



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:22 PM EDT

PDB ID : 7LRY  
Title : Structure of HIV-1 Reverse Transcriptase in complex with DNA, (-)FTC-TP, and CA(2+) ion  
Authors : Hoang, A.; Ruiz, F.X.; Arnold, E.  
Deposited on : 2021-02-17  
Resolution : 2.45 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

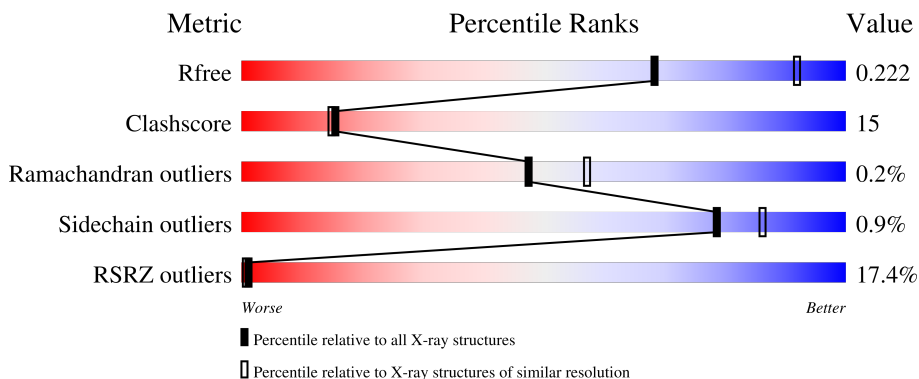
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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.



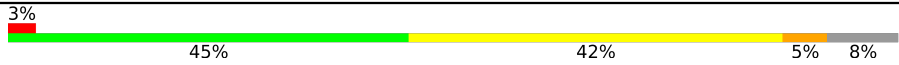
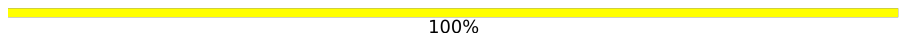
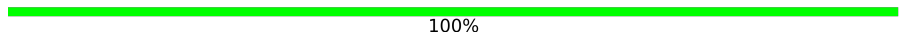
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	555	 13% 68% 31% .
1	C	555	 32% 68% 31% .
2	B	429	 8% 73% 24% .
2	D	429	 13% 70% 25% .
3	E	38	 53% 37% 8%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	F	38	
4	M	2	
4	N	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
6	GOL	A	602	-	-	-	X
7	PG4	A	603	-	-	X	-
8	NH4	A	604	-	-	-	X
8	NH4	C	602	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17811 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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
2	B	415	Total	C	N	O	S	0	1	0
			3440	2243	568	622	7			
2	D	410	Total	C	N	O	S	0	1	0
			3400	2217	562	614	7			

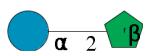
There are 4 discrepancies between the modelled and reference sequences:

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/RNA (38-MER).

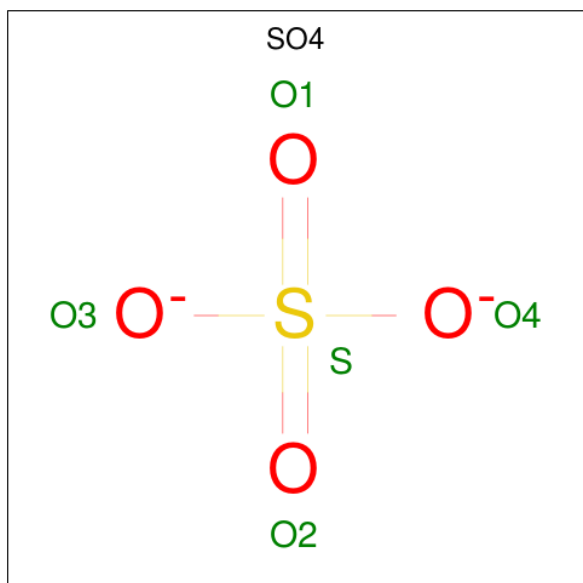
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	35	Total	C	N	O	P	0	0	0
			721	340	130	216	35			
3	E	35	Total	C	N	O	P	0	0	0
			721	340	130	216	35			

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



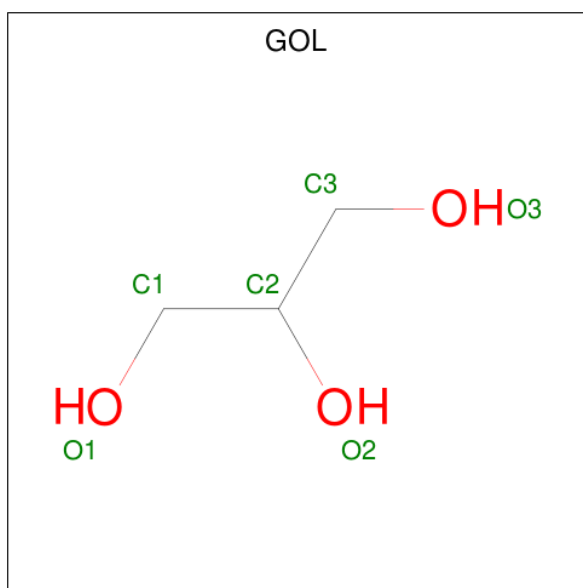
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	M	2	Total	C	O	0	0	0
			23	12	11			
4	N	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



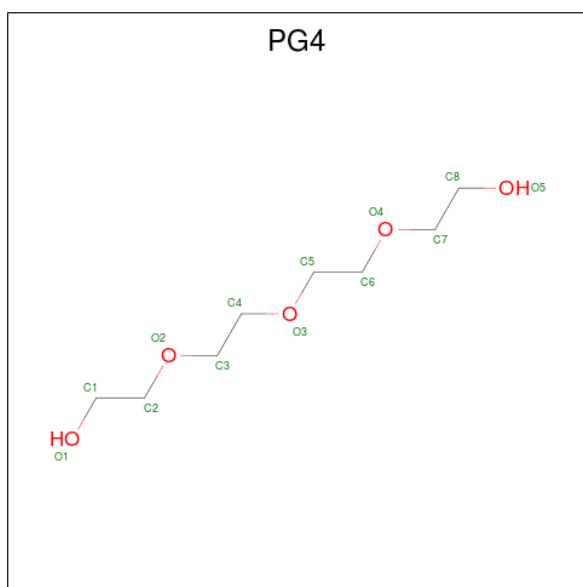
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		
5	B	1	Total	O S	0	0
			5	4 1		
5	C	1	Total	O S	0	0
			5	4 1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



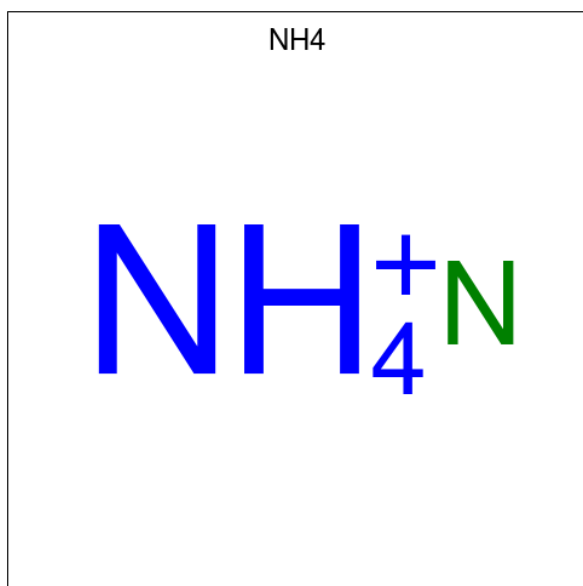
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0
6	D	1	Total C O 6 3 3	0	0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

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).

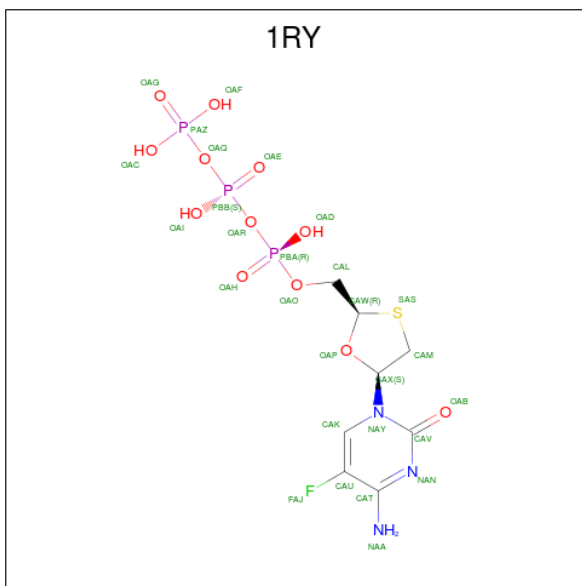


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	H	N	0	0
			5	4	1		
8	C	1	Total	H	N	0	0
			5	4	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Ca 1 1	0	0
9	C	1	Total Ca 1 1	0	0

- Molecule 10 is [[(2R,5S)-5-(4-azanyl-5-fluoranyl-2-oxidanylidene-pyrimidin-1-yl)-1,3-oxathiolan-2-yl]methoxy-oxidanyl-phosphoryl] phosphono hydrogen phosphate (three-letter code: 1RY) (formula: C<sub>8</sub>H<sub>13</sub>FN<sub>3</sub>O<sub>12</sub>P<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
10	A	1	Total	C	F	N	O	P	S	0	0
			28	8	1	3	12	3	1		
10	C	1	Total	C	F	N	O	P	S	0	0
			28	8	1	3	12	3	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	82	Total O 82 82	0	0
11	B	71	Total O 71 71	0	0
11	C	76	Total O 76 76	0	0
11	D	54	Total O 54 54	0	0
11	F	8	Total O 8 8	0	0

*Continued on next page...*



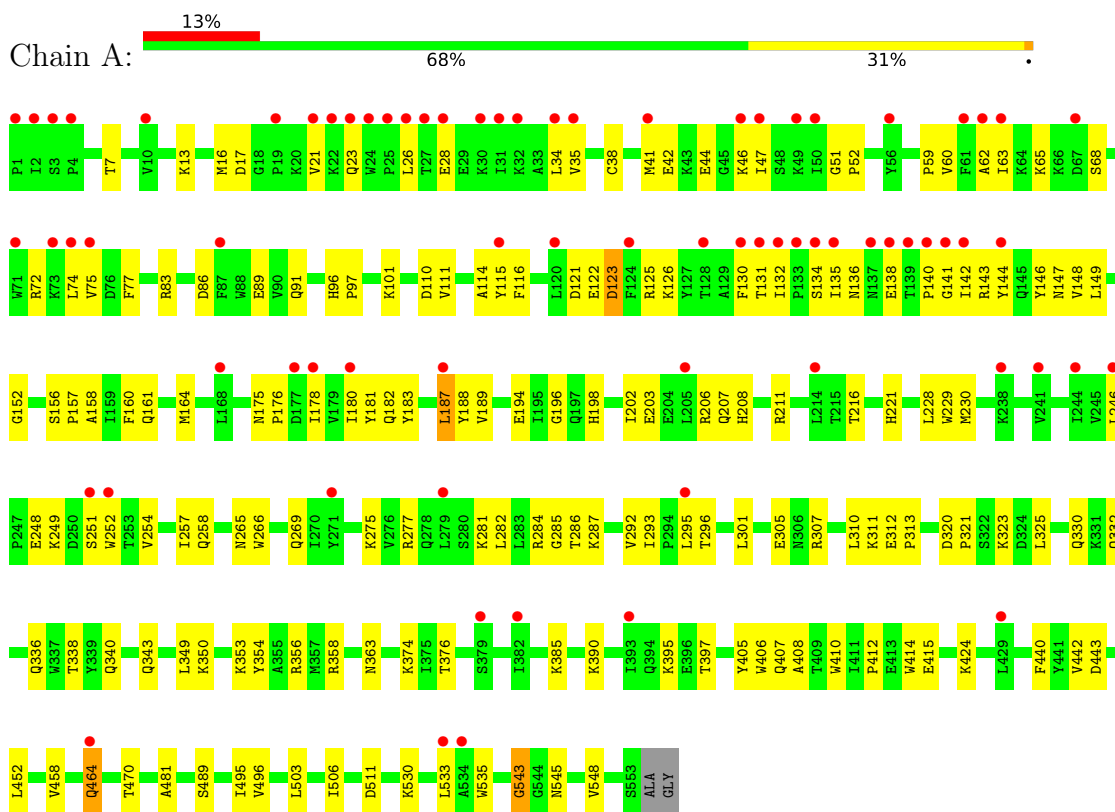
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
11	E	10	Total	O	0	0
			10	10		

