



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 10:17 AM BST

PDB ID : 6O9E
Title : Structure of HIV-1 Reverse Transcriptase in complex with DNA and INDOPY-1
Authors : Ruiz, F.X.; Hoang, A.; Das, K.; Arnold, E.
Deposited on : 2019-03-13
Resolution : 2.40 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 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

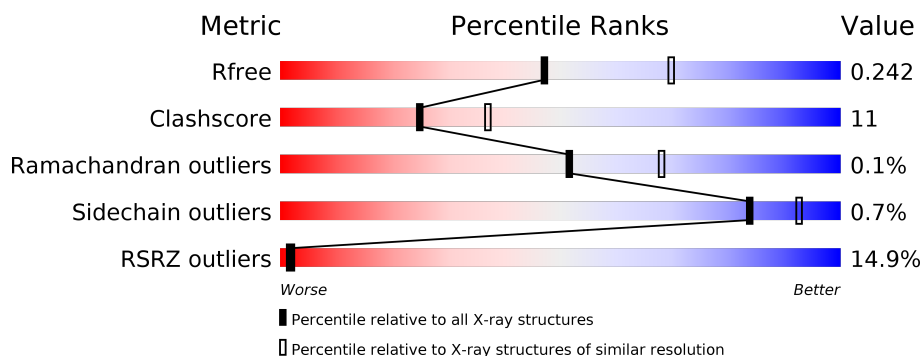
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 ≥ 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>13%</div> <div> <div>75%</div> <div>25%</div> </div> </div>
1	C	555	<div> <div>23%</div> <div> <div>76%</div> <div>23%</div> </div> </div>
2	B	429	<div> <div>10%</div> <div> <div>80%</div> <div>16%</div> </div> </div>
2	D	429	<div> <div>14%</div> <div> <div>78%</div> <div>17%</div> </div> </div>
3	E	38	<div> <div>32%</div> <div> <div>55%</div> <div>5%</div> <div>8%</div> </div> </div>
3	F	38	<div> <div>47%</div> <div> <div>39%</div> <div>5%</div> <div>8%</div> </div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GLC	H	1	-	-	X	-
5	SO4	B	502	-	-	X	-
6	NH4	A	603	-	-	-	X
6	NH4	C	604	-	-	-	X
8	PEG	B	506	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17591 atoms, of which 8 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 Reverse transcriptase p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	1	0
			4510	2920	751	832	7			
1	C	553	Total	C	N	O	S	0	0	0
			4504	2916	750	831	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366
A	498	ASN	ASP	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366
C	498	ASN	ASP	engineered mutation	UNP P03366

- Molecule 2 is a protein called Reverse transcriptase p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	415	Total	C	N	O	S	0	1	0
			3434	2239	567	621	7			
2	D	410	Total	C	N	O	S	0	2	0
			3409	2225	562	615	7			

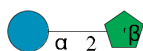
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	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).

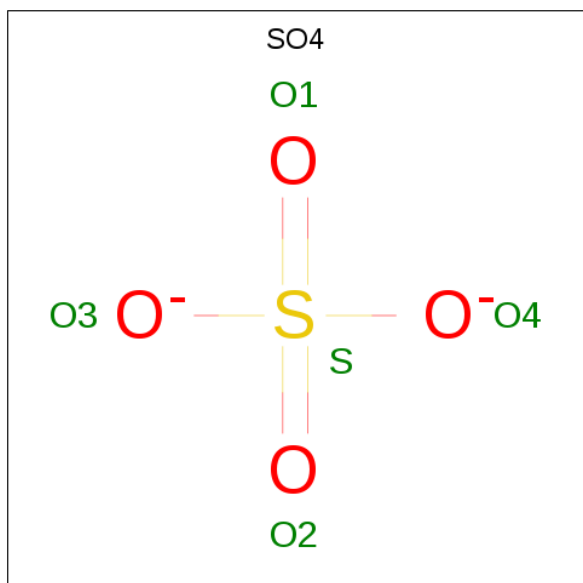
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	35	Total	C	N	O	P	0	0	0
			720	341	129	215	35			
3	E	35	Total	C	N	O	P	0	0	0
			720	341	129	215	35			

- 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			
4	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



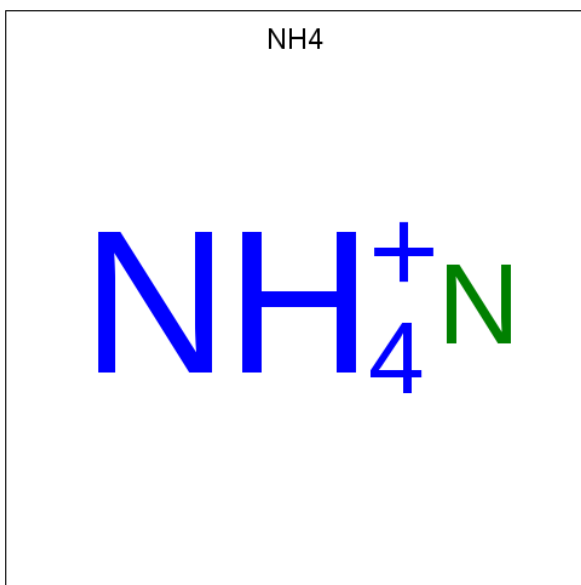
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 6 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



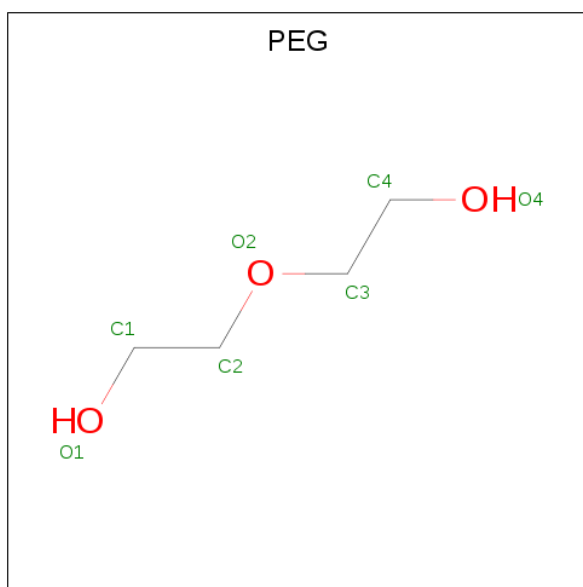
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	H	N	0	0
			5	4	1		
6	C	1	Total	H	N	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



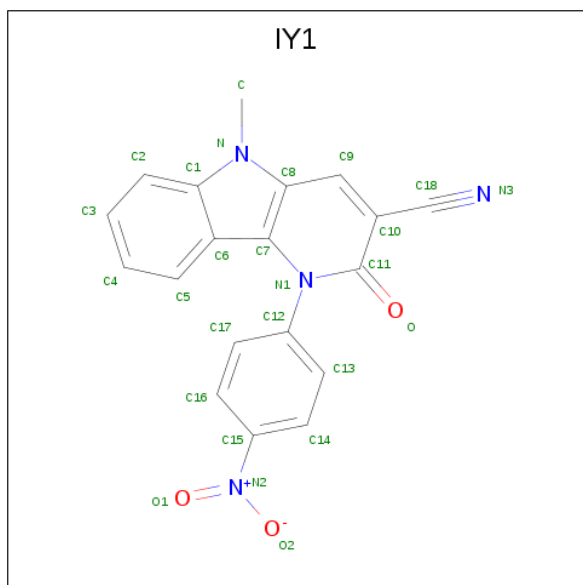
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		

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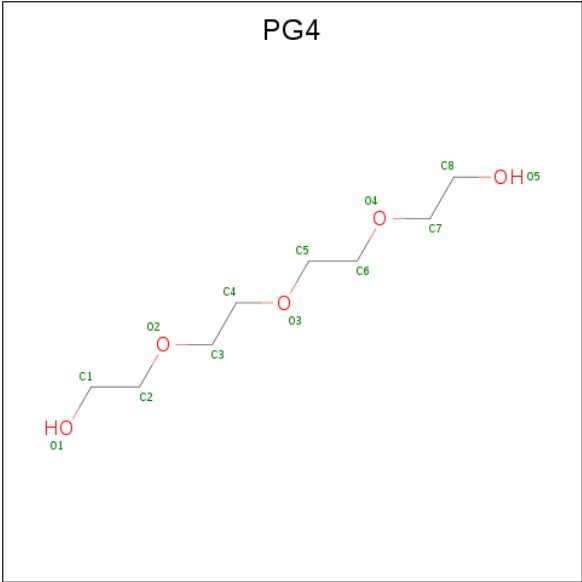
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 5-methyl-1-(4-nitrophenyl)-2-oxo-2,5-dihydro-1H-pyrido[3,2-b]indole-3-carbonitrile (three-letter code: IY1) (formula: C₁₉H₁₂N₄O₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	F	1	Total	C	N	O	0	0
			26	19	4	3		
9	E	1	Total	C	N	O	0	0
			26	19	4	3		

- Molecule 10 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	C	O	0	0
			13	8	5		

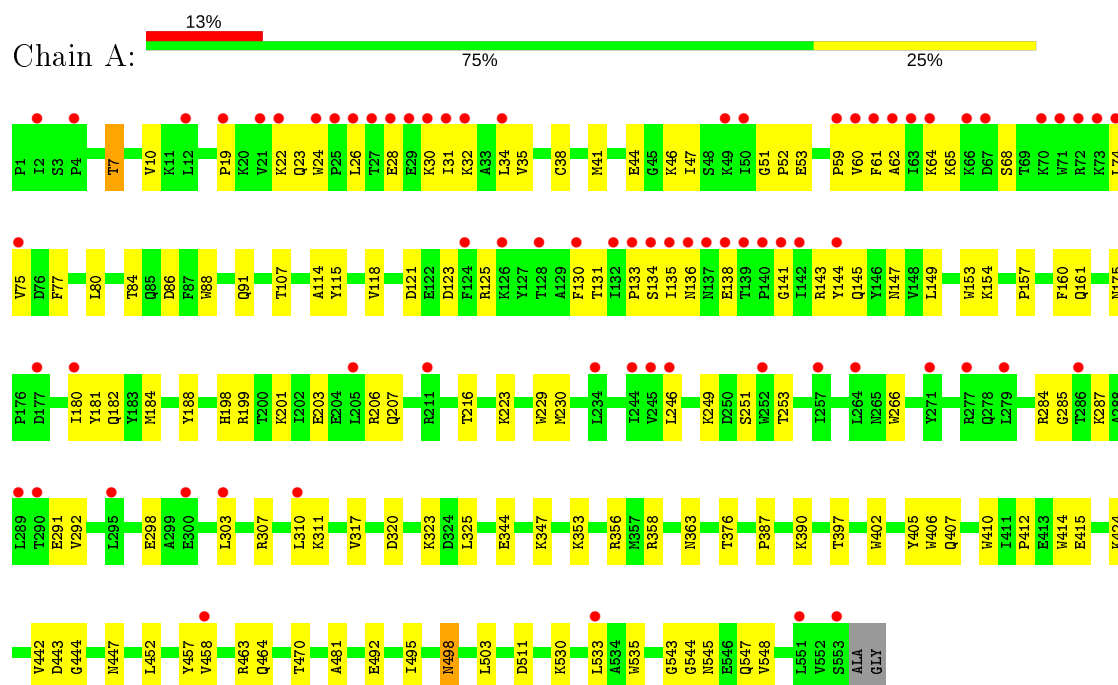
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	32	Total	O	0	0
			32	32		
11	B	35	Total	O	0	0
			35	35		
11	C	21	Total	O	0	0
			21	21		
11	D	15	Total	O	0	0
			15	15		
11	F	3	Total	O	0	0
			3	3		
11	E	5	Total	O	0	0
			5	5		

