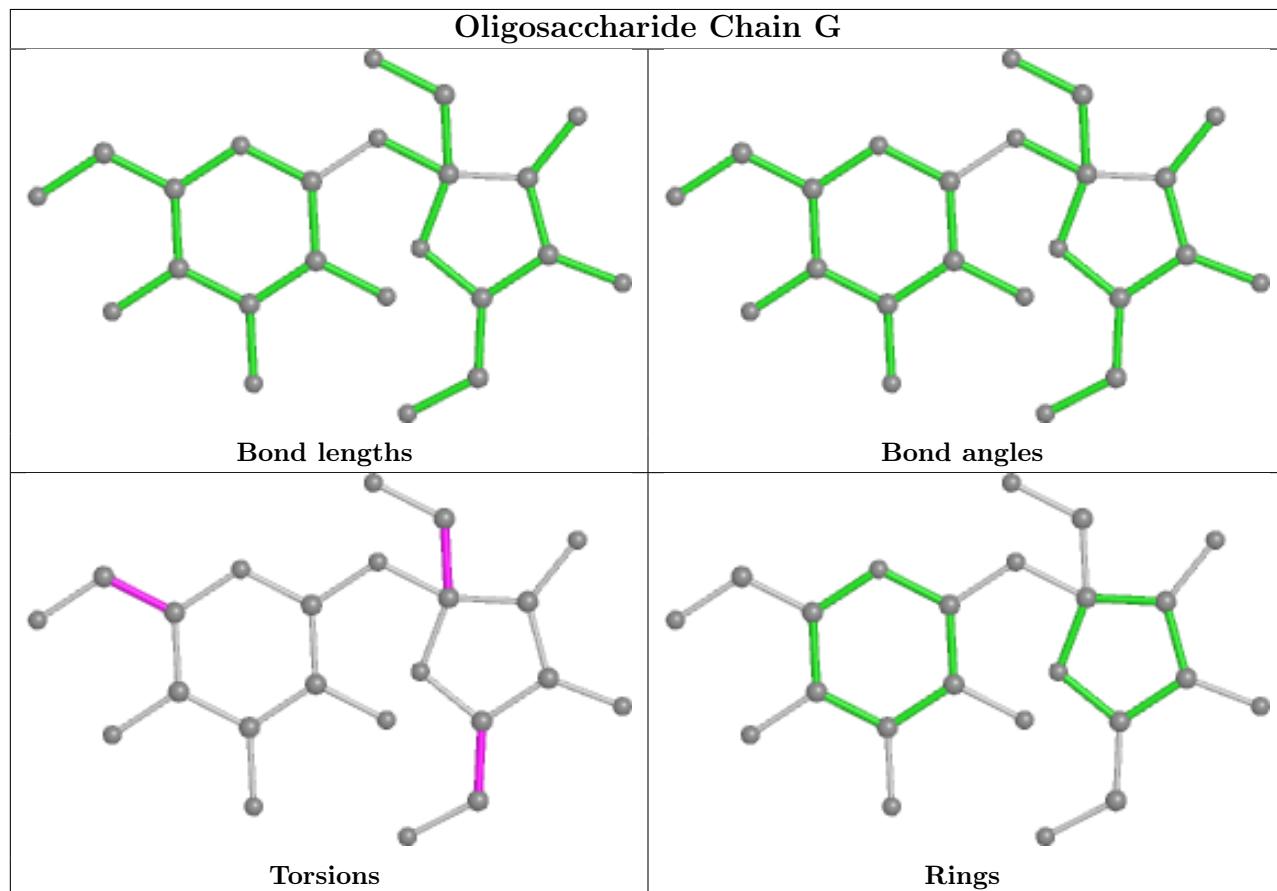
5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
7	GOL	A	603	-	5,5,5	0.37	0	5,5,5	0.28	0
7	GOL	D	502	-	5,5,5	0.38	0	5,5,5	0.31	0
7	GOL	D	501	-	5,5,5	0.36	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	DGT	C	602	5	26,33,33	3.78	13 (50%)	32,52,52	1.40	7 (21%)
6	DGT	A	602	5	26,33,33	3.78	13 (50%)	32,52,52	1.40	6 (18%)
7	GOL	B	501	-	5,5,5	0.38	0	5,5,5	0.33	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
7	GOL	A	603	-	-	2/4/4/4	-
7	GOL	D	502	-	-	0/4/4/4	-
7	GOL	D	501	-	-	2/4/4/4	-
6	DGT	C	602	5	-	5/18/34/34	0/3/3/3
6	DGT	A	602	5	-	4/18/34/34	0/3/3/3
7	GOL	B	501	-	-	2/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	602	DGT	O4'-C1'	8.94	1.62	1.42
6	A	602	DGT	O4'-C1'	8.88	1.62	1.42
6	A	602	DGT	O4'-C4'	-7.60	1.28	1.45
6	C	602	DGT	O4'-C4'	-7.54	1.28	1.45
6	C	602	DGT	C2'-C1'	-6.93	1.33	1.52
6	A	602	DGT	C2'-C1'	-6.92	1.33	1.52
6	C	602	DGT	C2-N3	6.03	1.47	1.33
6	A	602	DGT	C2-N3	5.99	1.47	1.33
6	A	602	DGT	C2-N2	5.60	1.47	1.34
6	C	602	DGT	C2-N2	5.49	1.47	1.34
6	C	602	DGT	C4-N3	5.41	1.50	1.37
6	A	602	DGT	C4-N3	5.41	1.50	1.37
