



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:56 AM BST

PDB ID : 5HRO  
Title : STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE In COMPLEX  
WITH A DNA aptamer and an Alpha-carboxy nucleoside phosphonate in-  
hibitor (alpha-CNP)  
Authors : Das, K.; Arnold, E.  
Deposited on : 2016-01-23  
Resolution : 2.75 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

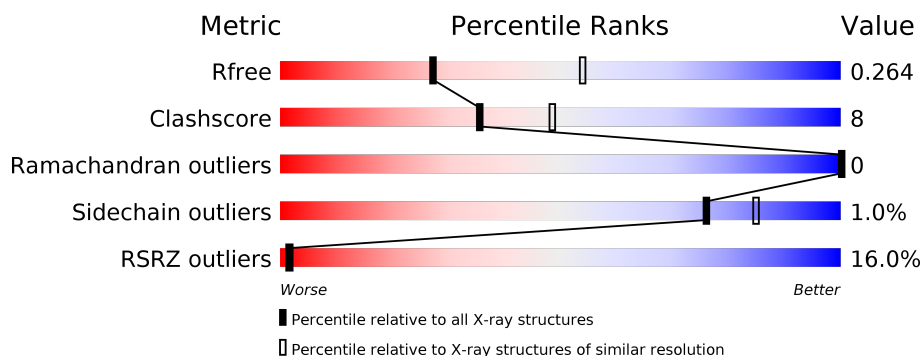
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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.




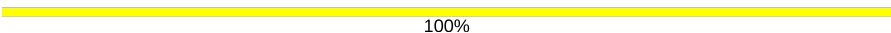
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	555	<div> <div>17%</div> <div> <div>76%</div> <div>23%</div> <div>.</div> </div> </div>
1	C	555	<div> <div>24%</div> <div> <div>75%</div> <div>24%</div> <div>..</div> </div> </div>
2	B	444	<div> <div>7%</div> <div> <div>78%</div> <div>14%</div> <div>7%</div> </div> </div>
2	D	444	<div> <div>12%</div> <div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
3	E	38	<div> <div>58%</div> <div>32%</div> <div>.</div> <div>8%</div> </div>
3	F	38	<div> <div>5%</div> <div> <div>55%</div> <div>29%</div> <div>8%</div> <div>8%</div> </div> </div>

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

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17349 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 HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4488	2905	747	829	7			
1	C	551	Total	C	N	O	S	0	0	0
			4488	2905	747	829	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P03366
B	-14	ALA	-	expression tag	UNP P03366
B	-13	HIS	-	expression tag	UNP P03366
B	-12	HIS	-	expression tag	UNP P03366
B	-11	HIS	-	expression tag	UNP P03366
B	-10	HIS	-	expression tag	UNP P03366
B	-9	HIS	-	expression tag	UNP P03366
B	-8	HIS	-	expression tag	UNP P03366
B	-7	ALA	-	expression tag	UNP P03366
B	-6	LEU	-	expression tag	UNP P03366

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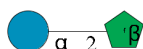
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	GLU	-	expression tag	UNP P03366
B	-4	VAL	-	expression tag	UNP P03366
B	-3	LEU	-	expression tag	UNP P03366
B	-2	PHE	-	expression tag	UNP P03366
B	-1	GLN	-	expression tag	UNP P03366
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	-15	MET	-	initiating methionine	UNP P03366
D	-14	ALA	-	expression tag	UNP P03366
D	-13	HIS	-	expression tag	UNP P03366
D	-12	HIS	-	expression tag	UNP P03366
D	-11	HIS	-	expression tag	UNP P03366
D	-10	HIS	-	expression tag	UNP P03366
D	-9	HIS	-	expression tag	UNP P03366
D	-8	HIS	-	expression tag	UNP P03366
D	-7	ALA	-	expression tag	UNP P03366
D	-6	LEU	-	expression tag	UNP P03366
D	-5	GLU	-	expression tag	UNP P03366
D	-4	VAL	-	expression tag	UNP P03366
D	-3	LEU	-	expression tag	UNP P03366
D	-2	PHE	-	expression tag	UNP P03366
D	-1	GLN	-	expression tag	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			
3	F	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			

- 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	C	O	0	0	0
			23	12	11			

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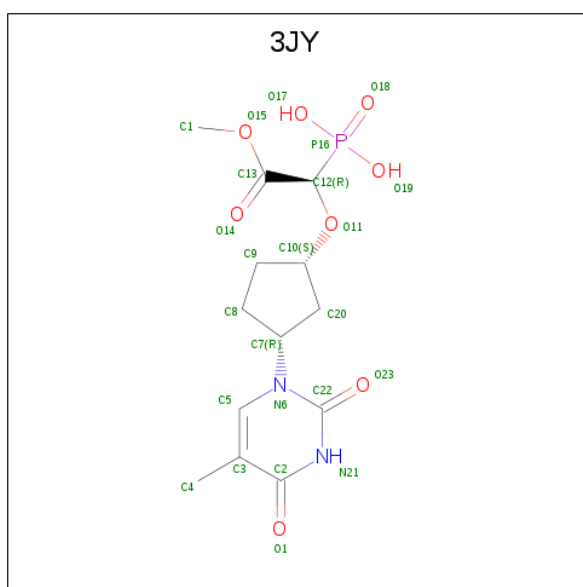
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	H	2	Total	C	O	0	0	0
			23	12	11			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Mg	0	0
			3	3		
5	C	3	Total	Mg	0	0
			3	3		

- Molecule 6 is [(1R)-2-methoxy-1-{[(1S,3R)-3-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)cyclopentyl]oxy}-2-oxoethyl]phosphonic acid (three-letter code: 3JY) (formula: C<sub>13</sub>H<sub>19</sub>N<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			23	12	2	8	1		
6	C	1	Total	C	N	O	P	0	0
			23	12	2	8	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

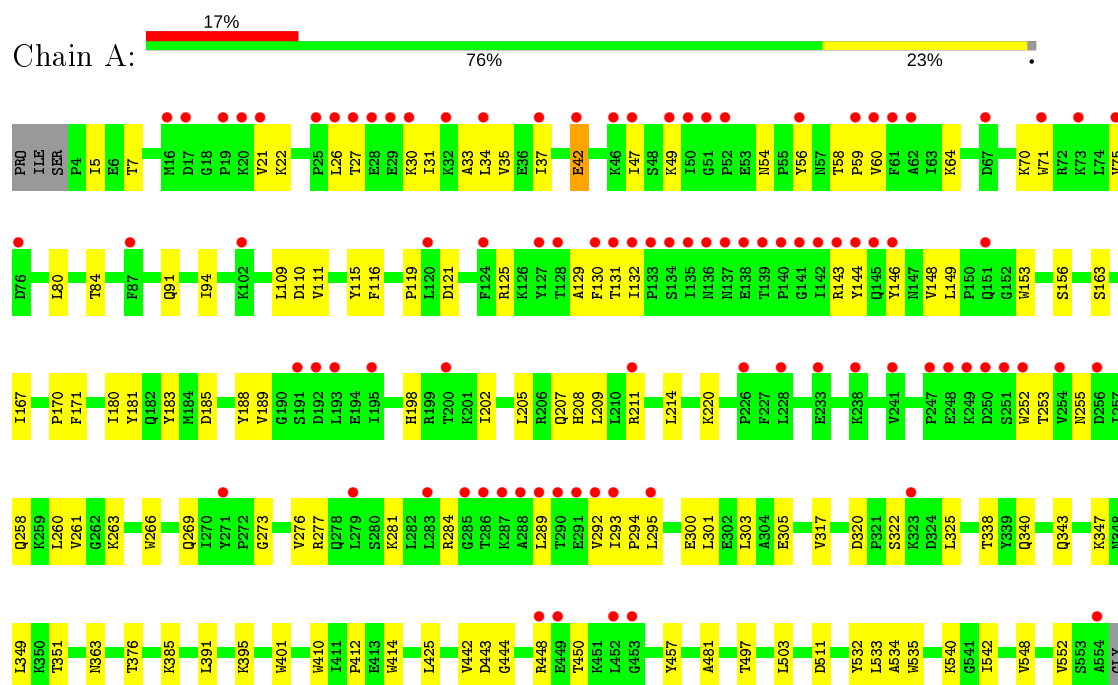
- Molecule 8 is water.

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

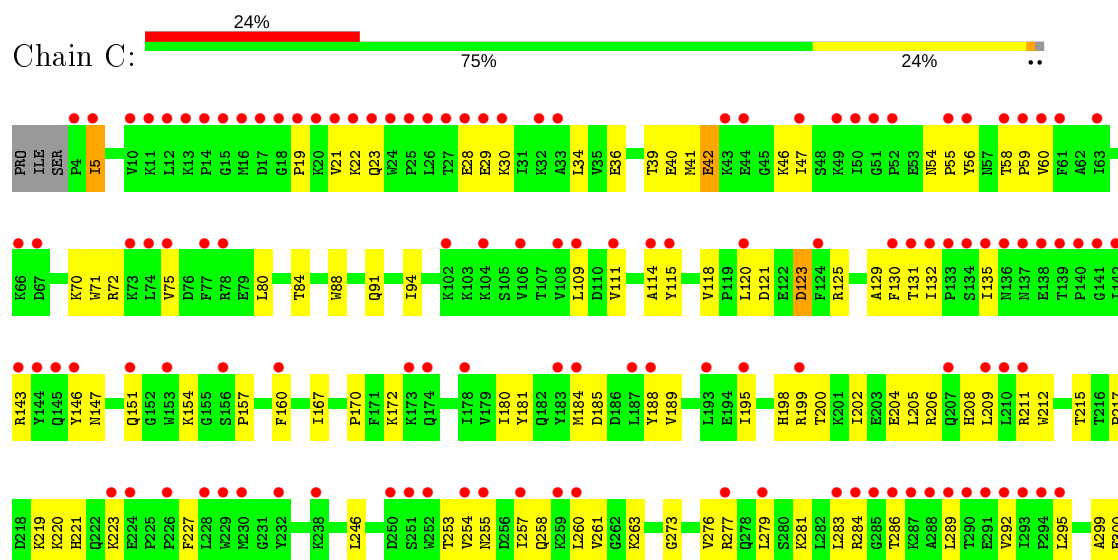
### 3 Residue-property plots

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.