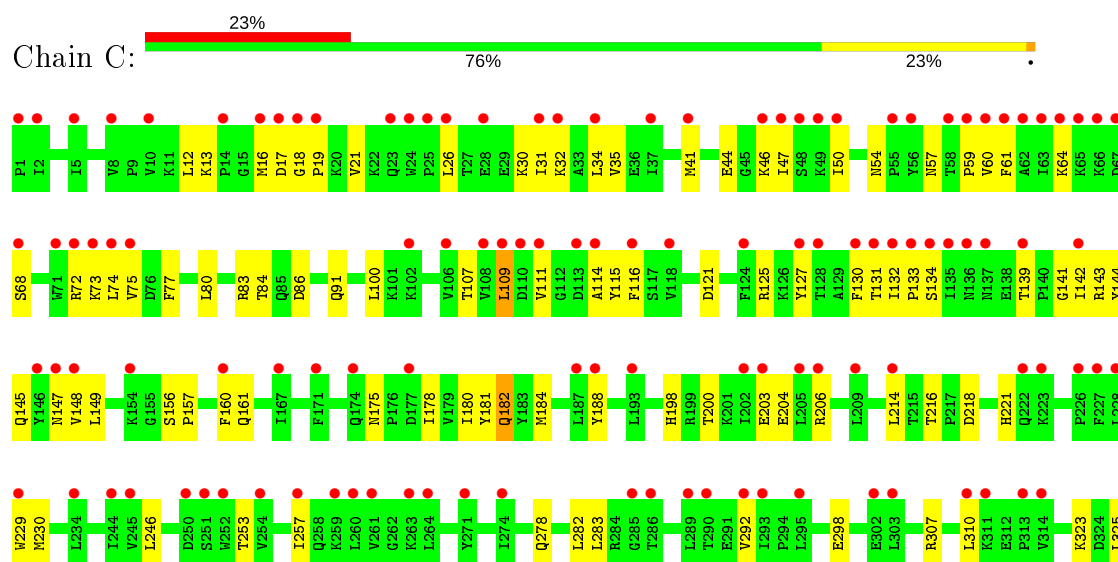
3 Residue-property plots

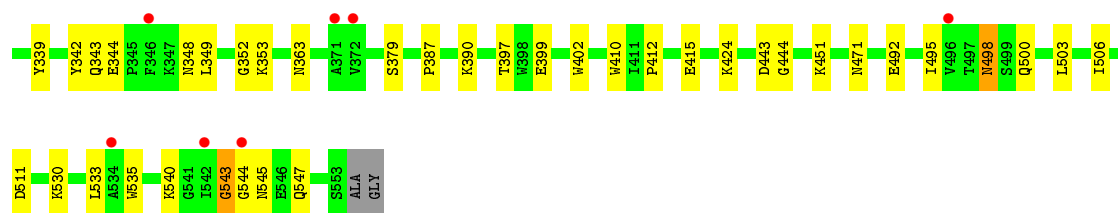
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reverse transcriptase p66

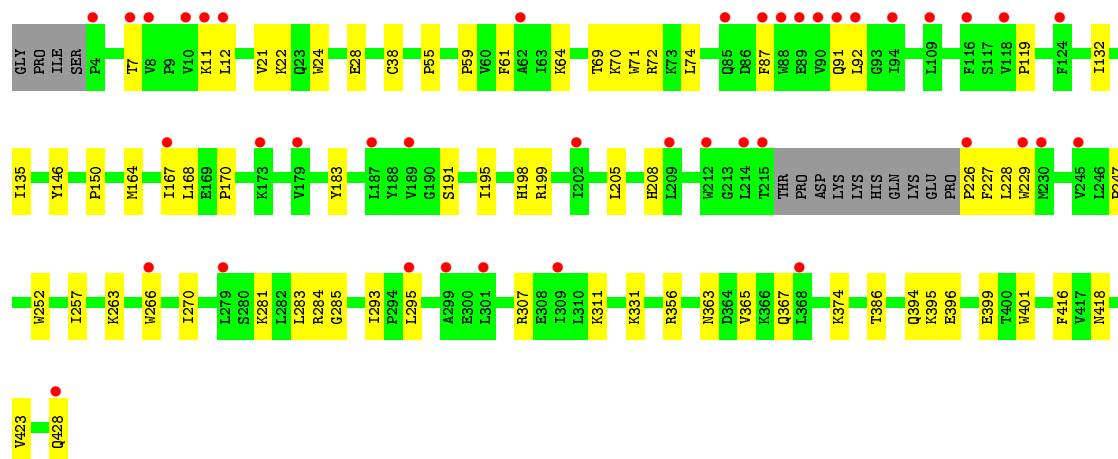
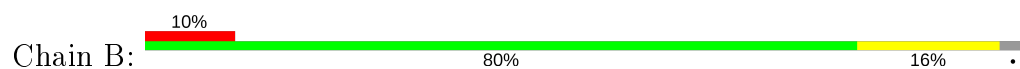


• Molecule 1: Reverse transcriptase p66

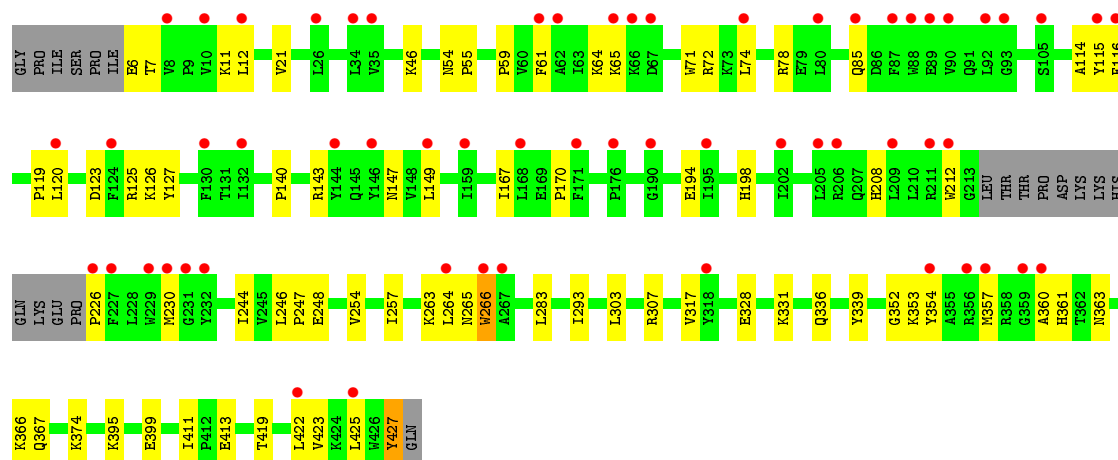
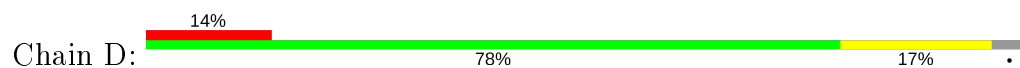




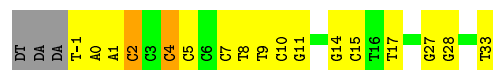
• Molecule 2: Reverse transcriptase p51



• Molecule 2: Reverse transcriptase p51



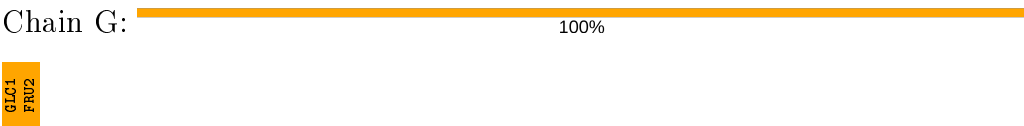
• Molecule 3: DNA (38-MER)



● 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, α , β , γ	89.76Å 127.66Å 131.61Å 90.00° 101.50° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 90.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.40) 99.8 (90.73-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.203 , 0.242 0.203 , 0.242	Depositor DCC
R_{free} test set	1998 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å ²)	73.6	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17591	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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, GLC, NH4, PG4, IY1, SO4, FRU, PEG

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	0.23	0/4631	0.42	0/6291
1	C	0.23	0/4622	0.42	0/6279
2	B	0.24	0/3534	0.41	0/4800
2	D	0.24	0/3515	0.41	0/4775
3	E	0.46	0/759	0.91	0/1170
3	F	1.76	13/759 (1.7%)	1.11	7/1170 (0.6%)
All	All	0.44	13/17820 (0.1%)	0.50	7/24485 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	-1	DT	C3'-C2'	-24.94	1.22	1.52
3	F	-1	DT	C5-C6	20.66	1.48	1.34
3	F	-1	DT	C2-N3	15.30	1.50	1.37
3	F	-1	DT	N1-C2	14.36	1.49	1.38
3	F	-1	DT	C2'-C1'	10.59	1.62	1.52
3	F	-1	DT	N1-C6	9.92	1.45	1.38
3	F	-1	DT	N3-C4	9.42	1.46	1.38
3	F	-1	DT	O4'-C1'	-9.38	1.31	1.42
3	F	-1	DT	C5'-C4'	-8.40	1.42	1.51
3	F	-1	DT	C4'-C3'	6.90	1.60	1.53
3	F	-1	DT	C3'-O3'	6.43	1.52	1.44
3	F	-1	DT	P-O5'	5.71	1.65	1.59
3	F	-1	DT	C5-C7	5.07	1.53	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	-1	DT	C2-N3-C4	-11.48	120.31	127.20
3	F	-1	DT	N1-C2-N3	8.47	119.68	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	-1	DT	N3-C4-C5	7.35	119.61	115.20
3	F	-1	DT	OP1-P-OP2	-7.15	108.87	119.60
3	F	-1	DT	C1'-O4'-C4'	-7.00	103.10	110.10
3	F	-1	DT	C5-C4-O4	-6.98	120.02	124.90
3	F	-1	DT	O4'-C1'-N1	5.68	111.97	108.00

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	4510	0	4575	117	0
1	C	4504	0	4567	99	0
2	B	3434	0	3465	62	0
2	D	3409	0	3438	64	0
3	E	720	0	398	27	0
3	F	720	0	398	16	0
4	G	23	0	21	5	0
4	H	23	0	21	9	0
5	A	10	0	0	0	0
5	B	10	0	0	3	0
5	C	10	0	0	0	0
6	A	1	4	0	0	0
6	C	1	4	0	0	0
7	B	12	0	16	1	0
7	C	6	0	8	1	0
8	B	14	0	20	7	0
9	E	26	0	0	1	0
9	F	26	0	0	2	0
10	E	13	0	18	2	0
11	A	32	0	0	0	0
11	B	35	0	0	1	0
11	C	21	0	0	1	0
11	D	15	0	0	1	0
11	E	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	3	0	0	0	0
All	All	17583	8	16945	367	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.