6	C	602	DGT	C6-N1	4.47	1.44	1.37
6	A	602	DGT	C6-N1	4.34	1.44	1.37
6	A	602	DGT	O6-C6	-4.15	1.14	1.23
6	C	602	DGT	O6-C6	-4.14	1.14	1.23
6	C	602	DGT	C5-C6	3.53	1.54	1.47
6	A	602	DGT	C5-C6	3.49	1.54	1.47
6	A	602	DGT	O3'-C3'	-3.08	1.36	1.43
6	C	602	DGT	O3'-C3'	-3.04	1.36	1.43
6	C	602	DGT	C2-N1	2.89	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	DGT	C2-N1	2.83	1.44	1.37
6	C	602	DGT	PA-O5'	2.46	1.69	1.59
6	A	602	DGT	PA-O5'	2.42	1.69	1.59
6	A	602	DGT	C5-C4	-2.28	1.37	1.43
6	C	602	DGT	C5-C4	-2.23	1.37	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	602	DGT	C5-C6-N1	3.51	120.15	113.95
6	C	602	DGT	C5-C6-N1	3.42	119.99	113.95
6	C	602	DGT	C2-N1-C6	-2.94	119.69	125.10
6	A	602	DGT	C2-N1-C6	-2.85	119.84	125.10
6	C	602	DGT	C8-N7-C5	2.72	108.17	102.99
6	A	602	DGT	C8-N7-C5	2.68	108.09	102.99
6	C	602	DGT	PB-O3B-PG	-2.44	124.44	132.83
6	A	602	DGT	PB-O3B-PG	-2.36	124.72	132.83
6	A	602	DGT	C2'-C1'-N9	-2.35	108.84	114.27
6	C	602	DGT	O6-C6-C5	-2.31	119.86	124.37
6	A	602	DGT	O6-C6-C5	-2.29	119.91	124.37
6	C	602	DGT	PA-O3A-PB	-2.06	125.76	132.83
6	C	602	DGT	C2'-C1'-N9	-2.04	109.56	114.27

