Full wwPDB X-ray Structure Validation Report (i)

Mar 1, 2026 – 01:11 PM UTC

PDB ID	:	6O9E / pdb_00006o9e
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

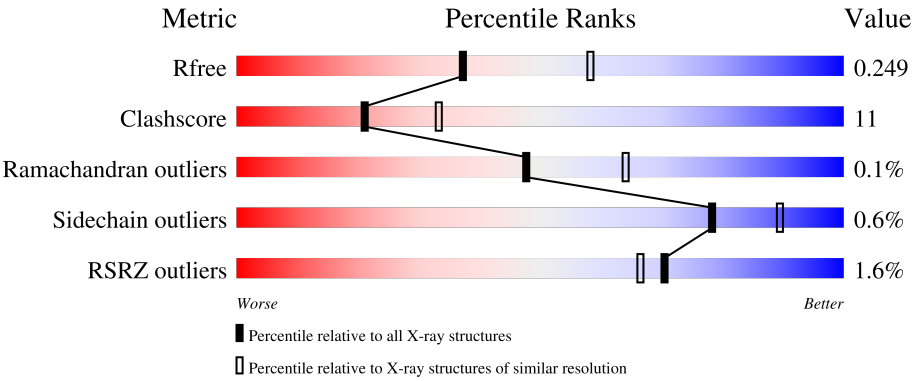
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	555	74% 25%
1	C	555	75% 24%
2	B	429	80% 17%
2	D	429	78% 17%
3	E	38	32% 55% 5% 8%

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Mol	Chain	Length	Quality of chain
3	F	38	
4	G	2	
4	H	2	

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	-
8	PEG	B	506	-	-	X	-

2 Entry composition (i)

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			

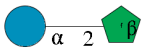
There are 4 discrepancies between the modelled and reference sequences:

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).

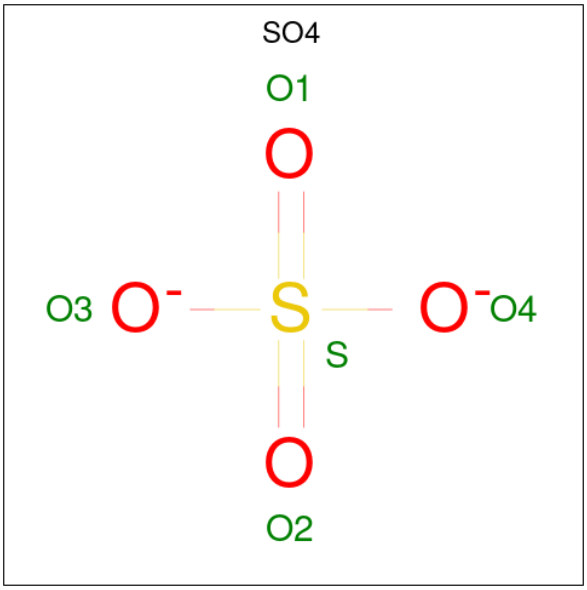
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	35	Total	C	N	O	P	0	0	0
			720	341	129	215	35			
3	E	35	Total	C	N	O	P	0	0	0
			720	341	129	215	35			

- 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 (CCD ID: SO4) (formula: O_4S).



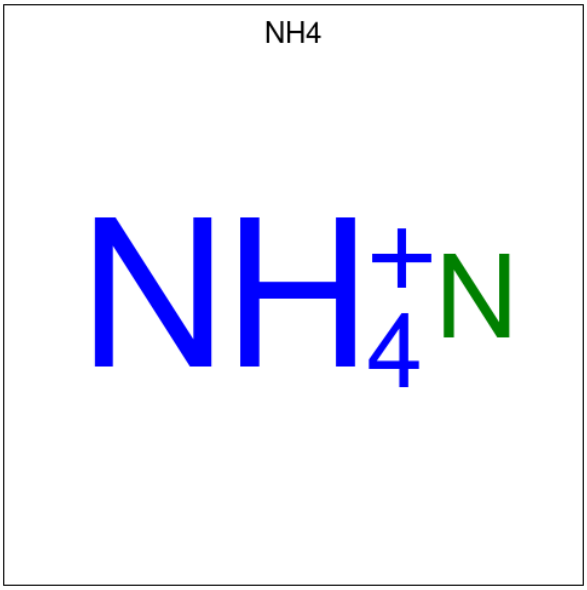
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

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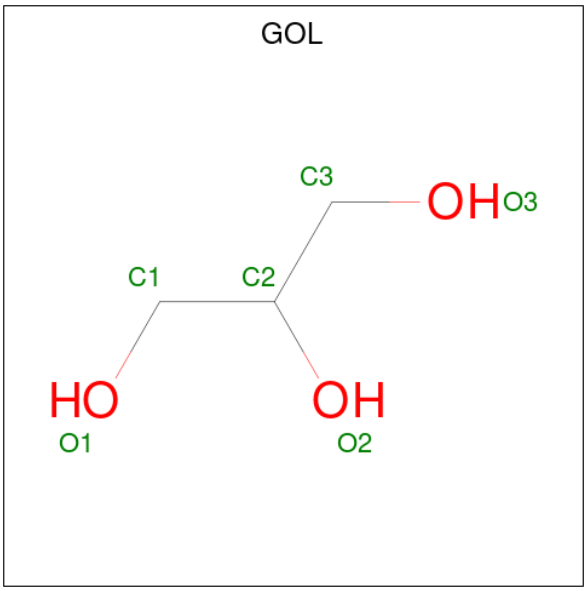
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0

- Molecule 6 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).



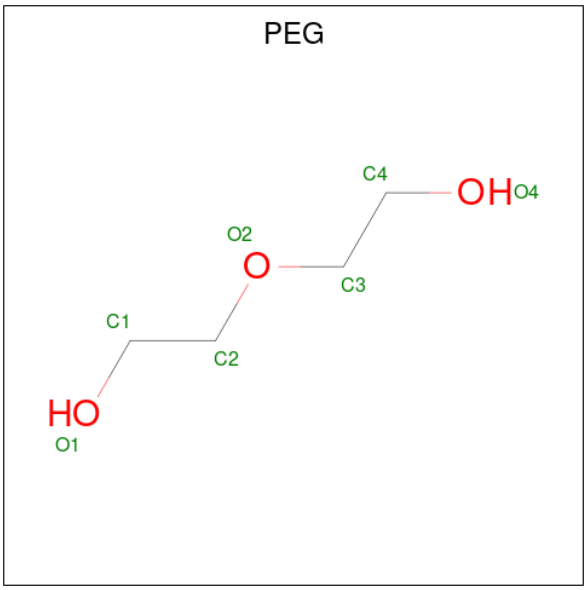
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total H N 5 4 1	0	0
6	C	1	Total H N 5 4 1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



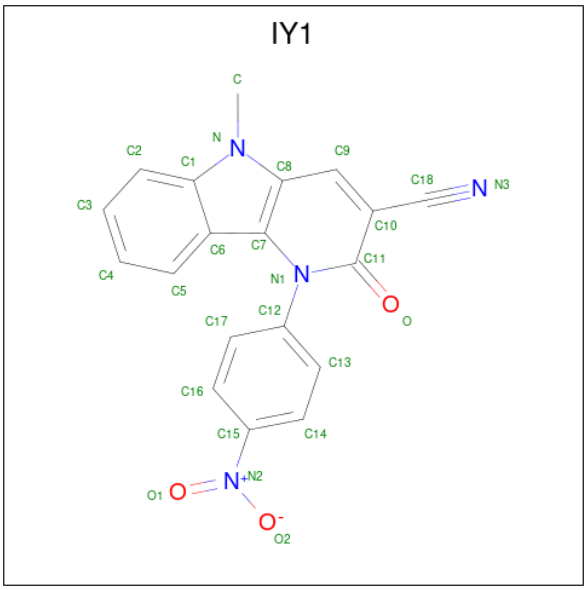
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 7 4 3	0	0

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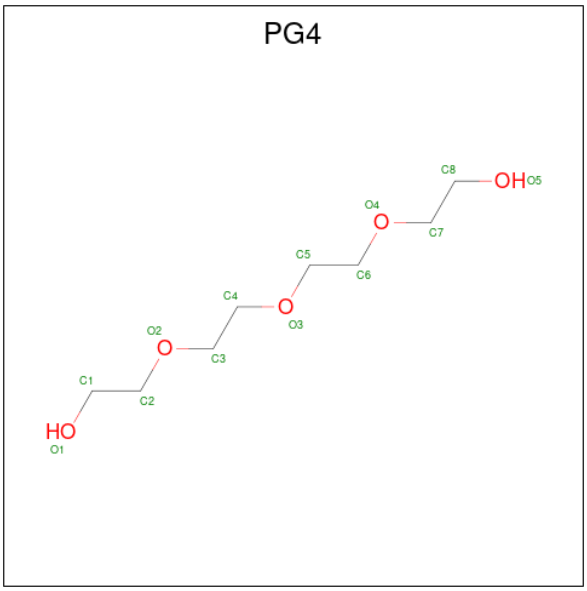
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 7 4 3	0	0

- Molecule 9 is 5-methyl-1-(4-nitrophenyl)-2-oxo-2,5-dihydro-1H-pyrido[3,2-b]indole-3-carbonitrile (CCD ID: IY1) (formula: $C_{19}H_{12}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 10 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 11 is water.