All (367) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:LYS:HE3	2:B:226:PRO:HD2	1.38	1.03
2:D:257:ILE:HD12	2:D:293:ILE:HD11	1.44	0.98
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.46	0.96
3:E:4:OMC:H5	3:E:30:DG:H1	1.16	0.91
1:C:246:LEU:HD13	1:C:307:ARG:HD3	1.54	0.90
1:A:199:ARG:HH12	1:A:223:LYS:HD3	1.40	0.86
1:C:246:LEU:HD11	1:C:310:LEU:HD12	1.56	0.86
2:D:360:ALA:HB3	2:D:366:LYS:HD3	1.60	0.83
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.60	0.83
2:D:120:LEU:H	2:D:125:ARG:HH21	1.23	0.82
3:F:17:DT:H5"	3:F:17:DT:H6	1.44	0.82
2:B:24:TRP:CE3	5:B:502:SO4:O3	2.34	0.80
2:D:64:LYS:HE3	2:D:71:TRP:CZ2	2.16	0.80
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.64	0.80
1:A:134:SER:OG	1:A:141:GLY:HA2	1.82	0.80
1:A:47:ILE:CG2	1:A:144:TYR:HB3	2.14	0.77
1:C:184:MET:SD	3:F:33:DT:H1'	2.26	0.75
2:B:374:LYS:NZ	8:B:506:PEG:H11	2.03	0.74
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.22	0.74
1:A:543:GLY:N	2:B:283:LEU:O	2.20	0.73
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.71	0.73
1:A:91:GLN:NE2	1:A:161:GLN:OE1	2.22	0.72
1:C:34:LEU:HD22	1:C:73:LYS:HG3	1.72	0.71
3:E:17:DT:H6	3:E:17:DT:H5"	1.54	0.71
1:A:320:ASP:OD2	1:A:323:LYS:NZ	2.23	0.71
1:C:114:ALA:HB3	9:F:101:IY1:O1	1.90	0.71
1:C:41:MET:HB3	1:C:46:LYS:HB2	1.73	0.70
1:A:284:ARG:NH2	3:E:8:DT:OP2	2.24	0.70
1:A:503:LEU:CD1	1:A:535:TRP:HB2	2.22	0.70
2:D:247:PRO:HG3	2:D:427:TYR:OH	1.93	0.69
1:A:203:GLU:O	1:A:207:GLN:HG2	1.93	0.69
2:B:374:LYS:HZ2	8:B:506:PEG:H11	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.74	0.68
2:D:65:LYS:HD3	2:D:230:MET:HE1	1.76	0.68
1:A:61:PHE:CZ	3:E:-1:DT:H2"	2.30	0.67
2:D:170:PRO:HB2	2:D:208:HIS:HE1	1.59	0.67
4:H:1:GLC:O6	4:H:1:GLC:H2	1.95	0.67
2:D:72:ARG:CG	2:D:226:PRO:HB3	2.25	0.66
2:B:70:LYS:CE	2:B:226:PRO:HD2	2.21	0.66
1:C:390:LYS:NZ	1:C:415:GLU:OE2	2.27	0.66
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.30	0.66
4:H:1:GLC:C6	4:H:1:GLC:H2	2.26	0.66
2:D:263:LYS:HA	2:D:423:VAL:HG11	1.77	0.65
1:A:74:LEU:HD22	3:E:0:DA:C6	2.31	0.65
4:H:1:GLC:O5	4:H:2:FRU:O6	2.12	0.65
1:A:28:GLU:OE2	1:A:136:ASN:ND2	2.30	0.65
1:A:74:LEU:HB2	3:E:0:DA:C2	2.30	0.65
2:B:7:THR:HG22	2:B:119:PRO:HB2	1.78	0.65
2:D:125:ARG:NH2	2:D:147:ASN:O	2.29	0.65
1:C:511:ASP:HB2	7:C:603:GOL:H11	1.78	0.65
1:A:458:VAL:HG23	1:A:464:GLN:HG2	1.79	0.64
2:D:78:ARG:CZ	4:H:2:FRU:H12	2.27	0.64
1:C:61:PHE:CZ	1:C:74:LEU:HD11	2.32	0.64
1:C:323:LYS:NZ	1:C:344:GLU:OE2	2.31	0.64
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.31	0.63
1:C:543:GLY:HA2	2:D:283:LEU:O	1.98	0.63
1:A:206:ARG:NH2	1:A:216:THR:O	2.32	0.63
2:D:72:ARG:HG3	2:D:226:PRO:HB3	1.80	0.63
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.39	0.63
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.80	0.62
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.81	0.62
2:D:78:ARG:NH1	4:H:2:FRU:H12	2.15	0.61
1:C:544:GLY:HA2	1:C:547:GLN:HG2	1.83	0.61
1:A:406:TRP:HD1	1:A:407[B]:GLN:HE21	1.45	0.61
2:B:24:TRP:CZ3	5:B:502:SO4:O3	2.52	0.61
2:B:266:TRP:HZ3	2:B:270:ILE:HD11	1.64	0.61
1:C:500:GLN:HG3	11:C:702:HOH:O	2.01	0.61
4:G:1:GLC:H61	4:G:2:FRU:O6	2.01	0.61
2:D:120:LEU:H	2:D:125:ARG:NH2	1.98	0.61
4:G:1:GLC:H4	4:G:2:FRU:O6	2.01	0.60
2:B:69:THR:HG22	11:B:620:HOH:O	2.00	0.60
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.82	0.60
1:A:28:GLU:HG2	1:A:136:ASN:OD1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:HG3	1:C:216:THR:OG1	2.02	0.60
10:E:101:PG4:H41	10:E:101:PG4:O4	2.02	0.60
3:E:4:OMC:H5	3:E:30:DG:N1	1.95	0.60
2:D:354:TYR:CE1	2:D:374:LYS:HD2	2.37	0.60
1:A:246:LEU:HD13	1:A:307:ARG:HD3	1.84	0.60
2:D:419:THR:HG23	2:D:419:THR:O	2.02	0.59
1:C:64:LYS:HE3	1:C:68:SER:O	2.02	0.59
1:A:253:THR:HA	1:A:292:VAL:HA	1.84	0.59
1:A:406:TRP:CD1	1:A:407[B]:GLN:HG2	2.38	0.59
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.83	0.59
2:B:167:ILE:O	2:B:208:HIS:NE2	2.27	0.59
2:B:191:SER:OG	2:B:198:HIS:ND1	2.26	0.59
1:C:34:LEU:CD2	1:C:73:LYS:HG3	2.33	0.59
1:C:498:ASN:OD1	1:C:545:ASN:OD1	2.21	0.59
2:D:6:GLU:OE1	2:D:6:GLU:N	2.36	0.59
2:B:266:TRP:HZ3	2:B:270:ILE:CD1	2.16	0.58
1:C:115:TYR:HB3	1:C:149:LEU:O	2.04	0.58
1:A:452:LEU:HD23	1:A:470:THR:HA	1.84	0.58
1:A:51:GLY:O	1:A:143:ARG:NH1	2.36	0.58
1:C:253:THR:HA	1:C:292:VAL:HA	1.86	0.58
2:D:11:LYS:HG2	2:D:85:GLN:OE1	2.04	0.57
7:B:504:GOL:O3	7:B:504:GOL:O1	2.03	0.57
1:C:100:LEU:HD11	1:C:229:TRP:CZ3	2.40	0.57
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.86	0.57
2:D:263:LYS:HE3	2:D:425:LEU:HA	1.87	0.57
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.39	0.57
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.86	0.57
1:C:46:LYS:O	1:C:147:ASN:HB2	2.03	0.57
1:C:353:LYS:NZ	3:F:7:DC:OP1	2.36	0.57
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.87	0.56
2:B:374:LYS:HZ2	8:B:506:PEG:H31	1.69	0.56
1:C:57:ASN:OD1	1:C:131:THR:HG23	2.04	0.56
2:D:254:VAL:HG13	2:D:283:LEU:HD22	1.86	0.56
3:E:1:DA:H2'	3:E:2:OMC:C6	2.41	0.56
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.40	0.56
1:C:12:LEU:HD11	1:C:127:TYR:CE1	2.41	0.56
2:B:307:ARG:O	2:B:311:LYS:HG3	2.05	0.56
3:F:14:DG:H2''	3:F:15:DC:C5	2.40	0.56
3:F:1:DA:H2'	3:F:2:OMC:C6	2.41	0.56
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.87	0.55
2:D:114:ALA:HB1	2:D:212:TRP:HZ3	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:357:MET:SD	2:D:361:HIS:NE2	2.79	0.55
1:C:257:ILE:HB	1:C:283:LEU:HD21	1.87	0.55
1:A:544:GLY:O	1:A:548:VAL:HG12	2.07	0.55
1:C:30:LYS:O	1:C:34:LEU:HG	2.06	0.55
2:B:374:LYS:NZ	8:B:506:PEG:H31	2.21	0.55
1:A:41:MET:HB3	1:A:46:LYS:HB2	1.88	0.55
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.42	0.55
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.08	0.54
2:B:281:LYS:HE2	2:B:284:ARG:HH21	1.72	0.54
1:A:358:ARG:NH2	2:B:394:GLN:HE22	2.06	0.54
4:H:1:GLC:C2	4:H:1:GLC:C6	2.85	0.54
1:A:107:THR:OG1	1:A:198:HIS:NE2	2.30	0.54
1:C:26:LEU:HD12	1:C:133:PRO:HD2	1.90	0.54
2:B:257:ILE:HD12	2:B:293:ILE:HD11	1.90	0.54
1:A:86:ASP:O	2:B:55:PRO:HB3	2.06	0.54
2:D:244:ILE:HD13	2:D:425:LEU:HD11	1.90	0.54
1:A:32:LYS:O	1:A:35:VAL:HG12	2.07	0.53
2:D:257:ILE:HD12	2:D:293:ILE:CD1	2.28	0.53
3:E:14:DG:H2''	3:E:15:DC:C5	2.44	0.53
1:A:358:ARG:NH2	2:B:394:GLN:NE2	2.56	0.53
1:C:19:PRO:HD3	1:C:80:LEU:HD13	1.89	0.53
1:A:31:ILE:HG23	1:A:133:PRO:O	2.09	0.53
1:A:397:THR:HG21	1:A:424:LYS:HA	1.91	0.53
2:B:263:LYS:HA	2:B:423:VAL:HG11	1.90	0.53
2:B:168:LEU:HD22	2:B:205:LEU:HD11	1.90	0.53
1:A:115:TYR:HB3	1:A:149:LEU:O	2.09	0.52
1:A:285:GLY:N	3:E:9:DT:OP1	2.42	0.52
1:C:132:ILE:CG2	1:C:142:ILE:HG12	2.39	0.52
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.09	0.52
1:A:199:ARG:NH1	1:A:223:LYS:HD3	2.16	0.52
2:B:247:PRO:HD3	2:B:428:GLN:OE1	2.07	0.52
1:C:75:VAL:HB	1:C:77:PHE:CE2	2.45	0.52
3:F:8:DT:H2'	3:F:9:DT:H71	1.91	0.52
1:A:61:PHE:CZ	1:A:74:LEU:HD11	2.45	0.52
1:A:543:GLY:HA2	2:B:285:GLY:O	2.09	0.52
1:C:31:ILE:HA	1:C:132:ILE:HD11	1.92	0.52
1:C:182:GLN:HG3	1:C:182:GLN:O	2.10	0.52
1:A:61:PHE:HZ	3:E:-1:DT:H2''	1.74	0.52
1:A:114:ALA:HB3	9:E:102:IY1:O1	2.09	0.52
2:D:61:PHE:CZ	2:D:74:LEU:HD23	2.45	0.51
1:C:19:PRO:HG3	1:C:80:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:15:DC:H2"	3:E:17:DT:H73	1.90	0.51
1:C:495:ILE:HB	1:C:533:LEU:HD23	1.93	0.51
1:C:13:LYS:HE3	1:C:84:THR:O	2.11	0.51
3:F:27:DG:H2"	3:F:28:DG:OP2	2.10	0.51
1:C:540:LYS:HE3	2:D:265:ASN:OD1	2.11	0.51
1:C:107:THR:OG1	1:C:198:HIS:NE2	2.36	0.51
1:A:182:GLN:HG3	1:A:182:GLN:O	2.11	0.51
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.46	0.50
1:C:503:LEU:CD2	1:C:535:TRP:HB2	2.37	0.50
1:A:74:LEU:HD22	3:E:0:DA:N1	2.26	0.50
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.47	0.50
1:A:303:LEU:O	1:A:307:ARG:HG2	2.12	0.50
1:A:307:ARG:O	1:A:311:LYS:HG3	2.12	0.50
1:C:134:SER:OG	1:C:139:THR:O	2.20	0.50
1:C:443:ASP:OD1	1:C:444:GLY:N	2.45	0.50
3:E:13:DT:H5"	11:E:202:HOH:O	2.12	0.50
1:A:65:LYS:HB3	1:A:68:SER:HB3	1.93	0.50
1:C:21:VAL:HB	1:C:59:PRO:HD3	1.93	0.50
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.47	0.50
1:A:358:ARG:HH22	2:B:394:GLN:HE22	1.59	0.50
1:A:30:LYS:O	1:A:34:LEU:HG	2.11	0.50
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.46	0.49
1:C:47:ILE:HG23	1:C:145:GLN:O	2.12	0.49
2:D:266:TRP:CE3	2:D:423:VAL:HB	2.47	0.49
1:C:132:ILE:HG21	1:C:142:ILE:HG12	1.94	0.49
1:A:180:ILE:HA	1:A:188:TYR:O	2.11	0.49
1:C:132:ILE:O	1:C:141:GLY:HA3	2.13	0.49
1:C:142:ILE:HD12	1:C:144:TYR:HE2	1.78	0.49
1:A:199:ARG:O	1:A:203:GLU:HG2	2.12	0.49
1:A:23:GLN:HE21	1:A:26:LEU:HD21	1.78	0.49
2:B:363:ASN:O	2:B:367:GLN:HG3	2.13	0.49
2:B:395:LYS:NZ	2:B:399:GLU:OE2	2.40	0.49
3:E:21:DA:C6	3:E:22:DC:N4	2.81	0.49
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.48	0.48
1:A:175:ASN:OD1	1:A:201:LYS:HE2	2.13	0.48
3:F:4:OMC:H2'	3:F:5:DC:C6	2.48	0.48
2:B:227:PHE:HB3	2:B:229:TRP:HD1	1.78	0.48
1:C:121:ASP:O	1:C:125:ARG:HG3	2.13	0.48
2:D:413:GLU:OE2	4:H:2:FRU:H3	2.14	0.48
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.95	0.48
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:GLN:OE1	2:B:396[A]:GLU:OE1	2.32	0.48
1:C:503:LEU:HD11	1:C:533:LEU:HB3	1.96	0.48
3:F:17:DT:H5"	3:F:17:DT:C6	2.35	0.48
1:A:131:THR:HG22	1:A:143:ARG:CG	2.32	0.48
1:C:402:TRP:O	2:D:331:LYS:NZ	2.45	0.48
2:D:72:ARG:HG2	2:D:226:PRO:HB3	1.96	0.48
1:C:50:ILE:HD13	1:C:145:GLN:HB3	1.95	0.48
3:F:0:DA:H8	3:F:0:DA:O5'	1.97	0.48
2:B:399:GLU:OE2	4:G:2:FRU:H12	2.14	0.47
2:D:120:LEU:HB3	2:D:125:ARG:HE	1.80	0.47
1:C:17:ASP:O	1:C:83:ARG:HD3	2.14	0.47
2:B:394:GLN:NE2	3:E:23:DC:OP1	2.47	0.47
2:B:164:MET:HE2	2:B:168:LEU:HD11	1.96	0.47
2:B:183:TYR:OH	2:B:386:THR:HG23	2.14	0.47
1:A:51:GLY:N	1:A:52:PRO:CD	2.78	0.47
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.78	0.47
2:D:7:THR:HG22	2:D:119:PRO:HB2	1.96	0.47
2:D:395:LYS:NZ	2:D:399:GLU:OE2	2.41	0.47
1:A:498:ASN:OD1	1:A:545:ASN:ND2	2.36	0.47
1:C:50:ILE:HD12	1:C:54:ASN:ND2	2.30	0.47
2:D:114:ALA:HB1	2:D:212:TRP:CZ3	2.49	0.47
1:C:91:GLN:OE1	1:C:161:GLN:NE2	2.45	0.47
3:E:21:DA:C5	3:E:22:DC:N4	2.82	0.47
3:F:10:DC:H2"	3:F:11:DG:C8	2.49	0.47
3:F:2:OMC:O5'	3:F:2:OMC:H6	1.97	0.47
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.97	0.47
1:C:41:MET:O	1:C:46:LYS:N	2.46	0.47
2:B:170:PRO:HB2	2:B:208:HIS:HE1	1.79	0.47
1:C:206:ARG:CG	1:C:216:THR:OG1	2.61	0.47
2:B:11:LYS:HG3	2:B:12:LEU:N	2.30	0.46
2:B:87:PHE:O	2:B:92:LEU:N	2.48	0.46
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.41	0.46
1:C:111:VAL:HG11	1:C:214:LEU:HD22	1.98	0.46
2:B:266:TRP:CZ3	2:B:270:ILE:HD11	2.47	0.46
1:A:118:VAL:HG11	1:A:149:LEU:HD11	1.97	0.46
1:A:246:LEU:HB3	1:A:307:ARG:NH1	2.30	0.46
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.50	0.46
1:C:156:SER:HB2	1:C:157:PRO:HD3	1.97	0.46
1:C:32:LYS:O	1:C:35:VAL:HG12	2.15	0.46
2:D:123:ASP:O	2:D:126:LYS:NZ	2.48	0.46
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:LEU:HD11	2:D:127:TYR:CE1	2.51	0.46
1:A:544:GLY:HA2	1:A:547:GLN:HG2	1.98	0.46
1:A:52:PRO:HD2	1:A:53:GLU:OE1	2.15	0.46
1:C:60:VAL:CG2	1:C:130:PHE:HB2	2.46	0.46
2:D:360:ALA:CB	2:D:366:LYS:HD3	2.39	0.46
2:B:24:TRP:CD2	5:B:502:SO4:O3	2.67	0.45
1:C:257:ILE:HD13	1:C:282:LEU:HD12	1.98	0.45
1:C:342:TYR:HB3	1:C:348:ASN:HA	1.97	0.45
1:C:161:GLN:HE21	2:D:140:PRO:HG3	1.81	0.45
2:D:194:GLU:O	2:D:198:HIS:N	2.45	0.45
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.81	0.45
1:A:7:THR:OG1	1:A:121:ASP:HA	2.16	0.45
2:B:374:LYS:HZ3	8:B:506:PEG:H11	1.78	0.45
2:D:317:VAL:O	2:D:317:VAL:HG23	2.16	0.45
1:A:121:ASP:O	1:A:125:ARG:HG3	2.17	0.45
1:A:47:ILE:HG23	1:A:145:GLN:O	2.17	0.45
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.47	0.45
2:D:248:GLU:HB3	11:D:602:HOH:O	2.16	0.45
1:A:44:GLU:CG	1:A:46:LYS:HE2	2.46	0.45
3:E:10:DC:H2''	3:E:11:DG:C8	2.52	0.45
4:G:1:GLC:O5	4:G:2:FRU:H4	2.16	0.45
1:A:75:VAL:HB	1:A:77:PHE:CE2	2.52	0.45
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.52	0.45
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.51	0.45
1:C:325:LEU:HB3	1:C:387:PRO:HB3	1.98	0.45
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.51	0.45
2:D:363:ASN:O	2:D:367:GLN:HG3	2.16	0.45
3:F:2:OMC:H1'	3:F:2:OMC:HM23	1.66	0.45
1:A:447:ASN:N	1:A:452:LEU:O	2.44	0.45
1:A:358:ARG:O	1:A:358:ARG:HG3	2.17	0.45
1:C:451:LYS:HB3	1:C:471:ASN:HA	1.98	0.45
1:C:506:ILE:HG21	1:C:533:LEU:HD11	1.99	0.45
1:A:325:LEU:HB3	1:A:387:PRO:HB3	1.99	0.44
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.52	0.44
2:D:246:LEU:CD1	2:D:264:LEU:HD21	2.46	0.44
3:E:27:DG:H2''	3:E:28:DG:OP2	2.17	0.44
1:C:131:THR:HG22	1:C:143:ARG:HG2	1.99	0.44
1:C:253:THR:HG22	1:C:292:VAL:HG22	1.98	0.44
2:B:28:GLU:HA	2:B:135:ILE:HD11	1.98	0.44
1:A:249:LYS:HG3	1:A:251:SER:H	1.82	0.44
2:B:87:PHE:HB3	2:B:92:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PRO:HG2	3:F:2:OMC:O4'	2.18	0.44
1:C:18:GLY:HA3	1:C:127:TYR:HD1	1.83	0.44
1:A:266:TRP:CE2	3:E:31:DG:H4'	2.53	0.44
1:A:88:TRP:HZ2	2:B:22:LYS:HA	1.83	0.44
1:C:200:THR:O	1:C:204:GLU:HG3	2.18	0.44
1:A:23:GLN:HG3	1:A:24:TRP:O	2.17	0.44
1:A:402:TRP:O	2:B:331:LYS:NZ	2.41	0.44
1:C:175:ASN:O	1:C:178:ILE:HG22	2.17	0.44
1:C:72:ARG:HH22	9:F:101:IY1:C8	2.31	0.44
3:E:21:DA:C4	3:E:22:DC:C4	3.05	0.44
2:B:11:LYS:HG3	2:B:12:LEU:O	2.18	0.43
1:C:125:ARG:HD3	1:C:147:ASN:HA	2.00	0.43
1:C:229:TRP:CE2	1:C:230:MET:HG2	2.53	0.43
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.99	0.43
2:D:65:LYS:HD3	2:D:230:MET:CE	2.45	0.43
2:D:336:GLN:OE1	2:D:353:LYS:HE3	2.18	0.43
1:A:157:PRO:HB3	1:A:184:MET:CE	2.49	0.43
1:A:443:ASP:OD1	1:A:444:GLY:N	2.49	0.43
1:A:287:LYS:HB3	1:A:291:GLU:OE1	2.17	0.43
1:A:405:TYR:CE2	1:A:407[A]:GLN:HB2	2.54	0.43
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.00	0.43
2:B:164:MET:CE	2:B:168:LEU:HD11	2.48	0.43
2:D:361:HIS:CD2	2:D:361:HIS:O	2.72	0.43
1:A:135:ILE:HG13	1:A:138:GLU:HB3	2.00	0.43
4:H:1:GLC:C1	4:H:2:FRU:C6	2.96	0.43
1:C:492:GLU:HG2	1:C:530:LYS:HB2	2.00	0.43
1:A:157:PRO:HB3	1:A:184:MET:HE1	2.01	0.43
2:B:374:LYS:HG2	8:B:506:PEG:H11	2.01	0.43
3:E:2:OMC:H1'	3:E:2:OMC:HM23	1.67	0.43
1:A:353:LYS:NZ	3:E:7:DC:OP1	2.50	0.43
3:E:4:OMC:H1'	3:E:4:OMC:HM22	1.55	0.43
1:C:109:LEU:HD23	1:C:221:HIS:NE2	2.33	0.42
1:A:10:VAL:HG11	1:A:153:TRP:HZ2	1.83	0.42
1:C:180:ILE:HA	1:C:188:TYR:O	2.20	0.42
1:C:86:ASP:O	2:D:55:PRO:HB3	2.19	0.42
2:D:354:TYR:CD1	2:D:374:LYS:HD2	2.53	0.42
2:D:247:PRO:CG	2:D:427:TYR:OH	2.64	0.42
2:B:72:ARG:HG2	2:B:226:PRO:HB3	2.02	0.42
2:D:339:TYR:CZ	2:D:352:GLY:HA3	2.54	0.42
1:C:503:LEU:HD23	2:D:422:LEU:HD22	2.01	0.42
3:E:24:DG:H2''	3:E:25:DA:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:GLU:OE1	1:C:206:ARG:NH2	2.53	0.42
1:A:84:THR:HB	1:A:154:LYS:HE2	2.01	0.42
1:C:278:GLN:HG3	1:C:298:GLU:HB3	2.00	0.42
3:F:4:OMC:H2'	3:F:5:DC:H6	1.84	0.42
1:A:51:GLY:H	1:A:52:PRO:HD3	1.85	0.42
1:A:406:TRP:HD1	1:A:407[B]:GLN:NE2	2.16	0.42
1:C:298:GLU:OE1	1:C:298:GLU:N	2.46	0.42
1:A:323:LYS:HE2	1:A:344:GLU:OE2	2.19	0.42
2:B:70:LYS:NZ	2:B:229:TRP:HE1	2.18	0.42
3:E:0:DA:H2''	3:E:1:DA:OP2	2.20	0.42
1:C:13:LYS:HB2	1:C:16:MET:SD	2.60	0.41
1:C:31:ILE:HG23	1:C:132:ILE:HD11	2.01	0.41
1:C:44:GLU:CG	1:C:46:LYS:HE2	2.50	0.41
2:D:115:TYR:O	2:D:149:LEU:HB2	2.20	0.41
4:G:1:GLC:H4	4:G:2:FRU:HO6	1.85	0.41
2:D:399:GLU:OE2	4:H:1:GLC:O3	2.38	0.41
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.85	0.41
2:D:78:ARG:HD3	2:D:411:ILE:O	2.21	0.41
1:A:412:PRO:O	1:A:414:TRP:HD1	2.03	0.41
2:D:120:LEU:HD23	2:D:125:ARG:HG2	2.02	0.41
2:B:227:PHE:CG	2:B:228:LEU:N	2.88	0.41
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.51	0.41
1:A:356:ARG:CZ	1:A:358:ARG:HH11	2.33	0.41
1:A:390:LYS:NZ	1:A:415:GLU:OE2	2.52	0.41
1:C:116:PHE:O	1:C:148:VAL:HG11	2.20	0.41
1:C:21:VAL:O	1:C:57:ASN:ND2	2.50	0.41
8:B:507:PEG:H31	8:B:507:PEG:H12	1.74	0.41
1:A:22:LYS:O	1:A:59:PRO:HG3	2.21	0.41
1:A:44:GLU:HG2	1:A:46:LYS:HE2	2.03	0.41
1:A:495:ILE:HB	1:A:533:LEU:HD23	2.02	0.41
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.56	0.41
1:A:407[B]:GLN:NE2	2:B:418:ASN:HA	2.36	0.41
10:E:101:PG4:H22	10:E:101:PG4:H41	1.46	0.41
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.81	0.41
1:A:23:GLN:NE2	1:A:26:LEU:HD21	2.36	0.41
2:B:91:GLN:NE2	1:C:343:GLN:O	2.54	0.41
2:D:328:GLU:O	2:D:339:TYR:HA	2.20	0.41
1:A:405:TYR:CE2	1:A:407[B]:GLN:HB2	2.56	0.41
1:A:284:ARG:NE	3:E:8:DT:OP1	2.54	0.41
2:D:167:ILE:O	2:D:208:HIS:NE2	2.41	0.40
1:C:397:THR:HG21	1:C:424:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:LYS:HD3	2:D:116:PHE:HB3	2.03	0.40
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.56	0.40
1:A:298:GLU:OE1	1:A:298:GLU:N	2.47	0.40
1:C:206:ARG:NH1	1:C:218:ASP:OD1	2.54	0.40
1:C:379:SER:CB	1:C:387:PRO:HD3	2.50	0.40
3:F:27:DG:C4	3:F:28:DG:N7	2.90	0.40
1:C:410:TRP:CH2	1:C:412:PRO:HA	2.57	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	552/555 (100%)	534 (97%)	18 (3%)	0	100	100
1	C	551/555 (99%)	536 (97%)	14 (2%)	1 (0%)	47	62
2	B	411/429 (96%)	398 (97%)	13 (3%)	0	100	100
2	D	408/429 (95%)	392 (96%)	16 (4%)	0	100	100
All	All	1922/1968 (98%)	1860 (97%)	61 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	543	GLY