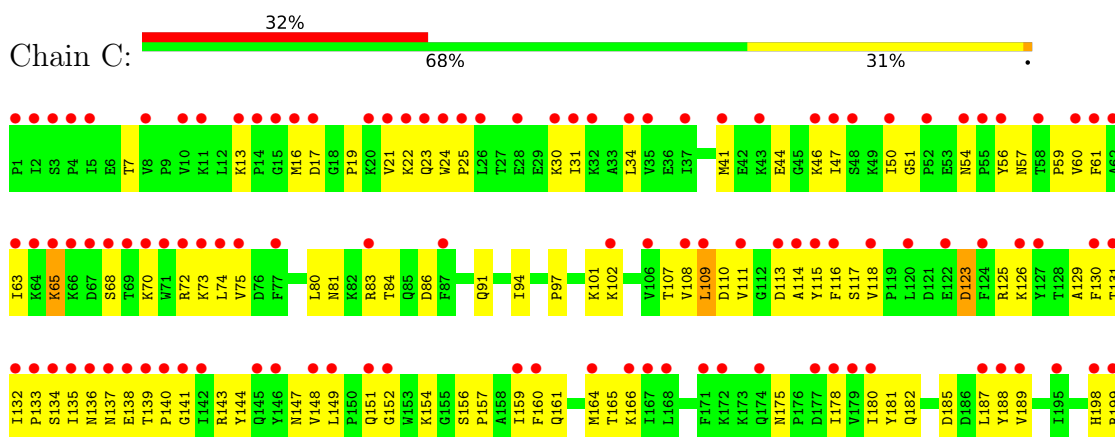
### 3 Residue-property plots

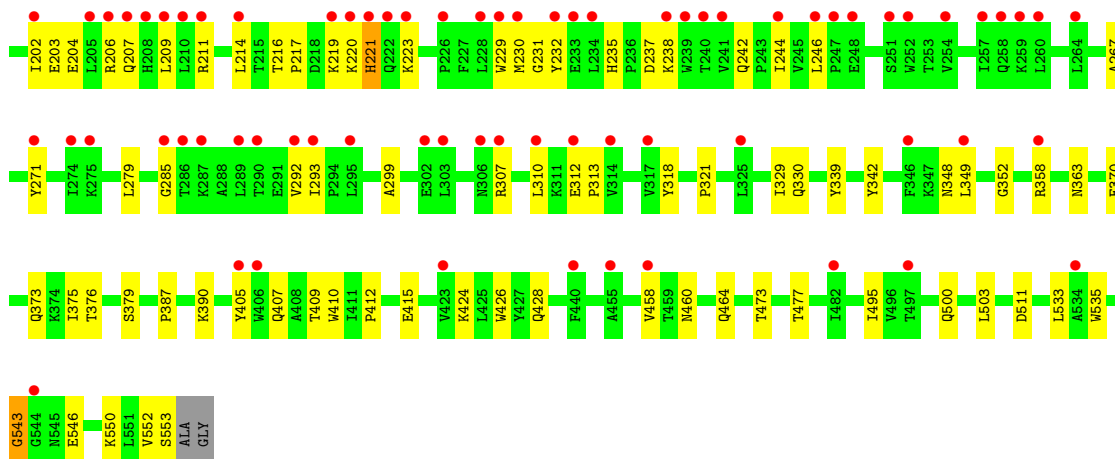
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

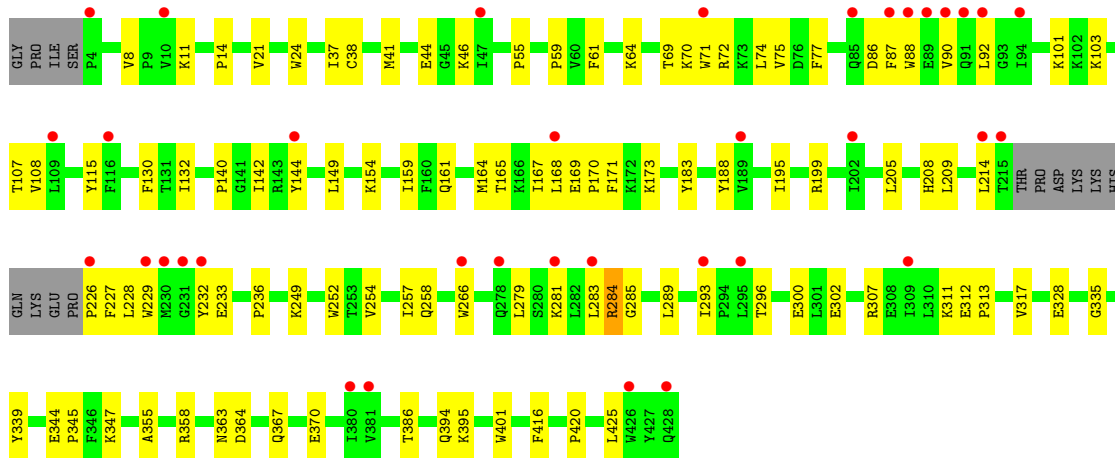


- Molecule 1: Reverse transcriptase p66

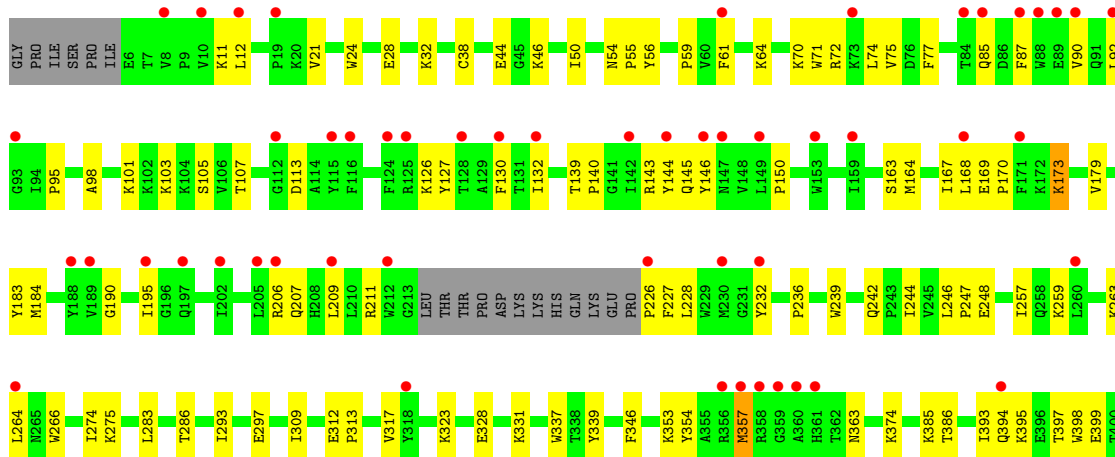


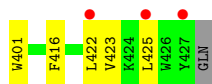


• Molecule 2: Reverse transcriptase p51

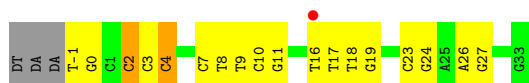


• Molecule 2: Reverse transcriptase p51

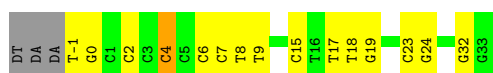




- Molecule 3: DNA/RNA (38-MER)



- Molecule 3: DNA/RNA (38-MER)



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.26Å 129.19Å 131.32Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	91.27 – 2.45 91.27 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (91.27-2.45) 99.6 (91.27-2.45)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.45Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.190 , 0.222 0.190 , 0.222	Depositor DCC
$R_{free}$ test set	1993 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 81.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17811	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, PG4, OMC, FRU, GLC, CA, NH4, 1RY

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	0.26	0/4631	0.44	0/6291
1	C	0.25	0/4622	0.44	0/6279
2	B	0.26	0/3543	0.45	0/4812
2	D	0.25	0/3502	0.44	0/4757
3	E	0.53	0/760	0.87	0/1172
3	F	0.53	0/760	0.88	0/1172
All	All	0.29	0/17818	0.50	0/24483

There are no bond length outliers.

There are no bond angle outliers.

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	150	0
1	C	4504	0	4567	163	0
2	B	3440	0	3474	91	0
2	D	3400	0	3429	105	0
3	E	721	0	397	15	0
3	F	721	0	397	19	0
4	M	23	0	21	1	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	23	0	21	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
6	A	6	0	8	1	0
6	B	36	0	48	5	0
6	D	24	0	32	6	0
6	F	6	0	8	0	0
7	A	13	0	18	7	0
8	A	1	4	0	0	0
8	C	1	4	0	0	0
9	A	1	0	0	0	0
9	C	1	0	0	0	0
10	A	28	0	12	2	0
10	C	28	0	11	2	0
11	A	82	0	0	11	0
11	B	71	0	0	5	0
11	C	76	0	0	11	0
11	D	54	0	0	6	0
11	E	10	0	0	2	0
11	F	8	0	0	2	0
All	All	17803	8	17018	510	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 15.

All (510) 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:281:LYS:HE3	2:B:284:ARG:NH2	1.43	1.34
2:D:257:ILE:HD12	2:D:293:ILE:HD11	1.35	1.08
1:A:208:HIS:HA	1:A:211:ARG:HE	1.14	1.06
1:C:246:LEU:HD11	1:C:310:LEU:HD12	1.38	1.03
1:A:458:VAL:HG23	1:A:464[B]:GLN:HG2	1.41	0.99
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.39	0.99
2:B:281:LYS:HE3	2:B:284:ARG:HH22	1.09	0.92
2:B:317:VAL:HG12	2:B:347:LYS:HD2	1.53	0.90
1:A:269:GLN:HB3	7:A:603:PG4:H32	1.56	0.88
1:C:75:VAL:HG12	11:C:720:HOH:O	1.75	0.87
1:A:44:GLU:HG2	1:A:46:LYS:HE2	1.59	0.85
1:C:131:THR:HG22	1:C:143:ARG:HG2	1.56	0.85

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:LYS:HG3	2:D:226:PRO:HD3	1.60	0.83
1:C:165:THR:HG23	1:C:182:GLN:HE22	1.43	0.83
1:A:65:LYS:HB2	1:A:68:SER:HB3	1.58	0.82
1:C:44:GLU:CG	1:C:46:LYS:HE2	2.09	0.82
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.62	0.82
1:C:101:LYS:HE3	1:C:321:PRO:HG2	1.62	0.81
1:A:208:HIS:HA	1:A:211:ARG:NE	1.93	0.81
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.62	0.80
2:D:164:MET:HE3	2:D:168:LEU:HD21	1.63	0.80
1:A:44:GLU:CG	1:A:46:LYS:HE2	2.11	0.80
1:A:135:ILE:HG13	1:A:138:GLU:HB2	1.63	0.80
1:C:135:ILE:HD11	1:C:139:THR:HG23	1.64	0.80
1:A:208:HIS:CB	1:A:211:ARG:HH21	1.96	0.79
1:A:208:HIS:HB2	1:A:211:ARG:HH21	1.47	0.79
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.65	0.79
2:B:195:ILE:HD12	2:B:195:ILE:H	1.48	0.77
2:B:266:TRP:CZ3	2:B:425:LEU:HD21	2.21	0.76
2:B:281:LYS:CE	2:B:284:ARG:HH22	1.95	0.76
1:C:44:GLU:HG3	1:C:46:LYS:HE2	1.68	0.76
2:D:195:ILE:H	2:D:195:ILE:HD12	1.51	0.75
2:D:164:MET:HE2	2:D:168:LEU:HD11	1.69	0.75
2:D:173:LYS:HE2	2:D:173:LYS:HA	1.67	0.75
2:B:281:LYS:HE3	2:B:284:ARG:CZ	2.16	0.75
2:B:296:THR:O	2:B:300:GLU:HG3	1.86	0.74
2:D:242:GLN:HE22	2:D:353:LYS:HE3	1.52	0.74
1:A:203:GLU:O	1:A:207:GLN:HG2	1.87	0.74
1:C:207:GLN:O	1:C:211:ARG:HG3	1.87	0.74
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.69	0.73
2:D:259:LYS:HG3	11:D:654:HOH:O	1.88	0.73
2:B:257:ILE:HD12	2:B:293:ILE:HD11	1.68	0.73
1:C:182:GLN:HE21	2:D:139:THR:HG23	1.53	0.73
1:C:41:MET:HB3	1:C:46:LYS:HB2	1.70	0.72
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.69	0.72
2:B:254:VAL:HG13	2:B:283:LEU:CD2	2.20	0.71
2:B:88:TRP:HZ2	1:C:390:LYS:HZ1	1.39	0.71
2:D:173:LYS:HA	2:D:173:LYS:CE	2.21	0.71
3:E:8:DT:H2'	3:E:9:DT:H71	1.72	0.71
1:A:281:LYS:O	1:A:284:ARG:HG2	1.89	0.70
1:C:182:GLN:NE2	2:D:139:THR:HG23	2.07	0.70
1:C:546:GLU:HG2	1:C:550:LYS:HE3	1.74	0.70
2:D:346:PHE:H	6:D:502:GOL:H12	1.55	0.70

