



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:09 AM BST

PDB ID : 6KDK  
Title : HIV-1 reverse transcriptase with Q151M/Y115F/F116Y:DNA:dCTP ternary complex  
Authors : Yasutake, Y.; Hattori, S.I.; Tamura, N.; Maeda, K.  
Deposited on : 2019-07-02  
Resolution : 2.56 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

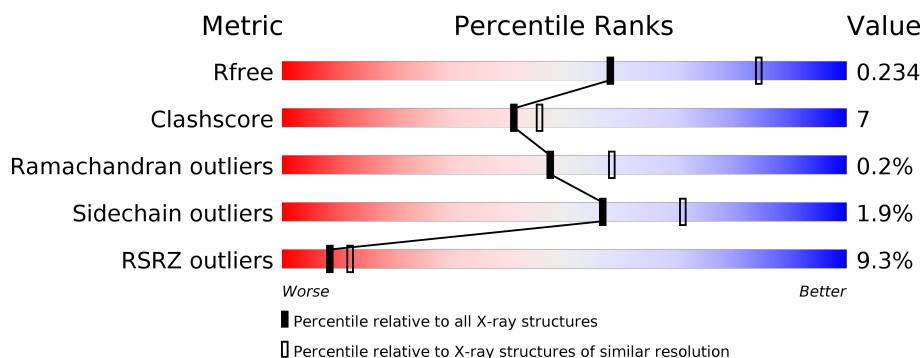
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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

Mol	Chain	Length	Quality of chain
1	A	557	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>••</div> </div> </div>
1	C	557	<div> <div>10%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>••</div> </div> </div>
2	B	444	<div> <div>13%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>• 9%</div> </div> </div>
2	D	444	<div> <div>7%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>• 9%</div> </div> </div>
3	E	38	<div> <div></div> <div> <div></div> <div>66%</div> <div>21%</div> <div>5%</div> <div>8%</div> </div> </div>
3	F	38	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17528 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 reverse transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4498	2911	750	829	8			
1	C	553	Total	C	N	O	S	0	0	0
			4498	2911	750	829	8			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP D3XFN5
A	0	VAL	-	expression tag	UNP D3XFN5
A	115	PHE	TYR	engineered mutation	UNP D3XFN5
A	116	TYR	PHE	engineered mutation	UNP D3XFN5
A	151	MET	GLN	engineered mutation	UNP D3XFN5
A	162	SER	CYS	engineered mutation	UNP D3XFN5
A	280	SER	CYS	engineered mutation	UNP D3XFN5
C	-1	MET	-	expression tag	UNP D3XFN5
C	0	VAL	-	expression tag	UNP D3XFN5
C	115	PHE	TYR	engineered mutation	UNP D3XFN5
C	116	TYR	PHE	engineered mutation	UNP D3XFN5
C	151	MET	GLN	engineered mutation	UNP D3XFN5
C	162	SER	CYS	engineered mutation	UNP D3XFN5
C	280	SER	CYS	engineered mutation	UNP D3XFN5

- Molecule 2 is a protein called HIV-1 RT p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	0	0
			3347	2178	557	606	6			
2	D	406	Total	C	N	O	S	0	0	0
			3347	2178	557	606	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	expression tag	UNP P12497
B	-14	ALA	-	expression tag	UNP P12497
B	-13	HIS	-	expression tag	UNP P12497
B	-12	HIS	-	expression tag	UNP P12497
B	-11	HIS	-	expression tag	UNP P12497
B	-10	HIS	-	expression tag	UNP P12497
B	-9	HIS	-	expression tag	UNP P12497
B	-8	HIS	-	expression tag	UNP P12497
B	-7	ALA	-	expression tag	UNP P12497
B	-6	LEU	-	expression tag	UNP P12497
B	-5	GLU	-	expression tag	UNP P12497
B	-4	VAL	-	expression tag	UNP P12497
B	-3	LEU	-	expression tag	UNP P12497
B	-2	PHE	-	expression tag	UNP P12497
B	-1	GLN	-	expression tag	UNP P12497
B	0	GLY	-	expression tag	UNP P12497
B	162	SER	CYS	engineered mutation	UNP P12497
B	280	SER	CYS	engineered mutation	UNP P12497
D	-15	MET	-	expression tag	UNP P12497
D	-14	ALA	-	expression tag	UNP P12497
D	-13	HIS	-	expression tag	UNP P12497
D	-12	HIS	-	expression tag	UNP P12497
D	-11	HIS	-	expression tag	UNP P12497
D	-10	HIS	-	expression tag	UNP P12497
D	-9	HIS	-	expression tag	UNP P12497
D	-8	HIS	-	expression tag	UNP P12497
D	-7	ALA	-	expression tag	UNP P12497
D	-6	LEU	-	expression tag	UNP P12497
D	-5	GLU	-	expression tag	UNP P12497
D	-4	VAL	-	expression tag	UNP P12497
D	-3	LEU	-	expression tag	UNP P12497
D	-2	PHE	-	expression tag	UNP P12497
D	-1	GLN	-	expression tag	UNP P12497
D	0	GLY	-	expression tag	UNP P12497
D	162	SER	CYS	engineered mutation	UNP P12497
D	280	SER	CYS	engineered mutation	UNP P12497

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

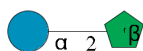
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			721	340	130	216	35			

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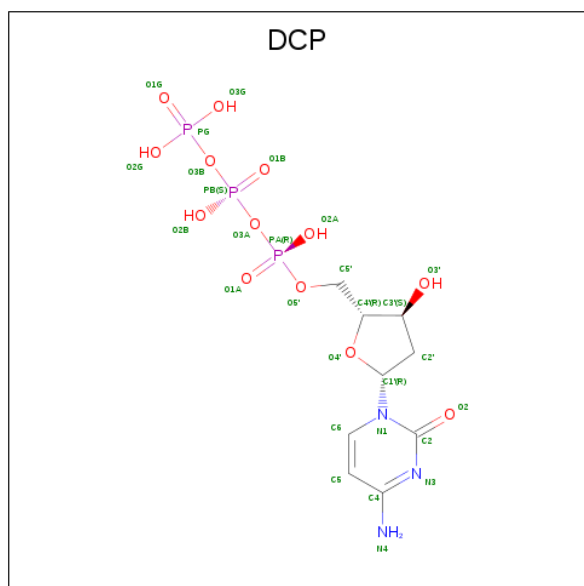
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	38	Total	C	N	O	P	0	0	0
			780	370	142	231	37			

- 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			

- Molecule 5 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by author).



