



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 01:46 AM UTC

PDB ID : 5HLF / pdb_00005hlf
Title : STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE In COMPLEX
WITH A 38-MER HAIRPIN TEMPLATE-PRIMER DNA APTAMER AND
AN ALPHA-CARBOXYPHOSPHONATE INHIBITOR
Authors : Das, K.; Arnold, E.
Deposited on : 2016-01-15
Resolution : 2.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

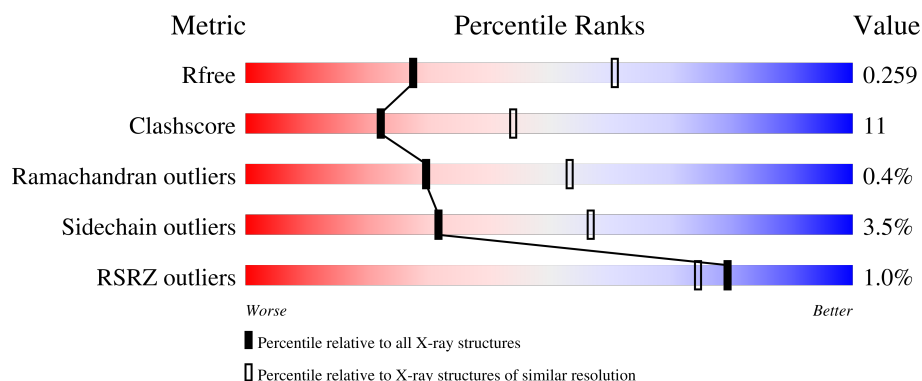
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	555	% 71% 26% .
1	C	555	2% 65% 32% .
2	B	444	78% 16% 6%
2	D	444	% 74% 18% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	38	47% 42% • 8%
3	F	38	45% 39% 8% 8%
4	G	2	50% 50%
4	H	2	50% 50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17429 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	554	Total	C	N	O	S	0	0	0
			4503	2915	749	832	7			
1	C	553	Total	C	N	O	S	0	0	0
			4495	2910	748	830	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	416	Total	C	N	O	S	0	1	0
			3436	2238	568	623	7			
2	D	410	Total	C	N	O	S	0	2	0
			3403	2222	559	615	7			

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

Continued on next page...

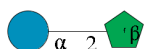
Continued from previous page...

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			

Continued on next page...

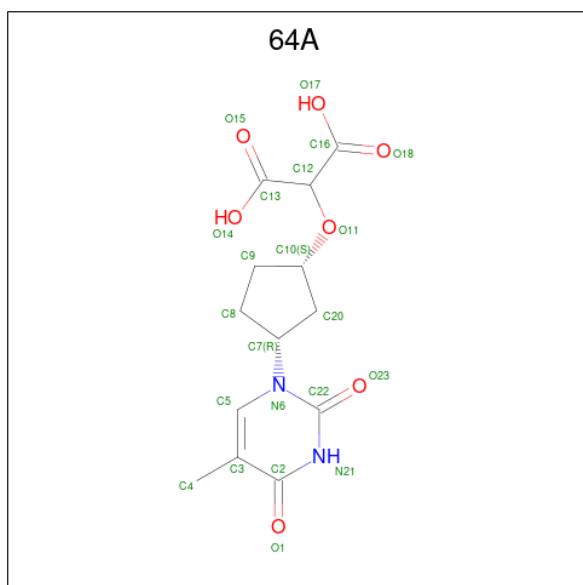
Continued from previous page...

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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is {[(1S,3R)-3-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)cyclopentyl]oxy}propanedioic acid (CCD ID: 64A) (formula: C₁₃H₁₆N₂O₇).



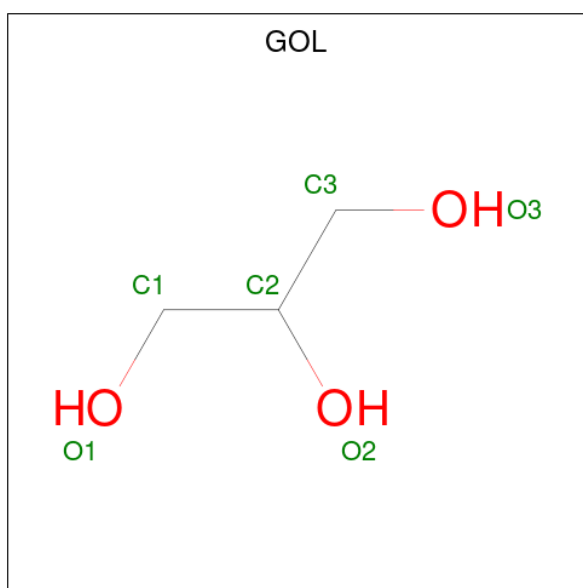
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			22	13	2	7		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