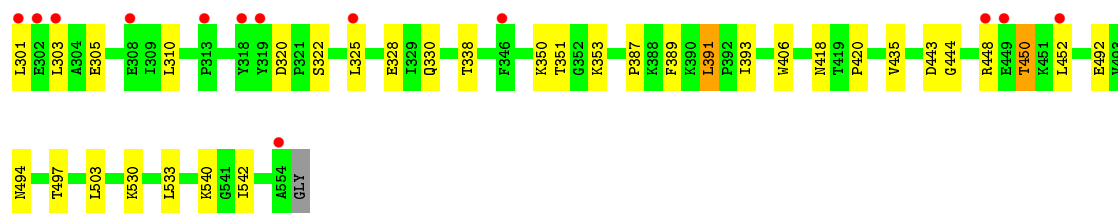
#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT



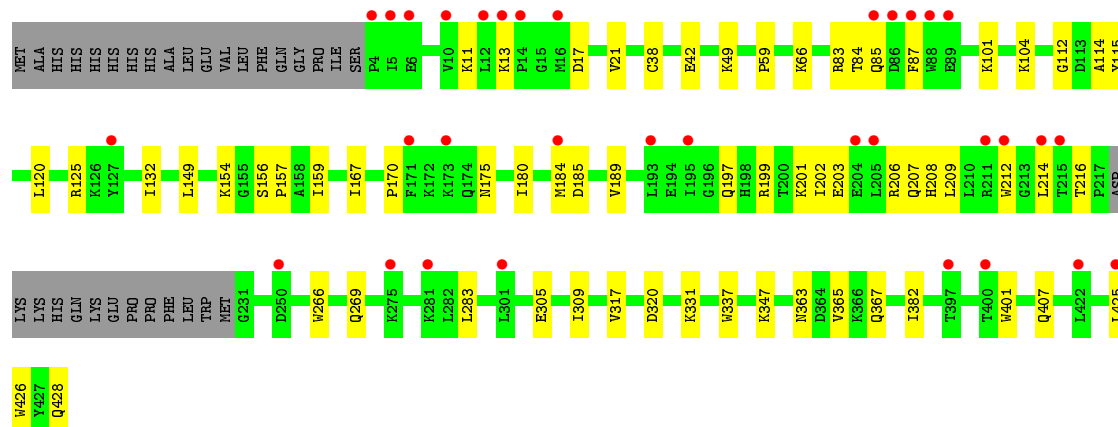
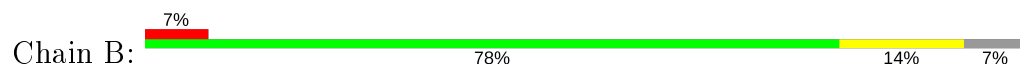
#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT



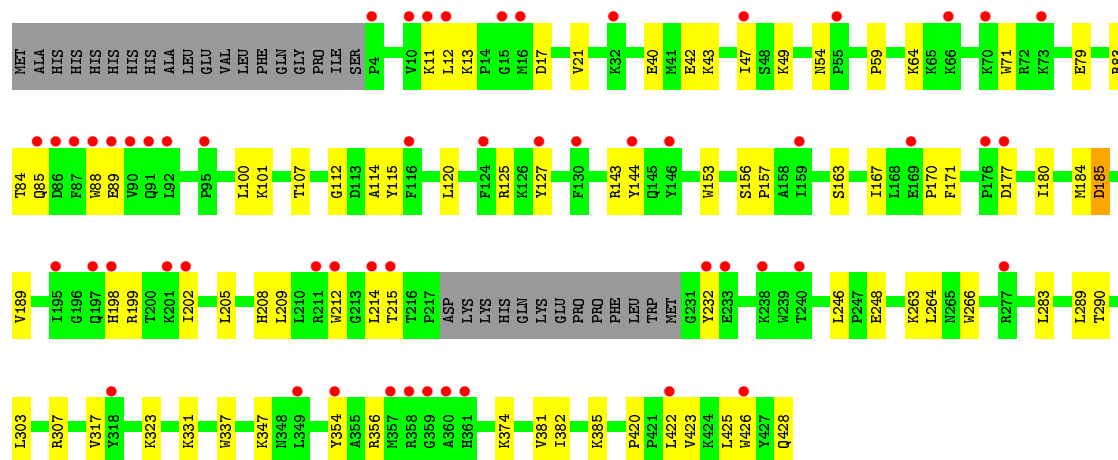
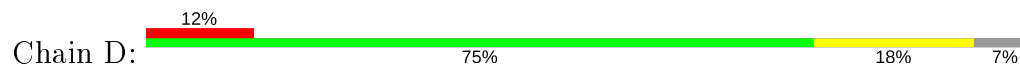




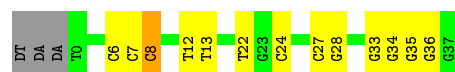
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



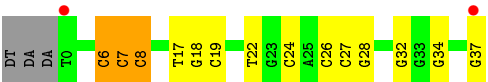
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 3: DNA (38-MER)



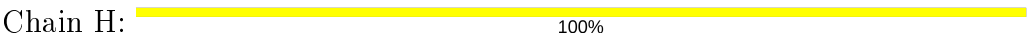
• Molecule 3: DNA (38-MER)



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.25Å 128.96Å 131.05Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	38.52 – 2.75 38.52 – 2.73	Depositor EDS
% Data completeness (in resolution range)	95.8 (38.52-2.75) 94.7 (38.52-2.73)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.72Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.235 , 0.265 0.235 , 0.264	Depositor DCC
$R_{free}$ test set	2960 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.1	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17349	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: OMC, MG, 3JY, GLC, SO4, FRU

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	0.28	0/4605	0.49	0/6255
1	C	0.28	0/4605	0.49	1/6255 (0.0%)
2	B	0.27	0/3497	0.47	0/4751
2	D	0.29	0/3497	0.49	0/4751
3	E	0.64	1/759 (0.1%)	1.01	0/1170
3	F	0.72	3/759 (0.4%)	1.01	2/1170 (0.2%)
All	All	0.33	4/17722 (0.0%)	0.56	3/24352 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	26	DC	C4'-O4'	7.28	1.52	1.45
3	F	19	DC	C4'-O4'	5.75	1.50	1.45
3	E	24	DC	C4'-O4'	5.24	1.50	1.45
3	F	24	DC	C4'-O4'	5.10	1.50	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	DC	O4'-C4'-C3'	-6.52	101.89	104.50
3	F	19	DC	O4'-C4'-C3'	-6.06	102.08	104.50
1	C	55	PRO	N-CA-C	5.21	125.65	112.10

There are no chirality outliers.

There are no planarity outliers.

## 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	4545	86	0
1	C	4488	0	4545	95	0
2	B	3400	0	3431	41	0
2	D	3400	0	3430	54	0
3	E	720	0	396	13	0
3	F	720	0	396	12	0
4	G	23	0	21	0	0
4	H	23	0	21	0	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0
6	A	23	0	14	0	0
6	C	23	0	14	4	0
7	A	5	0	0	0	0
7	B	20	0	0	0	0
7	C	5	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	3	0	0	0	0
All	All	17349	0	16813	277	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 8.