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

- Molecule 7 is GLYCEROL (three-letter code: 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
7	D	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	64	Total O 64 64	0	0
8	B	33	Total O 33 33	0	0
8	E	30	Total O 30 30	0	0
8	C	50	Total O 50 50	0	0

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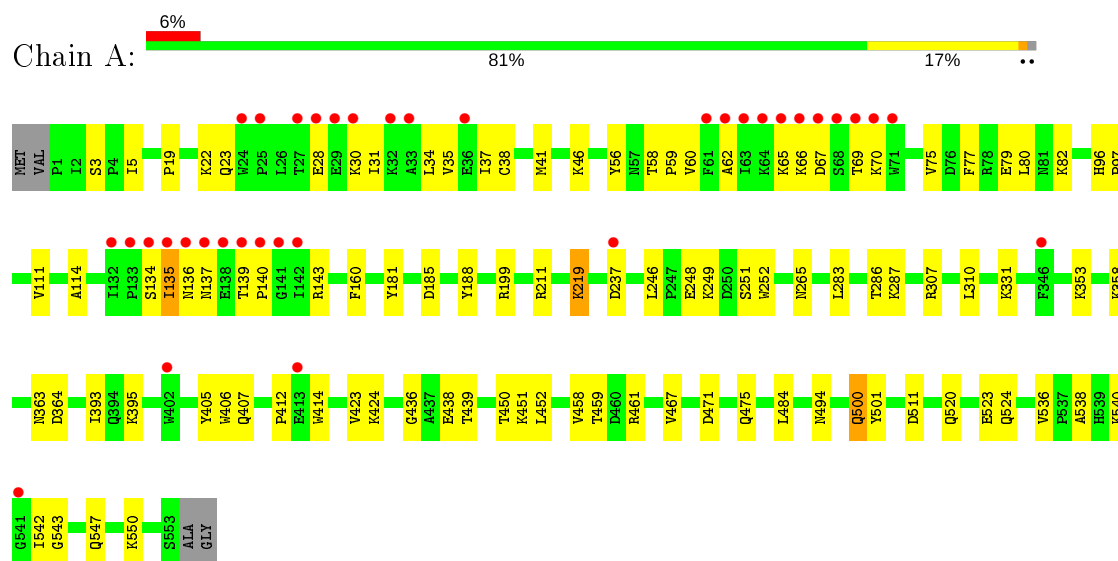
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	40	Total	O	0	0
			40	40		
8	F	15	Total	O	0	0
			15	15		



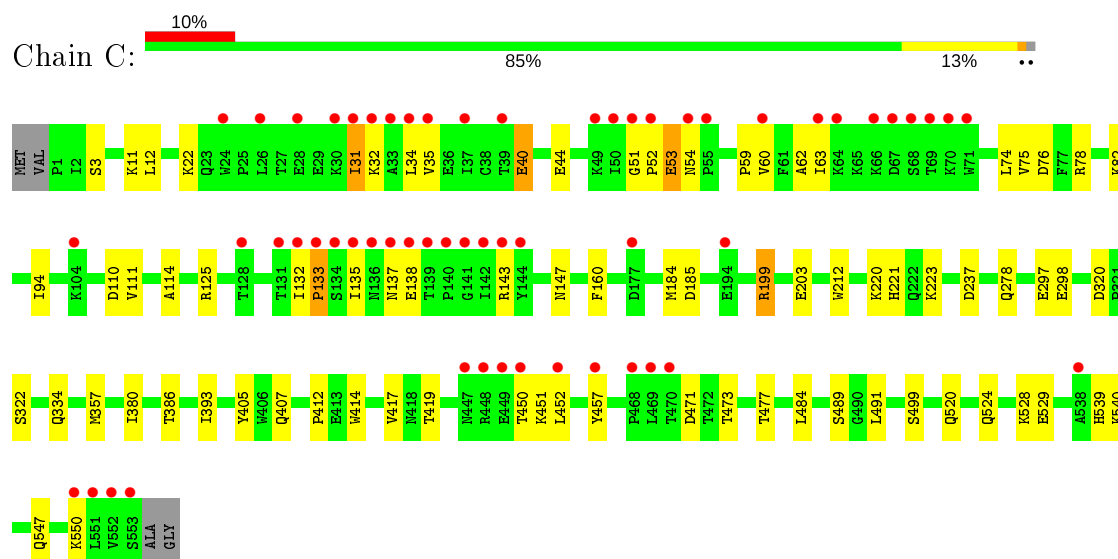
### 3 Residue-property plots [i](#)

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.

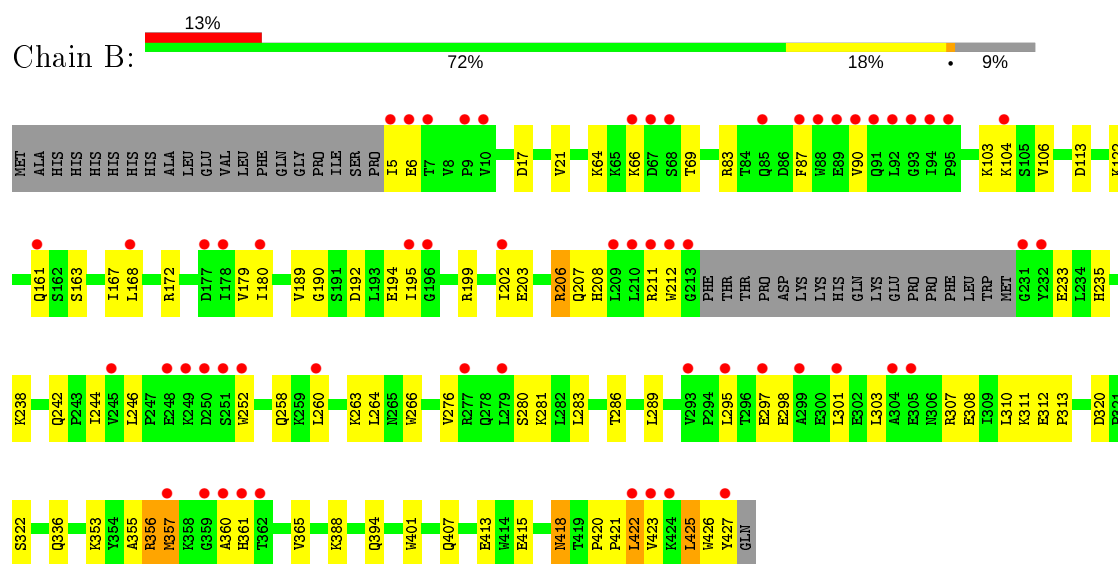
- Molecule 1: HIV-1 reverse transcriptase p66 subunit



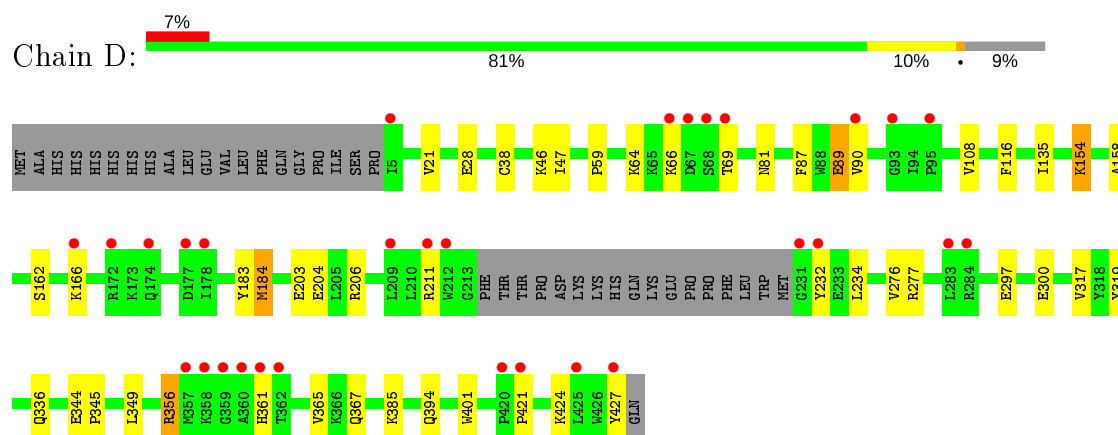
- Molecule 1: HIV-1 reverse transcriptase p66 subunit