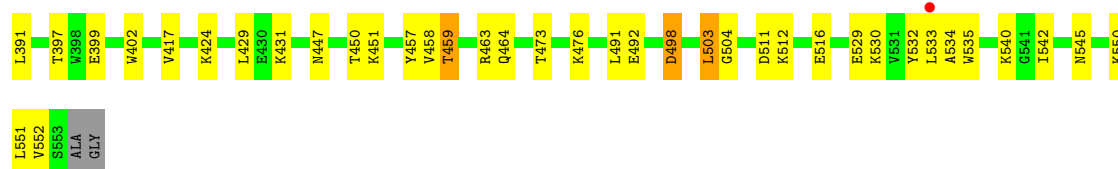
Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		
8	D	1	Total	C	O	0	0
			6	3	3		

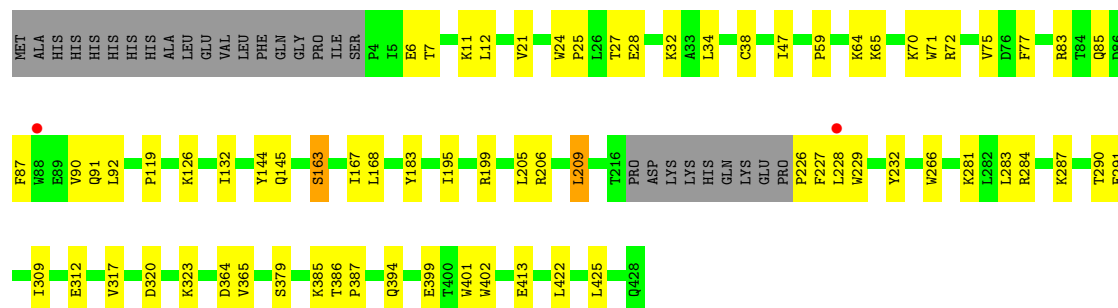
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	2	Total	O	0	0
			2	2		
9	C	3	Total	O	0	0
			3	3		



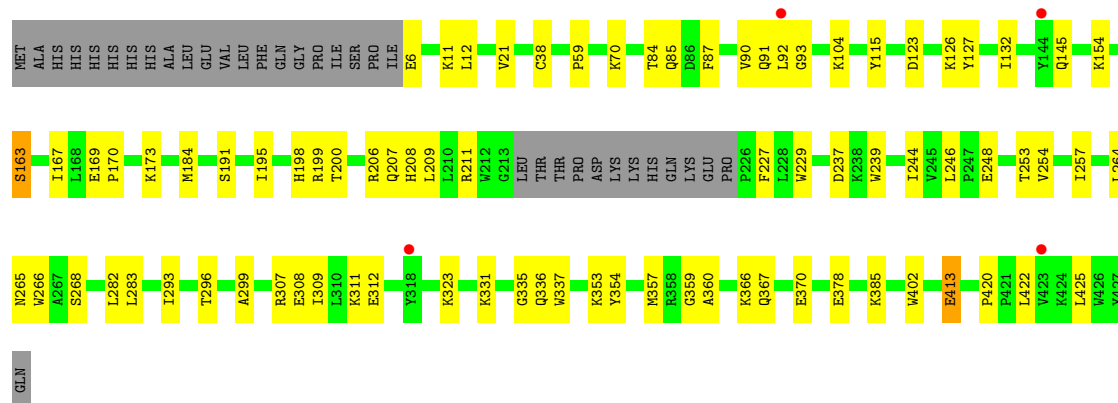
• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT

Chain B: 78% 16% 6%



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT

Chain D: 74% 18% 8%



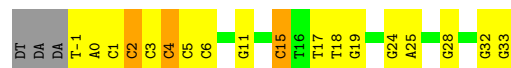
• Molecule 3: DNA (38-MER)

Chain E: 47% 42% 8%



• Molecule 3: DNA (38-MER)

Chain F: 45% 39% 8%



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

Chain G:  50% 50%



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

Chain H:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.06Å 128.56Å 132.41Å 90.00° 101.46° 90.00°	Depositor
Resolution (Å)	43.00 – 2.95 43.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	83.6 (43.00-2.95) 83.6 (43.00-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.257 0.213 , 0.259	Depositor DCC
R_{free} test set	2566 reflections (4.12%)	wwPDB-VP
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17429	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, GOL, FRU, SO4, 64A, MG, 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	0.39	0/4621	0.94	6/6279 (0.1%)
1	C	0.43	1/4613 (0.0%)	1.02	18/6268 (0.3%)
2	B	0.24	0/3537	0.70	0/4803
2	D	0.32	0/3509	0.94	5/4768 (0.1%)
3	E	0.42	1/759 (0.1%)	0.76	2/1170 (0.2%)
3	F	0.60	1/759 (0.1%)	0.62	2/1170 (0.2%)
All	All	0.38	3/17798 (0.0%)	0.90	33/24458 (0.1%)

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	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	15	DC	C4'-O4'	13.40	1.72	1.45
3	E	14	DG	C4'-O4'	5.42	1.56	1.45
1	C	59	PRO	N-CD	5.05	1.54	1.47