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.72	0.70
1:C:91:GLN:HB2	1:C:161:GLN:HE22	1.57	0.69
2:D:244:ILE:HD13	2:D:425:LEU:HD11	1.75	0.69
3:E:15:DC:H2'	11:E:106:HOH:O	1.92	0.69
1:A:275:LYS:HE3	11:A:779:HOH:O	1.90	0.69
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.74	0.69
1:A:152:GLY:H	3:E:0:DG:H21	1.41	0.69
2:D:263:LYS:HA	2:D:423:VAL:HG11	1.74	0.68
1:C:73:LYS:HB3	11:C:764:HOH:O	1.93	0.68
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.29	0.68
1:C:115:TYR:CZ	10:C:604:1RY:H9	2.29	0.68
1:C:458:VAL:HG23	1:C:464:GLN:HG2	1.74	0.68
1:C:113:ASP:HA	10:C:604:1RY:OAH	1.94	0.67
1:C:101:LYS:HE3	1:C:321:PRO:CG	2.24	0.67
2:D:309:ILE:O	2:D:312:GLU:HG2	1.93	0.67
1:C:390:LYS:NZ	1:C:415:GLU:OE2	2.28	0.67
2:B:164:MET:HE2	2:B:168:LEU:HD11	1.76	0.67
2:D:72:ARG:HG3	2:D:226:PRO:HB3	1.76	0.67
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.35	0.66
1:C:44:GLU:HG2	1:C:46:LYS:HE2	1.76	0.66
1:C:358:ARG:NH2	2:D:394[A]:GLN:OE1	2.28	0.66
1:A:91:GLN:NE2	1:A:161:GLN:OE1	2.28	0.66
2:B:70:LYS:HG3	2:B:226:PRO:HD3	1.77	0.66
1:C:358:ARG:HD3	1:C:370:GLU:OE2	1.96	0.66
1:C:135:ILE:O	1:C:135:ILE:HG13	1.96	0.66
1:C:72:ARG:HH21	1:C:151:GLN:HE22	1.43	0.66
1:C:178:ILE:HD11	1:C:189:VAL:CG1	2.26	0.66
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.30	0.66
3:E:18:DT:H4'	3:E:19:DG:C8	2.31	0.66
1:C:117:SER:HB2	11:C:705:HOH:O	1.96	0.65
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.78	0.65
1:C:139:THR:HB	1:C:140:PRO:HD2	1.79	0.65
1:A:206:ARG:HG2	1:A:216:THR:OG1	1.96	0.65
1:C:102:LYS:HE2	1:C:237:ASP:HA	1.79	0.64
1:A:101:LYS:HE2	1:A:321:PRO:CG	2.26	0.64
1:A:287:LYS:HE2	11:A:776:HOH:O	1.97	0.64
1:C:50:ILE:HG21	1:C:54:ASN:HB2	1.78	0.64
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.27	0.64
1:A:164:MET:HE2	1:A:164:MET:O	1.97	0.64
1:C:175:ASN:O	1:C:178:ILE:HG22	1.98	0.64
2:D:101:LYS:O	2:D:236:PRO:HB2	1.98	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:LYS:HG2	2:D:85:GLN:OE1	1.97	0.63
2:B:164:MET:CE	2:B:168:LEU:HD11	2.29	0.63
1:A:152:GLY:N	3:E:0:DG:H21	1.96	0.63
1:A:115:TYR:CZ	10:A:606:1RY:H9	2.34	0.63
2:D:357:MET:SD	2:D:357:MET:N	2.72	0.63
1:C:31:ILE:HG23	1:C:132:ILE:HD11	1.80	0.62
1:C:203:GLU:O	1:C:207:GLN:HG2	1.98	0.62
1:A:543:GLY:HA2	2:B:285:GLY:O	1.99	0.62
3:F:-1:DT:H2'	3:F:-1:DT:O2	1.99	0.62
1:A:47:ILE:CG2	1:A:144:TYR:HB3	2.30	0.62
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.34	0.62
2:D:257:ILE:HD12	2:D:293:ILE:CD1	2.22	0.62
4:M:1:GLC:H62	4:M:2:FRU:H61	1.79	0.62
1:C:110:ASP:HB3	1:C:220:LYS:HB3	1.82	0.62
1:C:152:GLY:N	3:F:0:DG:H21	1.98	0.62
2:B:101:LYS:O	2:B:236:PRO:HB2	1.99	0.61
1:C:22:LYS:O	1:C:59:PRO:HG3	2.00	0.61
1:A:115:TYR:OH	10:A:606:1RY:H9	1.99	0.61
1:C:123:ASP:O	1:C:126:LYS:HE3	2.00	0.61
1:C:543:GLY:HA3	11:D:635:HOH:O	1.99	0.60
2:D:61:PHE:CZ	2:D:74:LEU:HD23	2.36	0.60
1:A:287:LYS:HB2	11:A:736:HOH:O	2.00	0.60
1:C:24:TRP:HE3	1:C:25:PRO:HD2	1.67	0.60
1:C:285:GLY:N	3:F:9:DT:OP1	2.35	0.60
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.01	0.60
1:C:110:ASP:HB3	1:C:220:LYS:CB	2.32	0.60
1:C:198:HIS:O	1:C:202:ILE:HG12	2.01	0.60
1:A:17:ASP:O	1:A:83:ARG:HD3	2.02	0.60
2:B:164:MET:HE3	2:B:168:LEU:HD21	1.84	0.60
1:C:152:GLY:H	3:F:0:DG:H21	1.47	0.60
1:A:176:PRO:HA	11:A:711:HOH:O	2.02	0.60
1:C:410:TRP:CH2	1:C:412:PRO:HA	2.37	0.60
3:E:-1:DT:O2	3:E:-1:DT:H2'	2.01	0.60
2:B:142:ILE:HG12	11:B:638:HOH:O	2.00	0.59
1:C:156:SER:HB2	11:C:770:HOH:O	2.03	0.59
1:C:246:LEU:HD11	1:C:310:LEU:CD1	2.24	0.59
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.37	0.59
1:C:166:LYS:HD2	11:C:772:HOH:O	2.03	0.59
1:A:28:GLU:OE2	1:A:136:ASN:ND2	2.29	0.59
1:A:7:THR:HG21	1:A:121:ASP:HA	1.85	0.59
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.37	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:354:TYR:CE1	2:D:374:LYS:HD2	2.37	0.59
1:C:135:ILE:HG12	1:C:139:THR:OG1	2.02	0.59
1:C:180:ILE:HA	1:C:188:TYR:O	2.03	0.59
2:D:247:PRO:HD2	11:D:633:HOH:O	2.03	0.59
1:A:458:VAL:HG23	1:A:464[B]:GLN:CG	2.25	0.58
1:C:109:LEU:HD13	11:C:704:HOH:O	2.03	0.58
2:D:266:TRP:CE3	2:D:425:LEU:HD22	2.38	0.58
1:A:135:ILE:HB	1:A:138:GLU:OE1	2.03	0.58
1:A:332:GLN:OE1	1:A:338:THR:HG23	2.03	0.58
1:C:21:VAL:HB	1:C:59:PRO:HD3	1.86	0.58
1:A:533:LEU:O	6:A:602:GOL:H31	2.04	0.58
2:D:164:MET:CE	2:D:168:LEU:HD11	2.33	0.58
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.39	0.58
2:D:164:MET:HE3	2:D:168:LEU:CD2	2.32	0.58
1:C:358:ARG:HD3	1:C:370:GLU:CD	2.24	0.58
2:D:207:GLN:O	2:D:211:ARG:HG2	2.04	0.57
1:A:136:ASN:HB2	1:A:138:GLU:OE2	2.03	0.57
1:C:7:THR:HG22	11:C:735:HOH:O	2.04	0.57
1:C:204:GLU:HB3	11:C:768:HOH:O	2.05	0.57
2:D:183:TYR:OH	2:D:386:THR:HG23	2.05	0.57
2:B:209:LEU:HD13	2:B:228:LEU:CD2	2.34	0.57
1:C:206:ARG:HG2	1:C:216:THR:OG1	2.03	0.57
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.40	0.57
1:C:409:THR:OG1	6:D:501:GOL:H12	2.05	0.57
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.87	0.57
1:A:207:GLN:O	1:A:211:ARG:HG3	2.04	0.57
1:C:41:MET:O	1:C:46:LYS:N	2.35	0.57
2:D:266:TRP:CZ3	2:D:425:LEU:HD22	2.39	0.57
1:A:68:SER:HB2	11:A:704:HOH:O	2.05	0.56
1:A:390:LYS:NZ	1:A:415:GLU:OE2	2.37	0.56
1:A:452:LEU:HD22	1:A:470:THR:HG22	1.88	0.56
1:C:118:VAL:HB	1:C:149:LEU:HG	1.87	0.56
1:C:164:MET:CE	1:C:187:LEU:HD11	2.36	0.56
1:A:23:GLN:NE2	1:A:26:LEU:HD11	2.20	0.56
1:A:277:ARG:HD2	11:A:759:HOH:O	2.05	0.56
1:A:503:LEU:HD11	1:A:533:LEU:HB3	1.87	0.56
2:D:244:ILE:HD11	2:D:425:LEU:HD21	1.86	0.56
1:C:135:ILE:HG13	1:C:138:GLU:HB2	1.88	0.55
1:A:178:ILE:HD11	1:A:189:VAL:CG1	2.37	0.55
3:E:17:DT:H5'	11:E:110:HOH:O	2.06	0.55
2:B:317:VAL:CG1	2:B:347:LYS:HD2	2.33	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:HG3	1:A:46:LYS:HE2	1.89	0.55
2:B:64:LYS:O	6:B:505:GOL:H32	2.07	0.55
1:A:354:TYR:CE1	1:A:356:ARG:HB3	2.42	0.54
1:A:307:ARG:O	1:A:311:LYS:HG3	2.06	0.54
2:B:209:LEU:HD13	2:B:228:LEU:HD22	1.88	0.54
1:A:356:ARG:HD3	11:A:741:HOH:O	2.07	0.54
7:A:603:PG4:O5	7:A:603:PG4:H61	2.07	0.54
1:A:183:TYR:OH	3:E:32:DG:N3	2.36	0.54
2:B:72:ARG:HG2	2:B:226:PRO:HB3	1.90	0.54
2:D:146:TYR:CD2	2:D:150:PRO:HB3	2.43	0.54
1:A:23:GLN:HE21	1:A:26:LEU:HD21	1.73	0.54
1:C:108:VAL:C	1:C:109:LEU:HD12	2.28	0.54
1:A:51:GLY:N	1:A:52:PRO:CD	2.71	0.53
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.38	0.53
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.89	0.53
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.43	0.53
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.90	0.53
1:C:65:LYS:HB3	1:C:68:SER:HB3	1.89	0.53
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.44	0.53
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.43	0.53
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.91	0.53
2:B:64:LYS:HE3	2:B:71:TRP:CE2	2.43	0.53
1:A:149:LEU:HD12	1:A:160:PHE:HB2	1.90	0.53
1:C:132:ILE:HG13	1:C:133:PRO:HD2	1.91	0.53
1:A:132:ILE:CG2	1:A:142:ILE:HG13	2.38	0.52
7:A:603:PG4:H82	7:A:603:PG4:H31	1.92	0.52
2:B:107:THR:HA	2:B:232:TYR:O	2.10	0.52
2:B:317:VAL:HG12	2:B:347:LYS:CD	2.33	0.52
1:C:136:ASN:HB2	1:C:138:GLU:OE1	2.09	0.52
2:D:72:ARG:CG	2:D:226:PRO:HB3	2.39	0.52
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.90	0.52
1:A:358:ARG:HD2	11:A:741:HOH:O	2.08	0.52
1:A:374:LYS:NZ	7:A:603:PG4:H71	2.25	0.52
1:C:47:ILE:CG2	1:C:144:TYR:HB3	2.38	0.52
1:C:91:GLN:CB	1:C:161:GLN:HE22	2.20	0.52
1:C:189:VAL:HG23	11:C:704:HOH:O	2.08	0.52
2:D:95:PRO:HB2	11:D:648:HOH:O	2.08	0.52
1:A:312:GLU:HG2	1:A:313:PRO:HD2	1.91	0.52
1:C:182:GLN:HG3	2:D:140:PRO:HD3	1.91	0.52
2:D:75:VAL:HG11	2:D:77:PHE:CZ	2.45	0.52
2:B:86:ASP:OD1	2:B:154:LYS:NZ	2.43	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:399:GLU:O	6:D:504:GOL:H32	2.10	0.52
1:A:35:VAL:HG22	1:A:132:ILE:HD13	1.92	0.51
2:B:24:TRP:CD2	6:B:502:GOL:H31	2.45	0.51
2:D:346:PHE:H	6:D:502:GOL:C1	2.23	0.51
2:B:171:PHE:CD2	2:B:205:LEU:HD13	2.44	0.51
1:C:74:LEU:HD13	3:F:0:DG:C5	2.45	0.51
1:C:412:PRO:HB2	11:C:753:HOH:O	2.10	0.51
2:D:70:LYS:HG3	2:D:226:PRO:CD	2.35	0.51
1:A:47:ILE:HG21	1:A:144:TYR:HB3	1.92	0.51
2:B:363:ASN:O	2:B:367:GLN:HG3	2.11	0.51
1:C:30:LYS:O	1:C:34:LEU:HG	2.11	0.51
1:C:342:TYR:HB3	1:C:348:ASN:HA	1.92	0.51
1:C:500:GLN:HG2	2:D:422:LEU:HD12	1.91	0.51
1:A:35:VAL:HG22	1:A:132:ILE:CD1	2.40	0.51
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.46	0.51
2:B:183:TYR:OH	2:B:386:THR:HG23	2.11	0.51
2:D:11:LYS:O	2:D:85:GLN:HB3	2.11	0.51
1:A:350:LYS:HZ1	7:A:603:PG4:C5	2.23	0.51
1:A:206:ARG:NH2	1:A:216:THR:O	2.44	0.51
2:D:354:TYR:CD1	2:D:374:LYS:HD2	2.45	0.51
1:C:149:LEU:HD21	1:C:159:ILE:HG21	1.92	0.50
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.93	0.50
1:A:249:LYS:HG3	1:A:251:SER:H	1.77	0.50
1:A:7:THR:CG2	1:A:121:ASP:HA	2.42	0.50
2:B:44:GLU:HB2	2:B:46:LYS:HE2	1.92	0.50
1:A:506:ILE:HG21	1:A:533:LEU:HD11	1.93	0.50
2:B:281:LYS:CE	2:B:284:ARG:NH2	2.40	0.50
2:D:107:THR:HA	2:D:232:TYR:O	2.12	0.50
2:B:345:PRO:HA	6:B:507:GOL:O2	2.10	0.50
2:D:56:TYR:HE2	2:D:126:LYS:HD2	1.77	0.50
3:F:3:DC:H2'	3:F:4:OMC:C6	2.46	0.50
1:A:292:VAL:C	1:A:293:ILE:HD12	2.32	0.50
2:B:195:ILE:HD12	2:B:195:ILE:N	2.22	0.50
1:C:110:ASP:HB3	1:C:220:LYS:HG2	1.93	0.50
2:D:257:ILE:CD1	2:D:293:ILE:HD11	2.24	0.50
1:A:63:ILE:O	1:A:72:ARG:N	2.40	0.50
1:A:281:LYS:HG3	1:A:284:ARG:HE	1.76	0.50
2:B:69:THR:HG22	11:B:650:HOH:O	2.12	0.49
1:C:19:PRO:HD3	1:C:80:LEU:HD13	1.92	0.49
1:C:50:ILE:CG2	1:C:54:ASN:HB2	2.41	0.49
1:A:182:GLN:HG3	2:B:140:PRO:HD3	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PHE:HB3	2:B:92:LEU:HB2	1.93	0.49
2:B:281:LYS:O	2:B:284:ARG:HB2	2.13	0.49
1:C:50:ILE:HG21	1:C:54:ASN:CB	2.42	0.49
1:C:154:LYS:HB2	11:F:201:HOH:O	2.13	0.49
2:D:98:ALA:O	2:D:101:LYS:HE2	2.12	0.49
1:C:202:ILE:CG2	1:C:206:ARG:HH21	2.25	0.49
3:E:23:DC:H2'	3:E:24:DG:C8	2.47	0.49
1:C:114:ALA:HA	11:C:705:HOH:O	2.12	0.49
1:C:495:ILE:HB	1:C:533:LEU:HD23	1.94	0.49
1:A:142:ILE:HD12	1:A:144:TYR:CE2	2.47	0.49
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.94	0.49
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.47	0.49
1:C:107:THR:HG22	1:C:109:LEU:CD1	2.43	0.49
1:A:180:ILE:HG23	1:A:187:LEU:HD13	1.95	0.49
1:A:285:GLY:N	3:E:9:DT:OP1	2.46	0.49
2:B:307:ARG:O	2:B:311:LYS:HG2	2.12	0.49
1:C:329:ILE:HD11	1:C:375:ILE:HD12	1.93	0.49
2:D:195:ILE:H	2:D:195:ILE:CD1	2.24	0.49
1:A:374:LYS:HE2	3:E:6:DC:OP1	2.13	0.49
2:B:195:ILE:H	2:B:195:ILE:CD1	2.22	0.49
2:B:344:GLU:HG3	6:B:501:GOL:H31	1.95	0.49
1:C:221:HIS:CE1	1:C:223:LYS:HG2	2.48	0.49
2:D:209:LEU:HD23	2:D:209:LEU:O	2.12	0.49
2:D:394[B]:GLN:OE1	6:D:501:GOL:H31	2.13	0.49
2:B:312:GLU:HB2	2:B:313:PRO:HD2	1.95	0.49
2:D:242:GLN:NE2	2:D:353:LYS:HE3	2.24	0.49