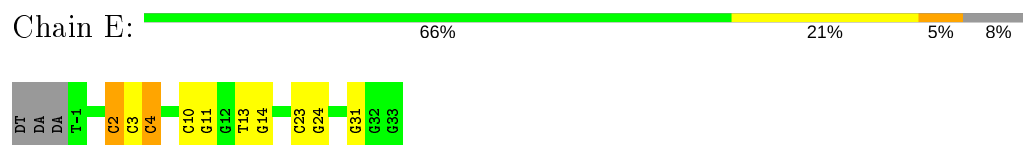
- Molecule 2: HIV-1 RT p51 subunit



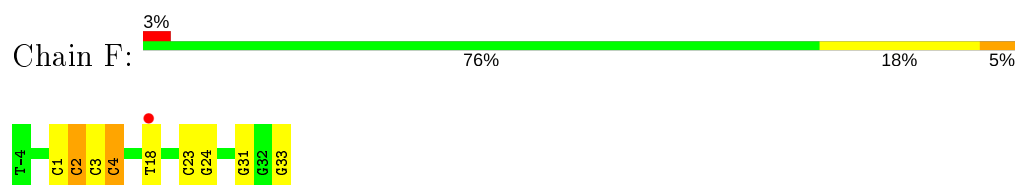
- Molecule 2: HIV-1 RT p51 subunit



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



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



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



GLC1  
FR02

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	284.85Å 284.85Å 95.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.74 – 2.56 48.74 – 2.56	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.74-2.56) 100.0 (48.74-2.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.25 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.14 _3260: ???)	Depositor
R, $R_{free}$	0.190 , 0.234 0.190 , 0.234	Depositor DCC
$R_{free}$ test set	4730 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17528	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, GOL, MG, GLC, FRU, DCP

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	0.30	0/4616	0.51	0/6268
1	C	0.28	0/4616	0.51	2/6268 (0.0%)
2	B	0.29	0/3441	0.51	0/4673
2	D	0.31	0/3441	0.52	2/4673 (0.0%)
3	E	0.48	0/760	0.96	1/1172 (0.1%)
3	F	0.51	0/827	0.98	2/1276 (0.2%)
All	All	0.32	0/17701	0.57	7/24330 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	18	DT	O4'-C1'-N1	6.14	112.30	108.00
3	F	31	DG	O4'-C4'-C3'	-5.57	102.27	104.50
1	C	133	PRO	N-CA-C	5.53	126.48	112.10
3	E	31	DG	O4'-C4'-C3'	-5.50	102.30	104.50
2	D	204	GLU	CA-CB-CG	5.07	124.55	113.40
2	D	204	GLU	OE1-CD-OE2	5.06	129.38	123.30
1	C	31	ILE	CG1-CB-CG2	-5.03	100.33	111.40

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	4498	0	4553	78	0
1	C	4498	0	4553	49	0
2	B	3347	0	3379	69	0
2	D	3347	0	3379	47	0
3	E	721	0	397	5	0
3	F	780	0	432	7	0
4	G	23	0	21	2	0
5	A	28	0	12	1	0
5	C	28	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	B	12	0	16	0	0
7	C	6	0	8	2	0
7	D	6	0	8	0	0
8	A	64	0	0	3	0
8	B	33	0	0	0	0
8	C	50	0	0	0	0
8	D	40	0	0	0	0
8	E	30	0	0	0	0
8	F	15	0	0	1	0
All	All	17528	0	16770	242	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 7.