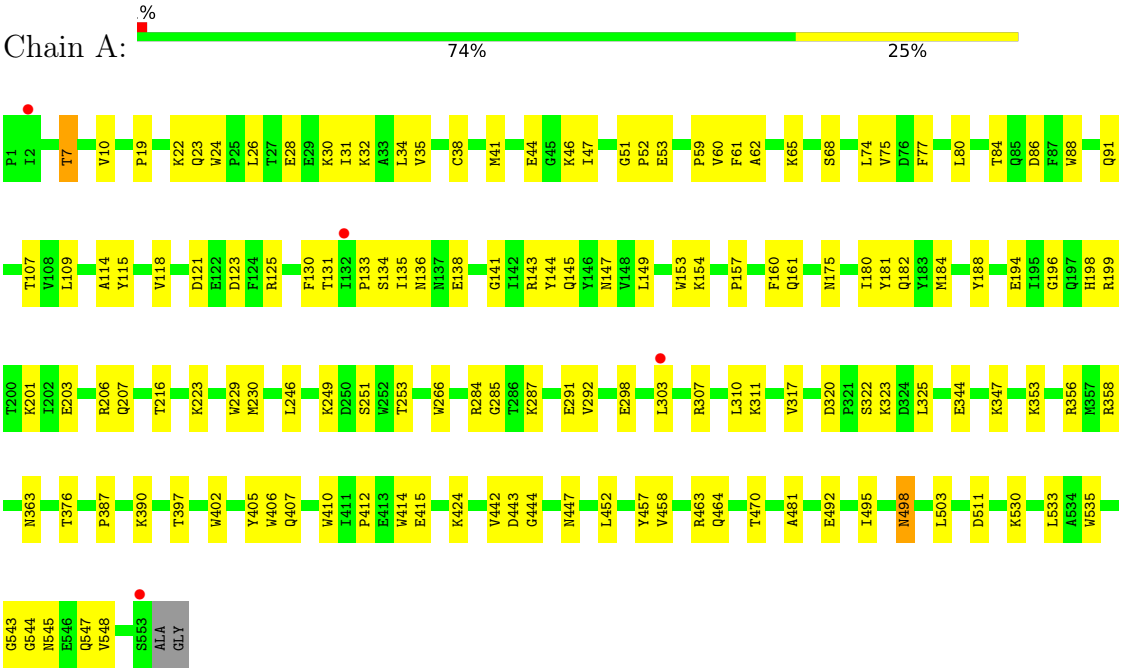
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	32	Total O 32 32	0	0
11	B	35	Total O 35 35	0	0
11	C	21	Total O 21 21	0	0
11	D	15	Total O 15 15	0	0
11	F	3	Total O 3 3	0	0
11	E	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

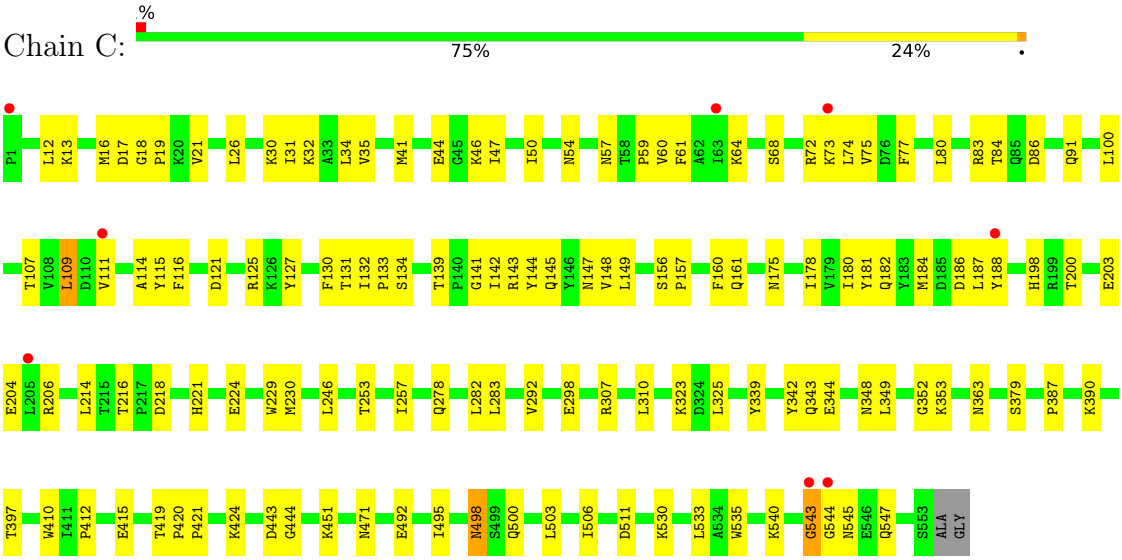
• Molecule 1: Reverse transcriptase p66

Chain A:



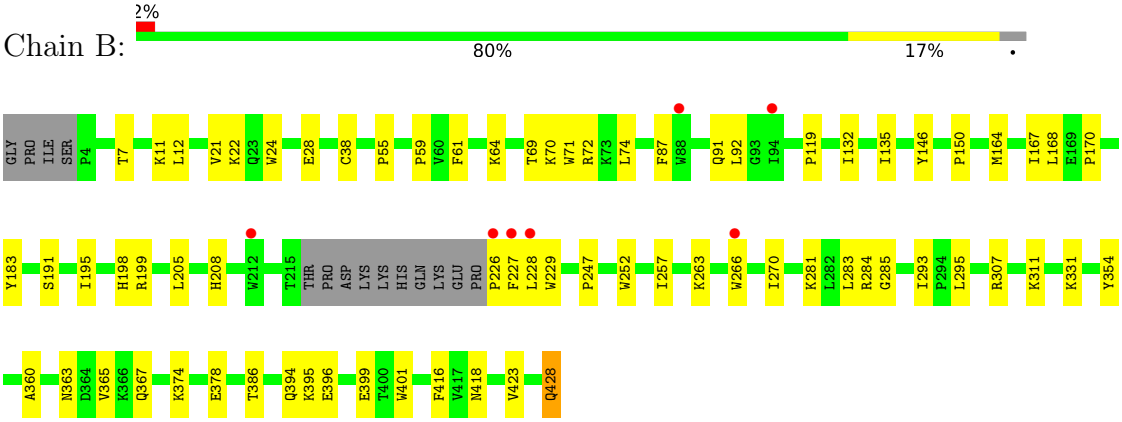
• Molecule 1: Reverse transcriptase p66

Chain C:



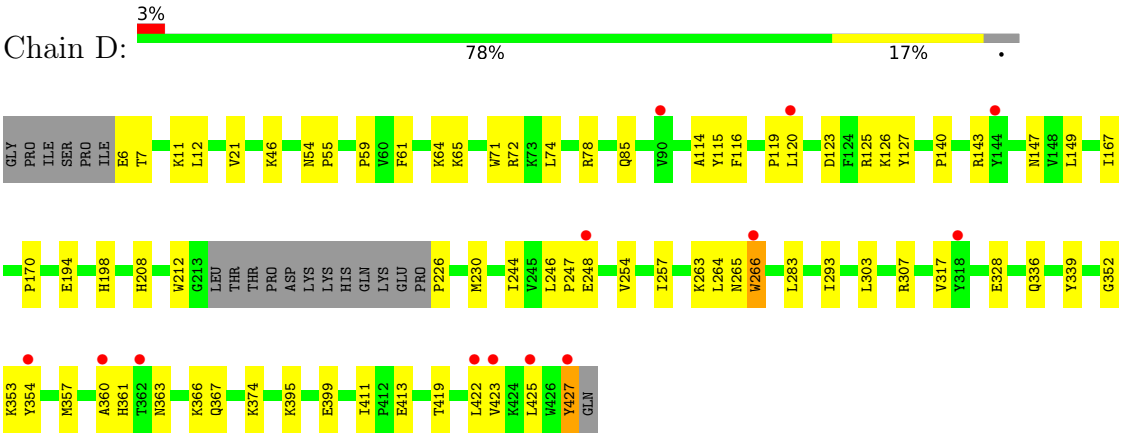
• Molecule 2: Reverse transcriptase p51

Chain B:



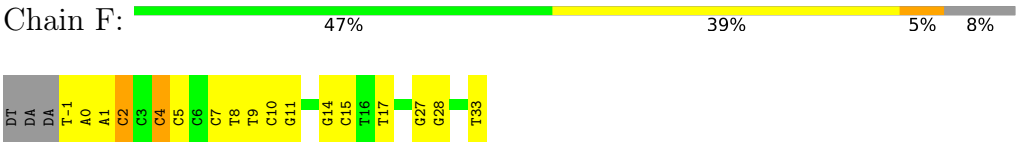
• Molecule 2: Reverse transcriptase p51

Chain D:



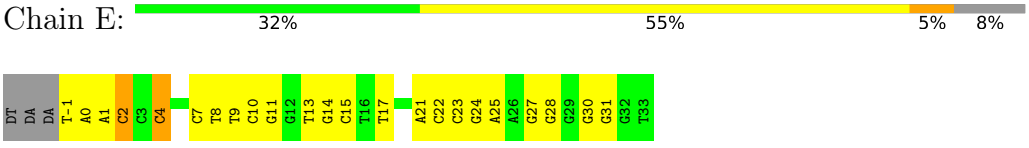
• Molecule 3: DNA (38-MER)

Chain F:



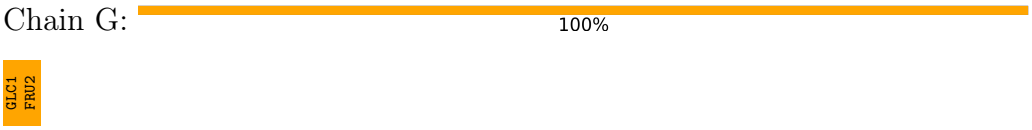
• Molecule 3: DNA (38-MER)

Chain E:



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

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

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 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.40) 99.8 (50.00-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.40Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.203 , 0.242 0.210 , 0.249	Depositor DCC
R_{free} test set	2000 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)	0.33 , 88.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FRU, NH4, SO4, GLC, OMC, PG4, GOL, IY1, 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	0.09	0/4631	0.27	0/6291
1	C	0.10	0/4622	0.30	2/6279 (0.0%)
2	B	0.09	0/3534	0.26	0/4800
2	D	0.10	0/3515	0.27	0/4775
3	E	0.18	0/759	0.37	0/1170
3	F	0.84	6/759 (0.8%)	0.46	0/1170
All	All	0.20	6/17820 (0.0%)	0.29	2/24485 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	-1	DT	C3'-C2'	-15.31	1.22	1.52
3	F	-1	DT	C5-C6	7.28	1.48	1.34
3	F	-1	DT	C2-N3	6.12	1.50	1.37
3	F	-1	DT	N1-C2	5.59	1.49	1.38
3	F	-1	DT	O4'-C1'	-5.42	1.31	1.41
3	F	-1	DT	C5'-C4'	-5.07	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	419	THR	CA-C-N	5.16	123.43	119.66
1	C	419	THR	C-N-CA	5.16	123.43	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4510	0	4575	122	0
1	C	4504	0	4567	100	0
2	B	3434	0	3465	62	0
2	D	3409	0	3438	63	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	6	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
11	F	3	0	0	0	0
All	All	17583	8	16945	373	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 (373) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:157:PRO:HB3	1:A:184:MET:HE1	1.57	0.86
2:B:374:LYS:HZ2	8:B:506:PEG:H11	1.42	0.85
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:D:65:LYS:HD3	2:D:230:MET:HE1	1.63	0.81
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:H5"	3:E:17:DT:H6	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:406:TRP:CD1	1:A:407[B]:GLN:HE21	2.10	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:164:MET:HE3	2:B:168:LEU:HD11	1.76	0.68
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.30	0.66
4:H:1:GLC:H2	4:H:1:GLC:C6	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:65:LYS:CD	2:D:230:MET:HE1	2.28	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
1:C:206:ARG:HG3	1:C:216:THR:OG1	2.02	0.60
3:E:4:OMC:H5	3:E:30:DG:N1	1.95	0.60
10:E:101:PG4:H41	10:E:101:PG4:O4	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	2:D:6:GLU:OE1	2.36	0.59
2:B:266:TRP:HZ3	2:B:270:ILE:CD1	2.16	0.58
2:D:419:THR:HG23	2:D:419:THR:O	2.02	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:64:LYS:HE3	2:D:71:TRP:CE2	2.39	0.57
2:D:263:LYS:HE3	2:D:425:LEU:HA	1.87	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
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
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:358:ARG:NH2	2:B:394:GLN:HE22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:1:GLC:C6	4:H:1:GLC:C2	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
2:B:374:LYS:HZ2	8:B:506:PEG:H31	1.75	0.52
1:C:31:ILE:HA	1:C:132:ILE:HD11	1.92	0.52
1:C:182:GLN:O	1:C:182:GLN:HG3	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
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:O	1:A:182:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:CYS:HB3	1:A:144:TYR:CE2	2.46	0.50
1:A:74:LEU:HD22	3:E:0:DA:N1	2.26	0.50
1:C:503:LEU:CD2	1:C:535:TRP:HB2	2.37	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:358:ARG:HH22	2:B:394:GLN:HE22	1.59	0.50
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.47	0.50
1:A:30:LYS:O	1:A:34:LEU:HG	2.11	0.50
1:C:47:ILE:HG23	1:C:145:GLN:O	2.12	0.49
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.46	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:23:GLN:HE21	1:A:26:LEU:HD21	1.78	0.49
1:A:199:ARG:O	1:A:203:GLU:HG2	2.12	0.49
2:B:363:ASN:O	2:B:367:GLN:HG3	2.13	0.49
3:E:21:DA:C6	3:E:22:DC:N4	2.81	0.49
1:A:320:ASP:OD1	1:A:322:SER:OG	2.29	0.48
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
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
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:O5'	3:F:0:DA:H8	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:394:GLN:NE2	3:E:23:DC:OP1	2.47	0.47
1:C:17:ASP:O	1:C:83:ARG:HD3	2.14	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:F:2:OMC:O5'	3:F:2:OMC:H6	1.97	0.47
3:F:10:DC:H2"	3:F:11:DG:C8	2.49	0.47
3:E:21:DA:C5	3:E:22:DC:N4	2.82	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:134:SER:HG	1:A:141:GLY:HA2	1.80	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:32:LYS:O	1:C:35:VAL:HG12	2.15	0.46
1:C:156:SER:HB2	1:C:157:PRO:HD3	1.97	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
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:161:GLN:HE21	2:D:140:PRO:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:TYR:HB3	1:C:348:ASN:HA	1.97	0.45
2:D:194:GLU:O	2:D:198:HIS:N	2.45	0.45
1:A:7:THR:OG1	1:A:121:ASP:HA	2.16	0.45
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.81	0.45
2:D:317:VAL:HG23	2:D:317:VAL:O	2.16	0.45
1:A:47:ILE:HG23	1:A:145:GLN:O	2.17	0.45
1:A:121:ASP:O	1:A:125:ARG:HG3	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
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:88:TRP:HZ2	2:B:22:LYS:HA	1.83	0.44
1:A:266:TRP:CE2	3:E:31:DG:H4'	2.53	0.44
2:B:360:ALA:HA	2:B:367:GLN:CD	2.43	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:194:GLU:CD	1:A:196:GLY:H	2.26	0.44
1:A:402:TRP:O	2:B:331:LYS:NZ	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:336:GLN:OE1	2:D:353:LYS:HE3	2.18	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
1:C:186:ASP:C	1:C:187:LEU:HD12	2.44	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
2:B:164:MET:HE3	2:B:168:LEU:CD1	2.46	0.43
4:H:1:GLC:C1	4:H:2:FRU:C6	2.96	0.43
2:B:354:TYR:OH	2:B:378:GLU:OE1	2.30	0.43
1:C:492:GLU:HG2	1:C:530:LYS:HB2	2.00	0.43
1:A:353:LYS:NZ	3:E:7:DC:OP1	2.50	0.43
2:B:374:LYS:HG2	8:B:506:PEG:H11	2.01	0.43
3:E:2:OMC:HM23	3:E:2:OMC:H1'	1.67	0.43
3:E:4:OMC:HM22	3:E:4:OMC:H1'	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:86:ASP:O	2:D:55:PRO:HB3	2.19	0.42
1:C:180:ILE:HA	1:C:188:TYR:O	2.20	0.42
2:D:247:PRO:CG	2:D:427:TYR:OH	2.64	0.42
2:D:354:TYR:CD1	2:D:374:LYS:HD2	2.53	0.42
2:B:72:ARG:HG2	2:B:226:PRO:HB3	2.02	0.42
1:C:503:LEU:HD23	2:D:422:LEU:HD22	2.01	0.42
2:D:339:TYR:CZ	2:D:352:GLY:HA3	2.54	0.42
3:E:24:DG:H2"	3:E:25:DA:C8	2.54	0.42
1:C:203:GLU:OE1	1:C:206:ARG:NH2	2.53	0.42
1:A:109:LEU:HD12	1:A:109:LEU:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:399:GLU:OE2	4:H:1:GLC:O3	2.38	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:C:420:PRO:HA	1:C:421:PRO:C	2.45	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:21:VAL:O	1:C:57:ASN:ND2	2.50	0.41
1:C:116:PHE:O	1:C:148:VAL:HG11	2.20	0.41
8:B:507:PEG:H12	8:B:507:PEG:H31	1.74	0.41
1:A:22:LYS:O	1:A:59:PRO:HG3	2.21	0.41
1:A:23:GLN:NE2	1:A:26:LEU:HD21	2.36	0.41
1:A:44:GLU:HG2	1:A:46:LYS:HE2	2.03	0.41
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.81	0.41
1:A:407[B]:GLN:NE2	2:B:418:ASN:HA	2.36	0.41
1:A:495:ILE:HB	1:A:533:LEU:HD23	2.02	0.41
2:B:91:GLN:NE2	1:C:343:GLN:O	2.54	0.41
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.56	0.41
2:D:328:GLU:O	2:D:339:TYR:HA	2.20	0.41
10:E:101:PG4:H41	10:E:101:PG4:H22	1.46	0.41
1:A:284:ARG:NE	3:E:8:DT:OP1	2.54	0.41
1:A:405:TYR:CE2	1:A:407[B]:GLN:HB2	2.56	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
2:D:46:LYS:HD3	2:D:116:PHE:HB3	2.03	0.40
1:A:28:GLU:CD	1:A:136:ASN:HD21	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	43 58
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%)	48 64