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	145	GLN	CB-CA-C	-7.78	93.73	110.45
3	E	14	DG	C5'-C4'-O4'	7.77	121.06	109.40
1	A	224	GLU	CA-C-N	7.69	125.27	119.66
1	A	224	GLU	C-N-CA	7.69	125.27	119.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	286	THR	N-CA-C	-7.47	101.06	111.81

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	306	ASN	Mainchain
1	C	542	ILE	Peptide

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	4503	0	4554	120	0
1	C	4495	0	4549	136	0
2	B	3436	0	3468	51	0
2	D	3403	0	3427	50	0
3	E	720	0	397	11	0
3	F	720	0	397	17	0
4	G	23	0	21	2	0
4	H	23	0	21	1	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
6	A	22	0	14	2	0
7	A	5	0	0	0	0
7	C	5	0	0	0	0
8	A	6	0	8	1	0
8	B	30	0	40	6	0
8	C	6	0	8	2	0
8	D	24	0	32	2	0
9	A	2	0	0	0	0
9	C	3	0	0	0	0
All	All	17429	0	16936	363	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 11.

The worst 5 of 363 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)
3:F:15:DC:C4'	3:F:15:DC:O4'	1.72	1.36
2:D:354:TYR:OH	2:D:378:GLU:OE1	1.88	0.91
1:C:60:VAL:HG21	1:C:130:PHE:CD2	2.12	0.84
1:C:23:GLN:OE1	1:C:131:THR:OG1	1.95	0.83
1:C:72:ARG:HH21	1:C:74:LEU:HD21	1.45	0.81

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	552/555 (100%)	525 (95%)	24 (4%)	3 (0%)	24	49
1	C	551/555 (99%)	511 (93%)	36 (6%)	4 (1%)	18	40
2	B	413/444 (93%)	400 (97%)	13 (3%)	0	100	100
2	D	408/444 (92%)	396 (97%)	12 (3%)	0	100	100
All	All	1924/1998 (96%)	1832 (95%)	85 (4%)	7 (0%)	30	53

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	551	LEU
1	A	282	LEU
1	A	135	ILE
1	A	313	PRO
1	C	249	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/495 (100%)	468 (95%)	25 (5%)	21	47
1	C	493/495 (100%)	464 (94%)	29 (6%)	18	41
2	B	377/403 (94%)	373 (99%)	4 (1%)	65	80
2	D	373/403 (93%)	370 (99%)	3 (1%)	73	85
All	All	1736/1796 (97%)	1675 (96%)	61 (4%)	32	57

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	413	GLU
1	C	498	ASP
1	C	61	PHE
1	C	459	THR
2	D	209	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	91	GLN
1	C	255	ASN
2	D	208	HIS
1	C	221	HIS
1	C	373	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	2	3	19,22,23	0.93	1 (5%)	25,31,34	0.86	0
3	OMC	E	4	3	19,22,23	0.92	1 (5%)	25,31,34	0.81	0
3	OMC	E	2	3	19,22,23	0.97	1 (5%)	25,31,34	0.88	0
3	OMC	F	4	3	19,22,23	0.92	1 (5%)	25,31,34	0.69	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	2	3	-	1/9/27/28	0/2/2/2
3	OMC	E	4	3	-	1/9/27/28	0/2/2/2
3	OMC	E	2	3	-	2/9/27/28	0/2/2/2
3	OMC	F	4	3	-	0/9/27/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	C4-N4	3.85	1.43	1.33
3	E	4	OMC	C4-N4	3.79	1.43	1.33
3	F	4	OMC	C4-N4	3.78	1.43	1.33
3	F	2	OMC	C4-N4	3.75	1.43	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	OMC	C1'-C2'-O2'-CM2
3	E	4	OMC	C1'-C2'-O2'-CM2
3	E	2	OMC	C1'-C2'-O2'-CM2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	2	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	OMC	1	0
3	F	4	OMC	1	0

5.5 Carbohydrates [i](#)

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	0.54	0	15,15,17	1.08	1 (6%)
4	FRU	G	2	4	11,12,12	0.60	0	10,18,18	0.78	0
4	GLC	H	1	4	11,11,12	0.56	0	15,15,17	0.79	0
4	FRU	H	2	4	11,12,12	0.60	0	10,18,18	1.06	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	-	2/2/19/22	0/1/1/1
4	FRU	G	2	4	-	3/5/24/24	0/1/1/1
4	GLC	H	1	4	-	2/2/19/22	0/1/1/1
4	FRU	H	2	4	-	5/5/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C1-O5-C5	2.76	115.88	112.19

There are no chirality outliers.