All (242) 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:D:64:LYS:HE2	2:D:69:THR:O	1.37	1.25
2:D:66:LYS:NZ	2:D:232:TYR:HD2	1.45	1.14
2:D:66:LYS:NZ	2:D:232:TYR:CD2	2.23	1.02
1:C:31:ILE:HD11	1:C:133:PRO:HD2	1.50	0.92
2:D:162:SER:O	2:D:166:LYS:HD3	1.72	0.89
1:A:459:THR:HG22	1:A:461:ARG:H	1.38	0.88
2:D:64:LYS:CE	2:D:69:THR:O	2.22	0.85
1:A:65:LYS:HB3	1:A:67:ASP:OD1	1.78	0.83
1:A:135:ILE:O	1:A:135:ILE:HG22	1.82	0.78
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.65	0.78
2:B:356:ARG:NH1	2:B:357:MET:HA	2.00	0.77
7:C:602:GOL:H11	2:D:394:GLN:HB2	1.66	0.77
2:D:356:ARG:HE	2:D:361:HIS:CB	1.97	0.76
2:B:422:LEU:N	2:B:422:LEU:HD23	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ARG:HD3	1:C:147:ASN:HA	1.68	0.75
1:A:540:LYS:HB2	1:A:542:ILE:HD11	1.69	0.75
1:C:31:ILE:CD1	1:C:133:PRO:HD2	2.16	0.74
2:B:87:PHE:HA	2:B:90:VAL:HG22	1.70	0.72
1:C:451:LYS:HD3	1:C:471:ASP:HA	1.72	0.72
1:A:451:LYS:HG3	1:A:471:ASP:H	1.53	0.71
2:D:90:VAL:HG21	2:D:158:ALA:HA	1.74	0.70
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.74	0.70
1:A:22:LYS:HD2	1:A:23:GLN:H	1.57	0.69
1:C:457:TYR:HE2	1:C:484:LEU:HD22	1.57	0.69
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.73	0.69
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.22	0.69
1:A:536:VAL:HG11	2:B:258:GLN:HE21	1.58	0.69
1:A:406:TRP:HE1	2:B:418:ASN:ND2	1.91	0.68
1:A:67:ASP:N	1:A:67:ASP:OD1	2.22	0.68
2:D:356:ARG:HE	2:D:361:HIS:HB3	1.58	0.68
1:A:31:ILE:HD13	1:A:135:ILE:H	1.58	0.67
1:A:56:TYR:O	1:A:143:ARG:NH2	2.28	0.67
2:D:276:VAL:HG23	2:D:277:ARG:HH11	1.62	0.65
1:A:199:ARG:NH1	8:A:701:HOH:O	2.30	0.65
1:A:520:GLN:O	1:A:524:GLN:HG3	1.97	0.65
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.79	0.65
1:A:406:TRP:HE1	2:B:418:ASN:HD21	1.44	0.64
3:F:3:DC:H2'	3:F:4:OMC:C6	2.32	0.64
1:C:473:THR:O	1:C:477:THR:HG23	1.97	0.64
2:D:276:VAL:HG23	2:D:277:ARG:NH1	2.13	0.64
2:B:298:GLU:HA	2:B:301:LEU:HD12	1.80	0.63
2:B:163:SER:O	2:B:167:ILE:HG13	1.99	0.62
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.80	0.62
1:C:32:LYS:HA	1:C:35:VAL:HG22	1.82	0.62
2:D:203:GLU:HA	2:D:206:ARG:HB2	1.82	0.62
2:B:266:TRP:CE3	2:B:425:LEU:HG	2.36	0.61
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.82	0.60
2:D:356:ARG:HE	2:D:361:HIS:HB2	1.64	0.60
1:C:520:GLN:O	1:C:524:GLN:HG3	2.02	0.60
2:D:66:LYS:CE	2:D:232:TYR:HD2	2.14	0.60
2:D:89:GLU:HG2	2:D:90:VAL:HG23	1.82	0.60
1:A:439:THR:HG21	2:B:289:LEU:CD1	2.32	0.60
1:A:451:LYS:HG3	1:A:471:ASP:N	2.18	0.59
1:A:31:ILE:O	1:A:35:VAL:HG23	2.03	0.59
2:D:108:VAL:HG21	2:D:232:TYR:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:GLN:NE2	1:C:334:GLN:OE1	2.35	0.59
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.85	0.58
3:E:3:DC:H2'	3:E:4:OMC:C6	2.38	0.58
1:C:60:VAL:HG12	1:C:75:VAL:HG22	1.83	0.58
2:D:28:GLU:HA	2:D:135:ILE:HD11	1.85	0.58
1:C:412:PRO:O	1:C:414:TRP:HD1	1.87	0.57
2:D:356:ARG:NE	2:D:361:HIS:HB2	2.18	0.57
2:B:208:HIS:CE1	2:B:212:TRP:HE1	2.23	0.57
2:B:260:LEU:HD21	2:B:303:LEU:HD13	1.87	0.57
2:D:81:ASN:O	2:D:154:LYS:NZ	2.38	0.56
2:D:87:PHE:HB3	2:D:89:GLU:OE2	2.04	0.56
1:A:412:PRO:O	1:A:414:TRP:HD1	1.87	0.56
2:D:356:ARG:C	2:D:356:ARG:HD2	2.26	0.55
1:A:500:GLN:CD	1:A:500:GLN:H	2.09	0.55
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.89	0.55
1:C:539:HIS:O	1:C:540:LYS:HD2	2.07	0.55
1:C:489:SER:OG	1:C:528:LYS:NZ	2.24	0.55
1:A:34:LEU:O	1:A:38:CYS:N	2.41	0.55
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.72	0.54
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.43	0.54
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.90	0.54
2:B:413:GLU:HG2	4:G:1:GLC:O6	2.08	0.54
2:B:244:ILE:HB	2:B:310:LEU:HD22	1.90	0.53
1:A:543:GLY:HA3	2:B:283:LEU:O	2.08	0.53
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.90	0.53
1:A:22:LYS:HD2	1:A:23:GLN:N	2.23	0.53
1:A:358:LYS:NZ	8:A:703:HOH:O	2.39	0.53
2:B:203:GLU:HA	2:B:206:ARG:HG2	1.90	0.53
2:B:235:HIS:HB2	2:B:238:LYS:HE2	1.90	0.53
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.42	0.53
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.91	0.53
1:C:35:VAL:HG12	1:C:132:ILE:HG21	1.91	0.52
1:C:380:ILE:HD11	1:C:386:THR:HG23	1.89	0.52
1:C:135:ILE:HG21	1:C:138:GLU:OE1	2.09	0.52
1:A:31:ILE:HG21	1:A:134:SER:HA	1.92	0.52
1:C:417:VAL:HG22	1:C:419:THR:HG23	1.92	0.51
2:B:106:VAL:HG22	2:B:190:GLY:HA3	1.91	0.51
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.92	0.51
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.93	0.51
2:B:252:TRP:HD1	2:B:295:LEU:HD11	1.76	0.51
1:C:3:SER:HB2	1:C:212:TRP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.46	0.51
1:A:331:LYS:NZ	1:C:297:GLU:OE2	2.33	0.51
2:B:353:LYS:HD2	2:B:427:TYR:OH	2.11	0.51
2:D:319:TYR:OH	2:D:385:LYS:HE2	2.10	0.50
3:F:1:DC:H2'	3:F:2:OMC:C6	2.46	0.50
1:C:78:ARG:O	1:C:82:LYS:HG3	2.11	0.50
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.46	0.50
1:C:450:THR:O	1:C:451:LYS:HB2	2.11	0.50
1:A:542:ILE:HD12	1:A:542:ILE:H	1.77	0.50
2:D:183:TYR:CE2	2:D:184:MET:HG3	2.47	0.50
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.44	0.50
2:B:168:LEU:O	2:B:172:ARG:HG3	2.11	0.50
1:C:457:TYR:CE2	1:C:484:LEU:HD22	2.43	0.49
1:A:135:ILE:O	1:A:137:ASN:N	2.42	0.49
2:B:303:LEU:O	2:B:307:ARG:HG3	2.12	0.49
2:B:64:LYS:HE2	2:B:69:THR:O	2.13	0.49
1:C:450:THR:HG23	1:C:452:LEU:H	1.78	0.49
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.94	0.49
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.13	0.49
2:D:297:GLU:HA	2:D:300:GLU:HG2	1.93	0.49
1:A:538:ALA:O	1:A:540:LYS:HG2	2.12	0.49
1:A:393:ILE:O	1:A:414:TRP:HZ3	1.95	0.48
2:D:66:LYS:NZ	2:D:232:TYR:CE2	2.71	0.48
2:D:421:PRO:O	2:D:424:LYS:HB2	2.12	0.48
3:E:10:DC:H2''	3:E:11:DG:C8	2.48	0.48
1:A:135:ILE:CG2	1:A:135:ILE:O	2.52	0.48
1:C:491:LEU:HB3	1:C:529:GLU:HG3	1.94	0.48
1:A:41:MET:HB3	1:A:46:LYS:HB2	1.95	0.48
2:B:5:ILE:HG22	2:B:6:GLU:H	1.78	0.48
2:D:66:LYS:HZ1	2:D:232:TYR:HD2	0.64	0.48