2:B:199:ARG:NE	2:B:233:GLU:OE2	2.46	0.48
2:D:12:LEU:HD11	2:D:127:TYR:CE1	2.49	0.48
2:D:248:GLU:OE1	2:D:248:GLU:HA	2.13	0.48
2:D:297:GLU:OE2	11:D:601:HOH:O	2.20	0.48
2:B:8:VAL:HG21	2:B:159:ILE:HG23	1.94	0.48
1:C:86:ASP:O	2:D:55:PRO:HB3	2.14	0.48
3:F:7:DC:H2'	3:F:8:DT:H71	1.95	0.48
2:B:167:ILE:O	2:B:208:HIS:NE2	2.41	0.48
1:C:363:ASN:HA	1:C:511:ASP:OD1	2.14	0.48
2:D:195:ILE:HD12	2:D:195:ILE:N	2.23	0.48
1:A:320:ASP:OD2	1:A:323:LYS:HE3	2.13	0.48
2:B:88:TRP:HZ2	1:C:390:LYS:NZ	2.10	0.48
2:B:249:LYS:HD2	2:B:252:TRP:CZ3	2.49	0.48
2:B:317:VAL:HG23	2:B:317:VAL:O	2.13	0.48
1:C:503:LEU:HD11	1:C:533:LEU:HB3	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:183:TYR:CE2	2:D:184:MET:HG2	2.49	0.48
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.49	0.47
7:A:603:PG4:H82	7:A:603:PG4:H51	1.96	0.47
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.49	0.47
1:C:129:ALA:HA	1:C:144:TYR:O	2.13	0.47
2:B:70:LYS:HG3	2:B:226:PRO:CD	2.43	0.47
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.49	0.47
1:C:110:ASP:HB3	1:C:220:LYS:CG	2.44	0.47
1:C:110:ASP:OD1	1:C:111:VAL:N	2.46	0.47
1:A:286:THR:O	1:A:286:THR:HG22	2.13	0.47
1:C:109:LEU:HD12	1:C:109:LEU:N	2.29	0.47
2:B:258:GLN:HG2	2:B:283:LEU:HD13	1.95	0.47
1:C:74:LEU:HD13	3:F:0:DG:N7	2.29	0.47
1:A:175:ASN:O	1:A:178:ILE:HG22	2.14	0.47
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.96	0.47
2:B:209:LEU:HD23	2:B:209:LEU:O	2.14	0.47
1:C:17:ASP:O	1:C:83:ARG:HD3	2.14	0.47
1:C:206:ARG:HG2	1:C:216:THR:CB	2.45	0.47
1:C:157:PRO:HG2	3:F:2:OMC:O4'	2.14	0.47
3:F:17:DT:H1'	11:F:204:HOH:O	2.13	0.47
1:A:545:ASN:HA	1:A:548:VAL:HG12	1.96	0.47
2:B:24:TRP:CE2	6:B:502:GOL:H31	2.50	0.47
2:D:246:LEU:CD1	2:D:264:LEU:HD21	2.39	0.47
3:F:18:DT:H4'	3:F:19:DG:C8	2.50	0.47
1:A:134:SER:HB2	1:A:141:GLY:HA2	1.95	0.46
1:A:41:MET:HB3	1:A:46:LYS:HB2	1.97	0.46
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.50	0.46
2:D:312:GLU:HB2	2:D:313:PRO:HD2	1.96	0.46
2:D:24:TRP:CD2	6:D:504:GOL:H2	2.51	0.46
1:A:265:ASN:OD1	1:A:353:LYS:HE3	2.15	0.46
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.44	0.46
2:B:37:ILE:O	2:B:41:MET:HG3	2.15	0.46
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.50	0.46
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.51	0.46
1:C:57:ASN:OD1	1:C:131:THR:HG23	2.16	0.46
1:C:221:HIS:NE2	1:C:223:LYS:HE2	2.30	0.46
1:C:13:LYS:HB2	1:C:16:MET:SD	2.56	0.46
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.81	0.46
2:B:214:LEU:O	2:B:214:LEU:HD23	2.14	0.45
1:C:149:LEU:HD11	1:C:159:ILE:HG22	1.98	0.45
1:A:142:ILE:HD12	1:A:144:TYR:HE2	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ILE:HD11	1:C:189:VAL:HG13	1.95	0.45
1:A:252:TRP:HB3	1:A:257:ILE:HD11	1.99	0.45
2:D:74:LEU:HD12	11:D:639:HOH:O	2.16	0.45
1:A:116:PHE:HA	1:A:148:VAL:CG2	2.47	0.45
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.52	0.45
2:B:72:ARG:CB	2:B:226:PRO:HG3	2.46	0.45
1:C:130:PHE:CE1	1:C:144:TYR:HB2	2.51	0.45
1:C:182:GLN:HA	1:C:187:LEU:HD23	1.98	0.45
1:C:246:LEU:HD13	1:C:307:ARG:HD3	1.98	0.45
2:B:161:GLN:HG2	11:B:663:HOH:O	2.17	0.45
1:C:81:ASN:HB3	1:C:154:LYS:HD3	1.96	0.45
3:F:16:DT:H3'	3:F:17:DT:H5''	1.99	0.45
1:A:51:GLY:H	1:A:52:PRO:HD3	1.82	0.45
1:A:194:GLU:CD	1:A:196:GLY:H	2.20	0.45
2:B:115:TYR:O	2:B:149:LEU:HB2	2.17	0.45
1:C:292:VAL:C	1:C:293:ILE:HD12	2.36	0.45
2:D:169:GLU:HB3	2:D:170:PRO:HD3	1.98	0.45
2:D:274:ILE:O	2:D:275:LYS:HD3	2.17	0.45
2:D:317:VAL:HG23	2:D:317:VAL:O	2.17	0.45
1:A:187:LEU:HD22	1:A:187:LEU:HA	1.83	0.45
2:B:14:PRO:HD2	11:B:652:HOH:O	2.16	0.45
1:A:38:CYS:O	1:A:42:GLU:HG3	2.17	0.44
1:A:208:HIS:CA	1:A:211:ARG:HH21	2.29	0.44
1:A:530:LYS:HA	11:A:709:HOH:O	2.18	0.44
1:A:354:TYR:CZ	1:A:356:ARG:HB3	2.52	0.44
2:D:393:ILE:HD13	2:D:398:TRP:HB2	1.99	0.44
3:F:10:DC:H2''	3:F:11:DG:C8	2.52	0.44
1:C:379:SER:CB	1:C:387:PRO:HD3	2.47	0.44
1:C:552:VAL:O	1:C:553:SER:HB2	2.17	0.44
1:A:110:ASP:OD2	1:A:111:VAL:N	2.50	0.44
1:A:350:LYS:HZ1	7:A:603:PG4:H52	1.81	0.44
2:B:41:MET:HA	2:B:46:LYS:HE3	2.00	0.44
2:B:165:THR:HG21	11:B:663:HOH:O	2.16	0.44
2:D:50:ILE:HD13	2:D:145:GLN:HB3	1.99	0.44
3:E:7:DC:H2'	3:E:8:DT:H71	1.99	0.44
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.00	0.44
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.99	0.44
1:C:543:GLY:N	2:D:283:LEU:O	2.51	0.44
2:D:130:PHE:CZ	2:D:144:TYR:HB2	2.52	0.44
2:B:72:ARG:HB2	2:B:226:PRO:HG3	1.99	0.44
2:D:103:LYS:HE3	2:D:179:VAL:HG23	2.00	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:OMC:HM23	3:E:4:OMC:H1'	1.76	0.44
1:A:13:LYS:HB2	1:A:16:MET:SD	2.58	0.44
1:A:543:GLY:N	2:B:283:LEU:O	2.50	0.44
2:B:11:LYS:HB3	2:B:11:LYS:HE3	1.80	0.44
1:C:13:LYS:HE3	1:C:84:THR:O	2.18	0.44
1:C:312:GLU:HG2	1:C:313:PRO:HD2	1.99	0.44
2:D:323:LYS:O	2:D:385:LYS:NZ	2.50	0.44
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.99	0.43
2:B:358:ARG:NE	2:B:370:GLU:OE1	2.51	0.43
1:C:134:SER:HB2	1:C:141:GLY:HA2	2.00	0.43
1:A:228:LEU:HD12	1:A:228:LEU:N	2.33	0.43
1:A:275:LYS:HB3	1:A:336:GLN:OE1	2.18	0.43
1:C:60:VAL:HG22	1:C:75:VAL:HG13	1.99	0.43
1:C:107:THR:HG22	1:C:109:LEU:HD12	1.99	0.43
1:A:443:ASP:HB2	1:A:548:VAL:HG13	2.00	0.43
1:C:156:SER:HB2	1:C:157:PRO:HD3	2.01	0.43
1:C:546:GLU:O	1:C:550:LYS:HG3	2.18	0.43
1:A:47:ILE:HD13	1:A:130:PHE:HZ	1.84	0.43
1:A:75:VAL:HB	1:A:77:PHE:CE2	2.54	0.43
1:A:358:ARG:HH22	2:B:394[A]:GLN:HE21	1.66	0.43
2:D:38:CYS:SG	2:D:132:ILE:HD11	2.58	0.43
2:D:173:LYS:HA	2:D:173:LYS:NZ	2.32	0.43
2:D:395:LYS:HG3	2:D:416:PHE:CE2	2.53	0.43
1:A:123:ASP:O	1:A:126:LYS:HE3	2.17	0.43
1:C:23:GLN:OE1	1:C:59:PRO:HA	2.18	0.43
1:C:116:PHE:HA	1:C:148:VAL:HG21	2.00	0.43
1:C:460:ASN:HA	2:D:286:THR:HG22	2.00	0.43
2:D:146:TYR:CG	2:D:150:PRO:HB3	2.54	0.43
1:A:149:LEU:CD1	1:A:160:PHE:HB2	2.49	0.43
1:A:164:MET:CE	1:A:164:MET:HA	2.49	0.43
1:A:397:THR:HG21	1:A:424:LYS:HA	2.01	0.43
2:B:328:GLU:O	2:B:339:TYR:HA	2.18	0.43
1:C:50:ILE:HG22	1:C:51:GLY:N	2.33	0.43
1:C:97:PRO:HD3	1:C:232:TYR:CE2	2.53	0.43
2:D:44:GLU:OE1	2:D:46:LYS:HE2	2.19	0.43
3:F:26:DA:H2''	3:F:27:DG:C8	2.53	0.43
1:A:125:ARG:HB3	1:A:146:TYR:O	2.19	0.43
1:C:61:PHE:HZ	3:F:0:DG:C8	2.36	0.43
1:C:91:GLN:HB2	1:C:161:GLN:NE2	2.28	0.43
1:C:115:TYR:HB3	1:C:149:LEU:O	2.18	0.43
2:D:28:GLU:CG	2:D:32:LYS:HE2	2.49	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:MET:HE3	2:D:168:LEU:CG	2.48	0.43
2:D:357:MET:O	2:D:357:MET:HG2	2.18	0.43
1:A:89:GLU:OE1	1:A:158:ALA:HB2	2.19	0.43
1:A:122:GLU:HB2	11:A:756:HOH:O	2.18	0.43
1:C:358:ARG:CZ	2:D:394[B]:GLN:HE21	2.32	0.43
1:A:74:LEU:HD13	3:E:0:DG:C5	2.54	0.43
1:C:199:ARG:HH12	1:C:223:LYS:HB3	1.84	0.43
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.01	0.42
1:C:244:ILE:HD12	1:C:267:ALA:HB2	2.01	0.42
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.01	0.42
1:A:198:HIS:O	1:A:202:ILE:HG12	2.19	0.42
1:A:325:LEU:HG	1:A:385:LYS:HE3	2.01	0.42
1:C:410:TRP:CZ2	1:C:412:PRO:HA	2.53	0.42
2:D:105:SER:O	2:D:190:GLY:HA2	2.18	0.42
1:A:164:MET:HA	1:A:164:MET:HE3	2.01	0.42
1:C:209:LEU:HB3	1:C:214:LEU:HB2	2.00	0.42
1:C:229:TRP:CE2	1:C:230:MET:HG2	2.54	0.42
1:A:248:GLU:HA	1:A:307:ARG:HH22	1.84	0.42
1:C:111:VAL:HB	1:C:185:ASP:HB2	2.01	0.42
1:C:135:ILE:HD11	1:C:139:THR:CG2	2.42	0.42
2:D:113:ASP:OD2	2:D:227:PHE:HE1	2.03	0.42
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.42	0.42
1:A:266:TRP:O	1:A:269:GLN:HG2	2.19	0.42
1:C:94:ILE:HG12	3:F:4:OMC:H1'	2.02	0.42
1:C:271:TYR:CD2	1:C:310:LEU:HD23	2.55	0.42
1:A:301:LEU:O	1:A:305:GLU:HG3	2.19	0.42
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.55	0.42
2:D:87:PHE:HB3	2:D:92:LEU:HB2	2.01	0.42
1:A:21:VAL:HG12	1:A:21:VAL:O	2.19	0.42
1:A:254:VAL:O	1:A:258:GLN:HG3	2.20	0.42
1:A:282:LEU:HD21	1:A:296:THR:HG23	2.02	0.42
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.55	0.42
3:F:-1:DT:O2	3:F:-1:DT:C2'	2.67	0.42
1:A:86:ASP:O	2:B:55:PRO:HB3	2.20	0.42
1:C:63:ILE:HD11	1:C:74:LEU:HD11	2.01	0.41
1:C:246:LEU:HB3	1:C:307:ARG:CZ	2.49	0.41
3:F:3:DC:H2'	3:F:4:OMC:H6	1.85	0.41
1:A:252:TRP:CD1	1:A:295:LEU:HD13	2.55	0.41
1:C:56:TYR:O	1:C:143:ARG:NH2	2.53	0.41
2:D:90:VAL:HG12	2:D:90:VAL:O	2.21	0.41
2:D:206:ARG:HA	2:D:228:LEU:HD21	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:GLY:O	1:C:242:GLN:HG3	2.20	0.41
2:B:169:GLU:OE2	2:B:173:LYS:HE3	2.21	0.41
1:C:24:TRP:CE3	1:C:25:PRO:HD2	2.52	0.41
1:C:473:THR:O	1:C:477:THR:HG23	2.20	0.41
2:D:328:GLU:O	2:D:339:TYR:HA	2.20	0.41
3:F:23:DC:H2''	3:F:24:DG:C8	2.55	0.41
2:D:163:SER:O	2:D:167:ILE:HG13	2.20	0.41
2:D:164:MET:CE	2:D:168:LEU:HD21	2.44	0.41
2:D:331:LYS:HB2	2:D:337:TRP:CZ3	2.55	0.41
1:A:216:THR:HG23	11:A:719:HOH:O	2.20	0.41
1:A:496:VAL:HG21	2:B:289:LEU:HD21	2.01	0.41
2:B:72:ARG:CG	2:B:226:PRO:HG3	2.50	0.41
2:D:64:LYS:HE3	2:D:71:TRP:NE1	2.35	0.41
2:D:209:LEU:HD23	2:D:209:LEU:C	2.41	0.41
1:C:235:HIS:HB2	1:C:238:LYS:O	2.20	0.41
1:C:279:LEU:HD23	1:C:299:ALA:HB1	2.03	0.41
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.55	0.41
1:C:503:LEU:HD12	1:C:503:LEU:HA	1.88	0.41
2:B:209:LEU:HD23	2:B:209:LEU:C	2.40	0.41
1:C:318:TYR:O	1:C:349:LEU:HD21	2.21	0.41
1:C:373:GLN:NE2	2:D:397:THR:OG1	2.45	0.41
2:D:297:GLU:OE2	2:D:297:GLU:HA	2.21	0.41
2:B:103:LYS:HA	2:B:103:LYS:HD3	1.91	0.41
1:C:134:SER:HB3	1:C:139:THR:O	2.21	0.41
2:B:90:VAL:HG12	2:B:90:VAL:O	2.20	0.40
2:B:281:LYS:CE	2:B:284:ARG:CZ	2.94	0.40
2:B:335:GLY:O	2:B:355:ALA:HA	2.21	0.40
1:C:70:LYS:HE3	1:C:219:LYS:HZ2	1.86	0.40
1:A:42:GLU:OE2	1:A:144:TYR:OH	2.35	0.40
2:B:227:PHE:HB3	2:B:229:TRP:HD1	1.87	0.40
2:B:266:TRP:CH2	2:B:425:LEU:HD21	2.55	0.40
1:C:110:ASP:O	1:C:217:PRO:HD2	2.21	0.40
2:D:28:GLU:HG2	2:D:32:LYS:HE2	2.03	0.40
2:D:183:TYR:CD2	2:D:184:MET:HG2	2.56	0.40
1:A:142:ILE:HD12	1:A:144:TYR:OH	2.21	0.40
2:D:236:PRO:HA	2:D:239:TRP:CD2	2.57	0.40
3:E:-1:DT:OP2	3:E:-1:DT:H4'	2.21	0.40
2:B:279:LEU:HG	2:B:302:GLU:OE1	2.22	0.40
1:C:410:TRP:CD1	2:D:363:ASN:HA	2.56	0.40
1:C:424:LYS:HE2	1:C:426:TRP:CH2	2.57	0.40
2:D:75:VAL:HG11	2:D:77:PHE:CE1	2.57	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:227:PHE:CG	2:D:228:LEU:N	2.89	0.40
1:C:110:ASP:OD1	1:C:110:ASP:C	2.60	0.40
1:C:133:PRO:HB3	1:C:137:ASN:ND2	2.36	0.40
1:C:376:THR:HG21	2:D:401:TRP:CH2	2.56	0.40
2:D:70:LYS:HE3	2:D:226:PRO:CD	2.52	0.40
2:D:173:LYS:HA	2:D:173:LYS:HZ3	1.87	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%)	532 (96%)	18 (3%)	2 (0%)	34	41
1	C	551/555 (99%)	534 (97%)	16 (3%)	1 (0%)	47	57
2	B	412/429 (96%)	398 (97%)	14 (3%)	0	100	100
2	D	407/429 (95%)	393 (97%)	14 (3%)	0	100	100
All	All	1922/1968 (98%)	1857 (97%)	62 (3%)	3 (0%)	47	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	543	GLY
1	C	543	GLY
1	A	140	PRO