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	496/495 (100%)	492 (99%)	4 (1%)	81	91
1	C	495/495 (100%)	491 (99%)	4 (1%)	81	91
2	B	377/390 (97%)	376 (100%)	1 (0%)	92	97
2	D	374/390 (96%)	371 (99%)	3 (1%)	81	91
All	All	1742/1770 (98%)	1730 (99%)	12 (1%)	84	92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	64	LYS
1	A	123	ASP
1	A	498	ASN
2	B	356	ARG
1	C	109	LEU
1	C	182	GLN
1	C	399	GLU
1	C	498	ASN
2	D	266	TRP
2	D	303	LEU
2	D	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	394	GLN
1	C	197	GLN
1	C	545	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	E	2	3	15,22,23	3.68	6 (40%)	17,31,34	1.26	2 (11%)
3	OMC	F	2	3	15,22,23	3.72	6 (40%)	17,31,34	1.28	2 (11%)
3	OMC	F	4	3	15,22,23	3.72	6 (40%)	17,31,34	1.26	2 (11%)
3	OMC	E	4	3	15,22,23	3.58	6 (40%)	17,31,34	1.27	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	E	2	3	-	1/7/27/28	0/2/2/2
3	OMC	F	2	3	-	1/7/27/28	0/2/2/2
3	OMC	F	4	3	-	1/7/27/28	0/2/2/2
3	OMC	E	4	3	-	1/7/27/28	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	OMC	C6-N1	9.10	1.47	1.35
3	F	2	OMC	C6-N1	9.04	1.47	1.35
3	E	2	OMC	C6-N1	8.90	1.46	1.35
3	E	4	OMC	C6-N1	8.55	1.46	1.35
3	F	2	OMC	C4-N3	7.04	1.46	1.35
3	E	2	OMC	C4-N3	6.99	1.46	1.35
3	F	4	OMC	C4-N3	6.94	1.46	1.35
3	E	4	OMC	C4-N3	6.75	1.46	1.35
3	E	4	OMC	C2-N3	5.71	1.49	1.38
3	F	2	OMC	C2-N3	5.69	1.49	1.38
3	F	4	OMC	C2-N3	5.66	1.49	1.38
3	E	2	OMC	C2-N3	5.63	1.49	1.38
3	F	4	OMC	C6-C5	5.47	1.50	1.38
3	F	2	OMC	C6-C5	5.42	1.50	1.38
3	E	2	OMC	C6-C5	5.39	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	C6-C5	5.17	1.49	1.38
3	E	2	OMC	C4-N4	2.82	1.43	1.35
3	E	4	OMC	C4-N4	2.81	1.43	1.35
3	F	4	OMC	C4-N4	2.81	1.43	1.35
3	F	2	OMC	C4-N4	2.78	1.43	1.35
3	F	4	OMC	C5-C4	2.31	1.46	1.41
3	E	2	OMC	C5-C4	2.21	1.46	1.41
3	F	2	OMC	C5-C4	2.21	1.46	1.41
3	E	4	OMC	C5-C4	2.16	1.46	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	OMC	C2-N3-C4	3.94	120.34	116.34
3	F	2	OMC	C2-N3-C4	3.92	120.32	116.34
3	E	2	OMC	C2-N3-C4	3.83	120.22	116.34
3	E	4	OMC	C2-N3-C4	3.57	119.95	116.34
3	E	4	OMC	N4-C4-N3	2.43	120.32	116.49
3	F	2	OMC	N4-C4-N3	2.19	119.95	116.49
3	E	2	OMC	N4-C4-N3	2.17	119.92	116.49
3	F	4	OMC	N4-C4-N3	2.16	119.91	116.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	OMC	2	0
3	F	2	OMC	4	0
3	F	4	OMC	2	0
3	E	4	OMC	3	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	0.29	0	15,15,17	1.28	2 (13%)
4	FRU	G	2	4	11,12,12	0.49	0	10,18,18	1.02	1 (10%)
4	GLC	H	1	4	11,11,12	0.30	0	15,15,17	1.43	3 (20%)
4	FRU	H	2	4	11,12,12	0.46	0	10,18,18	0.95	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	-	0/2/19/22	0/1/1/1
4	FRU	G	2	4	-	0/5/24/24	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 (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C1-O5-C5	3.23	116.58	112.19
4	H	1	GLC	O5-C5-C6	2.82	111.62	107.20
4	H	1	GLC	C1-O5-C5	2.70	115.86	112.19
4	H	1	GLC	C1-C2-C3	-2.70	106.35	109.67
4	G	2	FRU	O1-C1-C2	-2.22	107.15	111.86
4	G	1	GLC	C1-C2-C3	2.21	112.38	109.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