1:C:40:GLU:OE2	1:C:44:GLU:HG3	2.13	0.48
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.96	0.48
2:D:297:GLU:HA	2:D:300:GLU:CG	2.44	0.48
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.49	0.48
2:B:199:ARG:NH1	2:B:233:GLU:OE2	2.47	0.48
1:A:248:GLU:HG2	1:A:307:ARG:NH2	2.29	0.48
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.49	0.47
2:B:199:ARG:O	2:B:202:ILE:HB	2.14	0.47
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.95	0.47
2:B:103:LYS:NZ	2:B:190:GLY:O	2.42	0.47
2:B:320:ASP:OD1	2:B:322:SER:OG	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:HH2	2:B:426:TRP:CZ2	2.32	0.47
1:A:69:THR:HG22	1:A:69:THR:O	2.14	0.47
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.96	0.47
3:E:23:DC:H2"	3:E:24:DG:C8	2.49	0.47
1:C:184:MET:HG2	3:F:33:DG:H2"	1.96	0.47
1:A:23:GLN:OE1	1:A:59:PRO:HA	2.15	0.47
2:D:356:ARG:HB3	2:D:367:GLN:HG2	1.96	0.47
2:B:203:GLU:HA	2:B:206:ARG:CG	2.44	0.47
2:B:298:GLU:HA	2:B:301:LEU:HB2	1.96	0.47
2:D:64:LYS:HD3	2:D:69:THR:C	2.35	0.47
1:A:283:LEU:O	1:A:286:THR:OG1	2.31	0.47
1:C:221:HIS:NE2	1:C:223:LYS:HE2	2.29	0.47
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.50	0.46
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.97	0.46
2:D:297:GLU:HA	2:D:300:GLU:OE2	2.15	0.46
1:A:3:SER:HB3	1:A:5:ILE:HG22	1.97	0.46
2:B:21:VAL:HG11	4:G:2:FRU:H11	1.97	0.46
2:B:422:LEU:CD2	2:B:422:LEU:N	2.73	0.46
2:B:103:LYS:HZ1	2:B:179:VAL:N	2.14	0.46
1:A:66:LYS:N	1:A:66:LYS:HD3	2.30	0.46
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.50	0.46
1:A:500:GLN:H	1:A:500:GLN:NE2	2.14	0.46
2:B:208:HIS:HE1	2:B:212:TRP:HE1	1.64	0.46
1:C:393:ILE:O	1:C:414:TRP:HZ3	1.99	0.46
1:C:63:ILE:HG12	1:C:74:LEU:HD11	1.97	0.46
2:B:17:ASP:O	2:B:83:ARG:HD3	2.16	0.46
2:B:199:ARG:HA	2:B:202:ILE:CD1	2.42	0.46
2:B:356:ARG:HH11	2:B:357:MET:HA	1.77	0.46
2:B:203:GLU:HA	2:B:206:ARG:CD	2.46	0.45
2:B:297:GLU:HG2	2:B:298:GLU:OE1	2.15	0.45
1:C:51:GLY:N	1:C:53:GLU:OE1	2.38	0.45
7:C:602:GOL:H11	2:D:394:GLN:CB	2.42	0.45
1:A:265:ASN:OD1	1:A:353:LYS:HE3	2.17	0.45
2:D:46:LYS:HD3	2:D:116:PHE:HB3	1.98	0.45
1:C:237:ASP:N	1:C:237:ASP:OD2	2.38	0.45
1:C:298:GLU:CD	1:C:298:GLU:H	2.20	0.45
1:C:52:PRO:O	1:C:54:ASN:N	2.50	0.45
2:D:64:LYS:CD	2:D:69:THR:C	2.85	0.44
1:C:114:ALA:HB1	1:C:160:PHE:CE2	2.53	0.44
1:A:79:GLU:HA	1:A:82:LYS:HZ3	1.82	0.44
2:B:276:VAL:O	2:B:280:SER:OG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:GLU:OE1	2:B:308:GLU:HA	2.16	0.44
2:B:308:GLU:O	2:B:311:LYS:HB2	2.18	0.44
1:A:30:LYS:NZ	1:A:62:ALA:O	2.33	0.44
2:B:426:TRP:O	2:B:427:TYR:HD2	2.01	0.44
1:A:219:LYS:HE3	1:A:219:LYS:HB2	1.73	0.44
1:A:520:GLN:HA	1:A:523:GLU:HG2	1.99	0.44
1:C:524:GLN:O	1:C:528:LYS:HG2	2.18	0.44
2:D:344:GLU:HG2	2:D:345:PRO:HD2	1.99	0.44
1:A:60:VAL:HB	1:A:75:VAL:HG22	2.00	0.44
2:D:232:TYR:CD1	2:D:234:LEU:HD21	2.53	0.44
2:B:356:ARG:O	2:B:357:MET:SD	2.76	0.43
8:A:703:HOH:O	2:B:394:GLN:HB3	2.18	0.43
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.00	0.43
1:A:467:VAL:HG22	1:A:484:LEU:HD11	2.00	0.43
1:C:199:ARG:O	1:C:203:GLU:HG2	2.18	0.43
2:D:66:LYS:HB2	2:D:66:LYS:HE2	1.84	0.43
3:F:2:OMC:HM22	3:F:3:DC:O4'	2.18	0.43
2:D:277:ARG:HA	2:D:277:ARG:HD3	1.77	0.43
2:D:356:ARG:HH11	2:D:356:ARG:HG3	1.83	0.43
1:C:320:ASP:OD2	1:C:322:SER:HB3	2.19	0.43
2:B:263:LYS:HA	2:B:423:VAL:HG11	2.01	0.43
2:B:208:HIS:O	2:B:211:ARG:HB3	2.18	0.43
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.19	0.42
1:A:550:LYS:HA	1:A:550:LYS:HD3	1.83	0.42
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.49	0.42
1:A:37:ILE:O	1:A:41:MET:HG3	2.19	0.42
2:D:89:GLU:H	2:D:89:GLU:CD	2.23	0.42
2:D:38:CYS:HB3	2:D:47:ILE:HD11	2.02	0.42
1:A:28:GLU:OE2	1:A:28:GLU:N	2.51	0.42
1:C:539:HIS:C	1:C:540:LYS:HD2	2.40	0.42
1:C:22:LYS:HD2	1:C:22:LYS:N	2.35	0.42
2:D:64:LYS:CD	2:D:69:THR:O	2.66	0.42
1:A:451:LYS:HG3	1:A:471:ASP:HA	2.02	0.41
3:E:2:OMC:H1'	3:E:2:OMC:HM23	1.91	0.41
3:F:23:DC:H2''	3:F:24:DG:C8	2.56	0.41
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.19	0.41
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.56	0.41
3:F:23:DC:OP2	8:F:101:HOH:O	2.21	0.41
2:B:194:GLU:CD	2:B:195:ILE:H	2.24	0.41
2:B:66:LYS:H	2:B:407:GLN:HE22	1.68	0.41
1:A:65:LYS:HB2	1:A:70:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.55	0.41
2:B:203:GLU:O	2:B:207:GLN:HG2	2.20	0.41
2:B:252:TRP:CD1	2:B:295:LEU:HD21	2.54	0.41
1:C:110:ASP:HB3	1:C:220:LYS:HD3	2.03	0.41
2:B:360:ALA:O	2:B:361:HIS:HB2	2.21	0.41
1:C:11:LYS:HG3	1:C:12:LEU:O	2.20	0.41
1:A:450:THR:CG2	1:A:452:LEU:HD12	2.50	0.41
1:C:143:ARG:HG2	1:C:143:ARG:NH1	2.35	0.41
2:D:356:ARG:HH21	2:D:361:HIS:CD2	2.39	0.41
1:A:436:GLY:O	1:A:461:ARG:NH2	2.53	0.41
2:B:336:GLN:OE1	2:B:355:ALA:HB2	2.20	0.41
1:A:249:LYS:HB2	1:A:252:TRP:CE2	2.55	0.41
2:B:421:PRO:O	2:B:421:PRO:HG2	2.21	0.41
2:D:183:TYR:CD2	2:D:184:MET:HG3	2.56	0.41
3:E:13:DT:H2''	3:E:14:DG:C8	2.55	0.41
1:C:110:ASP:HB3	1:C:220:LYS:HB3	2.03	0.40
1:C:59:PRO:HG2	1:C:76:ASP:HB3	2.01	0.40
2:D:317:VAL:HG22	2:D:349:LEU:HD23	2.03	0.40
2:B:418:ASN:C	2:B:418:ASN:HD22	2.25	0.40
1:A:185:ASP:CG	5:A:601:DCP:H5'2	2.42	0.40
1:A:438:GLU:HG3	1:A:461:ARG:HD2	2.04	0.40
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.57	0.40
1:C:94:ILE:HG12	3:F:4:OMC:H1'	2.04	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	551/557 (99%)	532 (97%)	17 (3%)	2 (0%)	34 45
1	C	551/557 (99%)	529 (96%)	21 (4%)	1 (0%)	47 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	402/444 (90%)	388 (96%)	14 (4%)	0	100	100
2	D	402/444 (90%)	386 (96%)	16 (4%)	0	100	100
All	All	1906/2002 (95%)	1835 (96%)	68 (4%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	C	53	GLU
1	A	135	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/494 (100%)	484 (98%)	8 (2%)	62	76
1	C	492/494 (100%)	485 (99%)	7 (1%)	67	78
2	B	365/400 (91%)	354 (97%)	11 (3%)	41	53
2	D	365/400 (91%)	358 (98%)	7 (2%)	57	71
All	All	1714/1788 (96%)	1681 (98%)	33 (2%)	57	71