#### 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%)	489 (99%)	7 (1%)	67	77
1	C	495/495 (100%)	489 (99%)	6 (1%)	71	81
2	B	378/390 (97%)	377 (100%)	1 (0%)	92	95
2	D	373/390 (96%)	371 (100%)	2 (0%)	88	93
All	All	1742/1770 (98%)	1726 (99%)	16 (1%)	78	86

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ASP
1	A	187	LEU
1	A	221	HIS
1	A	330	GLN
1	A	340	GLN
1	A	464[A]	GLN
1	A	464[B]	GLN
2	B	284	ARG
1	C	65	LYS
1	C	109	LEU
1	C	123	ASP
1	C	221	HIS
1	C	330	GLN
1	C	428	GLN
2	D	173	LYS
2	D	357	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	221	HIS
1	C	91	GLN
1	C	161	GLN
1	C	182	GLN
2	D	242	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMC	F	2	3	19,22,23	3.06	7 (36%)	26,31,34	0.75	0
3	OMC	F	4	3	19,22,23	3.05	7 (36%)	26,31,34	0.73	0
3	OMC	E	4	3	19,22,23	3.04	7 (36%)	26,31,34	0.70	0
3	OMC	E	2	3	19,22,23	3.05	7 (36%)	26,31,34	0.77	0

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

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

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	C6-C5	6.53	1.50	1.35
3	E	4	OMC	C6-C5	6.51	1.50	1.35
3	F	2	OMC	C6-C5	6.47	1.50	1.35
3	F	2	OMC	C2-N3	6.45	1.49	1.36
3	F	4	OMC	C6-C5	6.43	1.50	1.35
3	F	4	OMC	C2-N3	6.39	1.49	1.36

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	C2-N3	6.39	1.49	1.36
3	E	2	OMC	C2-N3	6.39	1.49	1.36
3	F	2	OMC	C4-N3	6.15	1.46	1.34
3	F	4	OMC	C4-N3	6.11	1.46	1.34
3	E	2	OMC	C4-N3	6.10	1.46	1.34
3	E	4	OMC	C4-N3	6.01	1.46	1.34
3	E	4	OMC	C4-N4	4.09	1.43	1.33
3	F	4	OMC	C4-N4	4.05	1.43	1.33
3	E	2	OMC	C4-N4	4.04	1.43	1.33
3	F	2	OMC	C4-N4	4.03	1.43	1.33
3	F	4	OMC	C2-N1	3.92	1.48	1.40
3	F	2	OMC	C2-N1	3.87	1.48	1.40
3	E	2	OMC	C2-N1	3.83	1.48	1.40
3	E	4	OMC	C2-N1	3.83	1.48	1.40
3	F	2	OMC	C6-N1	3.73	1.47	1.38
3	E	2	OMC	C6-N1	3.72	1.47	1.38
3	F	4	OMC	C6-N1	3.69	1.46	1.38
3	E	4	OMC	C6-N1	3.66	1.46	1.38
3	F	4	OMC	O2-C2	-2.78	1.18	1.23
3	E	4	OMC	O2-C2	-2.76	1.18	1.23
3	F	2	OMC	O2-C2	-2.74	1.18	1.23
3	E	2	OMC	O2-C2	-2.72	1.18	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

## 5.5 Carbohydrates i

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GLC	M	1	4	11,11,12	0.60	0	15,15,17	0.71	0
4	FRU	M	2	4	11,12,12	0.51	0	10,18,18	0.58	0
4	GLC	N	1	4	11,11,12	0.66	0	15,15,17	0.73	0
4	FRU	N	2	4	11,12,12	0.52	0	10,18,18	0.84	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	M	1	4	-	1/2/19/22	0/1/1/1
4	FRU	M	2	4	-	5/5/24/24	0/1/1/1
4	GLC	N	1	4	-	0/2/19/22	0/1/1/1
4	FRU	N	2	4	-	5/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	2	FRU	O1-C1-C2-O2
4	N	2	FRU	O1-C1-C2-O2
4	M	2	FRU	O5-C5-C6-O6
4	N	2	FRU	O5-C5-C6-O6
4	M	2	FRU	C4-C5-C6-O6
4	N	2	FRU	C4-C5-C6-O6
4	M	2	FRU	O1-C1-C2-C3

*Continued on next page...*



Continued from previous page...

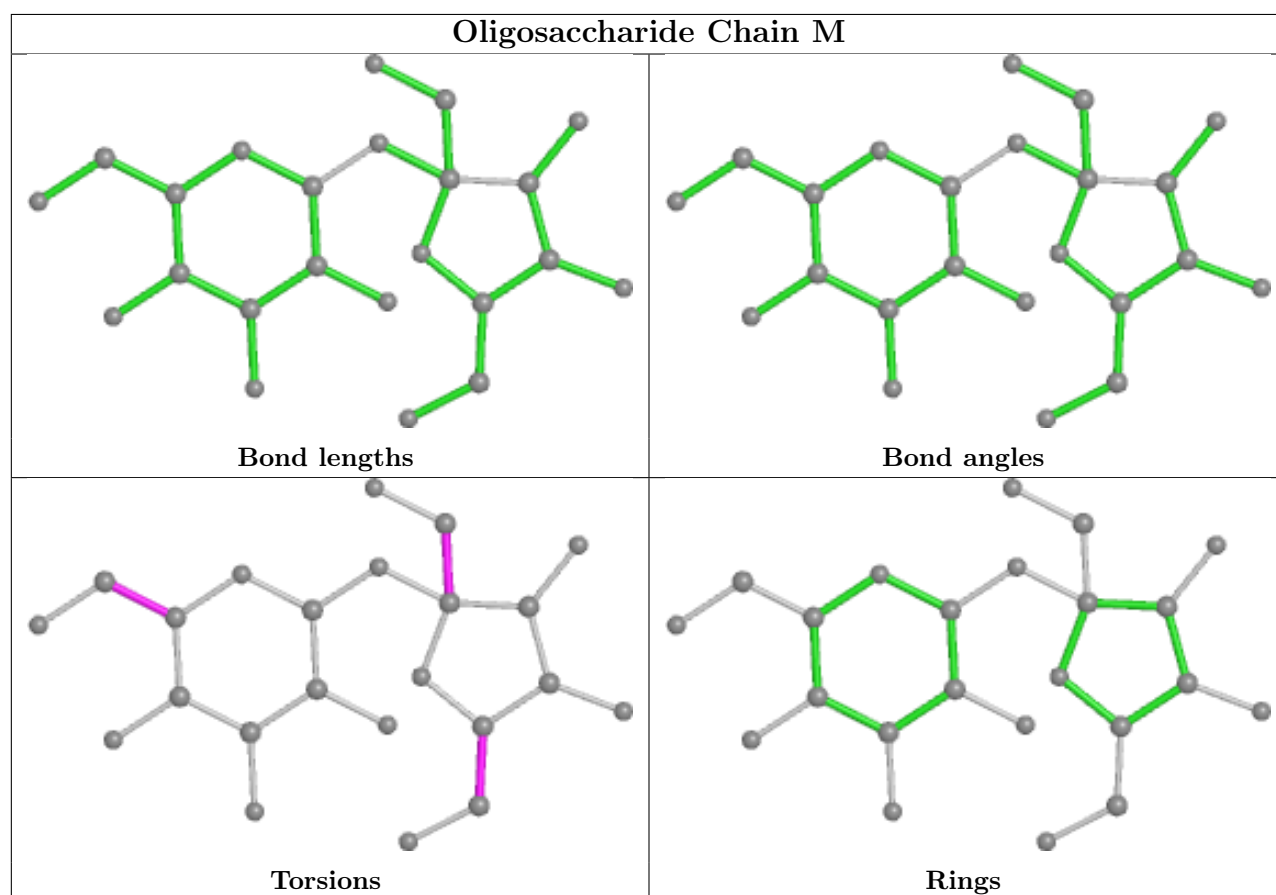
Mol	Chain	Res	Type	Atoms
4	N	2	FRU	O1-C1-C2-O5
4	M	1	GLC	C4-C5-C6-O6
4	M	2	FRU	O1-C1-C2-O5
4	N	2	FRU	O1-C1-C2-C3