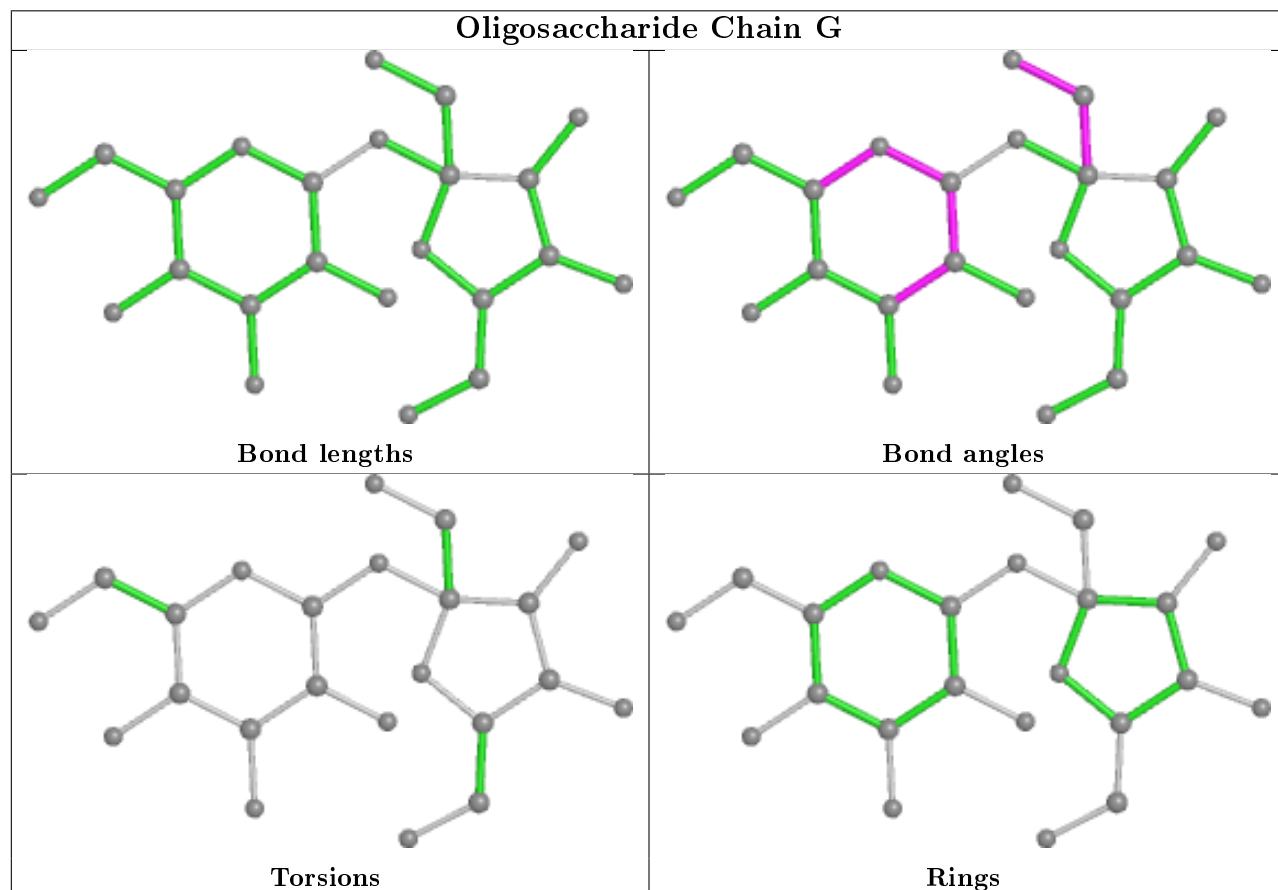
Mol	Chain	Res	Type	Atoms
4	H	1	GLC	O5-C5-C6-O6
4	H	1	GLC	C4-C5-C6-O6
4	H	2	FRU	C4-C5-C6-O6
4	H	2	FRU	O5-C5-C6-O6
4	H	2	FRU	O1-C1-C2-C3
4	H	2	FRU	O1-C1-C2-O5
4	H	2	FRU	O1-C1-C2-O2

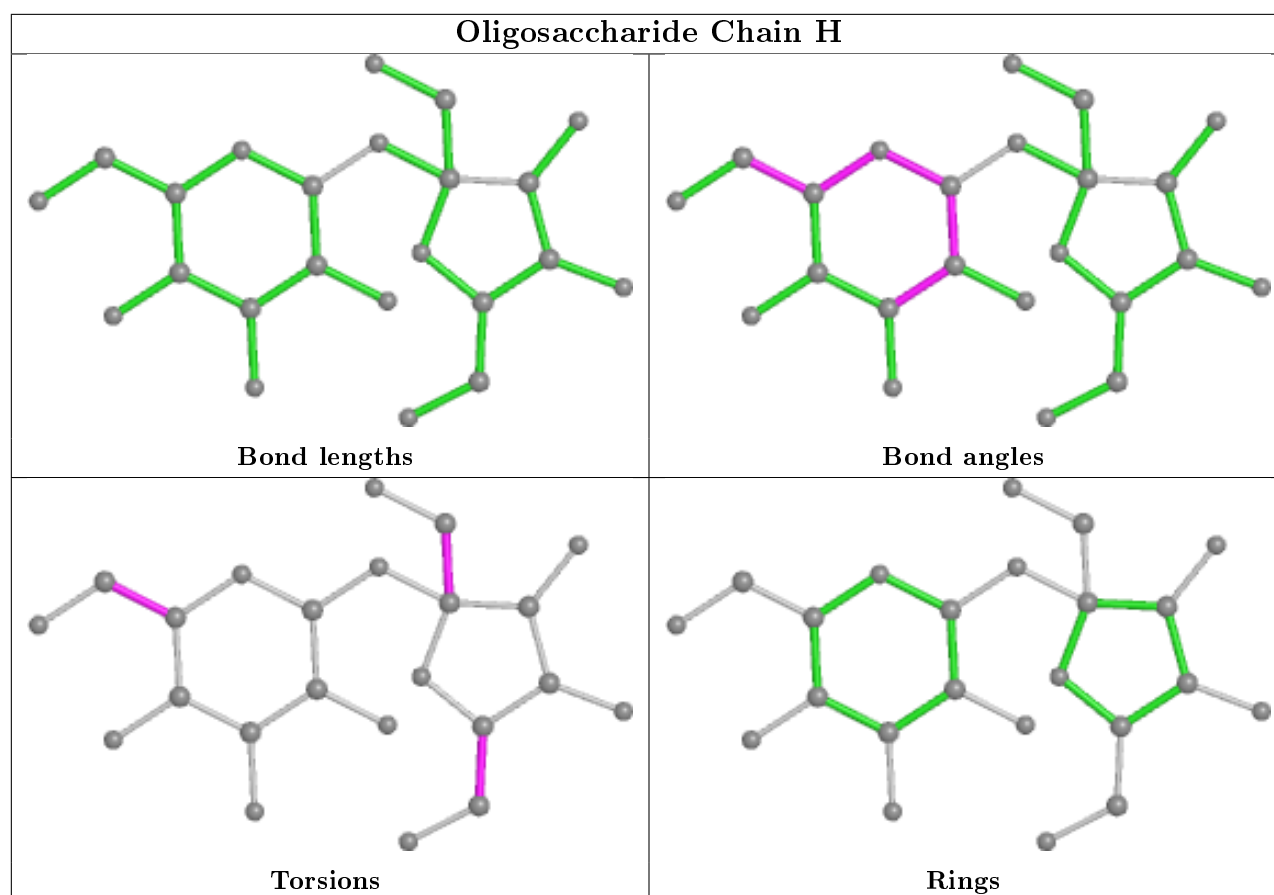
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	GLC	4	0
4	G	2	FRU	5	0
4	H	2	FRU	5	0
4	H	1	GLC	6	0