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%)	493 (99%)	3 (1%)	78 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	495/495 (100%)	492 (99%)	3 (1%)	78 89
2	B	377/390 (97%)	376 (100%)	1 (0%)	86 93
2	D	374/390 (96%)	371 (99%)	3 (1%)	73 86
All	All	1742/1770 (98%)	1732 (99%)	10 (1%)	78 89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	123	ASP
1	A	498	ASN
2	B	428	GLN
1	C	109	LEU
1	C	224	GLU
1	C	498	ASN
2	D	266	TRP
2	D	303	LEU
2	D	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	221	HIS
1	A	255	ASN
1	A	373	GLN
1	A	509	GLN
2	B	151	GLN
2	B	278	GLN
2	B	394	GLN
1	C	147	ASN
1	C	182	GLN
1	C	197	GLN
1	C	255	ASN
1	C	334	GLN
1	C	520	GLN
1	C	524	GLN
1	C	545	ASN
2	D	96	HIS
2	D	147	ASN

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	4	3	19,22,23	3.09	7 (36%)	25,31,34	0.74	0
3	OMC	E	4	3	19,22,23	3.04	7 (36%)	25,31,34	1.00	2 (8%)
3	OMC	F	2	3	19,22,23	3.08	7 (36%)	25,31,34	0.77	0
3	OMC	E	2	3	19,22,23	3.07	7 (36%)	25,31,34	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	F	4	3	-	1/9/27/28	0/2/2/2
3	OMC	E	4	3	-	3/9/27/28	0/2/2/2
3	OMC	F	2	3	-	1/9/27/28	0/2/2/2
3	OMC	E	2	3	-	1/9/27/28	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	C2-N3	6.62	1.49	1.36
3	F	2	OMC	C2-N3	6.60	1.49	1.36
3	F	4	OMC	C2-N3	6.57	1.49	1.36
3	E	2	OMC	C2-N3	6.54	1.49	1.36
3	F	4	OMC	C6-C5	6.50	1.50	1.35
3	F	2	OMC	C6-C5	6.45	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	C6-C5	6.42	1.50	1.35
3	F	2	OMC	C4-N3	6.27	1.46	1.34
3	E	2	OMC	C4-N3	6.23	1.46	1.34
3	E	4	OMC	C6-C5	6.21	1.49	1.35
3	F	4	OMC	C4-N3	6.20	1.46	1.34
3	E	4	OMC	C4-N3	6.03	1.46	1.34
3	E	4	OMC	C2-N1	4.17	1.48	1.40
3	F	4	OMC	C2-N1	4.09	1.48	1.40
3	E	2	OMC	C2-N1	3.99	1.48	1.40
3	F	2	OMC	C2-N1	3.99	1.48	1.40
3	E	2	OMC	C4-N4	3.96	1.43	1.33
3	E	4	OMC	C4-N4	3.95	1.43	1.33
3	F	4	OMC	C4-N4	3.94	1.43	1.33
3	F	2	OMC	C4-N4	3.90	1.43	1.33
3	F	4	OMC	C6-N1	3.77	1.47	1.38
3	F	2	OMC	C6-N1	3.74	1.47	1.38
3	E	2	OMC	C6-N1	3.66	1.46	1.38
3	E	4	OMC	C6-N1	3.48	1.46	1.38
3	E	4	OMC	O2-C2	-2.94	1.18	1.23
3	E	2	OMC	O2-C2	-2.75	1.18	1.23
3	F	2	OMC	O2-C2	-2.74	1.18	1.23
3	F	4	OMC	O2-C2	-2.72	1.18	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	4	OMC	C6-C5-C4	2.25	121.22	117.53
3	E	4	OMC	O2-C2-N3	-2.10	119.02	122.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	OMC	C1'-C2'-O2'-CM2
3	E	2	OMC	C1'-C2'-O2'-CM2
3	F	4	OMC	C1'-C2'-O2'-CM2
3	E	4	OMC	O4'-C1'-N1-C2
3	E	4	OMC	O4'-C1'-N1-C6
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	F	4	OMC	2	0
3	E	4	OMC	3	0
3	F	2	OMC	4	0
3	E	2	OMC	2	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	0.28	0	15,15,17	1.19	1 (6%)
4	FRU	G	2	4	11,12,12	0.51	0	10,18,18	0.99	1 (10%)
4	GLC	H	1	4	11,11,12	0.29	0	15,15,17	1.27	3 (20%)
4	FRU	H	2	4	11,12,12	0.49	0	10,18,18	0.94	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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	GLC	C1-O5-C5	3.27	116.58	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	1	GLC	C1-O5-C5	2.74	115.86	112.19
4	H	1	GLC	C1-C2-C3	-2.26	106.35	109.64
4	G	2	FRU	O1-C1-C2	-2.05	107.15	111.67
4	H	1	GLC	O5-C5-C6	2.03	111.62	107.66

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-O5
4	H	2	FRU	O1-C1-C2-C3
4	H	2	FRU	O1-C1-C2-O2

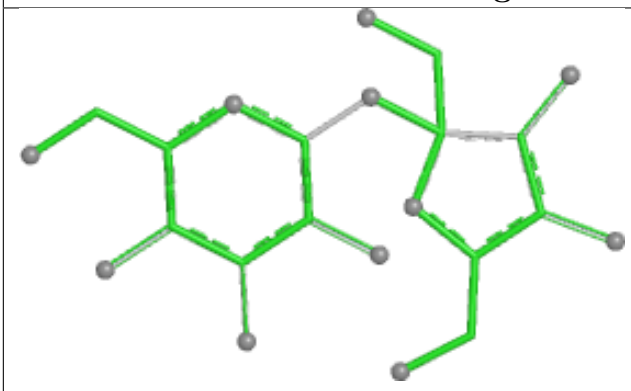
There are no ring outliers.