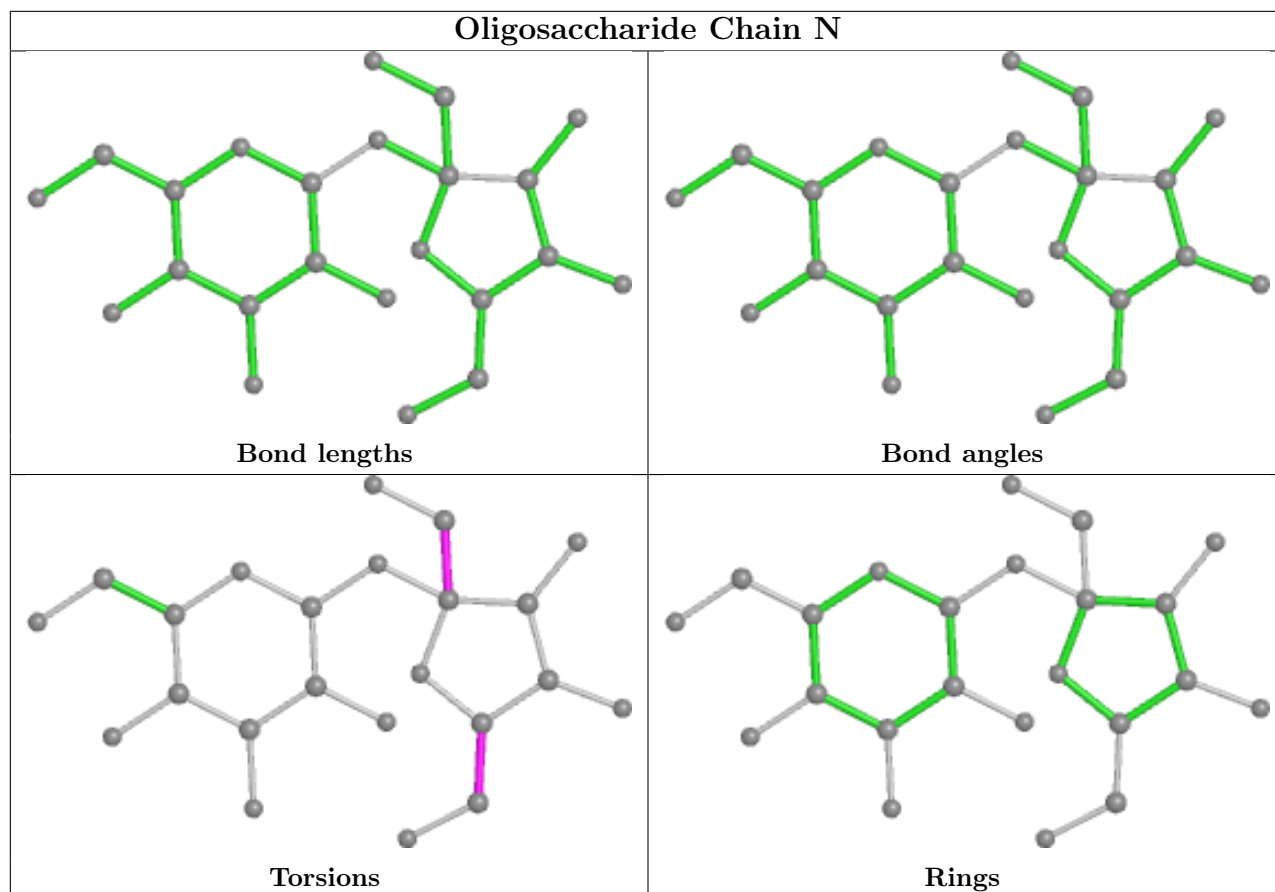
There are no ring outliers.

2 monomers are involved in 1 short contact:

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

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





## 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are modelled with single atom and 2 are monoatomic - leaving 18 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
5	SO4	B	506	-	4,4,4	0.13	0	6,6,6	0.05	0
6	GOL	A	602	-	5,5,5	0.96	0	5,5,5	0.97	0
5	SO4	A	601	-	4,4,4	0.13	0	6,6,6	0.06	0
6	GOL	B	504	-	5,5,5	1.03	0	5,5,5	0.97	0
6	GOL	B	507	-	5,5,5	0.96	0	5,5,5	0.92	0
6	GOL	F	101	-	5,5,5	0.89	0	5,5,5	0.99	0
6	GOL	D	504	-	5,5,5	0.91	0	5,5,5	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	C	601	-	4,4,4	0.15	0	6,6,6	0.05	0
10	1RY	C	604	9	25,29,29	0.41	0	35,45,45	0.94	1 (2%)
6	GOL	B	503	-	5,5,5	0.94	0	5,5,5	0.94	0
6	GOL	B	501	-	5,5,5	0.91	0	5,5,5	1.03	0
6	GOL	B	505	-	5,5,5	0.99	0	5,5,5	0.92	0
6	GOL	D	501	-	5,5,5	1.08	0	5,5,5	0.87	0
6	GOL	D	502	-	5,5,5	0.96	0	5,5,5	0.97	0
7	PG4	A	603	-	12,12,12	0.53	0	11,11,11	0.25	0
10	1RY	A	606	9	25,29,29	0.54	0	35,45,45	0.92	1 (2%)
6	GOL	D	503	-	5,5,5	0.90	0	5,5,5	1.00	0
6	GOL	B	502	-	5,5,5	0.95	0	5,5,5	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	A	602	-	-	3/4/4/4	-
6	GOL	B	507	-	-	3/4/4/4	-
6	GOL	B	504	-	-	2/4/4/4	-
6	GOL	F	101	-	-	2/4/4/4	-
6	GOL	D	504	-	-	0/4/4/4	-
10	1RY	C	604	9	-	8/22/31/31	0/2/2/2
6	GOL	B	503	-	-	2/4/4/4	-
6	GOL	B	501	-	-	2/4/4/4	-
6	GOL	B	505	-	-	1/4/4/4	-
6	GOL	D	501	-	-	2/4/4/4	-
6	GOL	D	502	-	-	0/4/4/4	-
7	PG4	A	603	-	-	7/10/10/10	-
10	1RY	A	606	9	-	5/22/31/31	0/2/2/2
6	GOL	D	503	-	-	4/4/4/4	-
6	GOL	B	502	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	604	1RY	OAO-PBA-OAH	4.08	125.01	109.07

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	606	1RY	OAO-PBA-OAH	3.63	123.27	109.07

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	GOL	O1-C1-C2-C3
6	B	502	GOL	O1-C1-C2-C3
6	B	502	GOL	C1-C2-C3-O3
6	D	501	GOL	O1-C1-C2-O2
6	D	501	GOL	O1-C1-C2-C3
6	D	503	GOL	C1-C2-C3-O3
10	A	606	1RY	CAL-OAO-PBA-OAD
10	C	604	1RY	CAL-OAO-PBA-OAR
7	A	603	PG4	C3-C4-O3-C5
7	A	603	PG4	C8-C7-O4-C6
6	A	602	GOL	O1-C1-C2-O2
6	B	502	GOL	O1-C1-C2-O2
7	A	603	PG4	O1-C1-C2-O2
6	B	503	GOL	C1-C2-C3-O3
6	B	507	GOL	O1-C1-C2-C3
6	F	101	GOL	O1-C1-C2-C3
6	B	502	GOL	O2-C2-C3-O3
6	B	507	GOL	O1-C1-C2-O2
6	D	503	GOL	O2-C2-C3-O3
10	A	606	1RY	PBA-OAR-PBB-OAE
10	C	604	1RY	PBA-OAR-PBB-OAE
6	B	504	GOL	O1-C1-C2-O2
6	D	503	GOL	O1-C1-C2-O2
6	F	101	GOL	O1-C1-C2-O2
10	C	604	1RY	PAZ-OAQ-PBB-OAR
7	A	603	PG4	C6-C5-O3-C4
6	B	507	GOL	O2-C2-C3-O3
10	A	606	1RY	CAL-OAO-PBA-OAR
10	A	606	1RY	OAO-CAL-CAW-OAP
10	C	604	1RY	CAW-CAL-OAO-PBA
7	A	603	PG4	C5-C6-O4-C7
10	A	606	1RY	PBB-OAR-PBA-OAD
6	B	501	GOL	O1-C1-C2-C3
6	B	501	GOL	C1-C2-C3-O3
6	B	505	GOL	O1-C1-C2-C3
6	B	503	GOL	O2-C2-C3-O3

*Continued on next page...*

*Continued from previous page...*

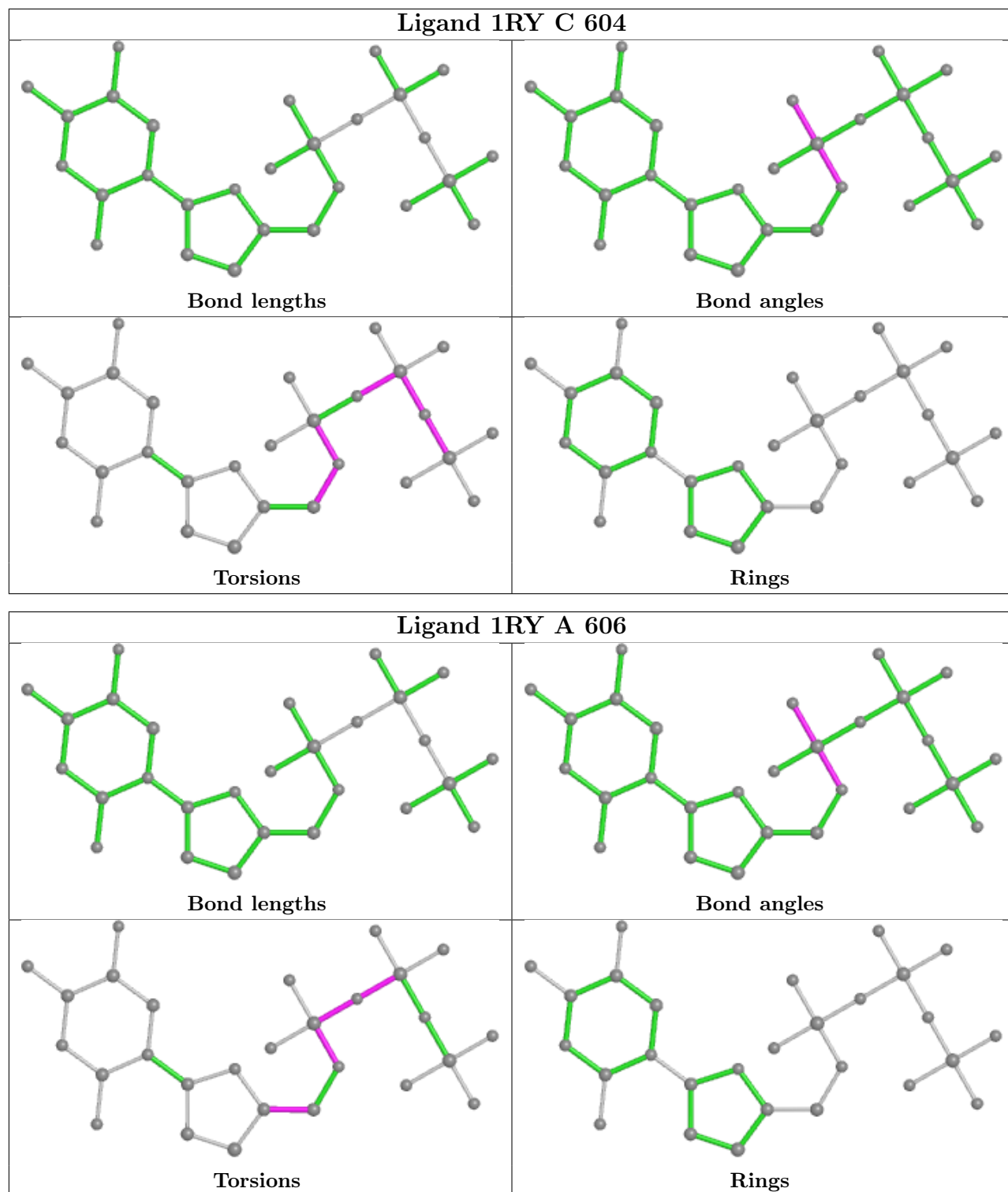
Mol	Chain	Res	Type	Atoms
10	C	604	1RY	PBB-OAQ-PAZ-OAF
7	A	603	PG4	O2-C3-C4-O3
10	C	604	1RY	PAZ-OAQ-PBB-OAE
10	C	604	1RY	PBA-OAR-PBB-OAI
6	A	602	GOL	C1-C2-C3-O3
6	B	504	GOL	O1-C1-C2-C3
6	D	503	GOL	O1-C1-C2-C3
10	C	604	1RY	CAL-OAO-PBA-OAH
7	A	603	PG4	O4-C7-C8-O5

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	602	GOL	1	0
6	B	507	GOL	1	0
6	D	504	GOL	2	0
10	C	604	1RY	2	0
6	B	501	GOL	1	0
6	B	505	GOL	1	0
6	D	501	GOL	2	0
6	D	502	GOL	2	0
7	A	603	PG4	7	0
10	A	606	1RY	2	0
6	B	502	GOL	2	0