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	ARG
1	A	219	LYS
1	A	237	ASP
1	A	251	SER
1	A	287	LYS
1	A	424	LYS
1	A	500	GLN
1	A	547	GLN
2	B	113	ASP

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Mol	Chain	Res	Type
2	B	122	LYS
2	B	161	GLN
2	B	206	ARG
2	B	242	GLN
2	B	281	LYS
2	B	356	ARG
2	B	357	MET
2	B	418	ASN
2	B	422	LEU
2	B	425	LEU
1	C	40	GLU
1	C	137	ASN
1	C	199	ARG
1	C	357	MET
1	C	499	SER
1	C	547	GLN
1	C	550	LYS
2	D	89	GLU
2	D	154	LYS
2	D	184	MET
2	D	211	ARG
2	D	336	GLN
2	D	356	ARG
2	D	427	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	GLN
1	A	464	GLN
1	A	483	HIS
1	A	500	GLN
1	A	509	GLN
1	A	524	GLN
2	B	151	GLN
2	B	161	GLN
2	B	208	HIS
2	B	235	HIS
2	B	258	GLN
2	B	269	GLN
2	B	418	ASN
1	C	207	GLN

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Mol	Chain	Res	Type
1	C	278	GLN
1	C	334	GLN
1	C	547	GLN
2	D	137	ASN
2	D	182	GLN
2	D	242	GLN
2	D	407	GLN
2	D	418	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	OMC	F	4	3	15,22,23	3.93	6 (40%)	17,31,34	1.60	2 (11%)
3	OMC	E	4	3	15,22,23	3.89	6 (40%)	17,31,34	1.51	2 (11%)
3	OMC	E	2	3	15,22,23	3.99	6 (40%)	17,31,34	1.54	2 (11%)
3	OMC	F	2	3	15,22,23	3.98	6 (40%)	17,31,34	1.50	1 (5%)

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	-	0/7/27/28	0/2/2/2
3	OMC	E	4	3	-	0/7/27/28	0/2/2/2
3	OMC	E	2	3	-	0/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	F	2	3	-	0/7/27/28	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	C6-N1	9.70	1.47	1.35
3	F	2	OMC	C6-N1	9.67	1.47	1.35
3	E	4	OMC	C6-N1	9.38	1.47	1.35
3	F	4	OMC	C6-N1	9.38	1.47	1.35
3	E	2	OMC	C4-N3	7.13	1.47	1.35
3	F	4	OMC	C4-N3	7.11	1.47	1.35
3	F	2	OMC	C4-N3	7.03	1.46	1.35
3	E	4	OMC	C4-N3	6.98	1.46	1.35
3	F	4	OMC	C2-N3	5.79	1.49	1.38
3	E	2	OMC	C2-N3	5.64	1.49	1.38
3	E	4	OMC	C2-N3	5.61	1.49	1.38
3	F	2	OMC	C2-N3	5.59	1.49	1.38
3	F	2	OMC	C6-C5	5.56	1.50	1.38
3	E	2	OMC	C6-C5	5.52	1.50	1.38
3	F	4	OMC	C6-C5	5.37	1.49	1.38
3	E	4	OMC	C6-C5	5.31	1.49	1.38
3	F	2	OMC	C4-N4	4.39	1.48	1.35
3	E	2	OMC	C4-N4	4.35	1.48	1.35
3	F	4	OMC	C4-N4	4.34	1.48	1.35
3	E	4	OMC	C4-N4	4.30	1.47	1.35
3	F	2	OMC	C5-C4	3.36	1.49	1.41
3	E	2	OMC	C5-C4	3.33	1.49	1.41
3	E	4	OMC	C5-C4	3.28	1.49	1.41
3	F	4	OMC	C5-C4	3.26	1.49	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	OMC	C2-N3-C4	5.33	121.75	116.34
3	E	4	OMC	C2-N3-C4	5.05	121.46	116.34
3	E	2	OMC	C2-N3-C4	5.05	121.46	116.34
3	F	2	OMC	C2-N3-C4	4.96	121.37	116.34
3	F	4	OMC	N4-C4-N3	2.37	120.23	116.49
3	E	2	OMC	N4-C4-N3	2.31	120.14	116.49
3	E	4	OMC	N4-C4-N3	2.23	120.02	116.49

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

## 5.5 Carbohydrates

2 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	0.56	0	15,15,17	0.83	1 (6%)
4	FRU	G	2	4	11,12,12	0.56	0	10,18,18	0.54	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	-	1/5/24/24	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	GLC	C1-O5-C5	2.21	115.19	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