There are no chirality outliers.

All (15) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
6	C	602	DGT	PB-O3B-PG-O2G
7	A	603	GOL	O1-C1-C2-C3
7	B	501	GOL	O1-C1-C2-C3
7	D	501	GOL	C1-C2-C3-O3
7	D	501	GOL	O2-C2-C3-O3
6	A	602	DGT	PB-O3A-PA-O2A
7	A	603	GOL	O1-C1-C2-O2
7	B	501	GOL	O1-C1-C2-O2
6	C	602	DGT	PA-O3A-PB-O1B
6	A	602	DGT	PB-O3B-PG-O1G
6	A	602	DGT	PA-O3A-PB-O1B
6	A	602	DGT	PB-O3A-PA-O1A
6	C	602	DGT	PA-O3A-PB-O2B
6	C	602	DGT	C5'-O5'-PA-O2A
6	C	602	DGT	PB-O3B-PG-O3G

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	603	GOL	1	0
7	D	501	GOL	1	0
6	C	602	DGT	1	0
6	A	602	DGT	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DGT C 602

Bond lengths

Bond angles

Torsions

Rings

Ligand DGT A 602

Bond lengths

Bond angles

Torsions

Rings
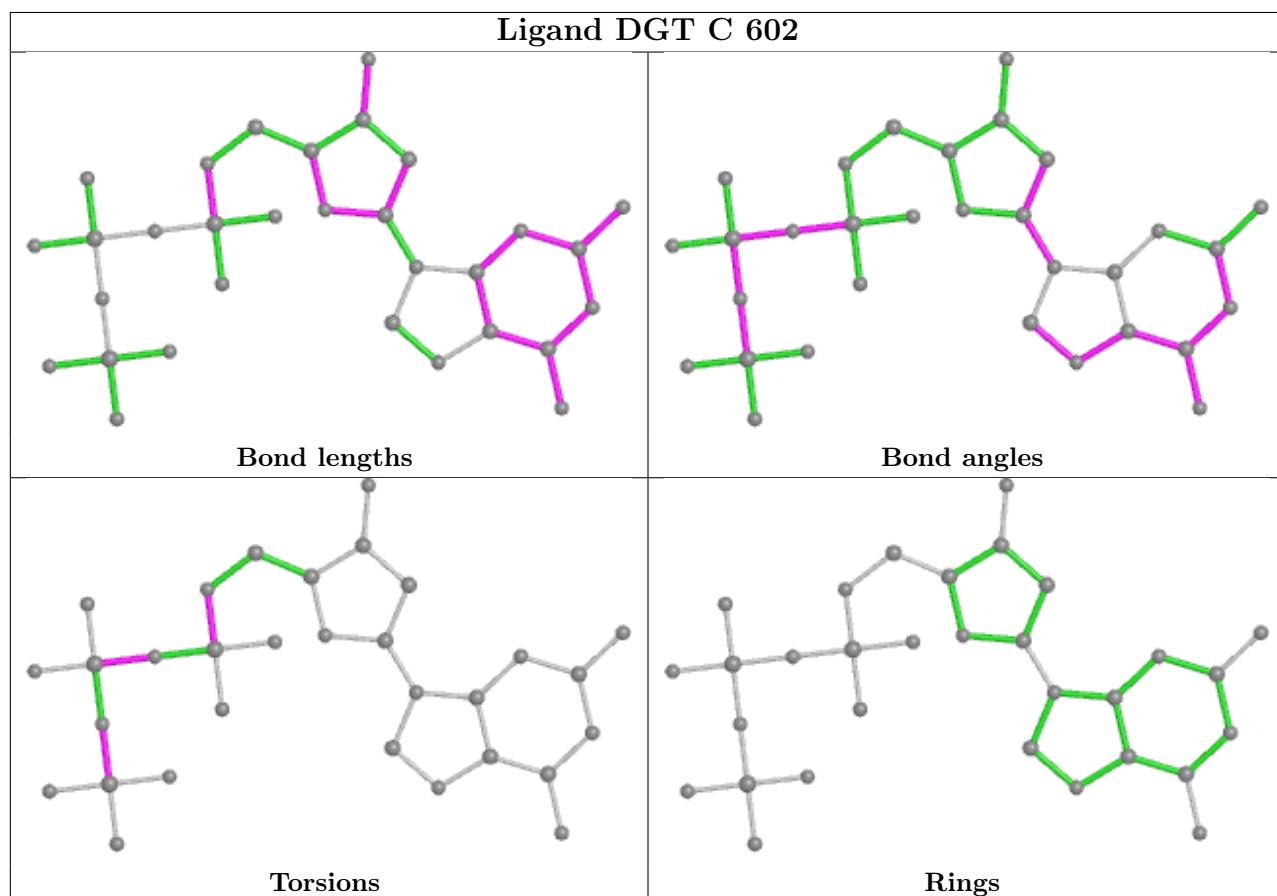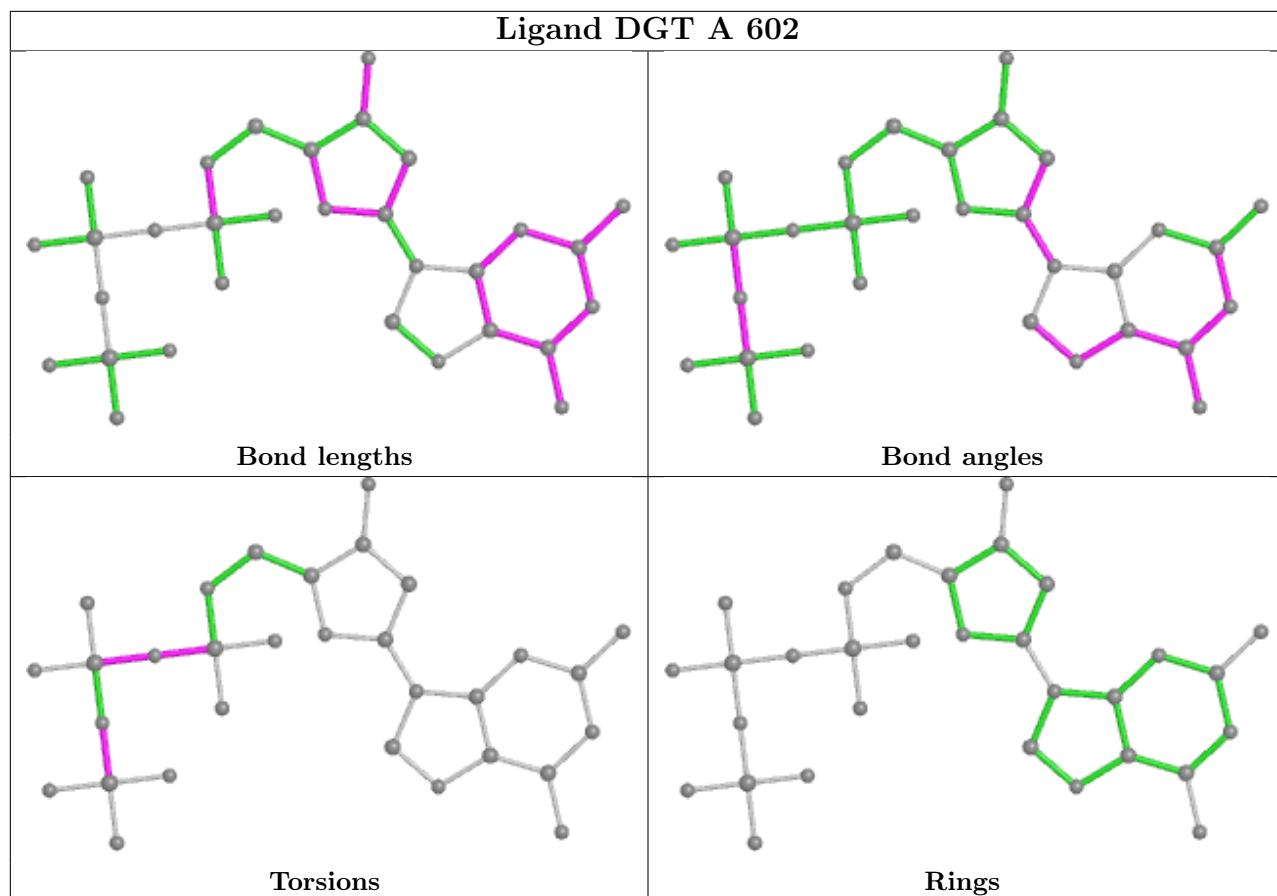