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



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	553/555 (99%)	1.12	74 (13%) 3 2	53, 117, 193, 276	0
1	C	553/555 (99%)	1.82	180 (32%) 0 0	56, 138, 236, 297	0
2	B	415/429 (96%)	0.85	36 (8%) 10 7	55, 98, 159, 212	0
2	D	410/429 (95%)	1.10	56 (13%) 3 2	59, 118, 185, 267	0
3	E	33/38 (86%)	0.02	0 100 100	90, 121, 151, 180	0
3	F	33/38 (86%)	0.02	1 (3%) 50 46	90, 135, 172, 197	0
All	All	1997/2044 (97%)	1.22	347 (17%) 1 1	53, 115, 210, 297	0

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	16.4
1	C	133	PRO	16.4
1	C	137	ASN	14.4
1	C	26	LEU	13.9
1	A	2	ILE	13.8
1	C	24	TRP	13.5
1	C	73	LYS	13.3
1	A	71	TRP	13.2
1	C	74	LEU	13.1
1	C	67	ASP	13.0
1	C	205	LEU	12.3
1	C	61	PHE	11.6
1	A	26	LEU	11.0
1	A	24	TRP	10.9
1	C	134	SER	10.6
2	D	226	PRO	10.3
1	C	25	PRO	10.2
1	C	66	LYS	9.2
2	B	88	TRP	9.1

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	132	ILE	9.1
2	D	92	LEU	8.9
2	D	90	VAL	8.7
1	C	68	SER	8.4
1	C	140	PRO	8.2
1	A	135	ILE	8.1
1	A	61	PHE	8.0
2	B	92	LEU	8.0
1	C	63	ILE	7.8
2	B	226	PRO	7.7
2	D	359	GLY	7.1
1	C	3	SER	7.1
1	C	229	TRP	7.1
2	D	358	ARG	7.0
1	C	142	ILE	7.0
2	D	10	VAL	7.0
1	C	22	LYS	7.0
2	D	212	TRP	7.0
1	A	1	PRO	6.8
1	C	108	VAL	6.8
1	A	139	THR	6.6
1	C	188	TYR	6.5
1	A	134	SER	6.3
1	C	2	ILE	6.2
1	C	47	ILE	6.2
2	D	202	ILE	6.1
1	C	228	LEU	6.1
2	D	232	TYR	6.0
1	C	136	ASN	6.0
1	C	71	TRP	5.9
1	A	25	PRO	5.8
1	A	28	GLU	5.8
1	C	69	THR	5.7
1	C	17	ASP	5.6
1	C	65	LYS	5.5
1	A	34	LEU	5.5
1	C	60	VAL	5.5
2	B	90	VAL	5.5
1	A	130	PHE	5.3
1	A	67	ASP	5.3
1	C	114	ALA	5.3
1	C	41	MET	5.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	230	MET	5.2
1	C	75	VAL	5.2
1	C	56	TYR	5.1
2	D	209	LEU	5.0
1	A	62	ALA	5.0
2	B	202	ILE	5.0
1	C	209	LEU	5.0
2	D	146	TYR	5.0
1	C	289	LEU	4.9
1	C	171	PHE	4.9
1	A	3	SER	4.8
2	D	206	ARG	4.8
1	C	124	PHE	4.8
1	C	28	GLU	4.8
1	C	46	LYS	4.8
1	C	72	ARG	4.7
1	C	135	ILE	4.7
1	A	30	LYS	4.7
1	C	292	VAL	4.7
1	C	109	LEU	4.7
1	C	312	GLU	4.6
1	C	214	LEU	4.6
1	C	139	THR	4.6
2	D	93	GLY	4.6
1	A	31	ILE	4.5
1	C	180	ILE	4.4
1	C	290	THR	4.4
2	D	85	GLN	4.4
1	C	145	GLN	4.4
1	C	286	THR	4.4
1	C	178	ILE	4.3
2	D	124	PHE	4.3
1	C	179	VAL	4.3
1	C	146	TYR	4.3
1	A	74	LEU	4.3
2	D	422	LEU	4.3
1	C	295	LEU	4.2
1	C	16	MET	4.1
2	B	89	GLU	4.1
1	C	202	ILE	4.1
1	C	232	TYR	4.1
1	A	21	VAL	4.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	87	PHE	4.0
1	C	174	GLN	4.0
1	A	295	LEU	3.9
1	C	5	ILE	3.9
1	C	21	VAL	3.9
2	B	87	PHE	3.9
1	C	54	ASN	3.9
1	C	115	TYR	3.9
1	C	50	ILE	3.9
2	B	214	LEU	3.8
1	C	1	PRO	3.8
1	C	246	LEU	3.8
1	A	132	ILE	3.8
1	A	140	PRO	3.8
1	C	70	LYS	3.7
1	C	293	ILE	3.7
1	C	222	GLN	3.7
1	C	52	PRO	3.7
1	C	206	ARG	3.7
1	C	138	GLU	3.7
2	D	144	TYR	3.7
2	D	130	PHE	3.6
2	D	356	ARG	3.6
2	B	109	LEU	3.6
2	D	132	ILE	3.6
1	C	141	GLY	3.6
2	D	357	MET	3.6
1	C	35	VAL	3.6
1	C	260	LEU	3.6
1	A	22	LYS	3.6
1	C	307	ARG	3.6
2	D	168	LEU	3.6
1	C	234	LEU	3.6
1	C	106	VAL	3.5
1	C	239	TRP	3.5
1	C	287	LYS	3.5
1	C	130	PHE	3.5
1	A	141	GLY	3.5
1	C	274	ILE	3.5
2	D	142	ILE	3.5
1	C	254	VAL	3.5
1	A	177	ASP	3.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	89	GLU	3.4
1	A	46	LYS	3.4
1	C	23	GLN	3.4
2	B	10	VAL	3.4
1	C	62	ALA	3.4
1	A	138	GLU	3.4
1	A	142	ILE	3.4
1	A	63	ILE	3.3
1	C	34	LEU	3.3
1	C	226	PRO	3.3
1	A	49	LYS	3.3
1	C	118	VAL	3.3
1	A	180	ILE	3.3
1	C	177	ASP	3.3
1	A	73	LYS	3.3
2	D	8	VAL	3.3
1	C	187	LEU	3.3
1	A	131	THR	3.3
2	D	116	PHE	3.3
1	C	48	SER	3.3
2	D	115	TYR	3.3
1	C	208	HIS	3.2
1	C	189	VAL	3.2
2	D	230	MET	3.2
1	C	455	ALA	3.1
2	D	360	ALA	3.1
1	C	14	PRO	3.1
1	C	247	PRO	3.1
2	D	84	THR	3.1
1	C	15	GLY	3.1
1	A	279	LEU	3.1
1	C	241	VAL	3.1
2	B	283	LEU	3.1
1	C	314	VAL	3.1
1	A	4	PRO	3.1
1	C	152	GLY	3.0
2	D	159	ILE	3.0
1	C	168	LEU	3.0
1	C	31	ILE	3.0
1	C	55	PRO	3.0
1	A	10	VAL	3.0
1	C	111	VAL	3.0

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	144	TYR	3.0
1	A	241	VAL	2.9
1	C	164	MET	2.9
2	D	189	VAL	2.9
1	C	195	ILE	2.9
1	C	258	GLN	2.9
1	A	124	PHE	2.9
2	D	88	TRP	2.9
2	D	205	LEU	2.9
1	C	37	ILE	2.9
2	D	12	LEU	2.9
1	C	160	PHE	2.8
1	C	310	LEU	2.8
2	B	85	GLN	2.8
1	C	87	PHE	2.8
1	A	214	LEU	2.8
2	B	71	TRP	2.8
2	D	125	ARG	2.8
1	A	19	PRO	2.8
1	C	122	GLU	2.8
1	C	223	LYS	2.8
1	C	167	ILE	2.8
1	C	257	ILE	2.8
2	B	47	ILE	2.7
2	B	281	LYS	2.7
1	C	131	THR	2.7
1	C	264	LEU	2.7
1	C	302	GLU	2.7
1	A	27	THR	2.7
1	A	246	LEU	2.7
2	B	116	PHE	2.7
1	C	248	GLU	2.6
1	A	56	TYR	2.6
1	A	32	LYS	2.6
2	B	229	TRP	2.6
1	C	30	LYS	2.6
1	C	199	ARG	2.6
2	D	188	TYR	2.6
1	A	178	ILE	2.6
1	C	346	PHE	2.6
1	C	207	GLN	2.6
1	C	10	VAL	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	32	LYS	2.6
1	C	259	LYS	2.6
2	D	197	GLN	2.6
1	C	102	LYS	2.6
2	D	112	GLY	2.6
1	C	58	THR	2.5
1	C	220	LYS	2.5
2	D	149	LEU	2.5
1	C	77	PHE	2.5
1	C	238	LYS	2.5
1	A	187	LEU	2.5
2	B	266	TRP	2.5
1	C	116	PHE	2.5
1	A	168	LEU	2.5
1	C	8	VAL	2.5
1	C	317	VAL	2.5
1	C	233	GLU	2.5
2	D	61	PHE	2.5
1	A	115	TYR	2.5
1	C	148	VAL	2.5
1	C	198	HIS	2.5
1	A	379	SER	2.4
1	C	349	LEU	2.4
1	C	458	VAL	2.4
1	C	83	ARG	2.4
1	C	306	ASN	2.4
2	B	426	TRP	2.4
1	C	166	LYS	2.4
1	A	137	ASN	2.4
2	B	231	GLY	2.4
2	D	394[A]	GLN	2.4
2	B	215	THR	2.4
1	C	149	LEU	2.4
2	D	195	ILE	2.4
2	B	144	TYR	2.4
1	A	534	ALA	2.4
2	D	153	TRP	2.4
1	C	303	LEU	2.3
2	B	295	LEU	2.3
2	D	128	THR	2.3
1	A	120	LEU	2.3
1	C	210	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	189	VAL	2.3
1	A	238	LYS	2.3
2	B	309	ILE	2.3
1	C	211	ARG	2.3
2	D	260	LEU	2.3
1	C	13	LYS	2.3
2	B	91	GLN	2.3
1	C	252	TRP	2.3
2	D	171	PHE	2.3
1	C	497	THR	2.3
1	C	11	LYS	2.3
1	A	251	SER	2.3
2	B	232	TYR	2.2
1	A	244	ILE	2.2
1	C	406	TRP	2.2
2	D	425	LEU	2.2
1	C	405	TYR	2.2
1	A	75	VAL	2.2
3	F	16	DT	2.2
1	C	221	HIS	2.2
2	B	293	ILE	2.2
1	C	43	LYS	2.2
2	D	264	LEU	2.2
2	B	278	GLN	2.2
1	A	382	ILE	2.2
2	B	380	ILE	2.2
1	A	87	PHE	2.2
1	C	64	LYS	2.2
1	C	544	GLY	2.2
1	C	127	TYR	2.2
1	C	20	LYS	2.1
1	A	128	THR	2.1
1	C	251	SER	2.1
1	C	113	ASP	2.1
1	C	482	ILE	2.1
1	A	429	LEU	2.1
1	A	23	GLN	2.1
1	A	252	TRP	2.1
1	A	464[A]	GLN	2.1
2	B	4	PRO	2.1
2	B	94	ILE	2.1
1	C	172	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	205	LEU	2.1
1	A	271	TYR	2.1
1	C	271	TYR	2.1
2	D	318	TYR	2.1
2	B	168	LEU	2.1
1	C	219	LYS	2.1
1	A	35	VAL	2.1
1	A	50	ILE	2.1
1	C	159	ILE	2.1
1	C	151	GLN	2.1
1	C	275	LYS	2.1
1	C	230	MET	2.0
1	C	534	ALA	2.0
1	C	423	VAL	2.0
1	A	47	ILE	2.0
1	C	120	LEU	2.0
1	C	325	LEU	2.0
1	C	440	PHE	2.0
2	B	428	GLN	2.0
2	B	381	VAL	2.0
2	D	361	HIS	2.0
1	A	393	ILE	2.0
1	C	126	LYS	2.0
1	C	244	ILE	2.0
2	D	427	TYR	2.0
1	A	41	MET	2.0
1	C	240	THR	2.0
2	D	73	LYS	2.0
2	D	147	ASN	2.0
1	C	285	GLY	2.0
1	C	358	ARG	2.0
1	A	533	LEU	2.0
1	C	4	PRO	2.0
2	D	19	PRO	2.0

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

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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OMC	F	2	21/22	0.90	0.16	128,137,147,150	0
3	OMC	E	2	21/22	0.91	0.19	102,122,132,136	0
3	OMC	F	4	21/22	0.93	0.15	104,115,129,141	0
3	OMC	E	4	21/22	0.97	0.18	81,91,103,105	0

### 6.3 Carbohydrates

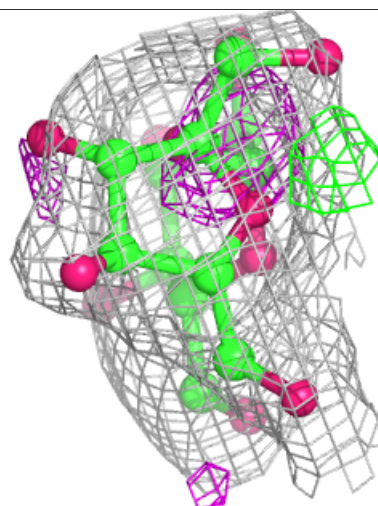
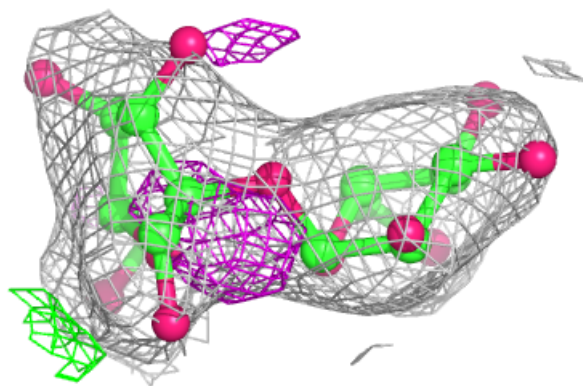
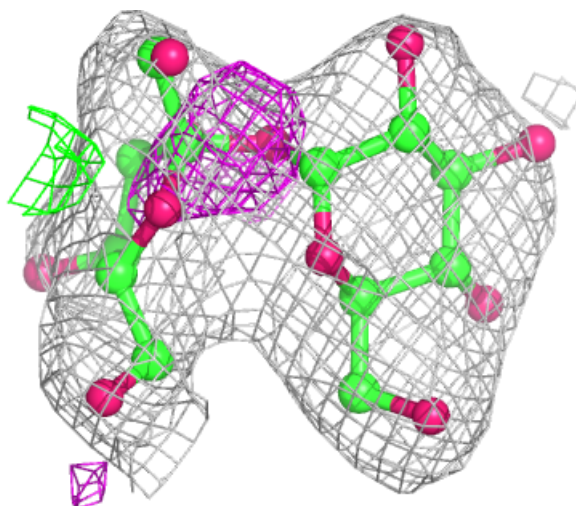
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