All (277) 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:255:ASN:HB2	1:A:289:LEU:HD21	1.27	1.09
1:A:255:ASN:HB2	1:A:289:LEU:CD2	1.98	0.92
1:C:221:HIS:HE1	1:C:223:LYS:HG3	1.39	0.88
1:A:255:ASN:CB	1:A:289:LEU:HD21	2.11	0.80
1:C:255:ASN:HB2	1:C:289:LEU:CD2	2.10	0.80
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.15	0.80
1:C:56:TYR:HB2	1:C:129:ALA:HB3	1.65	0.78
1:C:221:HIS:CE1	1:C:223:LYS:HG3	2.20	0.76
1:A:110:ASP:HB3	1:A:220:LYS:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ASN:HB2	1:C:289:LEU:HD21	1.71	0.71
6:C:605:3JY:H11	6:C:605:3JY:H6	1.73	0.70
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.72	0.70
1:C:172:LYS:HE2	1:C:180:ILE:HB	1.75	0.69
1:A:56:TYR:HB2	1:A:129:ALA:HB3	1.74	0.69
2:D:115:TYR:CD2	2:D:156:SER:HB3	2.28	0.69
1:C:72:ARG:NH1	6:C:605:3JY:O19	2.26	0.68
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.75	0.67
1:A:207:GLN:O	1:A:211:ARG:N	2.26	0.67
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.76	0.66
2:D:180:ILE:HG12	2:D:189:VAL:HG22	1.78	0.66
1:A:255:ASN:HD22	1:A:289:LEU:HD11	1.62	0.63
1:A:183:TYR:OH	3:E:36:DG:N3	2.29	0.63
1:C:60:VAL:HG22	1:C:75:VAL:HG13	1.79	0.63
1:C:41:MET:HB3	1:C:46:LYS:HB2	1.81	0.62
1:C:19:PRO:HB2	1:C:58:THR:HG23	1.79	0.62
1:A:94:ILE:HD11	3:E:35:DG:H21	1.65	0.62
3:E:27:DC:H2"	3:E:28:DG:C8	2.35	0.61
1:C:5:ILE:HG22	1:C:212:TRP:HD1	1.64	0.61
2:B:13:LYS:HD2	2:B:85:GLN:HB3	1.83	0.61
2:B:206:ARG:NH2	2:B:216:THR:O	2.33	0.61
1:A:64:LYS:HA	1:A:71:TRP:HA	1.83	0.61
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.82	0.60
1:A:448:ARG:HH21	3:E:22:DT:H5"	1.65	0.60
2:D:199:ARG:HA	2:D:202:ILE:HD12	1.84	0.60
1:C:184:MET:HG2	3:F:37:DG:H2"	1.83	0.59
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.84	0.59
1:A:253:THR:HA	1:A:292:VAL:HA	1.85	0.59
1:C:118:VAL:HG21	1:C:160:PHE:HD1	1.68	0.59
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.84	0.59
2:D:266:TRP:NE1	2:D:425:LEU:HD22	2.17	0.59
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.37	0.58
1:C:257:ILE:HB	1:C:283:LEU:HD21	1.85	0.58
2:B:157:PRO:HG3	2:B:184:MET:HA	1.85	0.58
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.38	0.58
1:A:70:LYS:HG2	1:A:71:TRP:H	1.69	0.58
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.86	0.57
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.87	0.57
1:C:180:ILE:HG23	1:C:189:VAL:HG22	1.87	0.57
1:C:125:ARG:HE	1:C:147:ASN:HA	1.68	0.57
2:B:170:PRO:HB2	2:B:208:HIS:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ILE:O	1:C:206:ARG:HG3	2.06	0.56
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.87	0.56
2:D:114:ALA:HB2	2:D:214:LEU:HD22	1.88	0.56
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.87	0.56
1:C:23:GLN:NE2	1:C:131:THR:O	2.38	0.56
1:C:219:LYS:HE2	1:C:220:LYS:HE2	1.88	0.56
1:C:5:ILE:HG22	1:C:212:TRP:CD1	2.40	0.55
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.87	0.55
1:C:23:GLN:HG3	1:C:131:THR:HG23	1.89	0.55
2:D:198:HIS:CD2	2:D:202:ILE:HD11	2.42	0.55
1:C:279:LEU:HD23	1:C:299:ALA:HB1	1.88	0.55
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.89	0.54
1:A:34:LEU:HD21	1:A:132:ILE:HD12	1.88	0.54
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.88	0.54
1:C:123:ASP:N	1:C:123:ASP:OD1	2.40	0.54
3:E:12:DT:H2'	3:E:13:DT:H71	1.89	0.54
1:A:395:LYS:NZ	1:A:414:TRP:O	2.40	0.54
2:B:363:ASN:O	2:B:367:GLN:HG3	2.08	0.54
2:B:17:ASP:O	2:B:83:ARG:NH1	2.40	0.54
1:C:253:THR:HA	1:C:292:VAL:HA	1.90	0.54
1:A:252:TRP:O	1:A:292:VAL:HG23	2.09	0.53
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.91	0.53
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.43	0.53
1:C:72:ARG:NH2	6:C:605:3JY:O19	2.42	0.53
1:C:255:ASN:HB2	1:C:289:LEU:HD23	1.89	0.53
1:C:258:GLN:CD	3:F:32:DG:H2''	2.28	0.53
1:A:281:LYS:O	1:A:284:ARG:HG2	2.07	0.53
1:C:281:LYS:O	1:C:284:ARG:HG2	2.09	0.53
2:B:87:PHE:HZ	2:B:159:ILE:HG13	1.73	0.53
1:C:60:VAL:HG21	1:C:130:PHE:CD2	2.44	0.53
1:A:180:ILE:HG23	1:A:189:VAL:HG22	1.89	0.53
1:C:255:ASN:CB	1:C:289:LEU:HD21	2.38	0.53
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.74	0.52
1:C:202:ILE:HG22	1:C:206:ARG:HD2	1.90	0.52
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.44	0.52
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.45	0.52
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.91	0.52
1:C:448:ARG:HH21	3:F:22:DT:H5''	1.73	0.52
1:A:94:ILE:HD11	3:E:35:DG:N2	2.25	0.52
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.90	0.52
2:B:203:GLU:O	2:B:207:GLN:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ILE:HD12	3:F:8:OMC:HM23	1.91	0.51
2:D:263:LYS:HA	2:D:423:VAL:HG21	1.92	0.51
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.93	0.51
1:A:27:THR:O	1:A:31:ILE:HG13	2.10	0.51
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.93	0.51
2:D:115:TYR:HD2	2:D:156:SER:HB3	1.75	0.51
2:D:266:TRP:CD1	2:D:425:LEU:HD13	2.46	0.51
2:D:13:LYS:HD2	2:D:85:GLN:HB3	1.93	0.51
1:A:47:ILE:HG13	1:A:144:TYR:HB3	1.94	0.50
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.93	0.50
1:A:503:LEU:HD11	1:A:533:LEU:HB3	1.92	0.50
2:B:197:GLN:O	2:B:201:LYS:HG2	2.12	0.50
2:D:84:THR:HG21	2:D:153:TRP:HZ2	1.77	0.50
2:D:425:LEU:HD23	2:D:426:TRP:CE2	2.47	0.50
3:E:7:DC:H2'	3:E:8:OMC:C6	2.47	0.50
3:E:7:DC:H2'	3:E:8:OMC:H6	1.77	0.49
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.94	0.49
2:B:209:LEU:HD13	2:B:214:LEU:HD23	1.94	0.49
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.47	0.49
2:D:209:LEU:HD13	2:D:214:LEU:HD23	1.94	0.49
1:A:293:ILE:HG13	1:A:294:PRO:HD2	1.95	0.49
1:C:260:LEU:HD21	1:C:303:LEU:HD13	1.94	0.49
1:A:47:ILE:HD12	1:A:146:TYR:HA	1.95	0.49
2:B:320:ASP:OD2	1:C:418:ASN:ND2	2.39	0.49
2:D:42:GLU:OE2	2:D:49:LYS:HG3	2.12	0.49
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.48
1:C:28:GLU:HB2	1:C:135:ILE:HD12	1.95	0.48
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.94	0.48
1:A:443:ASP:OD1	1:A:444:GLY:N	2.46	0.48
2:D:177:ASP:N	2:D:177:ASP:OD1	2.37	0.48
2:D:356:ARG:HG3	2:D:356:ARG:O	2.13	0.48
1:A:548:VAL:O	1:A:552:VAL:HG22	2.14	0.48
3:F:17:DT:H4'	3:F:18:DG:OP1	2.14	0.48
1:C:542:ILE:HG23	2:D:283:LEU:HD13	1.94	0.48
1:C:205:LEU:O	1:C:209:LEU:HG	2.14	0.48
2:D:167:ILE:HG23	2:D:212:TRP:CD1	2.49	0.48
1:A:110:ASP:HB3	1:A:220:LYS:CB	2.43	0.47
1:C:70:LYS:HG2	1:C:71:TRP:H	1.79	0.47
1:A:301:LEU:O	1:A:305:GLU:HG2	2.14	0.47
1:A:5:ILE:HD11	1:A:163:SER:HB3	1.96	0.47
2:B:317:VAL:HG12	2:B:347:LYS:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ASN:ND2	1:C:289:LEU:HD21	2.29	0.47
2:D:17:ASP:O	2:D:83:ARG:HD3	2.14	0.47
1:A:30:LYS:HG2	1:A:71:TRP:CZ3	2.50	0.47
1:C:254:VAL:HG13	1:C:283:LEU:HD22	1.94	0.47
1:C:391:LEU:HB3	1:C:393:ILE:HG22	1.97	0.47
2:D:428:GLN:HA	2:D:428:GLN:HE21	1.80	0.47
1:C:389:PHE:HB3	1:C:391:LEU:HD13	1.97	0.47
1:C:540:LYS:HA	1:C:540:LYS:HD3	1.68	0.47
2:D:100:LEU:HG	2:D:381:VAL:HG13	1.96	0.47
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.97	0.47
1:C:494:ASN:HB3	2:D:289:LEU:HD12	1.96	0.47
2:D:163:SER:O	2:D:167:ILE:HG13	2.15	0.47
1:A:167:ILE:O	1:A:170:PRO:HD2	2.14	0.47
1:C:263:LYS:HD2	3:F:34:DG:H4'	1.97	0.47
1:A:266:TRP:O	1:A:269:GLN:HG2	2.15	0.47
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.50	0.47
6:C:605:3JY:H3	6:C:605:3JY:H6	1.58	0.47
1:C:120:LEU:HD12	1:C:121:ASP:H	1.80	0.46
2:D:266:TRP:CD1	2:D:266:TRP:C	2.89	0.46
2:D:112:GLY:HA2	2:D:115:TYR:CD1	2.51	0.46
2:D:79:GLU:HG3	2:D:83:ARG:HE	1.80	0.46
3:F:17:DT:H2''	3:F:18:DG:C8	2.50	0.46
1:A:263:LYS:HD2	3:E:34:DG:H4'	1.97	0.46
1:A:31:ILE:O	1:A:35:VAL:HG23	2.14	0.46
2:B:115:TYR:O	2:B:149:LEU:HB2	2.16	0.46
1:A:121:ASP:O	1:A:125:ARG:HG3	2.15	0.46
2:B:66:LYS:NZ	2:B:407:GLN:OE1	2.39	0.46
1:C:125:ARG:NE	1:C:147:ASN:HA	2.30	0.46
1:C:131:THR:HB	1:C:143:ARG:HG2	1.98	0.46
1:C:29:GLU:HG3	1:C:30:LYS:N	2.31	0.46
1:C:167:ILE:O	1:C:170:PRO:HD2	2.16	0.46
1:C:200:THR:O	1:C:204:GLU:HG3	2.16	0.46
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.51	0.46
1:C:198:HIS:O	1:C:202:ILE:HG12	2.16	0.46
2:B:428:GLN:HA	2:B:428:GLN:HE21	1.80	0.45
1:C:34:LEU:HD21	1:C:132:ILE:HD12	1.98	0.45
2:D:12:LEU:HD11	2:D:127:TYR:CE1	2.50	0.45
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.98	0.45
1:A:7:THR:OG1	1:A:121:ASP:HA	2.16	0.45
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.56	0.45
1:C:273:GLY:HA2	1:C:338:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:O	1:A:143:ARG:NH2	2.49	0.45
2:B:154:LYS:HG2	2:B:184:MET:SD	2.57	0.45
1:A:5:ILE:HD12	1:A:167:ILE:HD11	1.99	0.45
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.98	0.45
1:C:211:ARG:HB2	1:C:212:TRP:CE3	2.52	0.45
1:C:184:MET:HE3	1:C:184:MET:HA	1.97	0.45
1:C:227:PHE:N	1:C:227:PHE:CD2	2.84	0.45
2:D:171:PHE:CD2	2:D:205:LEU:HD13	2.51	0.45
1:C:80:LEU:O	1:C:84:THR:OG1	2.33	0.45
1:A:116:PHE:O	1:A:148:VAL:HG11	2.17	0.45
1:A:295:LEU:HB3	1:A:300:GLU:HG2	1.99	0.45
2:D:40:GLU:HA	2:D:43:LYS:HG2	1.98	0.45
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.52	0.44
1:C:246:LEU:HD11	1:C:310:LEU:HD22	1.99	0.44
1:C:320:ASP:OD1	1:C:322:SER:OG	2.29	0.44
1:A:153:TRP:HB3	1:A:156:SER:OG	2.17	0.44
2:D:88:TRP:CE3	2:D:89:GLU:HG3	2.52	0.44
1:C:54:ASN:O	1:C:143:ARG:NH2	2.50	0.44
2:B:112:GLY:HA2	2:B:115:TYR:CD1	2.53	0.44
1:C:338:THR:HG22	1:C:353:LYS:HB3	2.00	0.44
2:D:303:LEU:HG	2:D:307:ARG:NH1	2.33	0.44
2:D:331:LYS:HB2	2:D:337:TRP:CZ3	2.53	0.44
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.53	0.44
1:C:258:GLN:NE2	3:F:32:DG:H2''	2.33	0.44
1:C:36:GLU:O	1:C:40:GLU:HG3	2.18	0.44
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.53	0.44
2:B:425:LEU:HD23	2:B:426:TRP:CE2	2.52	0.43
1:C:21:VAL:HG23	1:C:59:PRO:HD3	2.00	0.43
2:D:317:VAL:HG12	2:D:347:LYS:HB3	1.98	0.43
1:A:325:LEU:HD12	1:A:385:LYS:HG3	2.00	0.43
2:B:101:LYS:HD3	2:B:382:ILE:HG23	2.01	0.43
2:D:323:LYS:O	2:D:385:LYS:NZ	2.50	0.43
1:A:320:ASP:OD1	1:A:322:SER:OG	2.25	0.43
1:C:418:ASN:O	1:C:420:PRO:HD3	2.18	0.43
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.53	0.43
1:C:435:VAL:HG22	2:D:290:THR:HG21	2.00	0.43
2:D:47:ILE:HD12	2:D:144:TYR:CD2	2.53	0.43
1:A:70:LYS:HG2	1:A:71:TRP:N	2.32	0.43
1:C:91:GLN:O	3:F:7:DC:H4'	2.19	0.43
1:C:157:PRO:HG2	3:F:6:OMC:H1'	2.00	0.43
1:A:208:HIS:O	1:A:211:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:TYR:HD2	2:D:374:LYS:HD3	1.83	0.43
1:C:115:TYR:CD2	1:C:151:GLN:HG2	2.53	0.43
1:C:443:ASP:OD1	1:C:444:GLY:N	2.47	0.43
2:B:305:GLU:O	2:B:309:ILE:HG13	2.19	0.42
1:C:295:LEU:HB3	1:C:300:GLU:HG2	2.00	0.42
2:D:101:LYS:HD3	2:D:382:ILE:HG23	2.01	0.42
1:A:198:HIS:O	1:A:202:ILE:HG12	2.19	0.42
1:C:88:TRP:CD1	2:D:143:ARG:NH1	2.88	0.42
2:D:107:THR:HA	2:D:232:TYR:O	2.20	0.42
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.01	0.42
1:C:450:THR:HG22	1:C:452:LEU:HG	2.00	0.42
2:D:112:GLY:HA2	2:D:115:TYR:CE1	2.55	0.42
2:D:422:LEU:HG	2:D:423:VAL:HG12	2.00	0.42
3:F:8:OMC:HM23	3:F:8:OMC:H1'	1.83	0.42
1:A:115:TYR:HB3	1:A:149:LEU:O	2.18	0.42
2:D:185:ASP:OD1	2:D:185:ASP:N	2.50	0.42
1:C:254:VAL:HG21	1:C:286:THR:HG21	2.02	0.42
1:C:39:THR:O	1:C:42:GLU:HG3	2.20	0.42
1:A:457:TYR:HA	1:A:548:VAL:HG21	2.02	0.42
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.02	0.42
1:C:84:THR:HB	1:C:154:LYS:HE2	2.02	0.42
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.55	0.42
2:B:115:TYR:HE2	2:B:157:PRO:HA	1.85	0.42
1:A:91:GLN:O	3:E:7:DC:H4'	2.19	0.42
1:A:258:GLN:HB3	3:E:33:DG:H4'	2.02	0.42
1:A:22:LYS:HD3	1:A:22:LYS:HA	1.79	0.41
1:A:266:TRP:CE2	3:E:35:DG:H4'	2.55	0.41
1:A:33:ALA:O	1:A:37:ILE:HG12	2.21	0.41
1:A:5:ILE:CG2	1:A:119:PRO:HD2	2.50	0.41
2:B:104:LYS:HE2	2:B:104:LYS:HB3	1.77	0.41
2:B:42:GLU:OE2	2:B:49:LYS:HG3	2.20	0.41
3:F:27:DC:H2''	3:F:28:DG:C8	2.54	0.41
1:A:26:LEU:HD21	1:A:34:LEU:HD13	2.01	0.41
1:A:412:PRO:HD3	2:B:401:TRP:CZ2	2.55	0.41
1:C:22:LYS:HA	1:C:22:LYS:HD3	1.88	0.41
1:A:21:VAL:HG23	1:A:58:THR:HA	2.02	0.41
1:C:47:ILE:HD12	1:C:146:TYR:HA	2.02	0.41
2:D:157:PRO:HG3	2:D:184:MET:HA	2.03	0.41
2:B:185:ASP:N	2:B:185:ASP:OD1	2.54	0.41
1:A:94:ILE:CD1	3:E:35:DG:H21	2.33	0.41
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:CD1	1:A:163:SER:HB3	2.51	0.41
1:A:401:TRP:HB2	1:A:425:LEU:HD11	2.02	0.41
2:B:84:THR:HG22	2:B:87:PHE:HB3	2.03	0.41
1:C:325:LEU:HB3	1:C:387:PRO:HB3	2.03	0.41
1:C:195:ILE:O	1:C:199:ARG:HG3	2.20	0.41
2:D:422:LEU:HG	2:D:423:VAL:N	2.36	0.41
2:B:266:TRP:O	2:B:269:GLN:HG3	2.21	0.40
1:C:28:GLU:CB	1:C:135:ILE:HD12	2.51	0.40
1:C:350:LYS:NZ	1:C:351:THR:O	2.48	0.40
1:C:406:TRP:CZ2	2:D:420:PRO:HG3	2.57	0.40
2:D:214:LEU:HD12	2:D:215:THR:H	1.87	0.40
1:A:80:LEU:O	1:A:84:THR:OG1	2.32	0.40
1:A:131:THR:HB	1:A:143:ARG:HG2	2.03	0.40
2:B:175:ASN:OD1	2:B:201:LYS:HE2	2.22	0.40
1:C:255:ASN:CG	1:C:289:LEU:HD21	2.42	0.40
1:C:301:LEU:O	1:C:305:GLU:HG2	2.20	0.40
1:C:503:LEU:HD11	1:C:533:LEU:HB3	2.02	0.40
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.22	0.40
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.22	0.40
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.88	0.40
1:C:215:THR:O	1:C:217:PRO:HD3	2.22	0.40
1:C:328:GLU:HG2	1:C:330:GLN:NE2	2.36	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	549/555 (99%)	536 (98%)	13 (2%)	0	100	100
1	C	549/555 (99%)	533 (97%)	16 (3%)	0	100	100
2	B	408/444 (92%)	396 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	408/444 (92%)	396 (97%)	12 (3%)	0	100	100
All	All	1914/1998 (96%)	1861 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	492/495 (99%)	486 (99%)	6 (1%)	71	82
1	C	492/495 (99%)	483 (98%)	9 (2%)	59	75
2	B	374/403 (93%)	373 (100%)	1 (0%)	92	95
2	D	374/403 (93%)	372 (100%)	2 (0%)	88	92
All	All	1732/1796 (96%)	1714 (99%)	18 (1%)	76	85