5 of 12 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-O5
4	H	2	FRU	O1-C1-C2-C3
4	H	2	FRU	O1-C1-C2-O2
4	H	2	FRU	O1-C1-C2-O5

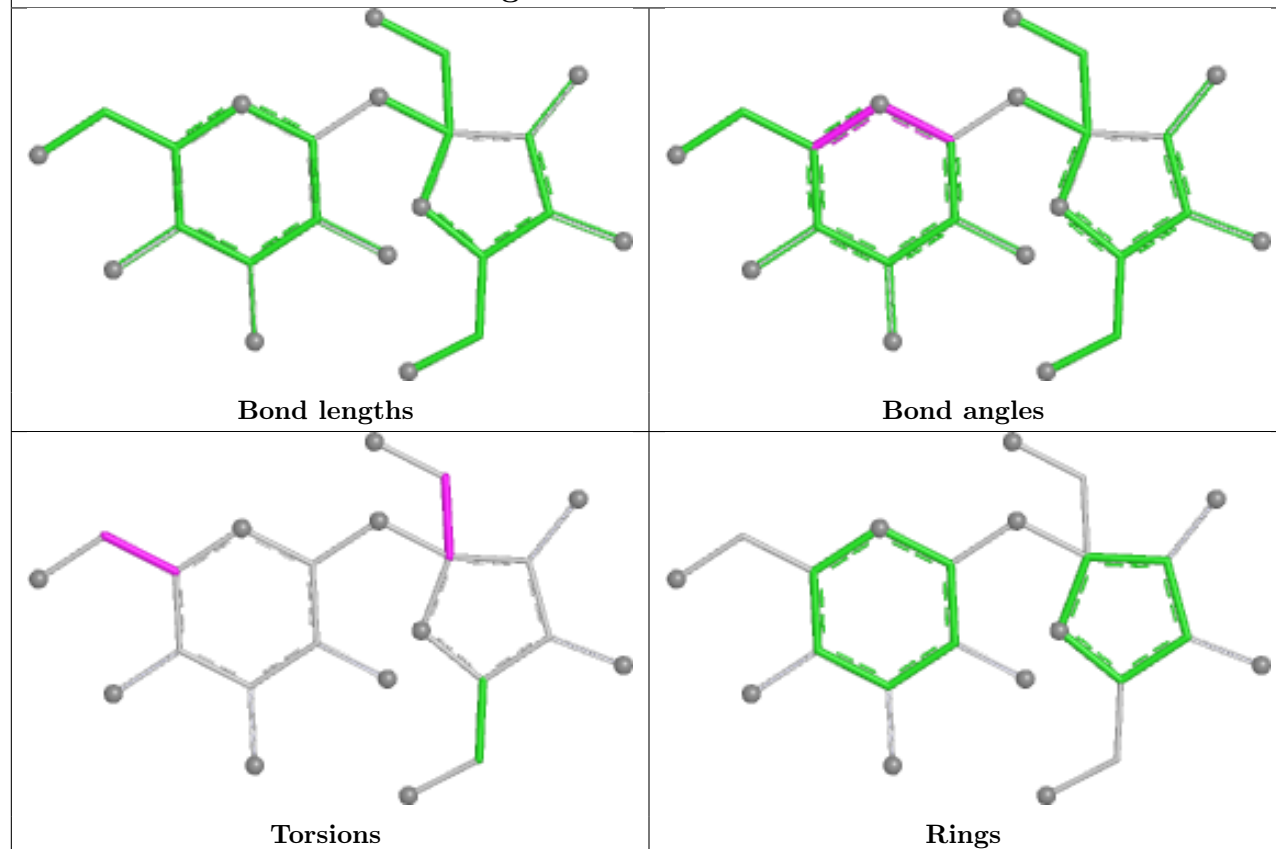
There are no ring outliers.

3 monomers are involved in 3 short contacts:

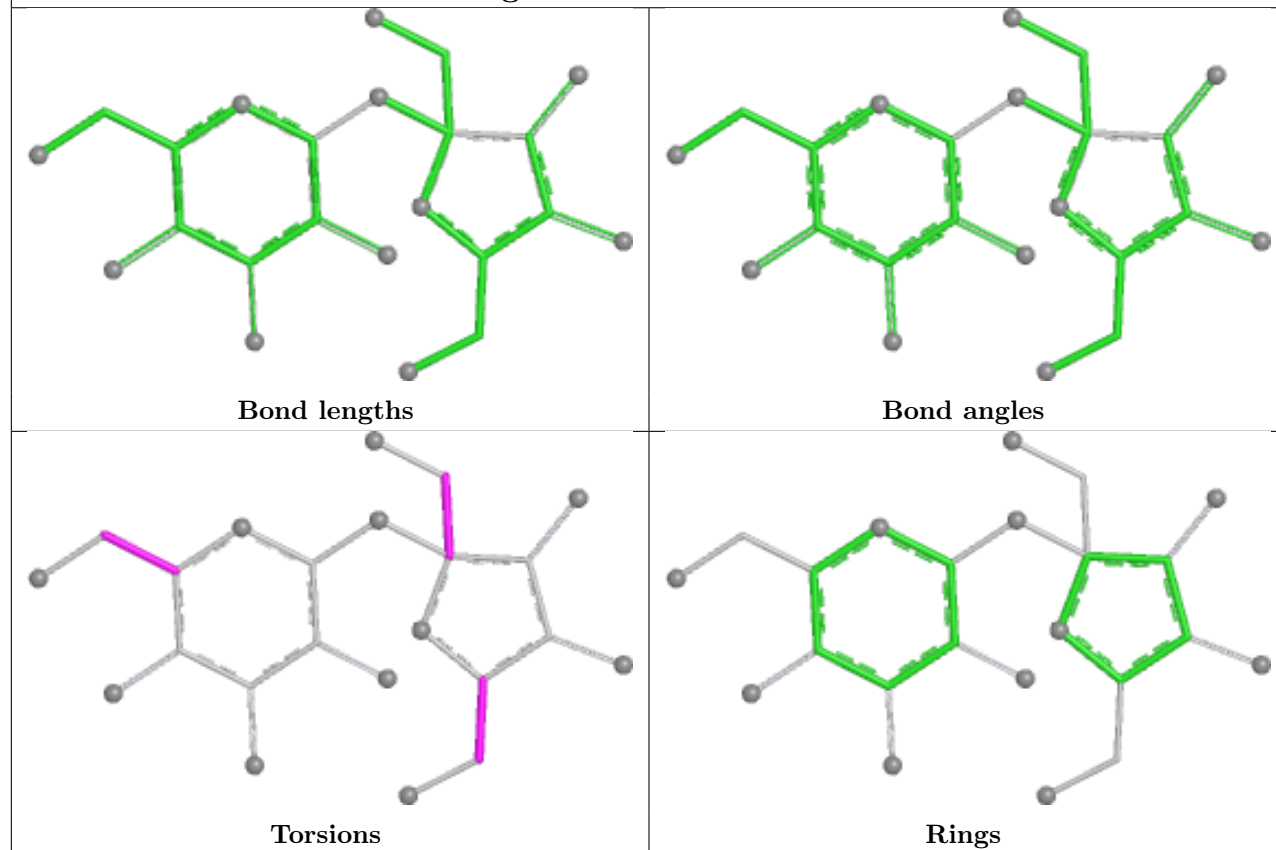
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1	GLC	1	0
4	G	1	GLC	1	0
4	G	2	FRU	2	0

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

Oligosaccharide Chain G



Oligosaccharide Chain H



5.6 Ligand geometry

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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
8	GOL	D	504	-	5,5,5	0.35	0	5,5,5	0.39	0
8	GOL	D	503	-	5,5,5	0.36	0	5,5,5	0.28	0
6	64A	A	602	5	23,23,23	3.15	14 (60%)	25,33,33	2.39	9 (36%)
8	GOL	B	2003	-	5,5,5	0.47	0	5,5,5	0.44	0
8	GOL	B	2005	-	5,5,5	0.38	0	5,5,5	0.49	0
8	GOL	B	2004	-	5,5,5	0.70	0	5,5,5	0.57	0
8	GOL	C	603	-	5,5,5	0.36	0	5,5,5	0.26	0
7	SO4	A	604	-	4,4,4	0.24	0	6,6,6	0.05	0
8	GOL	A	605	-	5,5,5	0.33	0	5,5,5	0.62	0
8	GOL	B	2002	-	5,5,5	0.37	0	5,5,5	0.67	0
8	GOL	D	502	-	5,5,5	0.37	0	5,5,5	0.26	0
8	GOL	D	505	-	5,5,5	0.38	0	5,5,5	0.27	0
8	GOL	B	2006	-	5,5,5	0.37	0	5,5,5	0.52	0
7	SO4	C	602	-	4,4,4	0.24	0	6,6,6	0.11	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
8	GOL	D	504	-	-	2/4/4/4	-
8	GOL	D	503	-	-	2/4/4/4	-
8	GOL	B	2003	-	-	4/4/4/4	-
8	GOL	C	603	-	-	2/4/4/4	-
8	GOL	B	2005	-	-	0/4/4/4	-
8	GOL	B	2004	-	-	4/4/4/4	-
8	GOL	A	605	-	-	2/4/4/4	-
8	GOL	B	2002	-	-	2/4/4/4	-
8	GOL	D	502	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	D	505	-	-	3/4/4/4	-
8	GOL	B	2006	-	-	0/4/4/4	-
6	64A	A	602	5	-	5/16/25/25	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	602	64A	O11-C10	-8.02	1.34	1.44
6	A	602	64A	O1-C2	5.68	1.34	1.23
6	A	602	64A	C12-C13	-4.41	1.46	1.52
6	A	602	64A	C12-C16	-4.33	1.46	1.52
6	A	602	64A	C2-C3	-3.62	1.38	1.44

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	602	64A	C3-C2-N21	4.77	119.47	115.32
6	A	602	64A	N21-C22-N6	4.66	120.95	114.89
6	A	602	64A	C2-N21-C22	-4.54	121.38	127.34
6	A	602	64A	O1-C2-C3	-4.13	120.19	124.92
6	A	602	64A	C3-C5-N6	-3.19	119.85	123.31

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	64A	C20-C10-O11-C12
8	A	605	GOL	C1-C2-C3-O3
8	B	2002	GOL	O1-C1-C2-C3
8	B	2003	GOL	O1-C1-C2-C3
8	B	2003	GOL	C1-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 13 short contacts:

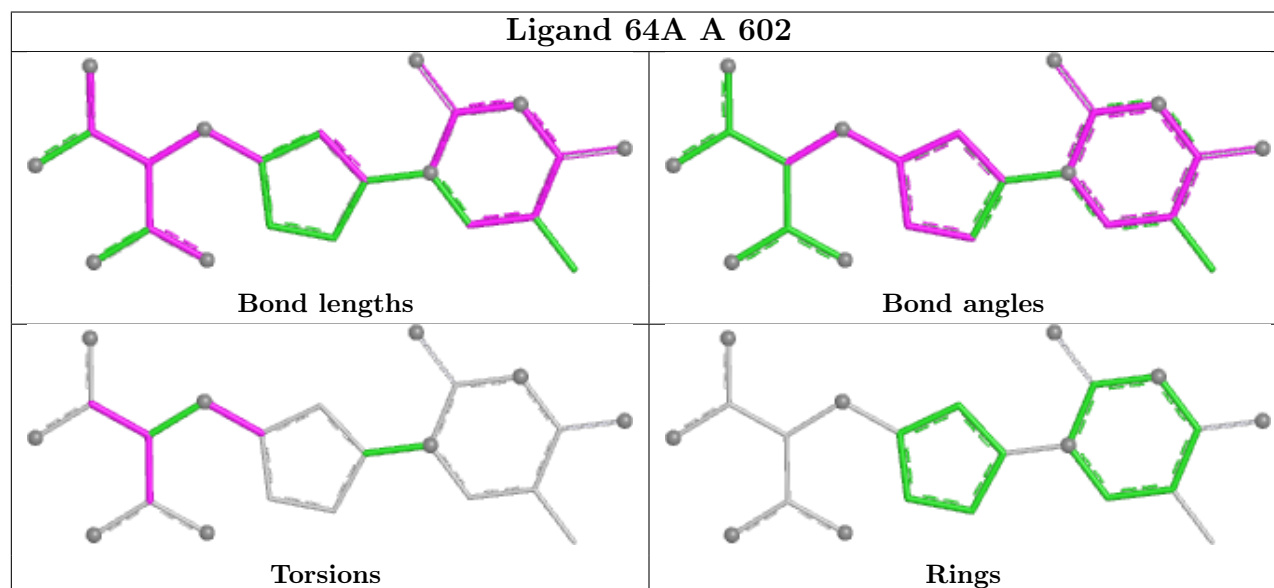
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	64A	2	0
8	B	2003	GOL	3	0
8	B	2005	GOL	1	0
8	B	2004	GOL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	603	GOL	2	0
8	A	605	GOL	1	0
8	D	502	GOL	1	0
8	D	505	GOL	1	0
8	B	2006	GOL	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 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	554/555 (99%)	-0.11	3 (0%) 87 83	44, 93, 169, 216	0
1	C	553/555 (99%)	0.05	10 (1%) 67 59	45, 127, 194, 218	0
2	B	416/444 (93%)	-0.26	2 (0%) 87 83	41, 80, 136, 170	1 (0%)
2	D	410/444 (92%)	-0.03	4 (0%) 79 74	48, 97, 152, 189	2 (0%)
3	E	33/38 (86%)	-0.15	0 100 100	111, 150, 171, 212	0
3	F	33/38 (86%)	-0.44	0 100 100	75, 108, 131, 169	0
All	All	1999/2074 (96%)	-0.09	19 (0%) 79 74	41, 95, 179, 218	3 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	73	LYS	3.5
1	A	62	ALA	3.3
2	B	88	TRP	3.1
1	A	63	ILE	3.0
2	D	318[A]	TYR	2.9

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.