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





5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are modelled with single atom - 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	$\# Z > 2$
10	PG4	E	101	-	12,12,12	0.52	0	11,11,11	0.24	0
5	SO4	C	602	-	4,4,4	0.44	0	6,6,6	0.04	0
8	PEG	B	507	-	6,6,6	0.11	0	5,5,5	0.08	0
9	IY1	F	101	-	26,29,29	1.12	4 (15%)	28,43,43	1.48	2 (7%)
5	SO4	A	602	-	4,4,4	0.14	0	6,6,6	0.04	0
7	GOL	C	603	-	5,5,5	0.35	0	5,5,5	0.24	0
5	SO4	C	601	-	4,4,4	0.14	0	6,6,6	0.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PEG	B	506	-	6,6,6	0.13	0	5,5,5	0.07	0
5	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.04	0
9	IY1	E	102	-	26,29,29	1.09	4 (15%)	28,43,43	1.49	2 (7%)
7	GOL	B	505	-	5,5,5	0.37	0	5,5,5	0.26	0
7	GOL	B	504	-	5,5,5	0.07	0	5,5,5	0.30	0
5	SO4	B	503	-	4,4,4	0.15	0	6,6,6	0.12	0
5	SO4	B	502	-	4,4,4	0.49	0	6,6,6	0.05	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
10	PG4	E	101	-	-	6/10/10/10	-
8	PEG	B	507	-	-	1/4/4/4	-
9	IY1	F	101	-	-	4/7/10/10	0/4/4/4
7	GOL	C	603	-	-	4/4/4/4	-
8	PEG	B	506	-	-	2/4/4/4	-
7	GOL	B	505	-	-	0/4/4/4	-
9	IY1	E	102	-	-	4/7/10/10	0/4/4/4
7	GOL	B	504	-	-	4/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	101	IY1	C11-N1	2.64	1.42	1.37
9	E	102	IY1	C11-N1	2.58	1.42	1.37
9	F	101	IY1	C7-N1	2.37	1.42	1.38
9	F	101	IY1	C6-C7	2.30	1.45	1.41
9	E	102	IY1	C7-N1	2.17	1.42	1.38
9	E	102	IY1	C6-C7	2.10	1.44	1.41
9	E	102	IY1	C7-C8	-2.10	1.39	1.44
9	F	101	IY1	C7-C8	-2.03	1.39	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	102	IY1	C9-C10-C11	6.08	121.40	117.58
9	F	101	IY1	C9-C10-C11	5.96	121.33	117.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	101	IY1	C2-C1-N	-2.28	129.53	132.29
9	E	102	IY1	C2-C1-N	-2.27	129.55	132.29

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	603	GOL	O1-C1-C2-C3
7	C	603	GOL	C1-C2-C3-O3
7	B	504	GOL	O1-C1-C2-C3
7	B	504	GOL	C1-C2-C3-O3
7	B	504	GOL	O2-C2-C3-O3
8	B	506	PEG	C1-C2-O2-C3
8	B	507	PEG	C1-C2-O2-C3
10	E	101	PG4	C4-C3-O2-C2
10	E	101	PG4	O2-C3-C4-O3
7	C	603	GOL	O2-C2-C3-O3
7	B	504	GOL	O1-C1-C2-O2
10	E	101	PG4	C6-C5-O3-C4
10	E	101	PG4	O4-C7-C8-O5
9	F	101	IY1	C17-C12-N1-C11
9	F	101	IY1	C17-C12-N1-C7
8	B	506	PEG	O2-C3-C4-O4
7	C	603	GOL	O1-C1-C2-O2
9	F	101	IY1	C13-C12-N1-C11
9	E	102	IY1	C17-C12-N1-C11
9	F	101	IY1	C13-C12-N1-C7
9	E	102	IY1	C17-C12-N1-C7
10	E	101	PG4	C3-C4-O3-C5
9	E	102	IY1	C13-C12-N1-C11
9	E	102	IY1	C13-C12-N1-C7
10	E	101	PG4	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	E	101	PG4	2	0
8	B	507	PEG	1	0
9	F	101	IY1	2	0
7	C	603	GOL	1	0

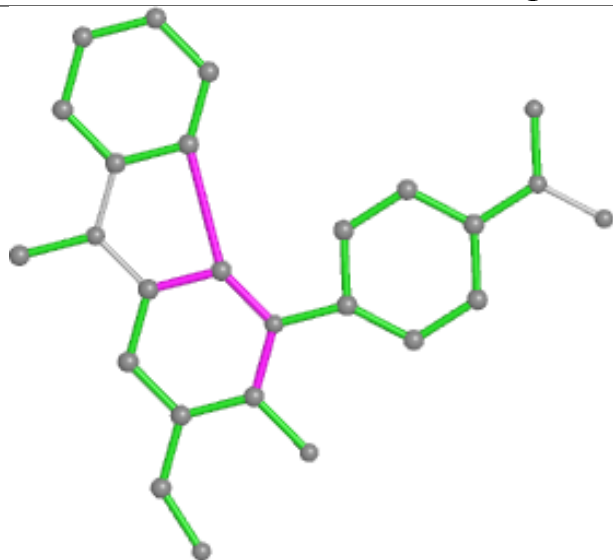
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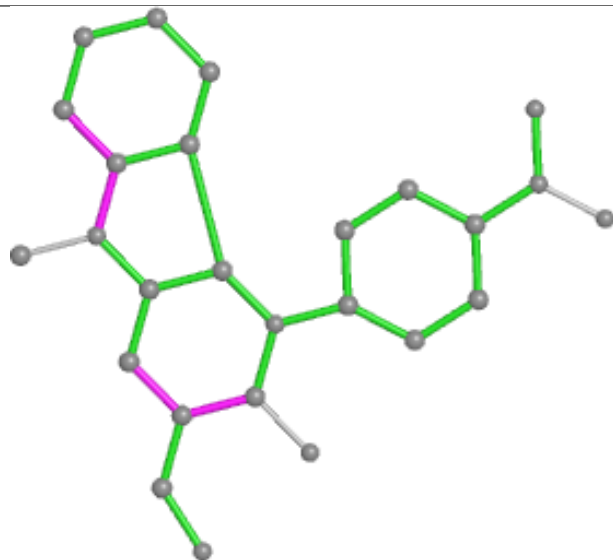
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	506	PEG	6	0
9	E	102	IY1	1	0
7	B	504	GOL	1	0
5	B	502	SO4	3	0

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.

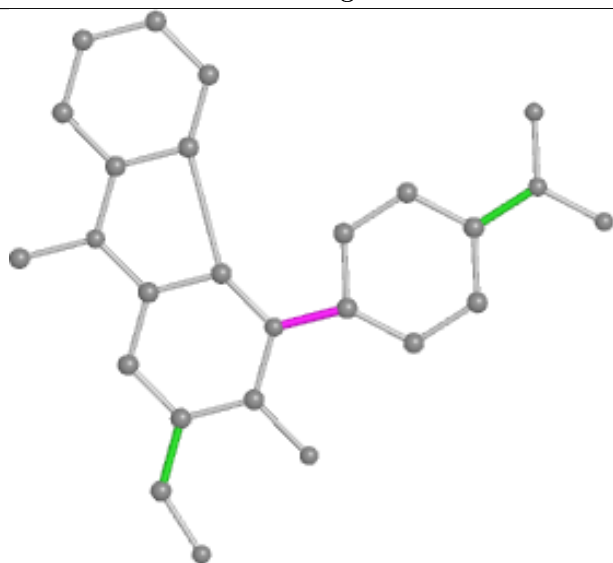
Ligand IY1 F 101



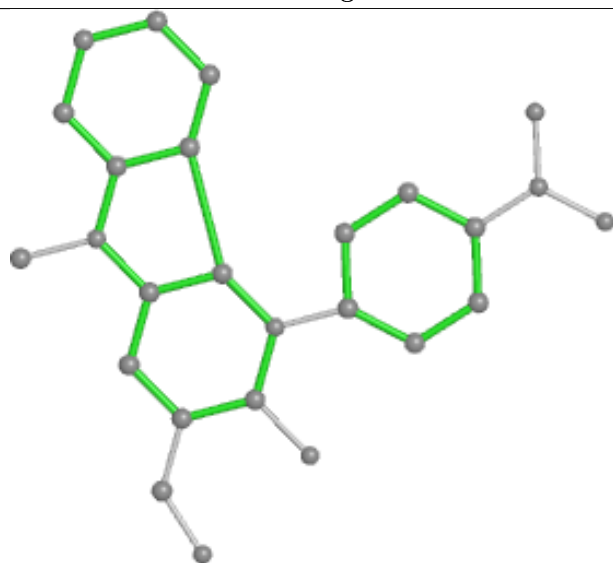
Bond lengths



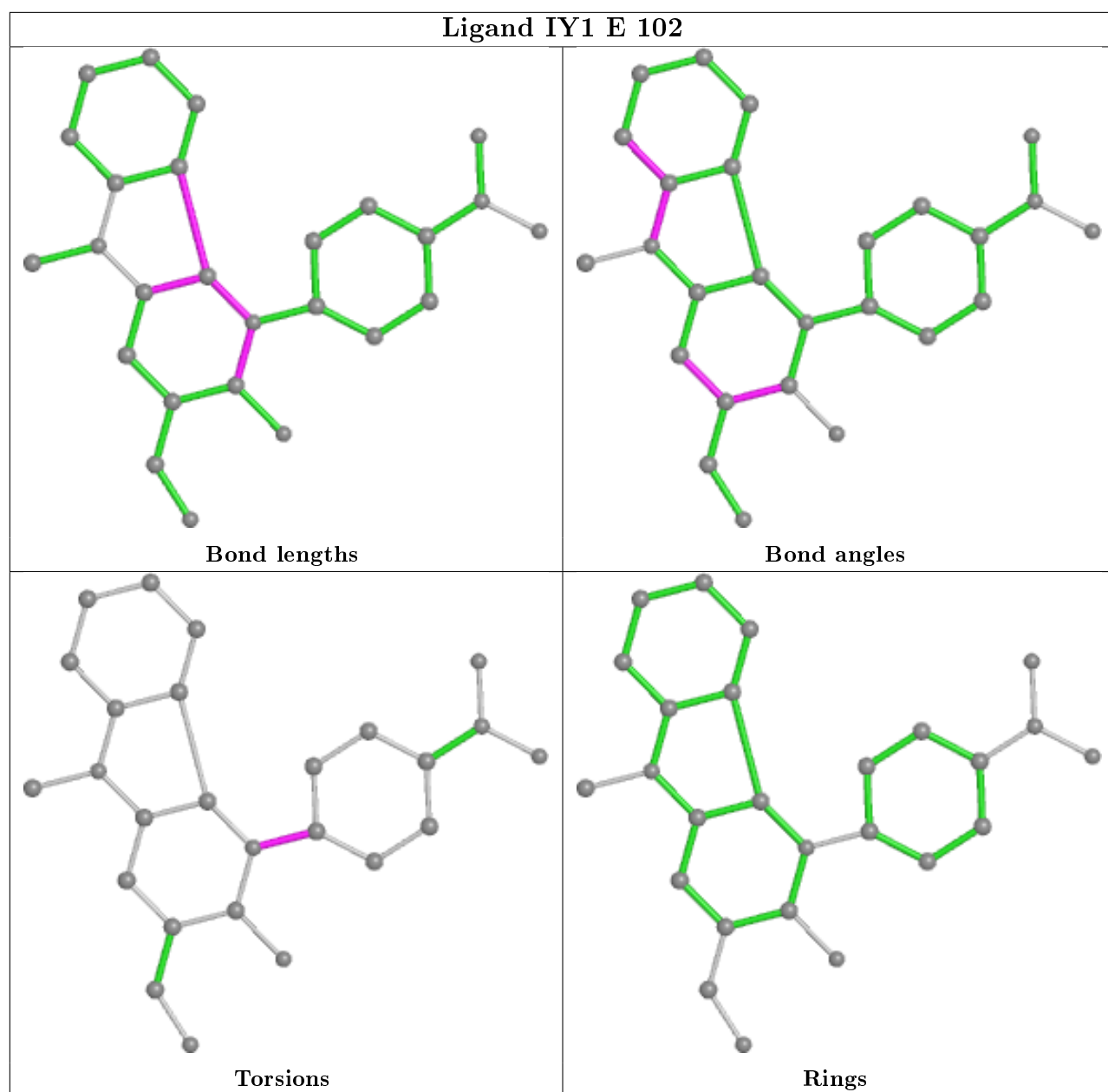
Bond angles



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(Å ²)	Q<0.9
1	A	553/555 (99%)	1.12	73 (13%) 3 3	56, 114, 216, 292	0
1	C	553/555 (99%)	1.31	125 (22%) 0 0	56, 137, 230, 292	0
2	B	415/429 (96%)	0.95	41 (9%) 7 6	60, 101, 176, 249	0
2	D	410/429 (95%)	1.10	59 (14%) 2 2	60, 123, 207, 256	0
3	E	33/38 (86%)	-0.07	0 100 100	81, 123, 187, 247	0
3	F	33/38 (86%)	-0.27	0 100 100	91, 145, 177, 223	0
All	All	1997/2044 (97%)	1.09	298 (14%) 2 2	56, 117, 217, 292	0