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	109	LEU
1	A	277	ARG
1	A	391	LEU
1	A	450	THR
1	A	497	THR
2	B	11	LYS
1	C	5	ILE
1	C	42	GLU
1	C	109	LEU
1	C	123	ASP
1	C	208	HIS
1	C	277	ARG
1	C	391	LEU
1	C	450	THR
1	C	497	THR

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Mol	Chain	Res	Type
2	D	11	LYS
2	D	185	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	GLN
2	B	428	GLN
1	C	221	HIS
1	C	255	ASN
1	C	487	GLN
1	C	507	GLN
2	D	208	HIS

### 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	8	3,2	15,22,23	0.91	1 (6%)	17,31,34	1.36	2 (11%)
3	OMC	E	8	3,2	15,22,23	0.86	1 (6%)	17,31,34	1.39	2 (11%)
3	OMC	E	6	3	15,22,23	0.93	1 (6%)	17,31,34	1.39	2 (11%)
3	OMC	F	6	3	15,22,23	0.94	1 (6%)	17,31,34	1.47	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	F	8	3,2	-	1/7/27/28	0/2/2/2
3	OMC	E	8	3,2	-	0/7/27/28	0/2/2/2
3	OMC	E	6	3	-	1/7/27/28	0/2/2/2
3	OMC	F	6	3	-	0/7/27/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	8	OMC	C4-N4	2.73	1.43	1.35
3	E	6	OMC	C4-N4	2.71	1.43	1.35
3	F	6	OMC	C4-N4	2.70	1.43	1.35
3	F	8	OMC	C4-N4	2.68	1.43	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	8	OMC	C2-N3-C4	4.47	120.87	116.34
3	F	6	OMC	C2-N3-C4	4.47	120.87	116.34
3	E	6	OMC	C2-N3-C4	4.43	120.83	116.34
3	F	8	OMC	C2-N3-C4	4.18	120.58	116.34
3	F	6	OMC	N4-C4-N3	2.36	120.21	116.49
3	E	8	OMC	N4-C4-N3	2.34	120.19	116.49
3	F	8	OMC	N4-C4-N3	2.27	120.07	116.49
3	E	6	OMC	N4-C4-N3	2.10	119.80	116.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	8	OMC	C1'-C2'-O2'-CM2
3	E	6	OMC	C1'-C2'-O2'-CM2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	8	OMC	2	0
3	E	8	OMC	2	0
3	F	6	OMC	1	0