5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	551/557 (98%)	0.52	36 (6%)	18	20	33, 59, 108, 198	0
1	C	551/557 (98%)	0.65	61 (11%)	5	6	37, 63, 114, 178	0
2	B	407/444 (91%)	0.95	62 (15%)	2	2	39, 75, 144, 187	0
2	D	407/444 (91%)	0.49	25 (6%)	21	23	37, 60, 113, 179	0
3	E	33/38 (86%)	0.07	0	100	100	41, 58, 90, 137	0
3	F	36/38 (94%)	0.04	1 (2%)	53	55	43, 68, 128, 161	0
All	All	1985/2078 (95%)	0.62	185 (9%)	8	9	33, 63, 121, 198	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4	PRO	12.5
2	B	88	TRP	10.5
2	D	67	ASP	10.4
2	B	93	GLY	10.1
2	D	231	GLY	10.0
2	B	212	TRP	9.8
1	A	140	PRO	9.5
1	A	34	LEU	9.4
2	B	90	VAL	9.0
2	B	92	LEU	8.7
1	A	69	THR	8.4
2	D	360	ALA	8.3
1	A	137	ASN	7.9
2	D	4	PRO	7.8
2	B	5	ILE	7.7
1	A	134	SER	7.6
2	B	301	LEU	7.5
1	A	139	THR	7.5
1	A	68	SER	7.3