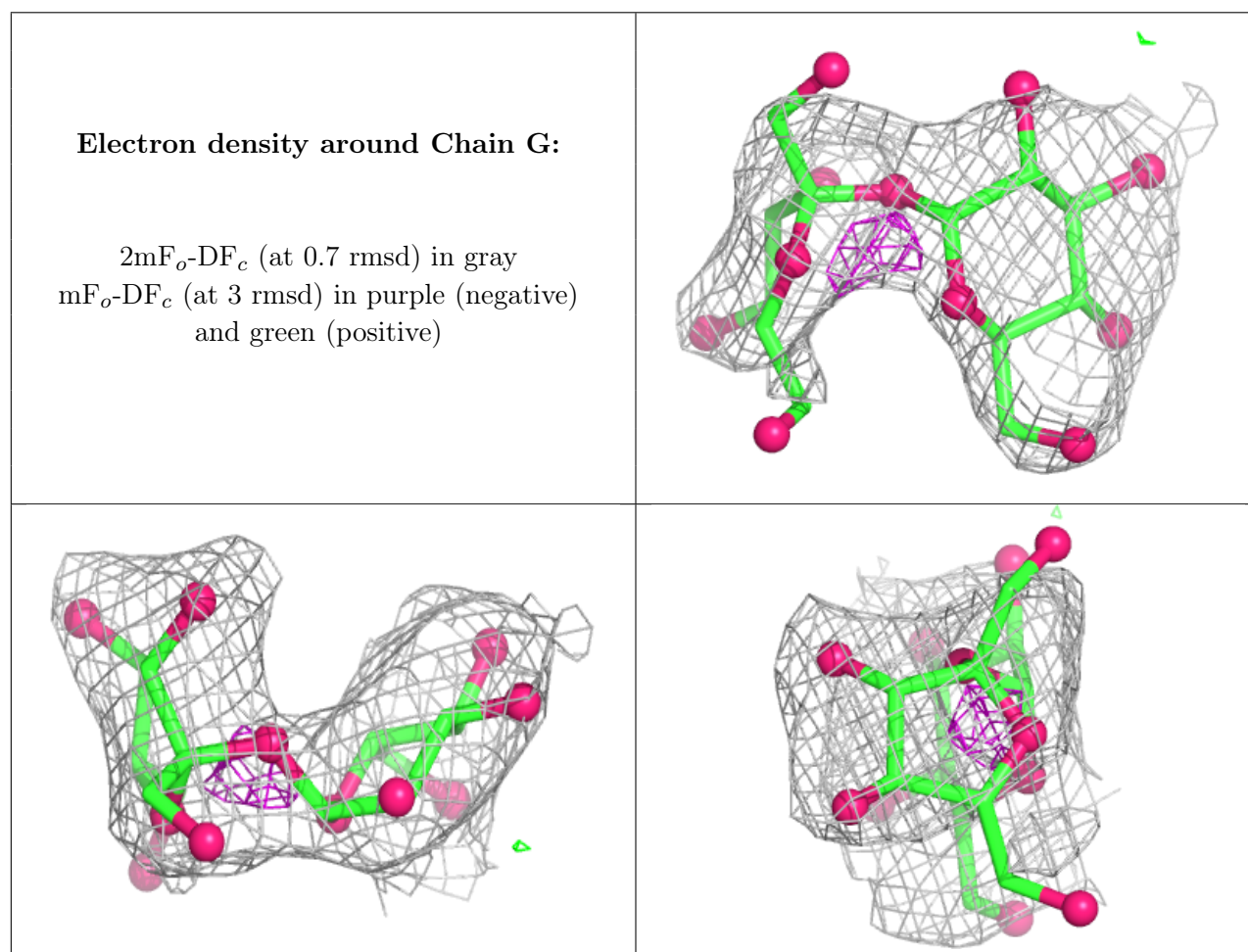
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OMC	E	2	21/22	0.79	0.10	147,150,154,159	0
3	OMC	E	4	21/22	0.87	0.11	127,138,145,157	0
3	OMC	F	2	21/22	0.94	0.08	86,96,102,111	0
3	OMC	F	4	21/22	0.96	0.09	70,76,81,83	0

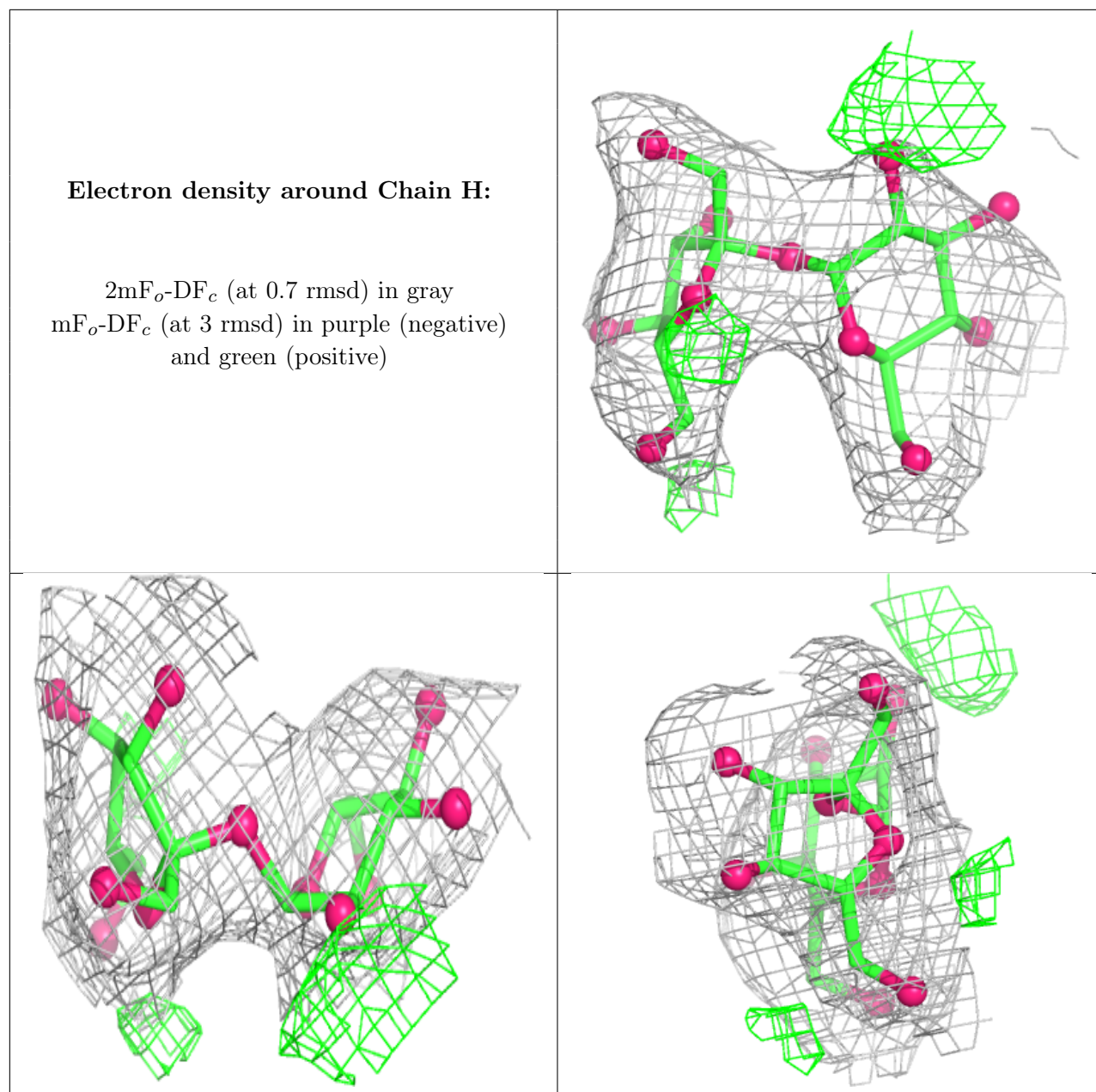
6.3 Carbohydrates [i](#)