## 5.5 Carbohydrates

4 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	0.61	0	15,15,17	0.83	1 (6%)
4	FRU	G	2	4	11,12,12	0.63	0	10,18,18	0.92	0
4	GLC	H	1	4	11,11,12	0.55	0	15,15,17	1.13	2 (13%)
4	FRU	H	2	4	11,12,12	0.67	0	10,18,18	1.16	1 (10%)

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	-	0/2/19/22	0/1/1/1
4	FRU	G	2	4	-	3/5/24/24	0/1/1/1
4	GLC	H	1	4	-	0/2/19/22	0/1/1/1
4	FRU	H	2	4	-	3/5/24/24	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	GLC	C1-C2-C3	2.51	112.75	109.67
4	G	1	GLC	C1-O5-C5	2.25	115.24	112.19
4	H	1	GLC	C1-O5-C5	2.22	115.20	112.19
4	H	2	FRU	C6-C5-C4	-2.17	109.85	115.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

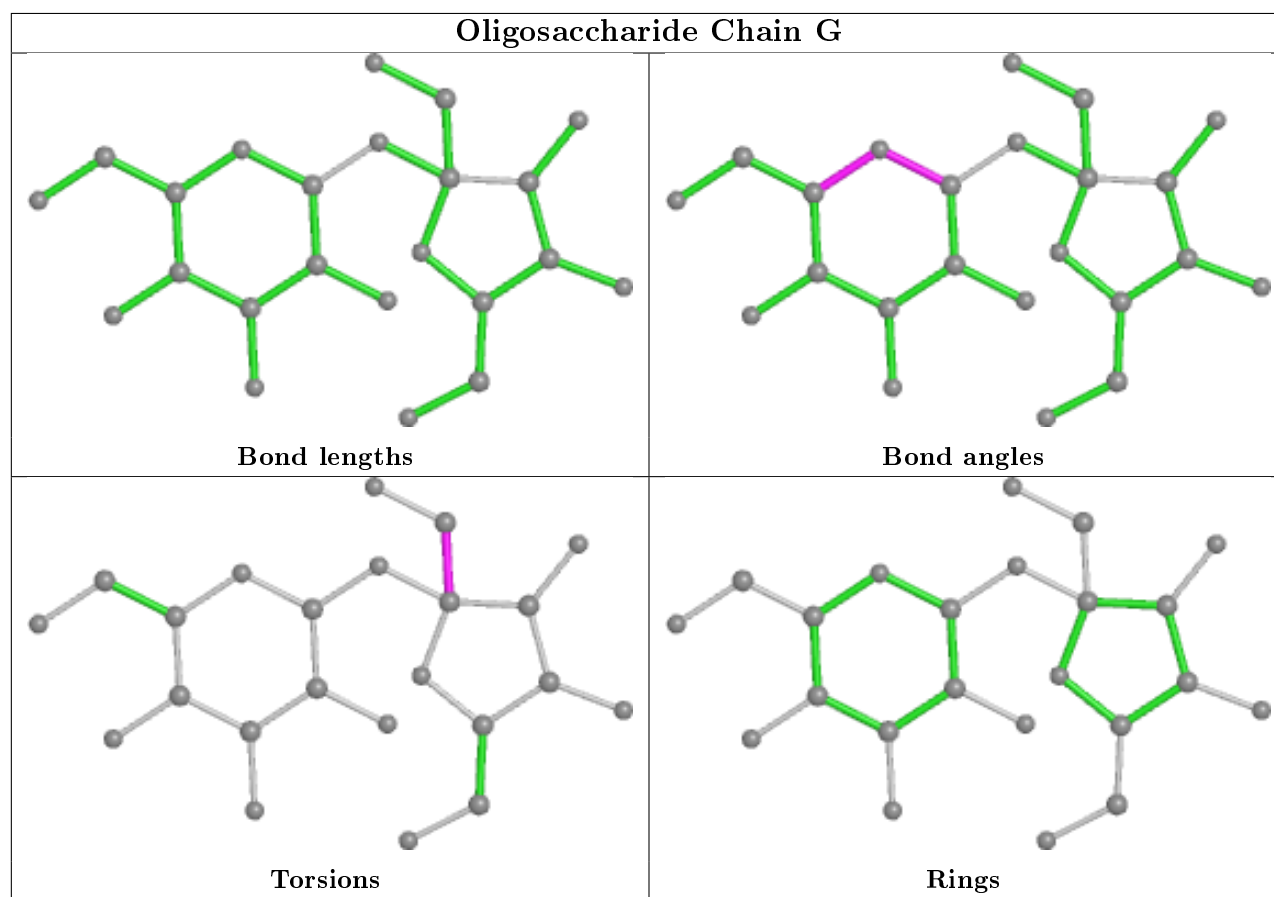


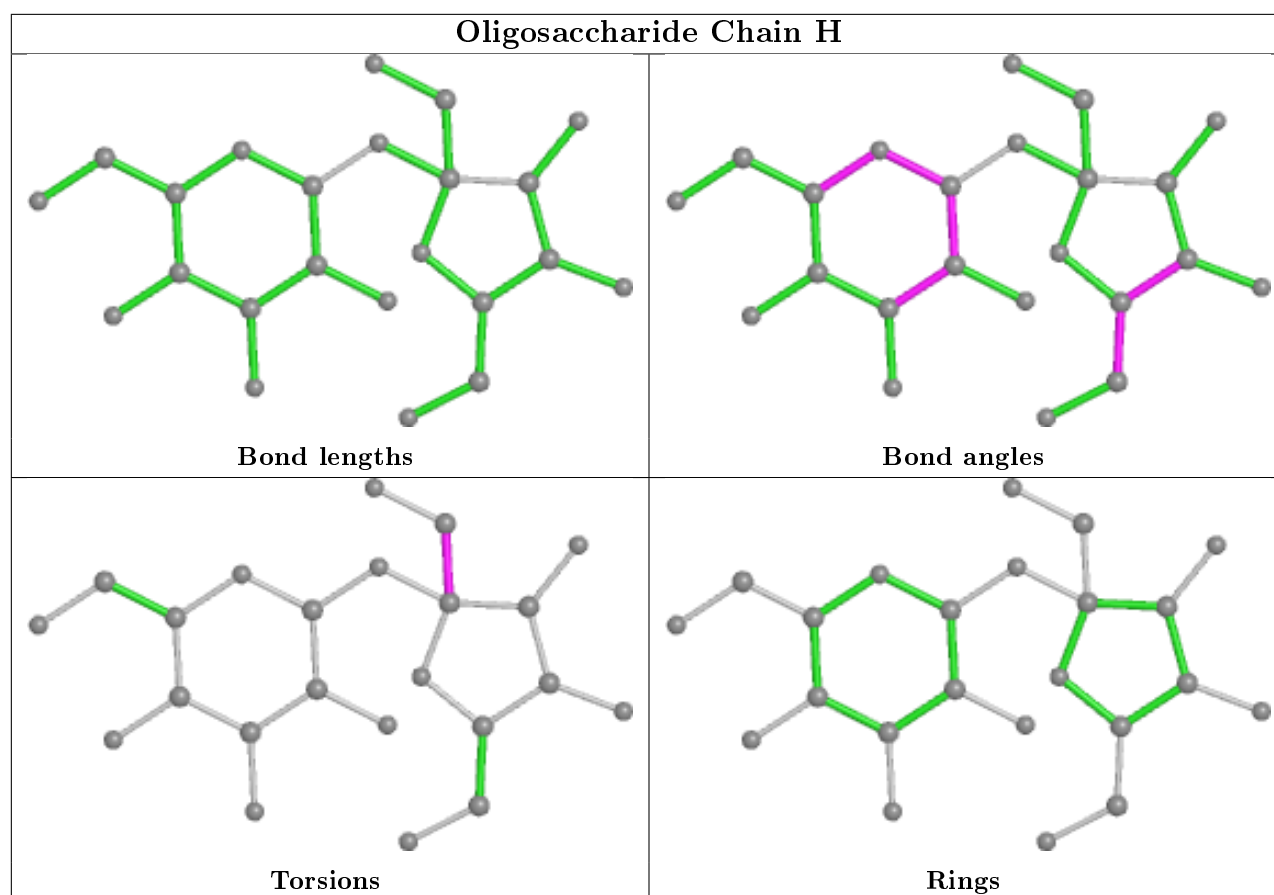
Mol	Chain	Res	Type	Atoms
4	G	2	FRU	O1-C1-C2-C3
4	G	2	FRU	O1-C1-C2-O2
4	G	2	FRU	O1-C1-C2-O5
4	H	2	FRU	O1-C1-C2-O2
4	H	2	FRU	O1-C1-C2-O5
4	H	2	FRU	O1-C1-C2-C3

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.





## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	$\# Z  > 2$
6	3JY	C	605	5	15,24,25	2.56	5 (33%)	16,36,37	2.47	5 (31%)
7	SO4	B	503	-	4,4,4	0.12	0	6,6,6	0.12	0
7	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.21	0
7	SO4	A	605	-	4,4,4	0.13	0	6,6,6	0.11	0
6	3JY	A	603	5	15,24,25	2.45	4 (26%)	16,36,37	2.82	6 (37%)
7	SO4	C	604	-	4,4,4	0.13	0	6,6,6	0.17	0
7	SO4	B	502	-	4,4,4	0.18	0	6,6,6	0.36	0
7	SO4	B	505	-	4,4,4	0.14	0	6,6,6	0.21	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
6	3JY	C	605	5	-	5/6/27/29	0/2/2/2
6	3JY	A	603	5	-	6/6/27/29	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	605	3JY	O11-C10	-7.50	1.34	1.44
6	A	603	3JY	O11-C10	-7.47	1.34	1.44
6	C	605	3JY	O1-C2	3.92	1.34	1.24
6	A	603	3JY	O1-C2	3.90	1.34	1.24
6	C	605	3JY	P16-O18	2.51	1.53	1.49
6	A	603	3JY	C22-N21	-2.37	1.33	1.38
6	C	605	3JY	C22-N21	-2.27	1.33	1.38
6	C	605	3JY	C20-C7	-2.15	1.50	1.53
6	A	603	3JY	C20-C7	-2.13	1.50	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	605	3JY	C2-N21-C22	7.63	121.58	115.14
6	A	603	3JY	C2-N21-C22	7.52	121.49	115.14
6	A	603	3JY	C12-O11-C10	5.61	135.79	115.39
6	C	605	3JY	C12-O11-C10	2.82	125.66	115.39
6	C	605	3JY	C10-C20-C7	2.62	108.66	102.43
6	A	603	3JY	O18-P16-C12	-2.59	108.20	113.35
6	A	603	3JY	C10-C20-C7	2.55	108.49	102.43
6	A	603	3JY	C20-C7-C8	2.49	106.53	102.76
6	A	603	3JY	C8-C9-C10	2.29	107.02	102.72
6	C	605	3JY	C8-C9-C10	2.21	106.86	102.72
6	C	605	3JY	C20-C7-C8	2.19	106.08	102.76

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	605	3JY	C20-C10-O11-C12
6	C	605	3JY	C13-C12-P16-O18

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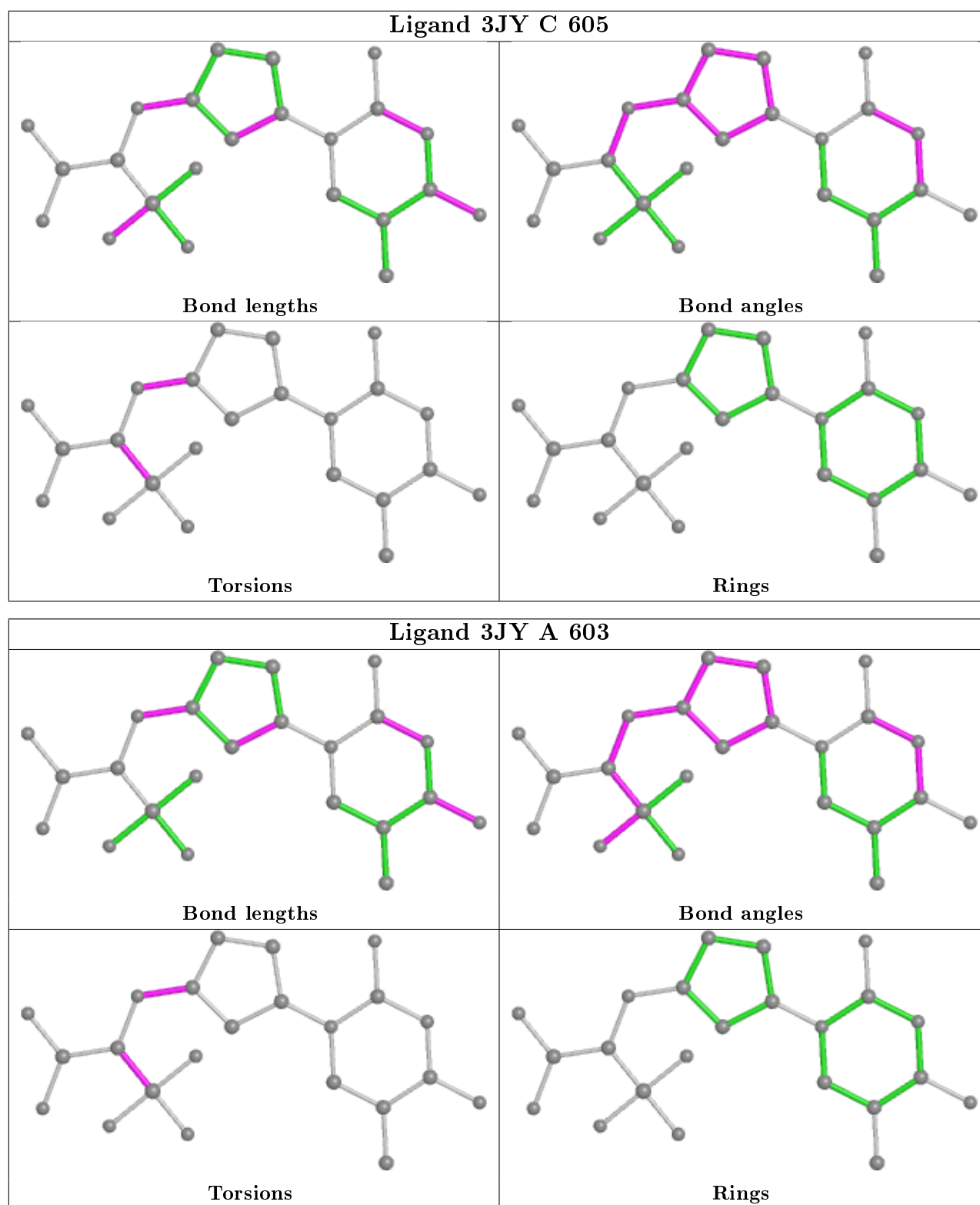
Mol	Chain	Res	Type	Atoms
6	C	605	3JY	C13-C12-P16-O19
6	C	605	3JY	C13-C12-P16-O17
6	C	605	3JY	O11-C12-P16-O18
6	A	603	3JY	C20-C10-O11-C12
6	A	603	3JY	C13-C12-P16-O18
6	A	603	3JY	C13-C12-P16-O19
6	A	603	3JY	C13-C12-P16-O17
6	A	603	3JY	O11-C12-P16-O18
6	A	603	3JY	C9-C10-O11-C12

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	605	3JY	4	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 than 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.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	551/555 (99%)	1.08	93 (16%) 1 1	41, 96, 151, 190	0
1	C	551/555 (99%)	1.34	135 (24%) 0 0	43, 113, 162, 182	0
2	B	412/444 (92%)	0.61	33 (8%) 12 15	41, 81, 127, 142	0
2	D	412/444 (92%)	0.85	55 (13%) 3 4	44, 92, 136, 160	0
3	E	33/38 (86%)	0.12	0 100 100	70, 97, 113, 152	0
3	F	33/38 (86%)	0.79	2 (6%) 21 26	82, 112, 131, 169	0
All	All	1992/2074 (96%)	0.98	318 (15%) 1 2	41, 93, 152, 190	0