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Mol	Chain	Res	Type	RSRZ
2	B	360	ALA	7.3
1	A	142	ILE	7.2
2	B	357	MET	6.9
2	B	94	ILE	6.8
1	C	141	GLY	6.7
2	D	5	ILE	6.6
1	C	142	ILE	6.5
2	B	359	GLY	6.4
1	C	138	GLU	6.4
1	C	132	ILE	6.3
2	B	91	GLN	6.1
1	A	35	VAL	6.0
2	B	231	GLY	6.0
1	C	133	PRO	6.0
2	B	361	HIS	5.9
1	C	34	LEU	5.9
1	C	140	PRO	5.9
2	B	95	PRO	5.9
1	C	50	ILE	5.7
2	D	232	TYR	5.5
2	B	281	LYS	5.5
1	C	469	LEU	5.5
1	A	32	LYS	5.3
2	B	232	TYR	5.3
1	A	136	ASN	5.3
1	C	68	SER	5.3
1	C	452	LEU	5.2
1	A	138	GLU	5.1
1	C	62	ALA	5.1
1	C	139	THR	5.0
1	C	28	GLU	5.0
1	C	52	PRO	4.9
1	C	135	ILE	4.9
1	A	67	ASP	4.9
1	A	141	GLY	4.8
1	A	135	ILE	4.8
1	C	553	SER	4.7
1	C	137	ASN	4.7
1	A	27	THR	4.6
2	D	66	LYS	4.6
1	C	67	ASP	4.5
1	C	69	THR	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	209	LEU	4.4
2	D	212	TRP	4.4
2	B	89	GLU	4.4
1	A	24	TRP	4.2
1	C	457	TYR	4.2
2	B	67	ASP	4.2
2	B	168	LEU	4.0
1	A	26	LEU	4.0
1	C	552	VAL	4.0
1	A	131	THR	4.0
1	A	132	ILE	3.9
1	C	71	TRP	3.9
2	B	295	LEU	3.9
1	C	550	LYS	3.8
1	C	551	LEU	3.8
2	B	297	GLU	3.8
2	D	361	HIS	3.8
1	C	54	ASN	3.7
2	B	296	THR	3.7
1	C	35	VAL	3.7
2	D	425	LEU	3.7
1	C	39	THR	3.6
2	B	250	ASP	3.6
1	A	36	GLU	3.6
1	A	62	ALA	3.6
2	B	66	LYS	3.6
2	B	245	VAL	3.6
2	B	248	GLU	3.5
2	B	7	THR	3.5
1	C	144	TYR	3.5
1	A	25	PRO	3.4
2	D	69	THR	3.4
1	A	29	GLU	3.4
2	B	279	LEU	3.4
1	C	70	LYS	3.3
2	B	423	VAL	3.3
2	B	427	TYR	3.3
2	D	209	LEU	3.3
2	B	213	GLY	3.3
1	C	450	THR	3.3
2	B	362	THR	3.3
1	A	133	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	32	LYS	3.3
2	B	252	TRP	3.2