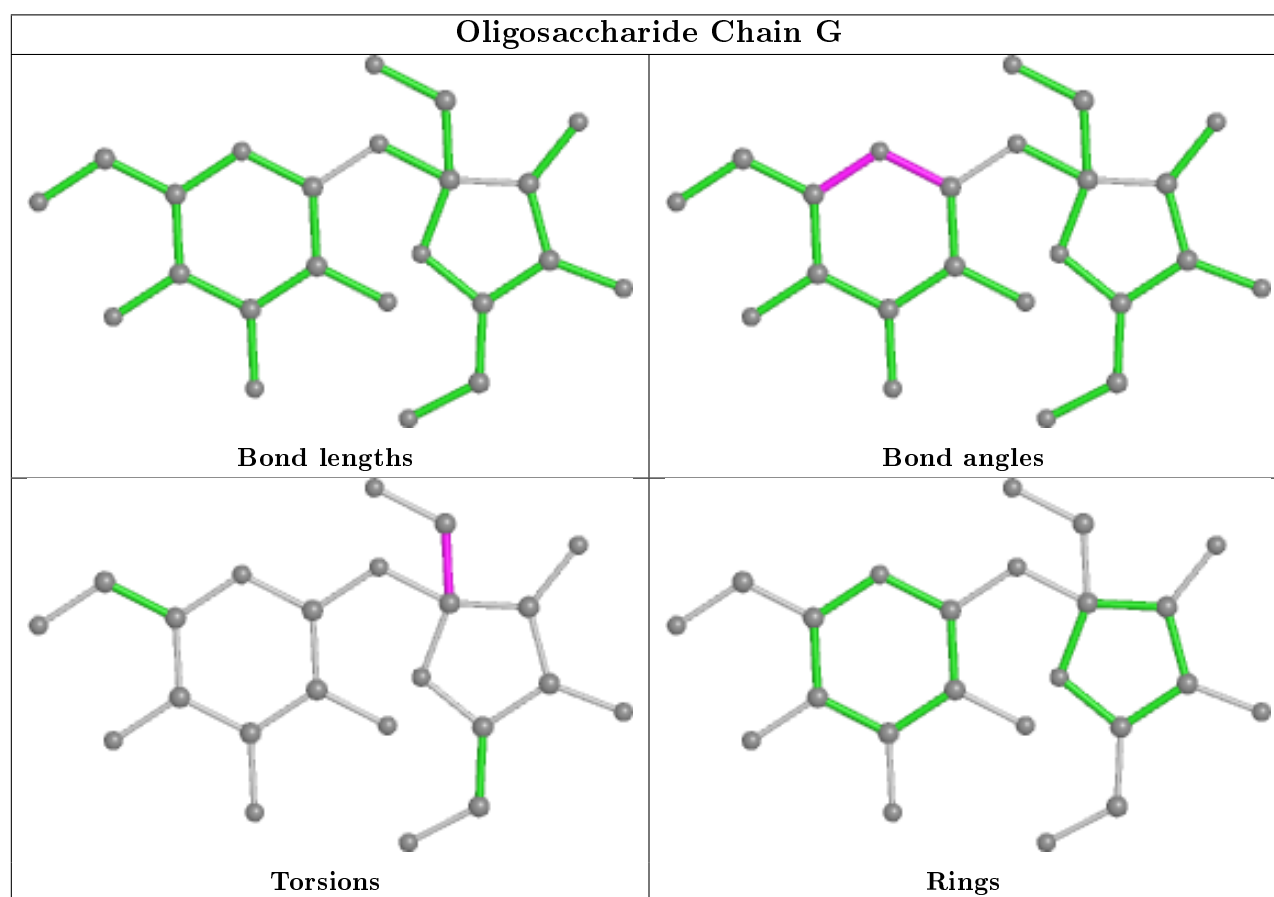
Mol	Chain	Res	Type	Atoms
4	G	2	FRU	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	GLC	1	0
4	G	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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
7	GOL	B	702	-	5,5,5	0.86	0	5,5,5	1.01	0
5	DCP	A	601	6	23,29,29	3.93	12 (52%)	30,45,45	1.42	4 (13%)
5	DCP	C	601	6	23,29,29	3.94	12 (52%)	30,45,45	1.30	4 (13%)
7	GOL	D	501	-	5,5,5	0.88	0	5,5,5	1.00	0
7	GOL	C	602	-	5,5,5	0.89	0	5,5,5	0.87	0
7	GOL	B	701	-	5,5,5	0.90	0	5,5,5	0.99	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
7	GOL	B	702	-	-	2/4/4/4	-
5	DCP	A	601	6	-	5/19/34/34	0/2/2/2
5	DCP	C	601	6	-	5/19/34/34	0/2/2/2
7	GOL	D	501	-	-	0/4/4/4	-
7	GOL	C	602	-	-	2/4/4/4	-
7	GOL	B	701	-	-	2/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	DCP	C6-N1	8.48	1.46	1.35
5	C	601	DCP	C6-N1	8.34	1.46	1.35
5	C	601	DCP	O4'-C4'	7.69	1.62	1.45
5	A	601	DCP	O4'-C4'	7.55	1.61	1.45
5	A	601	DCP	C3'-C4'	-6.45	1.35	1.53
5	C	601	DCP	C3'-C4'	-6.40	1.35	1.53
5	C	601	DCP	C4-N3	6.34	1.45	1.35
5	C	601	DCP	C2-N3	6.23	1.50	1.38
5	A	601	DCP	C4-N3	6.18	1.45	1.35
5	A	601	DCP	C2-N3	6.07	1.50	1.38
5	A	601	DCP	C6-C5	5.79	1.50	1.38
5	C	601	DCP	C6-C5	5.77	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	DCP	O4'-C1'	-5.17	1.30	1.42
5	C	601	DCP	O4'-C1'	-5.09	1.30	1.42
5	A	601	DCP	C4-N4	4.31	1.47	1.35
5	C	601	DCP	C4-N4	4.29	1.47	1.35
5	C	601	DCP	C5-C4	3.03	1.48	1.41
5	A	601	DCP	C5-C4	3.01	1.48	1.41
5	C	601	DCP	PA-O5'	2.47	1.69	1.59
5	A	601	DCP	PA-O5'	2.43	1.69	1.59
5	C	601	DCP	O3'-C3'	2.37	1.48	1.43
5	A	601	DCP	O3'-C3'	2.37	1.48	1.43
5	A	601	DCP	C2'-C1'	2.36	1.59	1.52
5	C	601	DCP	C2'-C1'	2.35	1.58	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	DCP	C2-N3-C4	5.05	121.45	116.34
5	C	601	DCP	C2-N3-C4	4.26	120.66	116.34
5	A	601	DCP	C2'-C1'-N1	-3.14	107.03	114.27
5	C	601	DCP	C2'-C1'-N1	-2.38	108.78	114.27
5	A	601	DCP	PB-O3B-PG	-2.34	124.79	132.83
5	C	601	DCP	PB-O3B-PG	-2.32	124.86	132.83
5	C	601	DCP	N4-C4-N3	2.16	119.91	116.49
5	A	601	DCP	N4-C4-N3	2.05	119.73	116.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	702	GOL	O1-C1-C2-C3
7	B	701	GOL	O1-C1-C2-C3
5	C	601	DCP	PB-O3B-PG-O2G
7	C	602	GOL	O1-C1-C2-O2
7	C	602	GOL	O1-C1-C2-C3
7	B	702	GOL	O1-C1-C2-O2
7	B	701	GOL	O1-C1-C2-O2
5	A	601	DCP	PB-O3B-PG-O1G
5	C	601	DCP	PA-O3A-PB-O2B
5	C	601	DCP	PB-O3B-PG-O1G
5	A	601	DCP	PB-O3B-PG-O2G
5	A	601	DCP	PB-O3B-PG-O3G
5	C	601	DCP	PB-O3B-PG-O3G