All (318) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	SER	14.5
1	C	60	VAL	12.0
1	C	132	ILE	11.7
1	A	131	THR	11.3
1	C	135	ILE	10.9
1	C	142	ILE	9.6
1	C	133	PRO	9.5
1	C	50	ILE	9.2
2	D	10	VAL	8.9
1	A	142	ILE	8.6
1	A	134	SER	7.9
1	C	67	ASP	7.9
1	A	133	PRO	7.5
1	A	136	ASN	7.3
2	B	214	LEU	7.2
1	C	26	LEU	7.1
1	A	135	ILE	7.1
1	A	26	LEU	7.0
1	A	137	ASN	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	28	GLU	6.4
1	C	25	PRO	6.3
1	C	24	TRP	6.2
1	C	138	GLU	6.1
1	A	138	GLU	5.9
1	C	17	ASP	5.8
1	A	28	GLU	5.7
1	C	131	THR	5.7
1	C	47	ILE	5.7
1	A	132	ILE	5.6
1	A	49	LYS	5.6
2	D	360	ALA	5.6
1	A	287	LYS	5.5
2	D	214	LEU	5.5
1	C	293	ILE	5.5
1	A	61	PHE	5.5
1	C	49	LYS	5.4
1	C	55	PRO	5.4
1	C	136	ASN	5.4
1	C	174	GLN	5.3
1	C	287	LYS	5.3
1	C	257	ILE	5.3
2	B	211	ARG	5.3
1	C	21	VAL	5.2
1	A	20	LYS	5.2
2	B	89	GLU	5.1
1	C	5	ILE	5.1
1	C	145	GLN	5.1
1	A	50	ILE	5.1
1	C	290	THR	5.0
1	C	288	ALA	5.0
1	A	27	THR	5.0
2	D	232	TYR	4.9
1	C	254	VAL	4.9
1	C	285	GLY	4.9
1	C	74	LEU	4.9
1	C	140	PRO	4.9
2	D	88	TRP	4.8
2	D	124	PHE	4.8
2	D	85	GLN	4.8
2	D	116	PHE	4.7
1	A	25	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	91	GLN	4.7
2	D	11	LYS	4.6
1	A	251	SER	4.6
1	C	43	LYS	4.6
2	B	301	LEU	4.6
1	C	16	MET	4.6
1	A	47	ILE	4.5
1	C	23	GLN	4.5
2	B	4	PRO	4.5
2	B	212	TRP	4.5
1	C	66	LYS	4.4
1	A	286	THR	4.4
1	A	139	THR	4.3
2	B	215	THR	4.3
1	A	21	VAL	4.3
1	A	193	LEU	4.3
1	C	228	LEU	4.3
2	D	357	MET	4.2
1	C	58	THR	4.2
1	A	143	ARG	4.2
1	A	288	ALA	4.2
1	C	124	PHE	4.2
1	C	14	PRO	4.1
1	C	193	LEU	4.1
1	C	295	LEU	4.1
1	A	75	VAL	4.1
2	D	89	GLU	4.1
1	C	139	THR	4.1
2	D	277	ARG	4.1
1	C	15	GLY	4.0
1	A	62	ALA	4.0
1	C	210	LEU	4.0
1	C	141	GLY	4.0
1	A	73	LYS	4.0
1	C	61	PHE	4.0
1	C	73	LYS	3.9
2	B	250	ASP	3.9
1	A	144	TYR	3.9
1	C	22	LYS	3.9
1	C	346	PHE	3.9
1	C	144	TYR	3.9
1	C	59	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	102	LYS	3.8
1	C	63	ILE	3.8
1	C	18	GLY	3.8
2	D	359	GLY	3.8
1	C	151	GLN	3.7
1	A	448	ARG	3.7
2	D	318	TYR	3.7
2	D	146	TYR	3.7
1	C	286	THR	3.7
2	D	361	HIS	3.7
2	D	358	ARG	3.6
1	A	252	TRP	3.6
1	C	13	LYS	3.6
1	A	59	PRO	3.6
1	A	293	ILE	3.6
2	B	88	TRP	3.6
1	A	71	TRP	3.6
1	C	20	LYS	3.6
1	C	211	ARG	3.6
2	B	16	MET	3.5
1	C	449	GLU	3.5
1	C	448	ARG	3.5
2	D	215	THR	3.5
1	C	109	LEU	3.5
1	A	250	ASP	3.5
1	C	143	ARG	3.5
2	D	87	PHE	3.5
1	A	247	PRO	3.4
1	C	250	ASP	3.4
1	C	173	LYS	3.4
1	C	289	LEU	3.4
2	B	12	LEU	3.4
1	A	290	THR	3.4
1	A	191	SER	3.3
1	C	114	ALA	3.3
1	C	75	VAL	3.3
2	D	86	ASP	3.3
1	C	56	TYR	3.3
1	A	228	LEU	3.3
1	C	251	SER	3.3
1	A	151	GLN	3.3
1	C	229	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	33	ALA	3.2
2	B	6	GLU	3.2
2	D	159	ILE	3.2
1	C	12	LEU	3.2
2	D	16	MET	3.2
1	A	30	LYS	3.2
1	C	319	TYR	3.2
2	D	195	ILE	3.2
1	C	104	LYS	3.1
1	A	295	LEU	3.1
2	B	87	PHE	3.1
2	D	4	PRO	3.1
2	D	212	TRP	3.1
1	C	260	LEU	3.0
1	A	19	PRO	3.0
1	C	32	LYS	3.0
1	C	283	LEU	3.0
1	A	16	MET	3.0
1	A	145	GLN	3.0
2	B	86	ASP	3.0
2	D	176	PRO	3.0
2	B	5	ILE	2.9
2	D	238	LYS	2.9
1	C	137	ASN	2.9
2	D	233	GLU	2.9
2	B	14	PRO	2.9
1	C	223	LYS	2.9
1	C	11	LYS	2.9
1	C	259	LYS	2.9
2	D	422	LEU	2.9
1	C	195	ILE	2.9
1	A	37	ILE	2.9
1	A	130	PHE	2.9
2	B	425	LEU	2.9
1	A	289	LEU	2.9
1	C	188	TYR	2.8
2	D	92	LEU	2.8
1	C	4	PRO	2.8
1	C	207	GLN	2.8
1	C	554	ALA	2.8
2	D	354	TYR	2.8
1	A	51	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	252	TRP	2.8
1	A	56	TYR	2.8
1	A	452	LEU	2.8
1	A	554	ALA	2.7
2	D	90	VAL	2.7
1	A	238	LYS	2.7
1	A	271	TYR	2.7
2	B	195	ILE	2.7
2	D	240	THR	2.7
1	A	226	PRO	2.7
1	C	52	PRO	2.7
1	C	160	PHE	2.7
2	D	426	TRP	2.7
1	C	77	PHE	2.7
1	C	146	TYR	2.7
1	A	17	ASP	2.6
1	C	27	THR	2.6
1	C	19	PRO	2.6
2	D	169	GLU	2.6
1	C	294	PRO	2.6
1	A	141	GLY	2.6
1	A	128	THR	2.6
1	C	292	VAL	2.6
1	A	279	LEU	2.6
3	F	0	DT	2.6
2	D	95	PRO	2.6
1	A	60	VAL	2.6
1	C	303	LEU	2.6
1	C	130	PHE	2.6
2	D	15	GLY	2.6
1	A	120	LEU	2.5
1	A	127	TYR	2.5
1	A	256	ASP	2.5
1	C	78	ARG	2.5
1	A	52	PRO	2.5
1	C	232	TYR	2.5
2	B	10	VAL	2.5
1	A	200	THR	2.5
1	C	115	TYR	2.5
1	C	44	GLU	2.5
2	B	205	LEU	2.5
2	D	177	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	146	TYR	2.5
1	A	285	GLY	2.5
2	B	173	LYS	2.4
2	B	127	TYR	2.4
1	C	301	LEU	2.4
1	C	184	MET	2.4
1	A	140	PRO	2.4
1	A	233	GLU	2.4
1	C	187	LEU	2.4
2	B	193	LEU	2.4
2	B	184	MET	2.4
1	A	254	VAL	2.4
1	C	29	GLU	2.3
1	C	318	TYR	2.3
1	C	156	SER	2.3
1	A	449	GLU	2.3
2	B	400	THR	2.3
1	A	195	ILE	2.3
1	C	108	VAL	2.3
2	B	13	LYS	2.3
2	D	201	LYS	2.3
1	A	283	LEU	2.3
1	C	30	LYS	2.3
1	C	51	GLY	2.3
2	B	281	LYS	2.3
2	D	73	LYS	2.3
1	C	291	GLU	2.3
1	A	211	ARG	2.3
1	A	46	LYS	2.3
1	A	124	PHE	2.3
1	A	76	ASP	2.3
1	A	249	LYS	2.3
2	D	130	PHE	2.2
1	A	102	LYS	2.2
1	C	238	LYS	2.2
2	D	211	ARG	2.2
2	D	144	TYR	2.2
1	C	226	PRO	2.2
2	D	55	PRO	2.2
2	D	202	ILE	2.2
1	C	199	ARG	2.2
2	B	422	LEU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	127	TYR	2.2
1	A	34	LEU	2.2
2	D	349	LEU	2.2
1	C	230	MET	2.2
1	A	32	LYS	2.1
1	C	10	VAL	2.1
1	C	106	VAL	2.1
1	C	277	ARG	2.1
1	C	183	TYR	2.1
1	A	192	ASP	2.1
1	A	453	GLY	2.1
1	A	29	GLU	2.1
2	B	171	PHE	2.1
2	D	32	LYS	2.1
1	C	284	ARG	2.1
1	A	241	VAL	2.1
1	C	120	LEU	2.1
1	C	178	ILE	2.1
1	C	279	LEU	2.1
1	C	325	LEU	2.1
2	B	204	GLU	2.1
1	C	111	VAL	2.1
2	D	70	LYS	2.1
1	A	67	ASP	2.1
1	A	248	GLU	2.1
1	C	224	GLU	2.1
1	C	302	GLU	2.1
1	A	292	VAL	2.1
2	B	85	GLN	2.1
1	C	255	ASN	2.1
1	A	291	GLU	2.1
1	C	153	TRP	2.1
1	C	209	LEU	2.0
2	D	12	LEU	2.0
2	D	66	LYS	2.0
3	F	37	DG	2.0
1	C	308	GLU	2.0
1	A	323	LYS	2.0
2	D	198	HIS	2.0
2	D	47	ILE	2.0
1	A	42	GLU	2.0
2	B	275	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	87	PHE	2.0
1	C	313	PRO	2.0
2	B	397	THR	2.0
2	D	197	GLN	2.0
1	C	452	LEU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	OMC	F	6	21/22	0.90	0.24	85,98,111,120	0
3	OMC	F	8	21/22	0.92	0.25	95,103,106,118	0
3	OMC	E	8	21/22	0.94	0.23	67,73,76,90	0
3	OMC	E	6	21/22	0.97	0.20	82,91,95,98	0

## 6.3 Carbohydrates [i](#)

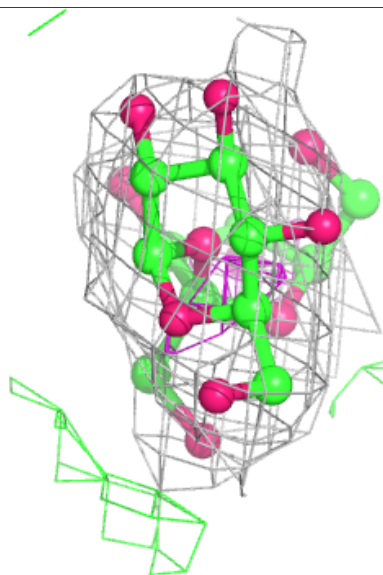
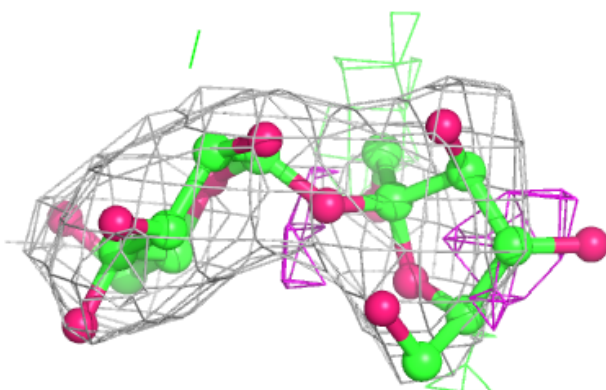
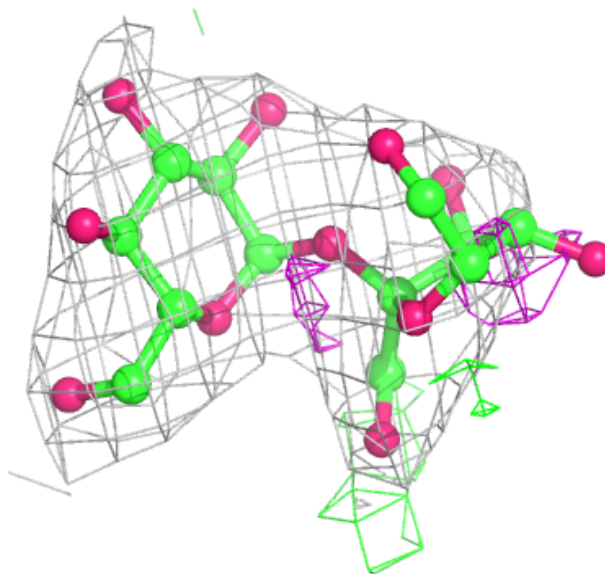
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FRU	G	2	12/12	0.86	0.21	82,97,108,109	0
4	GLC	H	1	11/12	0.93	0.13	82,92,96,101	0
4	FRU	H	2	12/12	0.93	0.17	93,101,102,104	0
4	GLC	G	1	11/12	0.95	0.15	67,77,86,87	0