1	A	31	ILE	3.2
1	C	64	LYS	3.2
2	D	68	SER	3.2
1	A	66	LYS	3.2
1	C	136	ASN	3.1
1	C	37	ILE	3.1
2	D	357	MET	3.1
2	B	238	LYS	3.1
1	A	64	LYS	3.1
2	D	356	ARG	3.1
1	C	63	ILE	3.1
1	A	33	ALA	3.1
2	B	251	SER	3.0
1	C	31	ILE	3.0
2	D	424	LYS	3.0
1	C	49	LYS	3.0
1	C	24	TRP	3.0
2	B	166	LYS	3.0
1	C	36	GLU	2.9
1	A	22	LYS	2.9
1	C	449	GLU	2.9
1	C	26	LEU	2.9
1	A	550	LYS	2.9
2	B	277	ARG	2.9
2	B	358	LYS	2.9
2	D	283	LEU	2.8
1	C	448	ARG	2.8
2	B	172	ARG	2.8
2	B	299	ALA	2.7
1	C	451	LYS	2.7
2	B	6	GLU	2.7
2	D	358	LYS	2.7
1	A	37	ILE	2.7
2	B	211	ARG	2.7
1	A	61	PHE	2.7
2	B	305	GLU	2.7
2	B	303	LEU	2.7
1	C	467	VAL	2.6
1	A	551	LEU	2.6
1	C	104	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	211	ARG	2.6
2	B	249	LYS	2.6
1	C	131	THR	2.5
2	B	422	LEU	2.5
2	B	68	SER	2.5
1	C	27	THR	2.5
2	B	278	GLN	2.5
1	A	21	VAL	2.5
2	D	315	HIS	2.5
1	C	33	ALA	2.4
2	B	104	LYS	2.4
1	C	51	GLY	2.4
1	C	38	CYS	2.4
3	F	18	DT	2.4
2	B	260	LEU	2.4
1	C	134	SER	2.4
2	B	274	ILE	2.4
2	D	421	PRO	2.4
2	D	174	GLN	2.4
1	C	56	TYR	2.3
1	C	143	ARG	2.3
1	C	25	PRO	2.3
2	D	172	ARG	2.3
2	B	425	LEU	2.3
1	C	470	THR	2.3
1	C	55	PRO	2.2
2	B	11	LYS	2.2
2	D	210	LEU	2.2
1	C	195	ILE	2.2
1	A	63	ILE	2.2
2	B	64	LYS	2.2
1	C	30	LYS	2.2
1	C	59	PRO	2.2
2	B	284	ARG	2.1
1	C	60	VAL	2.1
2	D	266	TRP	2.1
2	B	87	PHE	2.1
2	B	177	ASP	2.1
2	B	116	PHE	2.0
2	B	161	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	OMC	E	2	21/22	0.96	0.20	36,42,49,52	0
3	OMC	F	2	21/22	0.96	0.17	51,56,64,68	0
3	OMC	F	4	21/22	0.97	0.20	38,46,51,52	0
3	OMC	E	4	21/22	0.98	0.21	34,42,46,47	0