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	SER	20.3
1	A	135	ILE	14.7
2	B	226	PRO	13.2
1	A	30	LYS	12.4
1	C	26	LEU	12.4
1	A	133	PRO	11.5
2	D	226	PRO	11.0
2	B	88	TRP	10.6
2	B	215	THR	10.4
1	A	63	ILE	10.0
1	C	137	ASN	9.1
1	C	71	TRP	8.8
1	A	24	TRP	8.8
1	C	142	ILE	8.7
1	A	132	ILE	8.6
2	B	230	MET	8.5
2	B	4	PRO	8.5
1	A	26	LEU	8.4
1	A	137	ASN	8.2

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Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	7.9
2	D	230	MET	7.7
1	C	205	LEU	7.4
2	D	209	LEU	7.4
2	B	89	GLU	7.3
1	C	58	THR	7.3
1	C	66	LYS	7.2
2	D	116	PHE	7.2
2	B	90	VAL	7.0
1	C	134	SER	6.9
2	D	90	VAL	6.8
2	D	357	MET	6.8
1	C	74	LEU	6.7
2	D	212	TRP	6.7
1	C	2	ILE	6.6
1	A	22	LYS	6.4
1	C	24	TRP	6.3
2	D	120	LEU	6.2
1	C	60	VAL	6.0
1	A	62	ALA	6.0
1	A	289	LEU	5.9
2	D	124	PHE	5.9
1	C	132	ILE	5.9
2	D	195	ILE	5.8
1	C	111	VAL	5.8
1	A	142	ILE	5.8
1	C	25	PRO	5.8
1	C	133	PRO	5.7
1	A	34	LEU	5.7
2	D	168	LEU	5.7
1	A	67	ASP	5.7
1	C	135	ILE	5.7
2	D	85	GLN	5.7
2	B	92	LEU	5.6
2	B	87	PHE	5.5
1	C	131	THR	5.5
2	D	92	LEU	5.4
1	C	229	TRP	5.3
2	D	232	TYR	5.3
1	A	64	LYS	5.2
1	A	60	VAL	5.2
2	D	12	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	5	ILE	5.1
1	C	50	ILE	5.1
2	D	87	PHE	5.1
1	A	71	TRP	5.1
1	C	56	TYR	5.1
1	C	109	LEU	5.1
1	C	124	PHE	5.0
1	A	66	LYS	5.0
1	A	29	GLU	4.9
1	A	74	LEU	4.8
2	D	88	TRP	4.8
1	A	61	PHE	4.8
1	C	34	LEU	4.8
2	B	214	LEU	4.8
2	D	10	VAL	4.8
1	C	62	ALA	4.7
2	D	130	PHE	4.7
1	C	28	GLU	4.7
1	C	257	ILE	4.7
1	C	310	LEU	4.6
1	C	244	ILE	4.5
2	B	91	GLN	4.5
1	C	226	PRO	4.5
1	C	48	SER	4.5
1	C	17	ASP	4.5
2	D	66	LYS	4.4
1	C	61	PHE	4.4
1	C	346	PHE	4.4
1	A	141	GLY	4.3
2	D	89	GLU	4.3
2	B	266	TRP	4.3
1	C	251	SER	4.3
1	A	136	ASN	4.2
1	C	214	LEU	4.2
1	C	75	VAL	4.2
2	B	94	ILE	4.2
2	B	209	LEU	4.2
1	C	202	ILE	4.2
1	C	127	TYR	4.2
1	C	146	TYR	4.2
2	B	212	TRP	4.1
2	B	116	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	130	PHE	4.1
2	D	227	PHE	4.1
2	D	144	TYR	4.1
1	A	139	THR	4.0
1	C	63	ILE	4.0
1	C	108	VAL	4.0
1	C	295	LEU	4.0
2	D	360	ALA	3.9
1	A	27	THR	3.9
1	A	75	VAL	3.9
1	A	279	LEU	3.9
1	C	193	LEU	3.9
1	A	50	ILE	3.8
1	A	70	LYS	3.8
1	C	68	SER	3.7
2	D	159	ILE	3.7
1	C	245	VAL	3.7
2	B	301	LEU	3.7
1	C	59	PRO	3.7
1	A	138	GLU	3.6
1	A	140	PRO	3.6
1	A	303	LEU	3.6
1	A	31	ILE	3.6
1	C	136	ASN	3.6
1	C	19	PRO	3.6
1	C	23	GLN	3.6
1	C	1	PRO	3.6
1	C	313	PRO	3.5
1	C	188	TYR	3.5
1	A	205	LEU	3.5
2	D	146	TYR	3.5
1	C	228	LEU	3.5
1	C	72	ARG	3.4
1	C	67	ASP	3.4
2	D	356	ARG	3.4
1	C	118	VAL	3.3
1	C	8	VAL	3.3
1	C	130	PHE	3.3
1	A	21	VAL	3.3
2	D	115	TYR	3.3
1	A	12	LEU	3.2
1	C	160	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	205	LEU	3.2
1	A	49	LYS	3.2
2	B	309	ILE	3.2
1	A	73	LYS	3.2
1	C	187	LEU	3.2
2	B	109	LEU	3.2
2	D	35	VAL	3.2
2	D	359	GLY	3.1
1	C	64	LYS	3.1
1	C	254	VAL	3.1
1	C	289	LEU	3.1
1	C	290	THR	3.1
2	D	354	TYR	3.1
1	C	227	PHE	3.1
1	C	314	VAL	3.1
1	C	274	ILE	3.1
1	A	286	THR	3.1
1	C	14	PRO	3.1
1	C	252	TRP	3.0
2	B	8	VAL	3.0
1	C	311	LYS	3.0
2	B	10	VAL	3.0
2	D	266	TRP	3.0
1	C	46	LYS	3.0
2	D	229	TRP	3.0
1	A	28	GLU	2.9
1	A	32	LYS	2.9
1	A	144	TYR	2.9
1	A	177	ASP	2.9
2	B	12	LEU	2.9
2	D	149	LEU	2.9
1	C	285	GLY	2.9
2	D	318[A]	TYR	2.9
1	C	147	ASN	2.9
2	D	171	PHE	2.9
1	C	260	LEU	2.9
1	A	295	LEU	2.9
1	C	223	LYS	2.9
1	A	271	TYR	2.9
1	C	16	MET	2.8
1	A	72	ARG	2.8
1	C	116	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	47	ILE	2.8
2	D	105	SER	2.8
1	C	102	LYS	2.8
1	C	18	GLY	2.8
1	C	41	MET	2.8
2	D	80	LEU	2.8
2	B	229	TRP	2.8
2	D	422	LEU	2.7
1	A	4	PRO	2.7
1	C	293	ILE	2.7
1	C	110	ASP	2.7
1	C	171	PHE	2.7
1	C	106	VAL	2.7
2	B	118	VAL	2.7
1	C	113	ASP	2.7
1	C	234	LEU	2.7
1	A	128	THR	2.6
1	C	49	LYS	2.6
1	C	271	TYR	2.6
1	C	292	VAL	2.6
1	A	244	ILE	2.6
1	C	372	VAL	2.6
1	A	533	LEU	2.6
2	D	176	PRO	2.6
2	B	428	GLN	2.6
1	C	177	ASP	2.6
1	C	10	VAL	2.6
2	D	132	ILE	2.6
1	A	252	TRP	2.5
2	D	231	GLY	2.5
2	B	11	LYS	2.5
1	C	73	LYS	2.5
1	C	209	LEU	2.5
2	D	190	GLY	2.5
2	B	85	GLN	2.5
1	A	257	ILE	2.5
1	A	211	ARG	2.4
1	C	174	GLN	2.4
1	C	286	THR	2.4
1	A	246	LEU	2.4
1	C	203	GLU	2.4
1	A	25	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	277	ARG	2.4
2	D	211	ARG	2.4
1	C	154	LYS	2.4
1	C	259	LYS	2.4
2	D	8	VAL	2.4
1	A	264	LEU	2.4
2	D	34	LEU	2.4
2	B	279	LEU	2.3
1	C	222	GLN	2.3
2	B	62	ALA	2.3
2	B	7	THR	2.3
2	B	295	LEU	2.3
2	D	67	ASP	2.3
2	B	179	VAL	2.3
1	A	290	THR	2.3
2	D	425	LEU	2.3
2	D	202	ILE	2.3
1	C	114	ALA	2.3
2	D	26	LEU	2.3
2	D	74	LEU	2.3
1	C	55	PRO	2.3
1	C	206	ARG	2.3
1	C	37	ILE	2.3
2	B	173	LYS	2.2
1	C	167	ILE	2.2
1	C	544	GLY	2.2
1	C	148	VAL	2.2
1	A	553	SER	2.2
1	C	31	ILE	2.2
2	D	62	ALA	2.2
1	A	19	PRO	2.2
1	A	551	LEU	2.2
2	D	267	ALA	2.2
1	A	234	LEU	2.2
1	A	310	LEU	2.2
1	A	458	VAL	2.2
1	C	65	LYS	2.2
2	D	206	ARG	2.2
1	A	300	GLU	2.2
2	D	93	GLY	2.2
2	B	202	ILE	2.1
1	A	59	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	124	PHE	2.1
1	C	303	LEU	2.1
1	C	263	LYS	2.1
2	B	189	VAL	2.1
1	C	542	ILE	2.1
2	D	264	LEU	2.1
1	C	250	ASP	2.1
1	A	126	LYS	2.1
1	C	534	ALA	2.1
2	B	167	ILE	2.1
2	D	61	PHE	2.1
1	C	302	GLU	2.1
1	C	261	VAL	2.1
2	B	299	ALA	2.1
1	C	496	VAL	2.1
2	B	245	VAL	2.1
1	A	180	ILE	2.1
2	D	65	LYS	2.1
1	C	264	LEU	2.1
1	C	371	ALA	2.0
1	A	124	PHE	2.0
2	B	368	LEU	2.0
1	C	128	THR	2.0
1	C	139	THR	2.0
1	C	32	LYS	2.0
1	A	245	VAL	2.0
2	B	187	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, 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	F	2	21/22	0.91	0.13	135,146,151,153	0
3	OMC	F	4	21/22	0.93	0.17	114,128,141,154	0
3	OMC	E	4	21/22	0.95	0.19	71,84,97,118	0
3	OMC	E	2	21/22	0.96	0.19	92,106,115,118	0