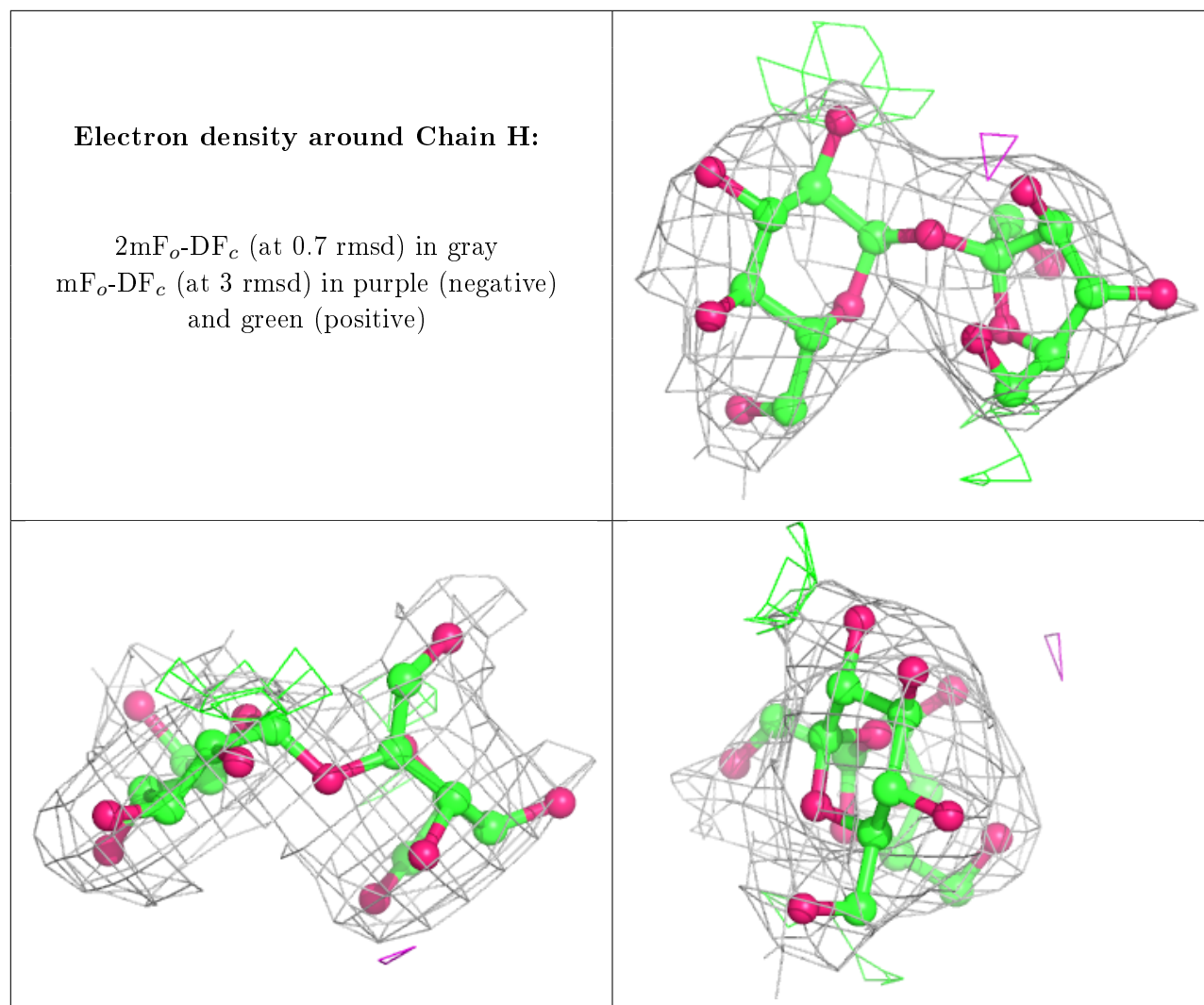
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	MG	C	603	1/1	0.56	0.14	172,172,172,172	0
7	SO4	B	505	5/5	0.81	0.40	78,78,84,111	0
6	3JY	C	605	23/24	0.84	0.24	98,119,137,145	0
5	MG	A	602	1/1	0.85	0.15	114,114,114,114	0
7	SO4	B	504	5/5	0.85	0.40	87,98,102,121	0
7	SO4	B	502	5/5	0.85	0.21	78,79,85,101	0
7	SO4	B	503	5/5	0.85	0.17	94,100,109,113	0
7	SO4	C	604	5/5	0.88	0.24	84,92,112,112	0

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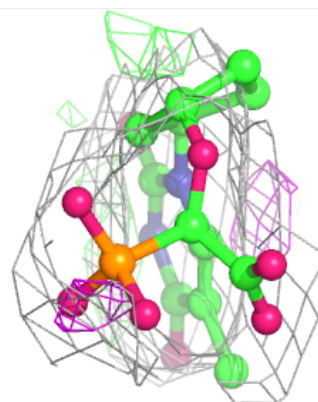
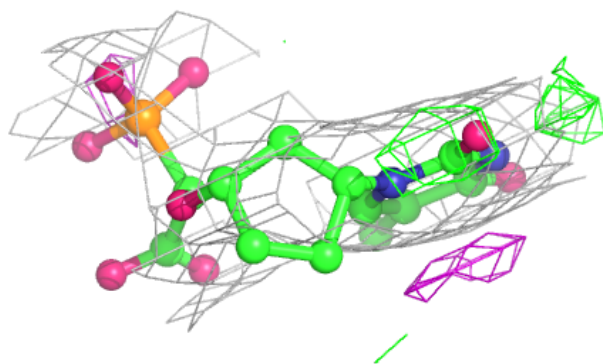
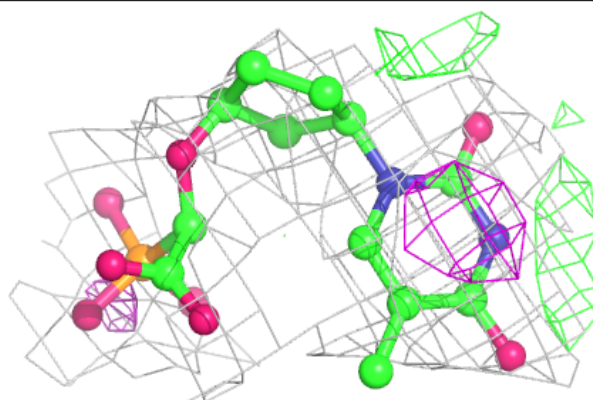
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	A	604	1/1	0.92	0.14	70,70,70,70	0
6	3JY	A	603	23/24	0.94	0.20	103,107,123,129	0
7	SO4	A	605	5/5	0.95	0.12	98,102,110,116	0
5	MG	C	602	1/1	0.95	0.19	70,70,70,70	0
5	MG	C	601	1/1	0.96	0.28	122,122,122,122	0
5	MG	A	601	1/1	0.97	0.20	114,114,114,114	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.

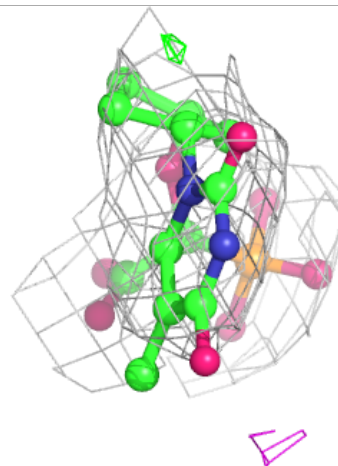
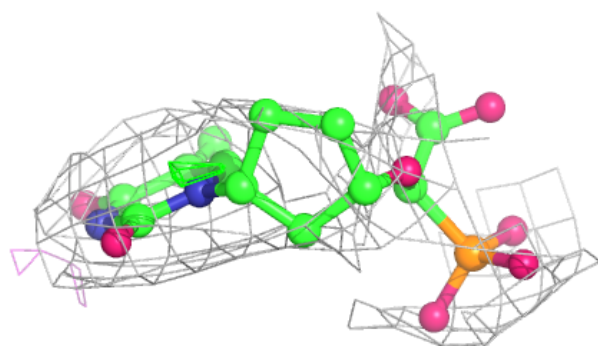
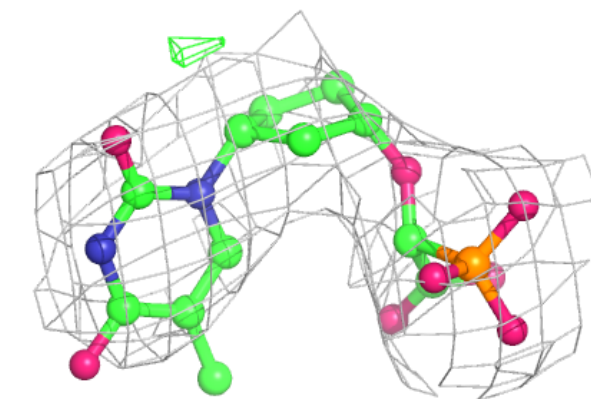
**Electron density around 3JY C 605:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 3JY A 603:**

$2mF_o-DF_c$  (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.