4 monomers are involved in 14 short contacts:

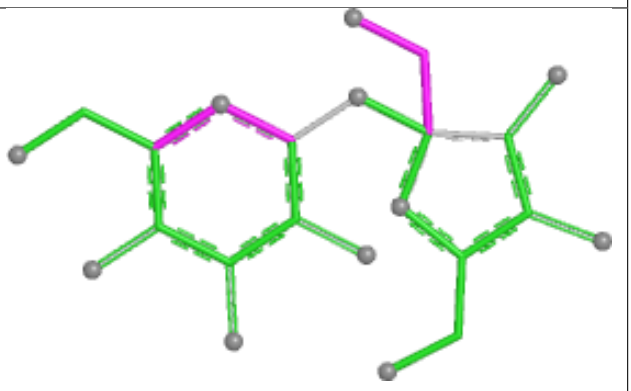
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	GLC	4	0
4	H	1	GLC	6	0
4	G	2	FRU	5	0
4	H	2	FRU	5	0

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

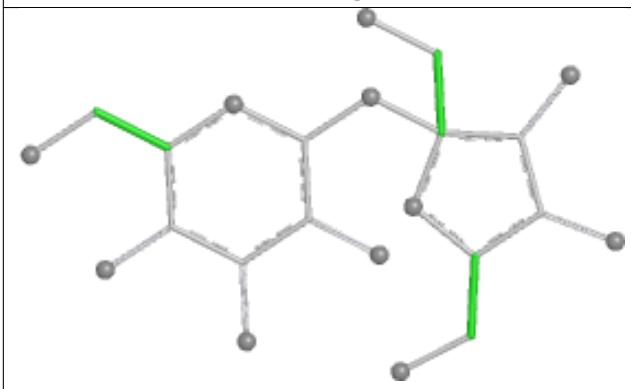
Oligosaccharide Chain G



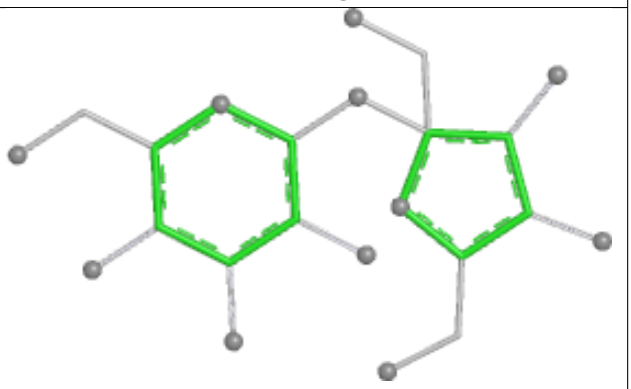
Bond lengths



Bond angles

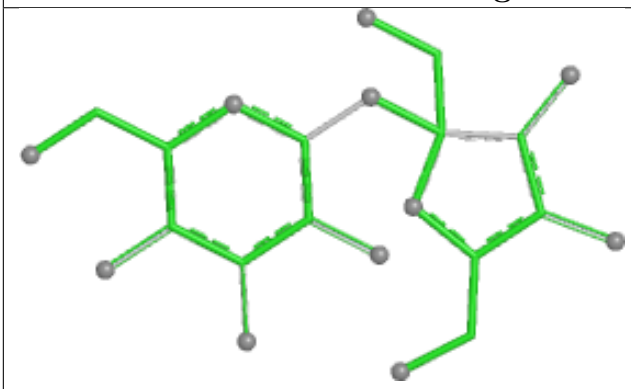


Torsions

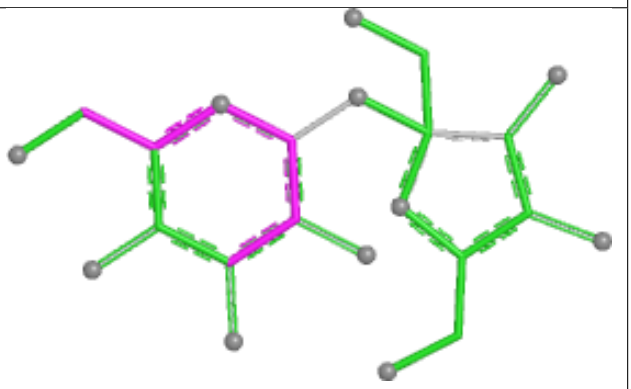


Rings

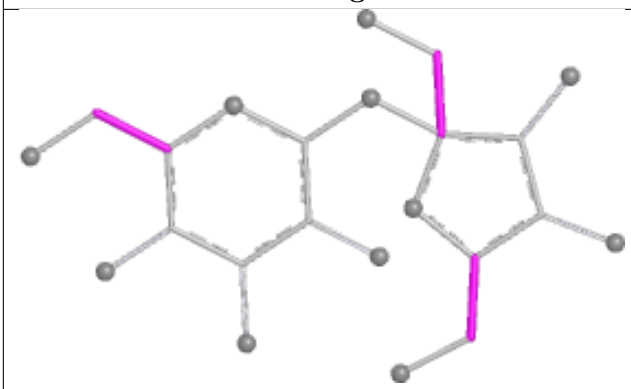
Oligosaccharide Chain H



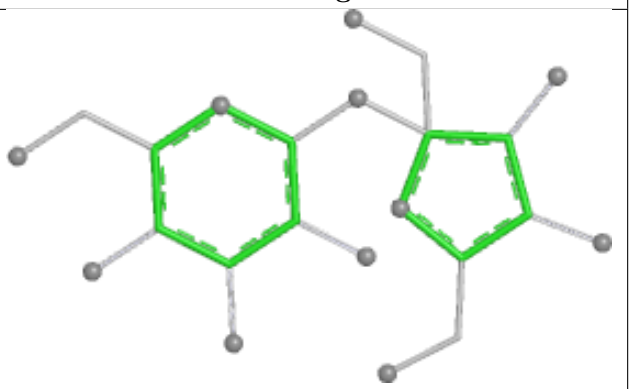
Bond lengths



Bond angles



Torsions



Rings

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	$\#\|Z\| > 2$
9	IY1	F	101	-	29,29,29	0.51	0	35,43,43	1.19	2 (5%)
8	PEG	B	507	-	6,6,6	0.11	0	5,5,5	0.08	0
10	PG4	E	101	-	12,12,12	0.54	0	11,11,11	0.23	0
5	SO4	A	601	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	C	601	-	4,4,4	0.23	0	6,6,6	0.07	0
7	GOL	C	603	-	5,5,5	0.35	0	5,5,5	0.27	0
9	IY1	E	102	-	29,29,29	0.50	0	35,43,43	1.17	2 (5%)
7	GOL	B	505	-	5,5,5	0.37	0	5,5,5	0.30	0
5	SO4	B	503	-	4,4,4	0.26	0	6,6,6	0.12	0
5	SO4	C	602	-	4,4,4	0.38	0	6,6,6	0.08	0
5	SO4	B	502	-	4,4,4	0.42	0	6,6,6	0.08	0
7	GOL	B	504	-	5,5,5	0.07	0	5,5,5	0.29	0
8	PEG	B	506	-	6,6,6	0.13	0	5,5,5	0.07	0
5	SO4	A	602	-	4,4,4	0.23	0	6,6,6	0.07	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
9	IY1	F	101	-	-	0/6/10/10	0/4/4/4
10	PG4	E	101	-	-	6/10/10/10	-
9	IY1	E	102	-	-	0/6/10/10	0/4/4/4
7	GOL	C	603	-	-	4/4/4/4	-
7	GOL	B	505	-	-	0/4/4/4	-
8	PEG	B	507	-	-	1/4/4/4	-
7	GOL	B	504	-	-	4/4/4/4	-
8	PEG	B	506	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	101	IY1	C9-C8-N	5.93	132.53	128.97
9	E	102	IY1	C9-C8-N	5.79	132.45	128.97
9	F	101	IY1	C6-C7-N1	2.56	132.68	126.88
9	E	102	IY1	C6-C7-N1	2.52	132.57	126.88

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	504	GOL	O1-C1-C2-C3
7	B	504	GOL	C1-C2-C3-O3
7	B	504	GOL	O2-C2-C3-O3
7	C	603	GOL	O1-C1-C2-C3
7	C	603	GOL	C1-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	B	504	GOL	O1-C1-C2-O2
7	C	603	GOL	O2-C2-C3-O3
10	E	101	PG4	C6-C5-O3-C4
10	E	101	PG4	O4-C7-C8-O5
8	B	506	PEG	O2-C3-C4-O4
7	C	603	GOL	O1-C1-C2-O2
10	E	101	PG4	C3-C4-O3-C5
10	E	101	PG4	O1-C1-C2-O2

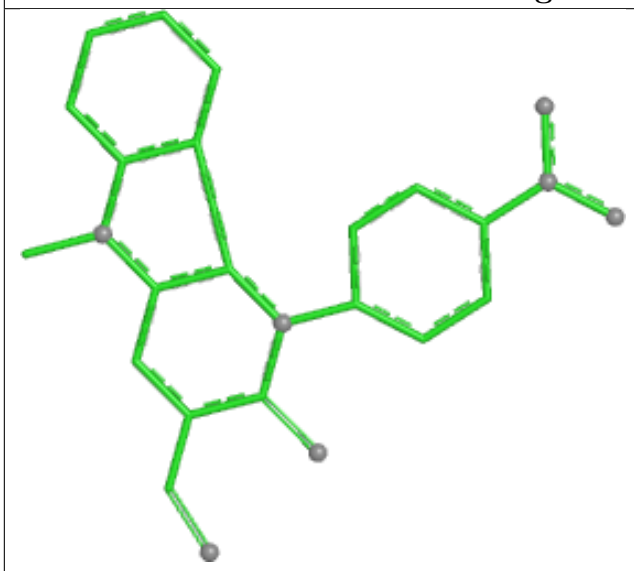
There are no ring outliers.