6.3 Carbohydrates

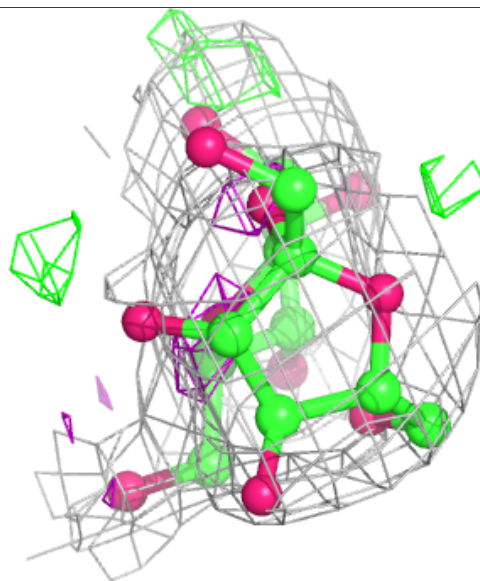
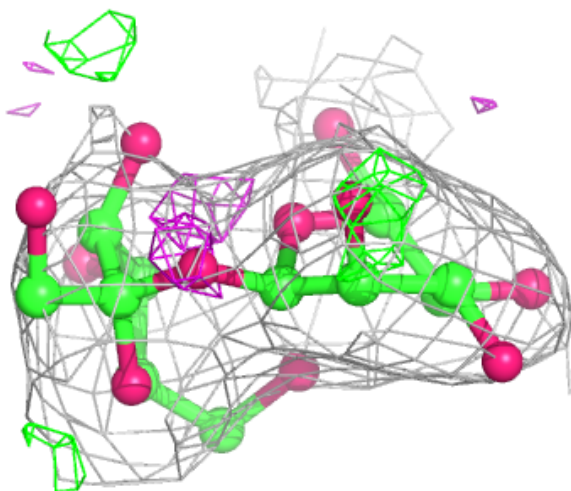
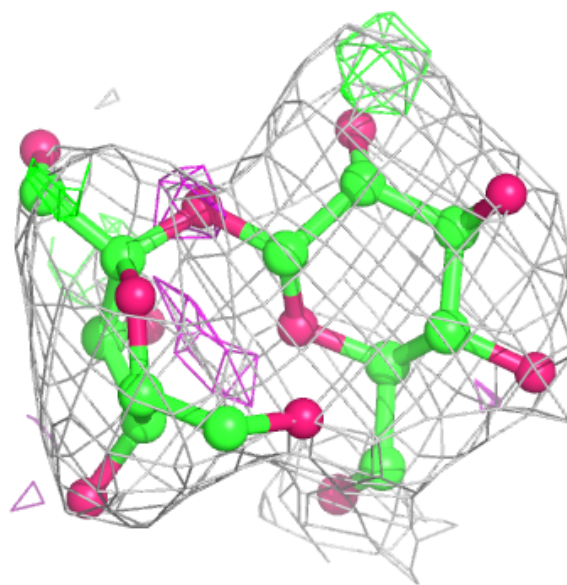
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

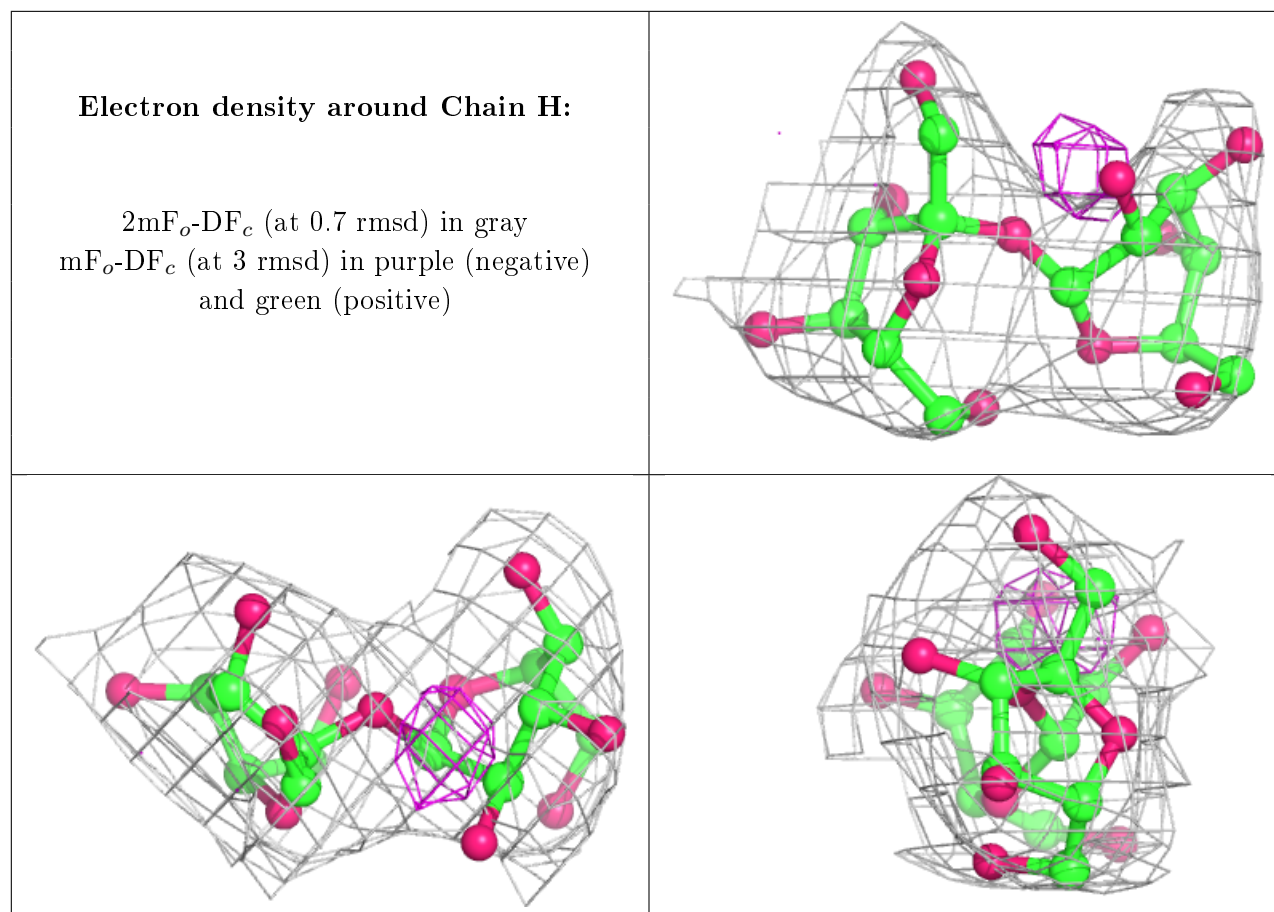
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FRU	G	2	12/12	0.80	0.27	138,151,156,161	0
4	GLC	H	1	11/12	0.84	0.20	132,137,151,157	0
4	FRU	H	2	12/12	0.87	0.15	135,157,166,170	0
4	GLC	G	1	11/12	0.87	0.20	102,114,127,132	0

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
6	NH4	A	603	1/1	0.29	0.62	130,156,156,156	0
8	PEG	B	507	7/7	0.65	0.38	168,187,201,203	0
6	NH4	C	604	1/1	0.66	0.57	104,125,125,125	0
10	PG4	E	101	13/13	0.72	0.14	125,144,149,150	0
5	SO4	A	601	5/5	0.76	0.28	166,171,173,176	0
7	GOL	B	504	6/6	0.76	0.18	91,113,121,126	0
8	PEG	B	506	7/7	0.77	0.21	92,100,103,109	0
9	IY1	F	101	26/26	0.80	0.36	169,182,210,216	0
7	GOL	B	505	6/6	0.80	0.51	89,95,106,107	0
5	SO4	B	503	5/5	0.81	0.22	190,190,193,194	0
5	SO4	B	502	5/5	0.81	0.34	137,137,138,150	0
5	SO4	C	602	5/5	0.82	0.12	188,191,192,196	0

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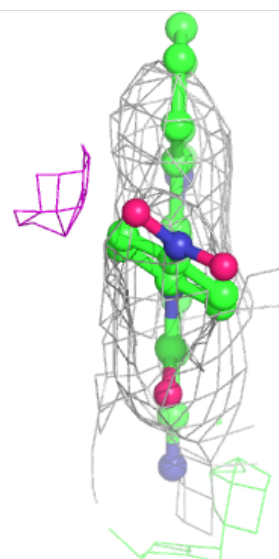
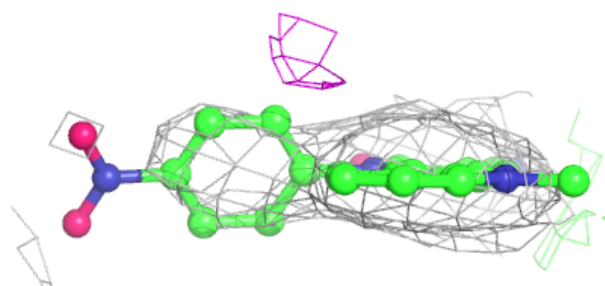
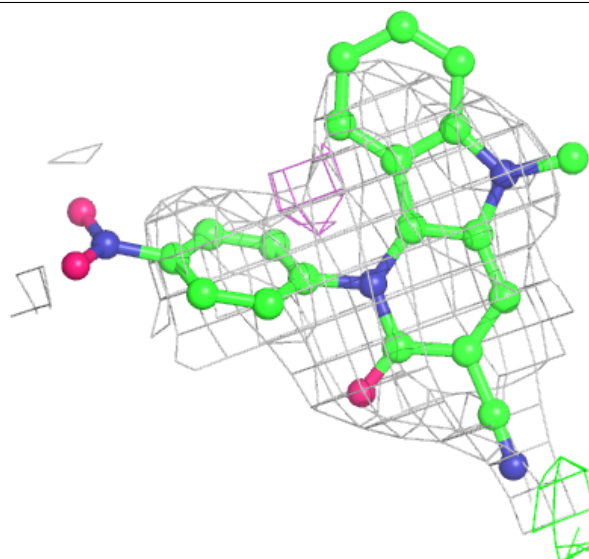
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	C	603	6/6	0.82	0.20	115,119,121,124	0
5	SO4	A	602	5/5	0.84	0.27	178,182,184,184	0
9	IY1	E	102	26/26	0.84	0.27	144,158,178,183	0
5	SO4	C	601	5/5	0.96	0.12	159,161,162,163	0

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.

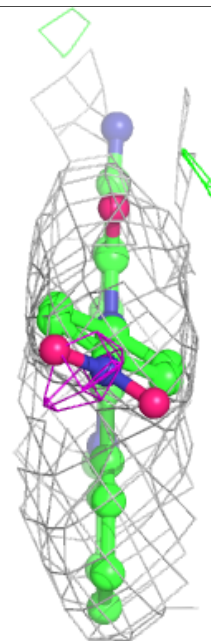
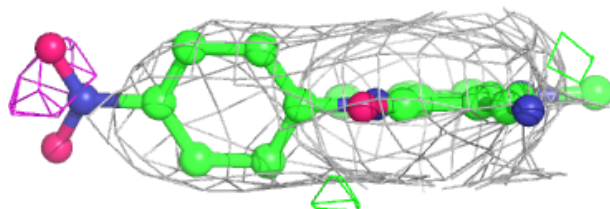
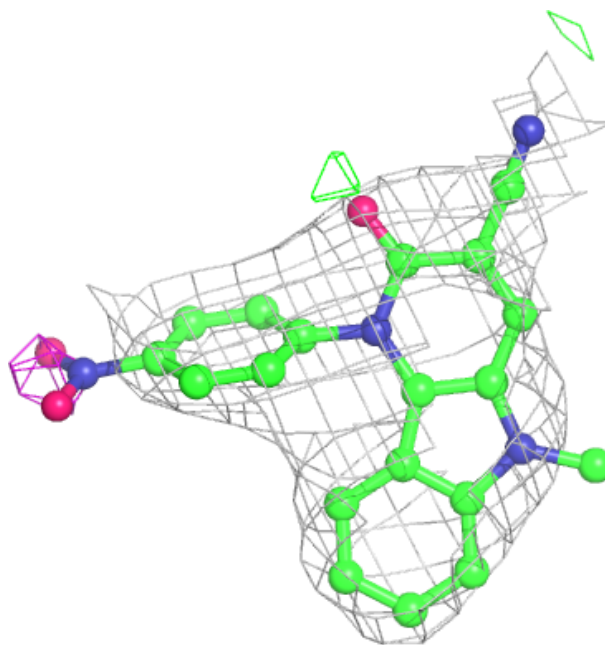
Electron density around IY1 F 101:

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 IY1 E 102:

$2mF_o-DF_c$ (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.