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($\text{\AA}^2$)	Q<0.9
4	GLC	H	1	11/12	0.83	0.10	75,94,96,103	0
4	FRU	H	2	12/12	0.90	0.09	87,97,105,105	0
4	FRU	G	2	12/12	0.94	0.11	75,91,96,98	0
4	GLC	G	1	11/12	0.95	0.10	71,79,93,93	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.





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	D	505	6/6	0.79	0.15	75,82,92,92	0
6	64A	A	602	22/22	0.84	0.10	93,110,118,119	0
8	GOL	D	502	6/6	0.86	0.16	81,87,88,93	0

Continued on next page...

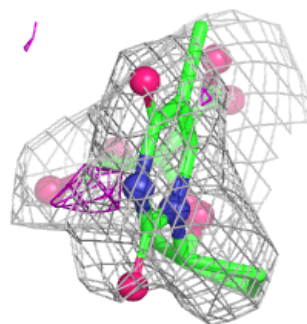
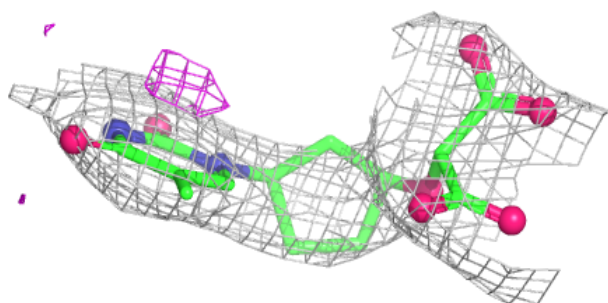
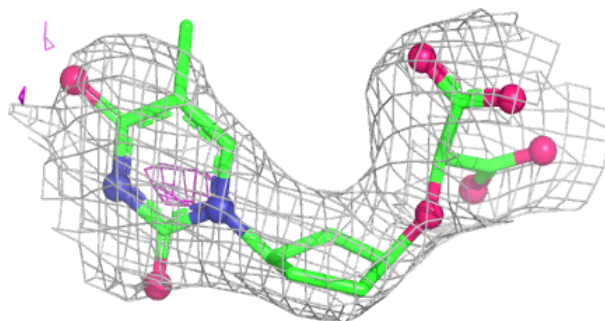
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	A	604	5/5	0.87	0.10	100,118,133,135	0
8	GOL	B	2002	6/6	0.87	0.12	57,69,71,76	0
7	SO4	C	602	5/5	0.88	0.10	104,121,122,131	0
8	GOL	C	603	6/6	0.88	0.14	112,126,133,133	0
8	GOL	D	504	6/6	0.91	0.10	79,98,104,106	0
5	MG	A	603	1/1	0.91	0.08	82,82,82,82	0
5	MG	A	601	1/1	0.92	0.08	109,109,109,109	0
8	GOL	D	503	6/6	0.92	0.16	66,75,83,83	0
8	GOL	B	2006	6/6	0.92	0.16	59,64,74,82	0
8	GOL	A	605	6/6	0.92	0.09	61,82,84,89	0
8	GOL	B	2005	6/6	0.93	0.14	60,64,66,72	0
8	GOL	B	2004	6/6	0.94	0.14	70,76,80,96	0
8	GOL	B	2003	6/6	0.95	0.11	56,59,64,73	0
5	MG	C	601	1/1	0.96	0.04	81,81,81,81	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 64A 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.