8 monomers are involved in 16 short contacts:

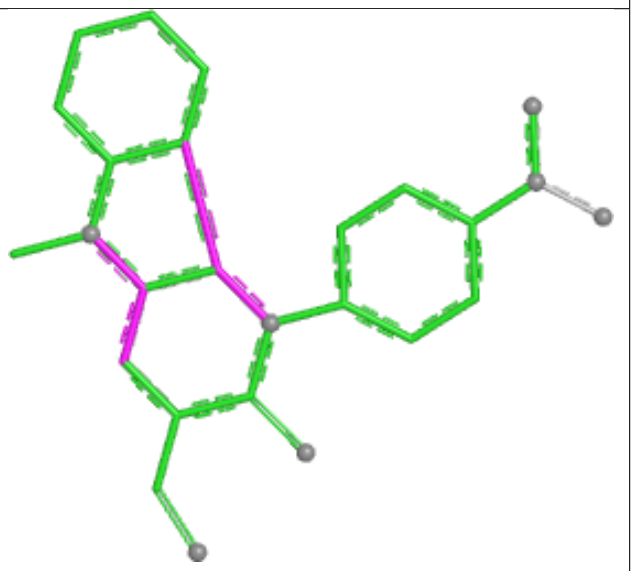
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	101	IY1	2	0
8	B	507	PEG	1	0
10	E	101	PG4	2	0
7	C	603	GOL	1	0
9	E	102	IY1	1	0
5	B	502	SO4	3	0
7	B	504	GOL	1	0
8	B	506	PEG	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