6.3   Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FRU	G	2	12/12	0.54	0.39	103,121,123,124	0
4	GLC	G	1	11/12	0.78	0.23	55,78,89,100	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.
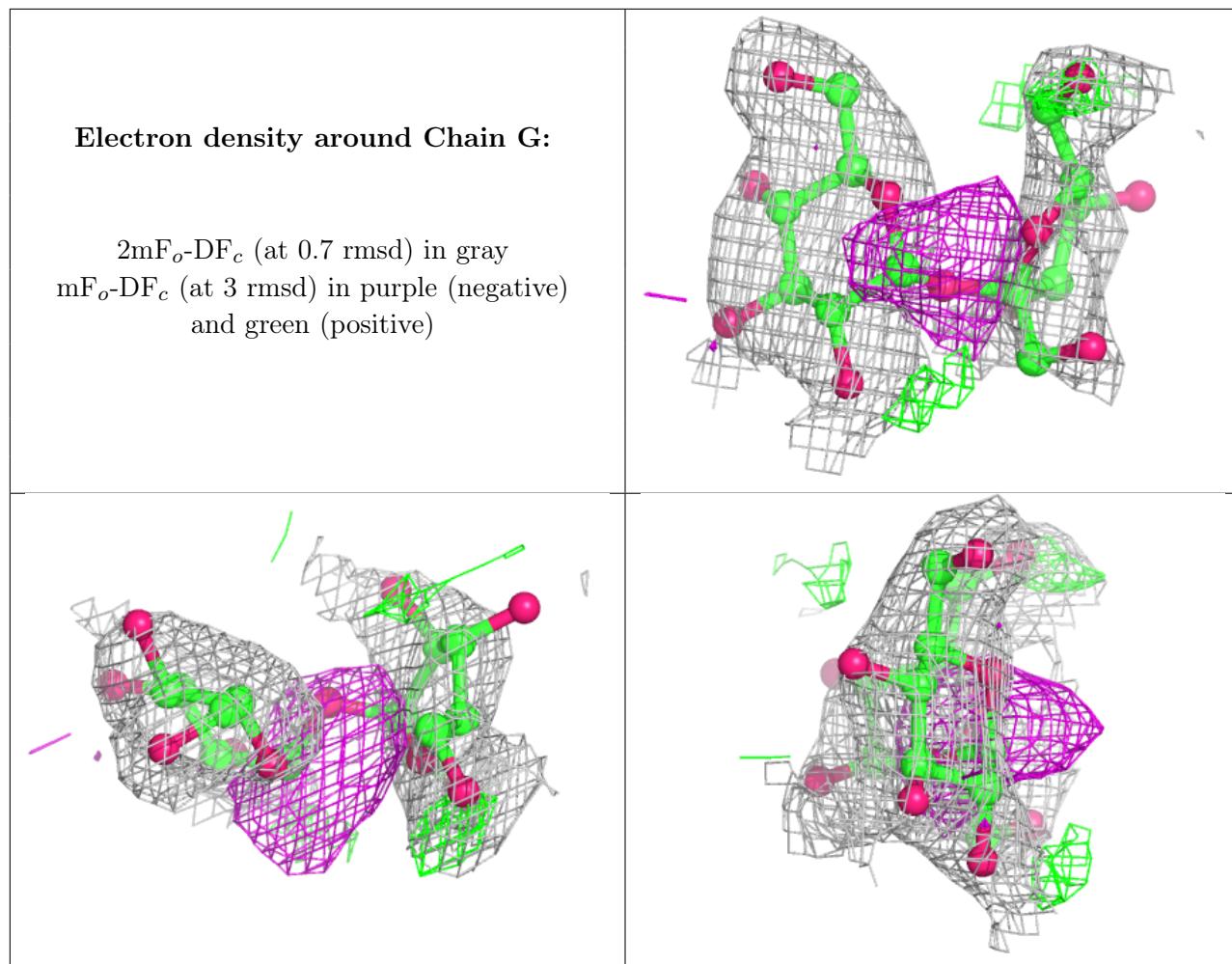
Electron density around Chain G:

$2mF_o$-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, 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
5	MG	C	601	1/1	0.80	0.11	60,60,60,60	0
7	GOL	A	603	6/6	0.89	0.21	61,66,70,73	0
7	GOL	D	502	6/6	0.90	0.23	56,65,69,70	0
5	MG	A	601	1/1	0.91	0.12	59,59,59,59	0
6	DGT	A	602	31/31	0.91	0.17	53,65,80,85	0
6	DGT	C	602	31/31	0.92	0.14	61,74,92,97	0
7	GOL	B	501	6/6	0.93	0.25	53,59,60,63	0
7	GOL	D	501	6/6	0.94	0.20	47,58,59,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DGT A 602:

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

Electron density around DGT C 602:

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

6.5 Other polymers (i)

There are no such residues in this entry.