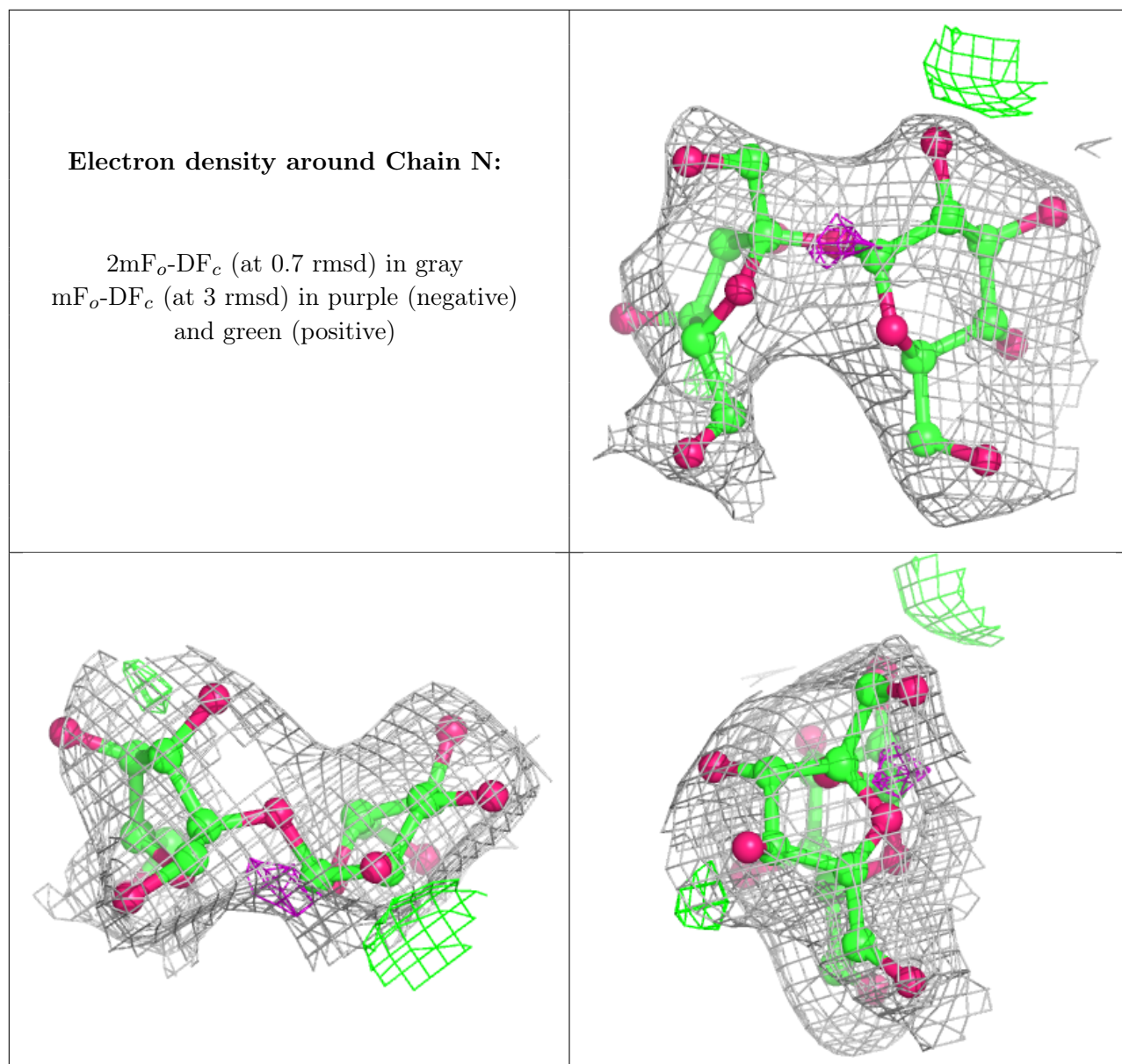
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FRU	N	2	12/12	0.84	0.18	92,126,129,130	0
4	GLC	N	1	11/12	0.89	0.19	91,111,125,129	0
4	GLC	M	1	11/12	0.90	0.25	78,104,114,114	0
4	FRU	M	2	12/12	0.90	0.23	79,116,126,127	0

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 M:**

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





## 6.4 Ligands [i](#)

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

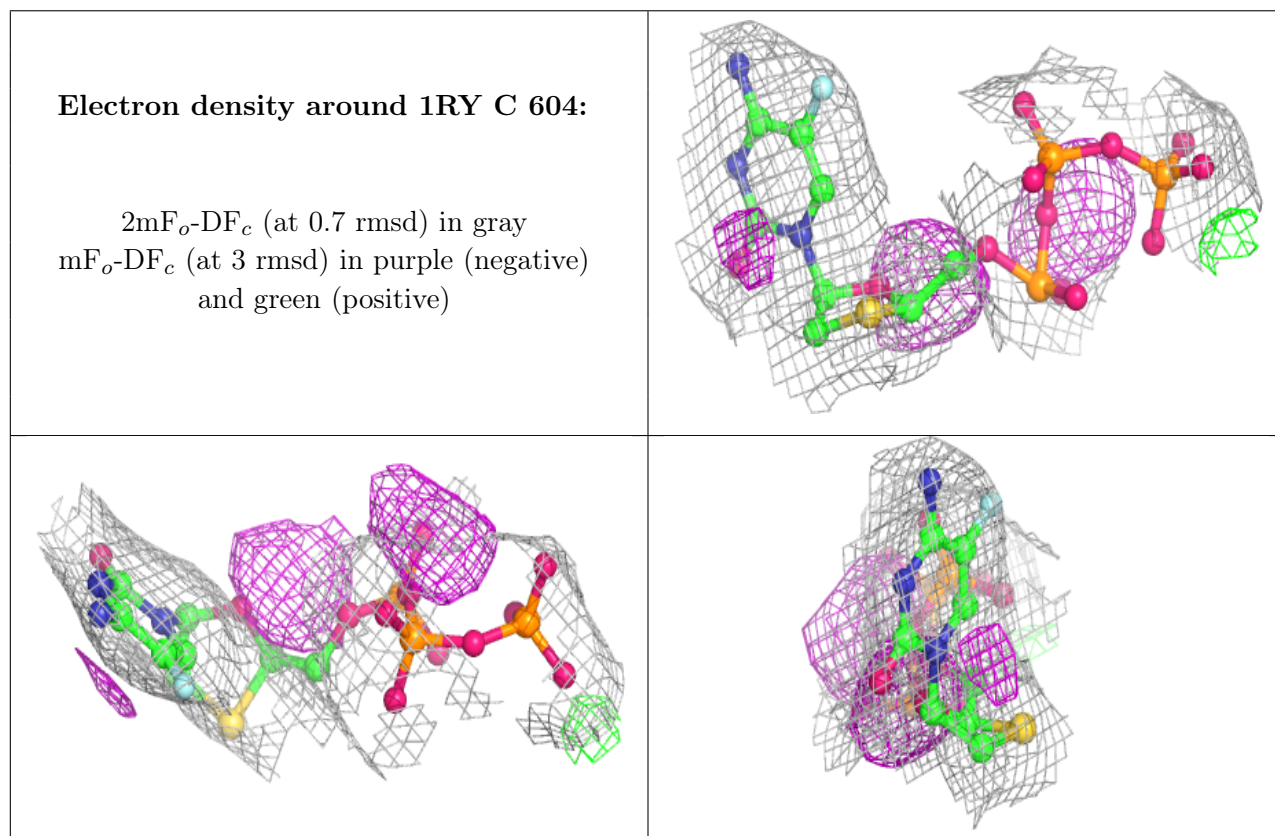
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	NH4	A	604	1/1	0.63	0.46	108,130,130,130	0
8	NH4	C	602	1/1	0.66	0.50	70,84,84,84	0
7	PG4	A	603	13/13	0.75	0.32	101,109,117,122	0
6	GOL	A	602	6/6	0.76	0.68	64,104,117,126	0
6	GOL	D	504	6/6	0.77	0.38	100,104,111,115	0

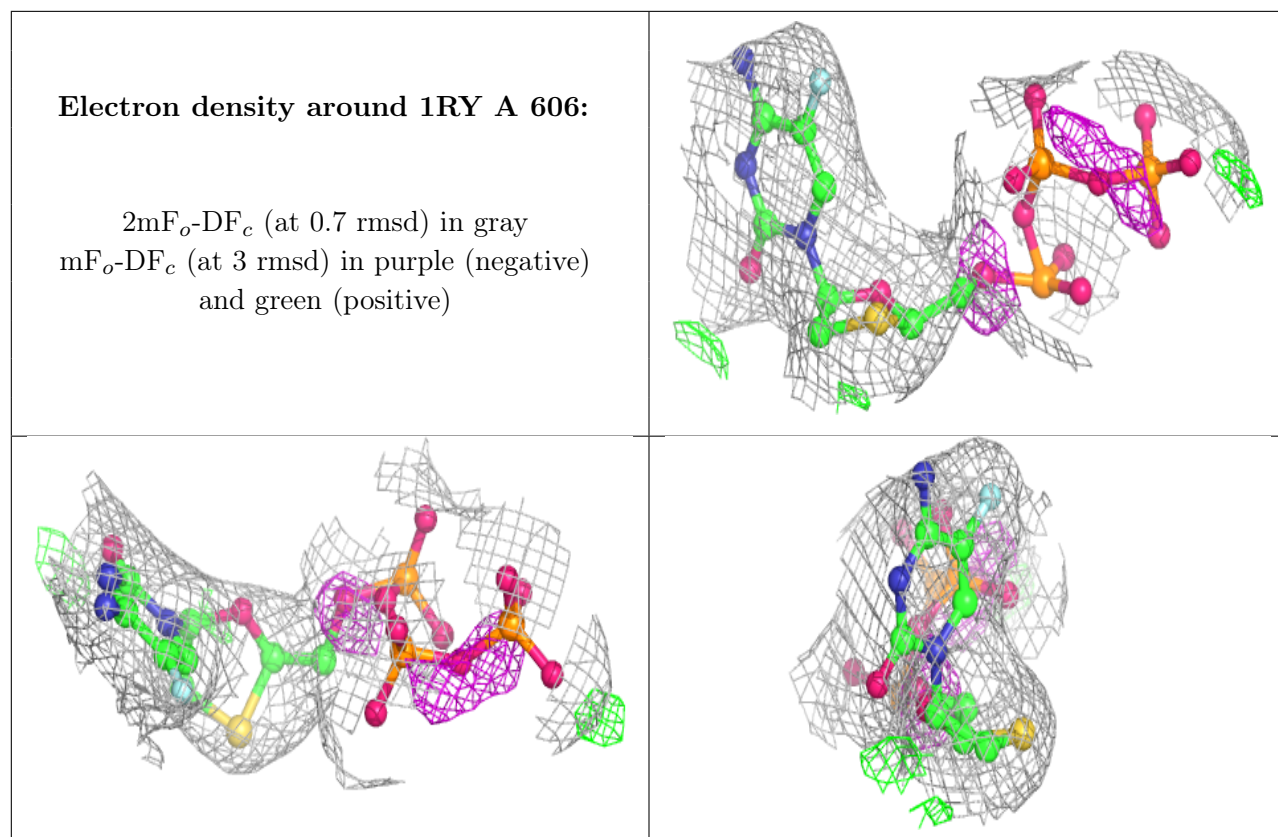
*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	D	501	6/6	0.80	0.53	76,82,93,97	0
6	GOL	B	505	6/6	0.80	0.30	69,90,94,107	0
6	GOL	F	101	6/6	0.80	0.38	116,121,125,128	0
10	1RY	C	604	28/28	0.81	0.17	142,181,211,216	0
6	GOL	B	503	6/6	0.84	0.24	80,91,94,103	0
6	GOL	B	507	6/6	0.86	0.23	90,97,101,102	0
10	1RY	A	606	28/28	0.87	0.14	127,143,171,175	0
5	SO4	A	601	5/5	0.88	0.18	93,115,128,139	0
9	CA	A	605	1/1	0.88	0.10	146,146,146,146	0
6	GOL	B	501	6/6	0.89	0.19	74,83,100,107	0
6	GOL	D	502	6/6	0.89	0.27	87,96,105,105	0
6	GOL	B	502	6/6	0.91	0.19	77,89,93,94	0
6	GOL	D	503	6/6	0.91	0.23	95,104,111,113	0
9	CA	C	603	1/1	0.92	0.08	186,186,186,186	0
5	SO4	B	506	5/5	0.93	0.25	136,146,161,164	0
6	GOL	B	504	6/6	0.97	0.22	63,71,80,84	0
5	SO4	C	601	5/5	0.98	0.15	98,101,111,123	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.