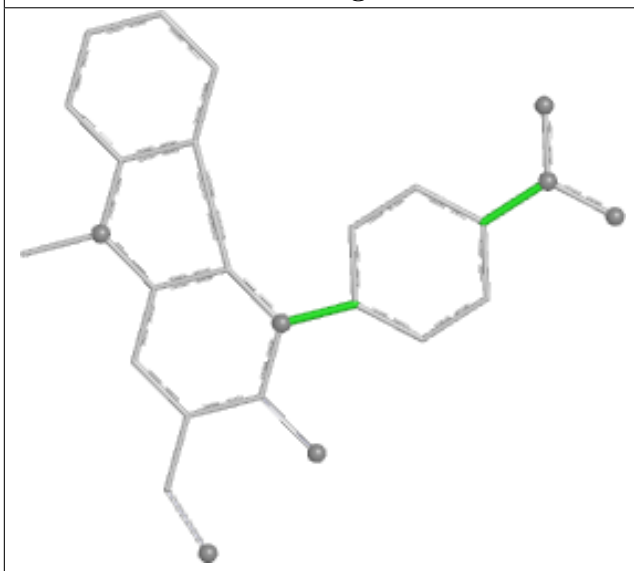
Ligand IY1 F 101



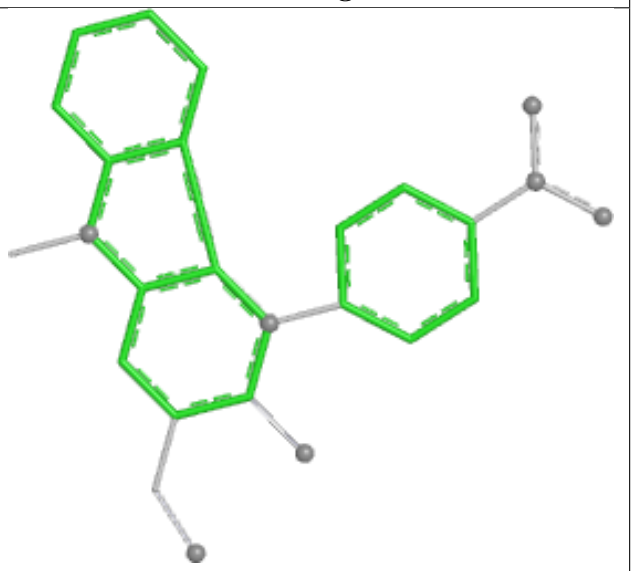
Bond lengths



Bond angles

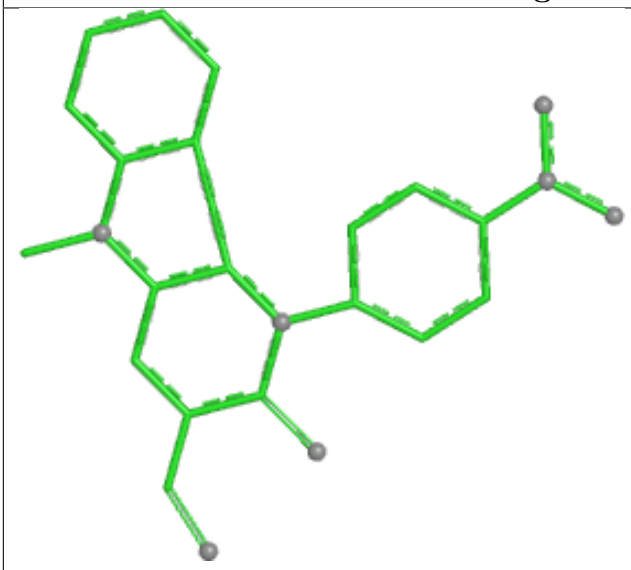


Torsions

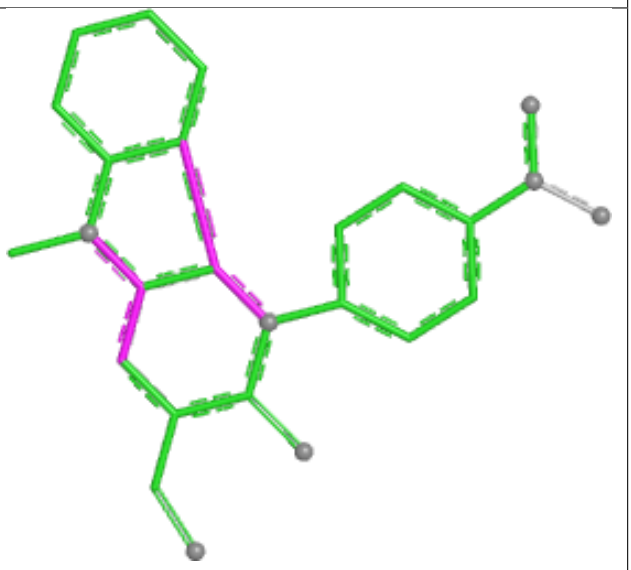


Rings

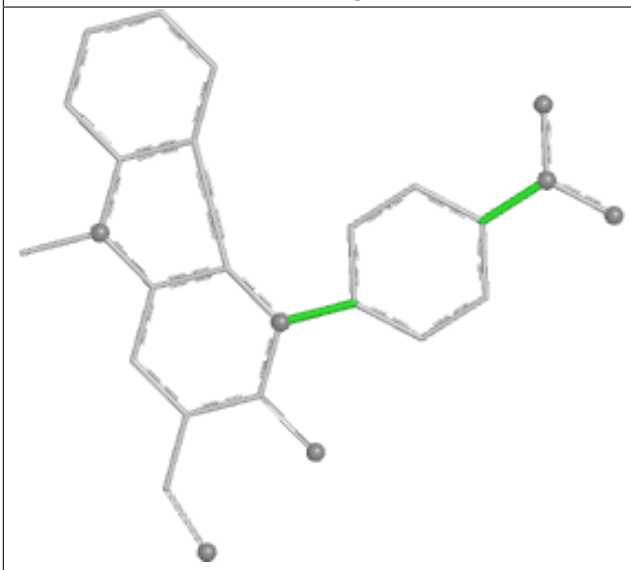
Ligand IY1 E 102



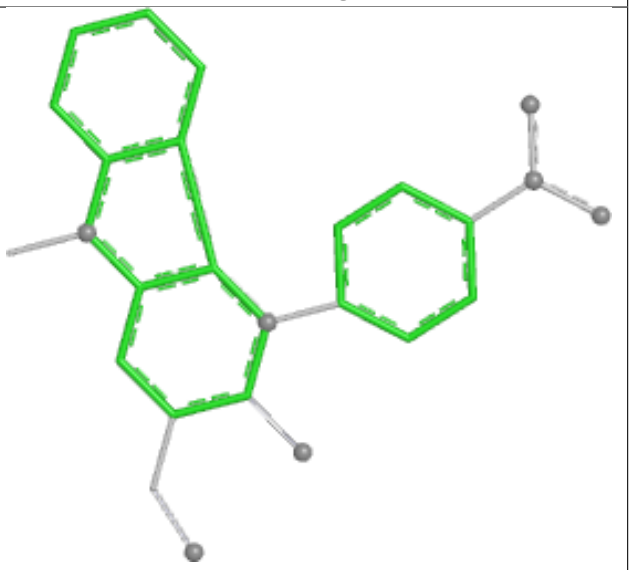
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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%)	0.10	4 (0%) 84 81	39, 114, 216, 292	1 (0%)
1	C	553/555 (99%)	0.14	8 (1%) 73 69	56, 137, 230, 292	0
2	B	415/429 (96%)	-0.01	7 (1%) 69 65	60, 101, 176, 249	0
2	D	410/429 (95%)	0.20	13 (3%) 50 46	51, 123, 207, 256	2 (0%)
3	E	33/38 (86%)	-0.39	0 100 100	81, 123, 187, 247	0
3	F	33/38 (86%)	-0.45	0 100 100	91, 145, 177, 223	0
All	All	1997/2044 (97%)	0.09	32 (1%) 70 66	39, 117, 217, 292	3 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	226	PRO	4.0
2	D	266	TRP	3.8
2	B	266	TRP	3.5
1	C	544	GLY	3.1
2	B	228	LEU	3.0
2	D	423	VAL	2.8
1	C	1	PRO	2.8
2	B	212	TRP	2.8
1	A	2	ILE	2.8
2	D	360	ALA	2.7
2	B	227	PHE	2.7
1	C	63	ILE	2.6
2	D	425	LEU	2.6
2	D	427	TYR	2.6
1	C	205	LEU	2.5
1	C	543	GLY	2.5
2	D	354	TYR	2.4
2	B	88	TRP	2.4
2	D	422	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	362	THR	2.3
2	D	248	GLU	2.2
1	C	188	TYR	2.2
1	A	132	ILE	2.2
2	B	94	ILE	2.2
1	A	553	SER	2.2
1	A	303	LEU	2.1
2	D	318[A]	TYR	2.1
2	D	144	TYR	2.1
1	C	73	LYS	2.1
1	C	111	VAL	2.1
2	D	90	VAL	2.0
2	D	120	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^{th} 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	0.93	0.07	135,146,151,153	0
3	OMC	F	4	21/22	0.93	0.09	114,128,141,154	0
3	OMC	E	4	21/22	0.93	0.11	71,84,97,118	0
3	OMC	E	2	21/22	0.95	0.08	92,106,115,118	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^{th} 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.

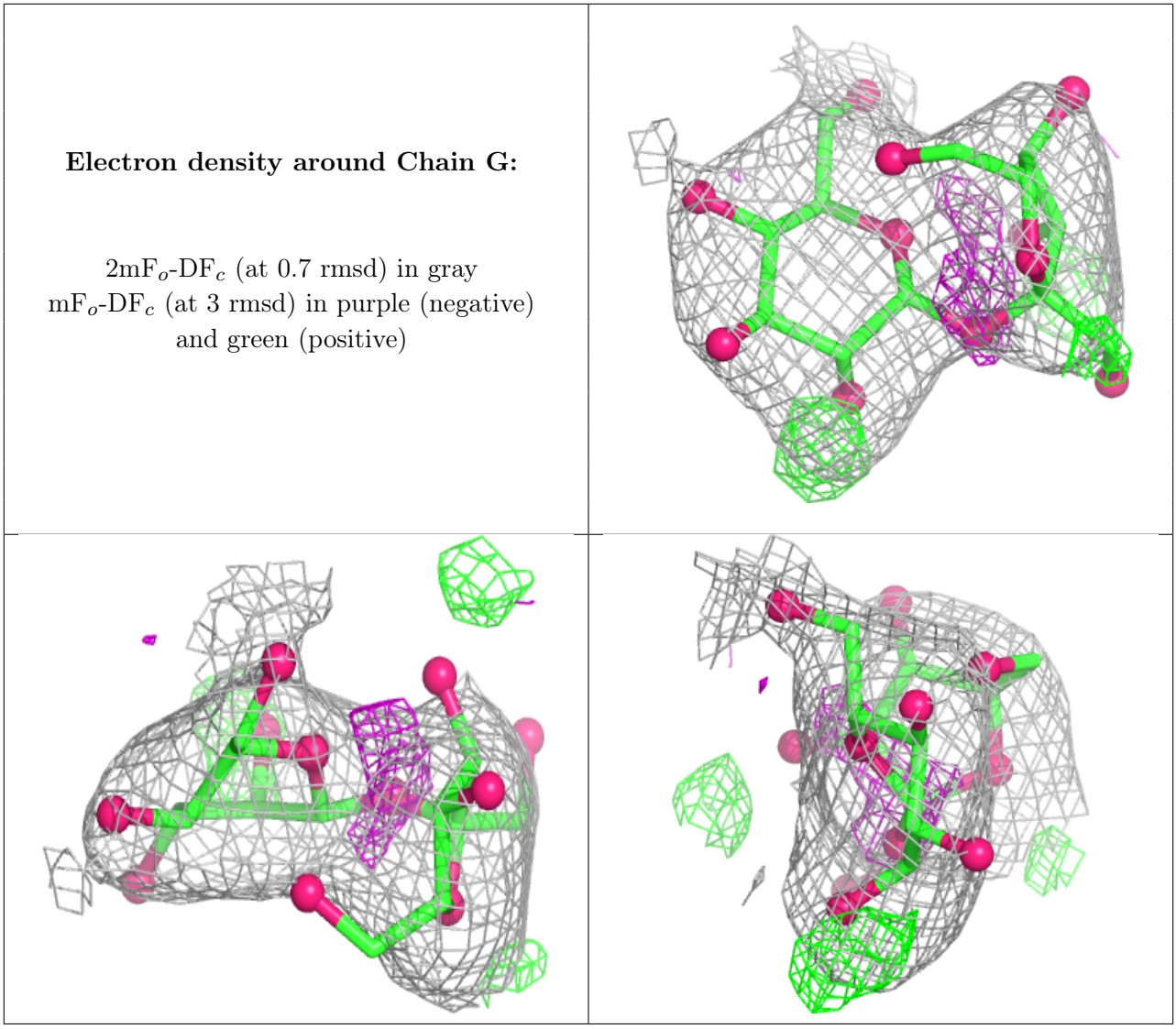
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FRU	G	2	12/12	0.81	0.18	138,151,156,161	0
4	FRU	H	2	12/12	0.83	0.11	135,157,166,170	0
4	GLC	G	1	11/12	0.85	0.12	102,114,127,132	0
4	GLC	H	1	11/12	0.88	0.12	132,137,151,157	0

The following is a graphical depiction of the model fit to experimental electron density for oligosac-

charide. Each fit is shown from different orientation to approximate a three-dimensional view.

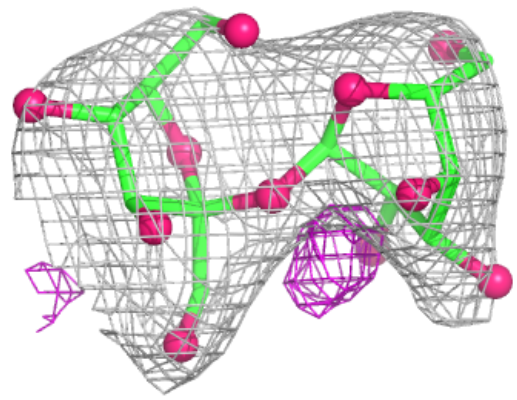
Electron density around Chain G:

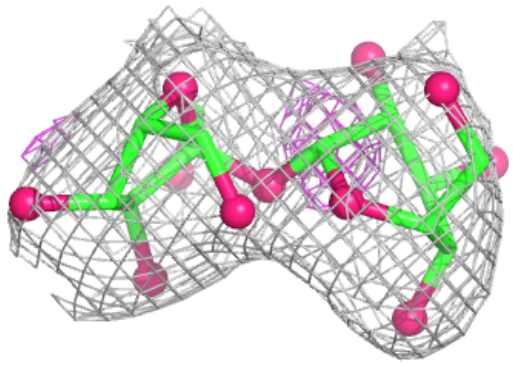
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

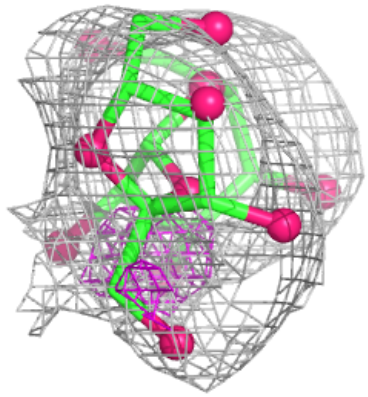


Electron density around Chain H:

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







6.4 Ligands

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^{th} 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	0.50	0.28	130,156,156,156	0
5	SO4	C	602	5/5	0.61	0.08	188,191,192,196	0
5	SO4	A	601	5/5	0.63	0.11	166,171,173,176	0
9	IY1	F	101	26/26	0.64	0.14	169,182,210,216	0
6	NH4	C	604	1/1	0.73	0.26	104,125,125,125	0
5	SO4	B	503	5/5	0.73	0.10	190,190,193,194	0
5	SO4	C	601	5/5	0.76	0.10	159,161,162,163	0
10	PG4	E	101	13/13	0.81	0.15	125,144,149,150	0
9	IY1	E	102	26/26	0.85	0.11	144,158,178,183	0
7	GOL	B	504	6/6	0.85	0.13	91,113,121,126	0
7	GOL	C	603	6/6	0.87	0.10	115,119,121,124	0
8	PEG	B	507	7/7	0.88	0.42	168,187,201,203	0
5	SO4	B	502	5/5	0.89	0.11	137,137,138,150	0

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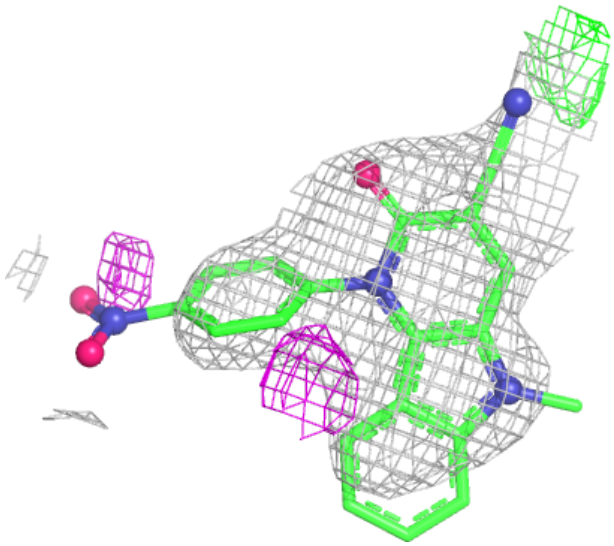
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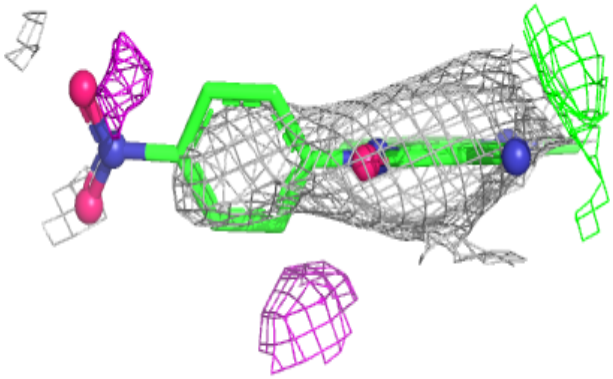
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	B	505	6/6	0.90	0.22	89,95,106,107	0
8	PEG	B	506	7/7	0.91	0.12	92,100,103,109	0
5	SO4	A	602	5/5	0.92	0.09	178,182,184,184	0

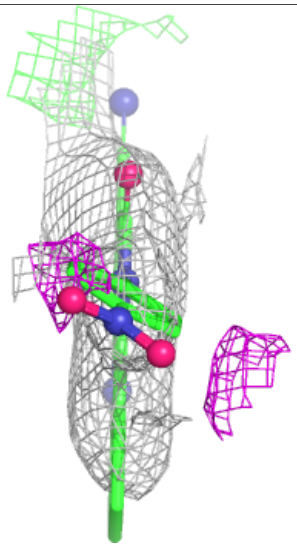
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

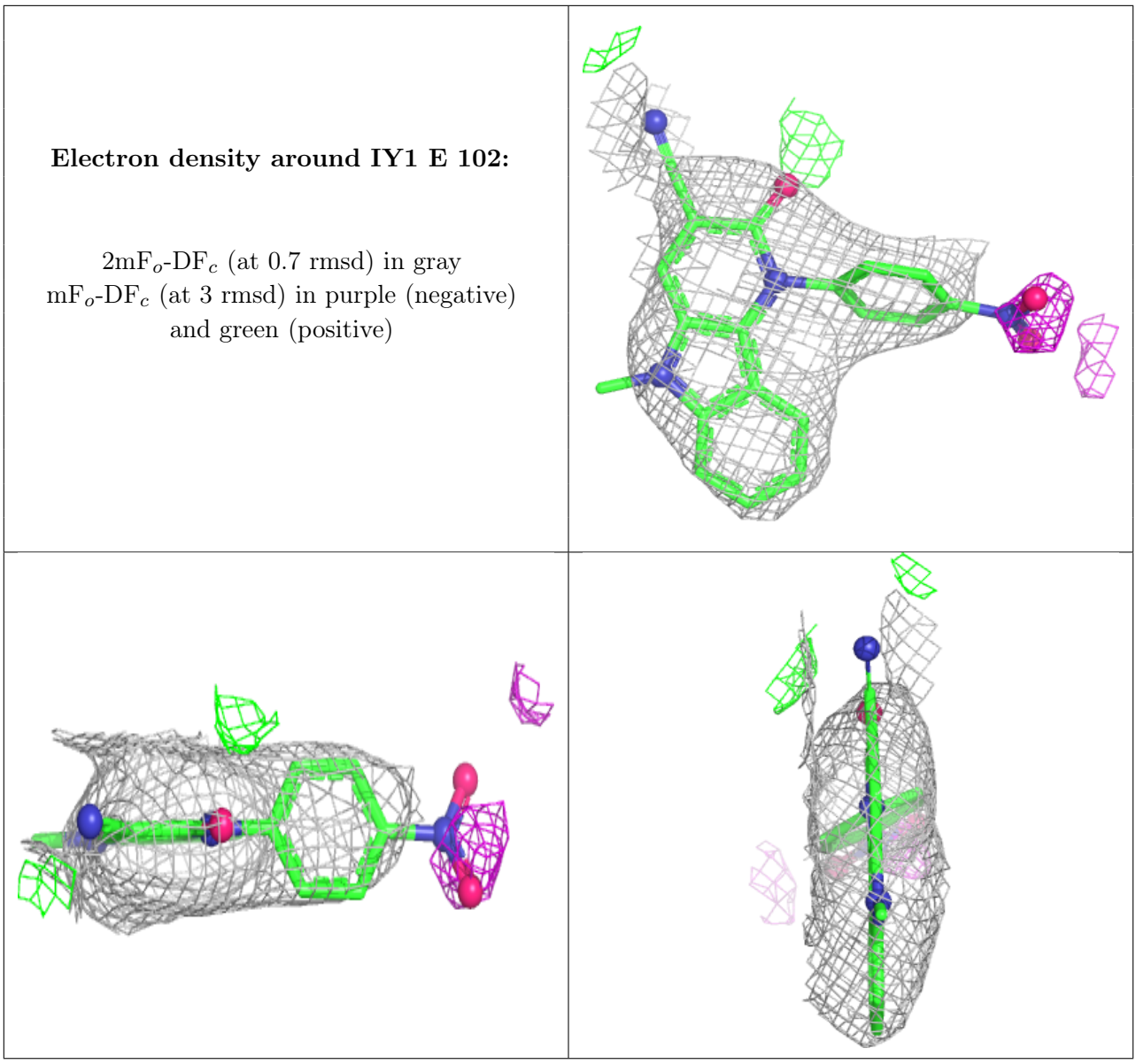






Electron density around IY1 E 102:

$2mF_o$-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

There are no such residues in this entry.