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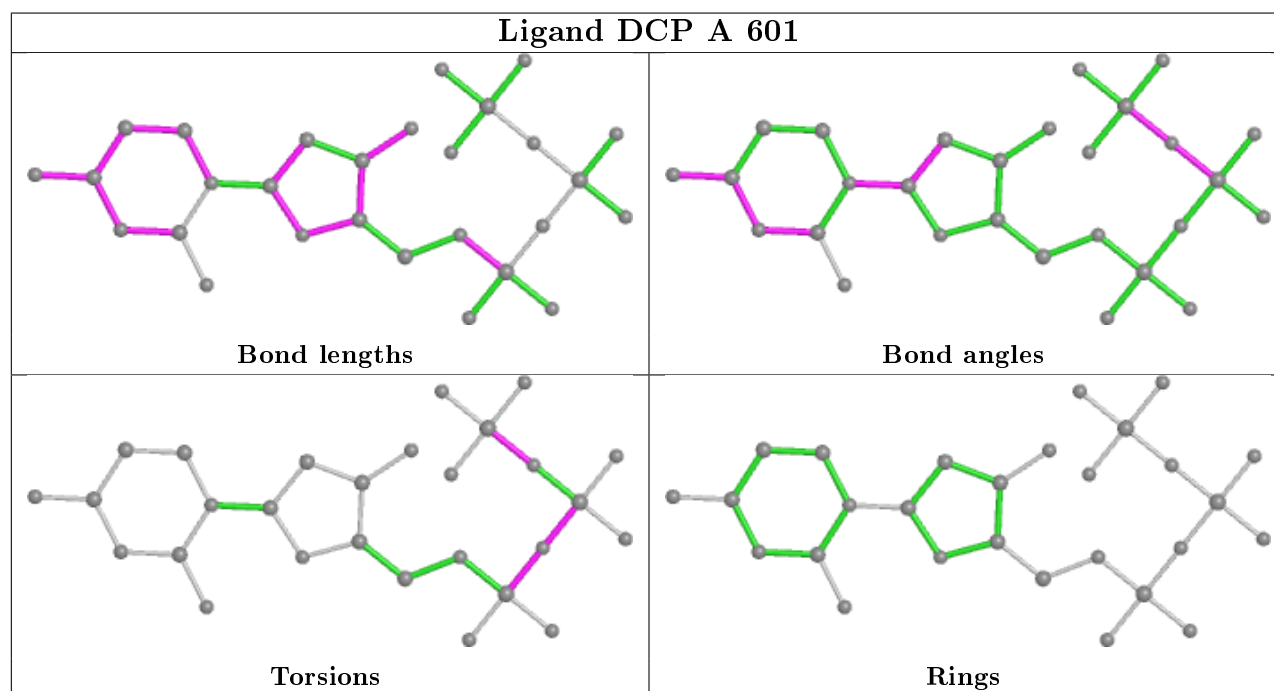
Mol	Chain	Res	Type	Atoms
5	A	601	DCP	PB-O3A-PA-O1A
5	A	601	DCP	PA-O3A-PB-O1B
5	C	601	DCP	PA-O3A-PB-O1B

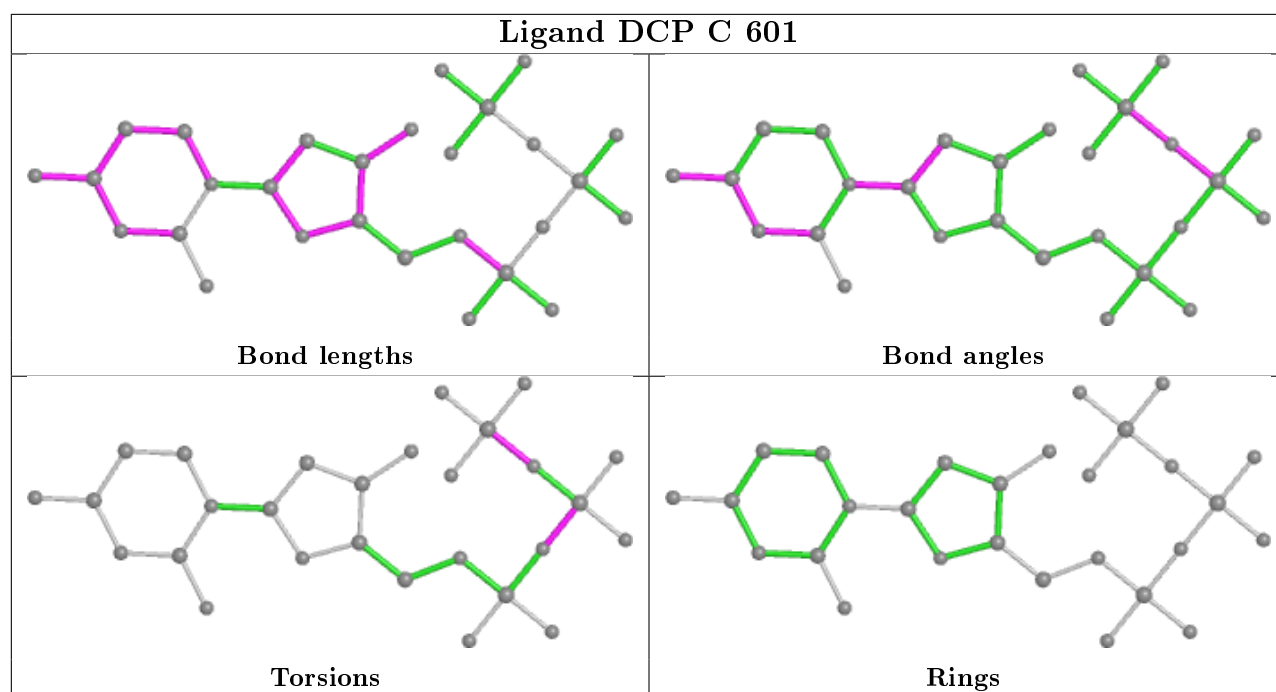
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	DCP	1	0
7	C	602	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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	553/557 (99%)	0.52	36 (6%) 18 23	39, 64, 101, 141	0
1	C	553/557 (99%)	0.73	58 (10%) 6 9	39, 67, 106, 165	0
2	B	406/444 (91%)	0.97	59 (14%) 2 3	40, 79, 123, 139	0
2	D	406/444 (91%)	0.49	30 (7%) 14 19	34, 60, 96, 116	0
3	E	33/38 (86%)	0.02	0 100 100	40, 64, 94, 128	0
3	F	36/38 (94%)	0.19	1 (2%) 53 62	43, 72, 125, 146	0
All	All	1987/2078 (95%)	0.65	184 (9%) 8 12	34, 66, 113, 165	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	9.3
2	B	88	TRP	8.7
2	D	360	ALA	7.8
1	C	69	THR	7.7
1	C	136	ASN	7.3
1	C	137	ASN	7.3
2	B	212	TRP	6.8
1	C	133	PRO	6.7
1	A	27	THR	6.7
2	B	427	TYR	6.6
2	B	360	ALA	6.5
1	A	140	PRO	6.3
1	A	28	GLU	6.3
1	A	69	THR	6.3
1	C	135	ILE	6.3
2	D	361	HIS	6.3
1	C	140	PRO	6.3
1	C	139	THR	6.2
2	B	92	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	C	141	GLY	6.1
1	A	137	ASN	6.1
2	D	359	GLY	6.1
1	C	553	SER	6.0
2	B	301	LEU	6.0
1	C	31	ILE	5.9
2	B	94	ILE	5.8
2	B	357	MET	5.8
2	B	91	GLN	5.6
2	B	213	GLY	5.4
2	B	361	HIS	5.4
2	D	231	GLY	5.4
2	B	93	GLY	5.3
2	B	359	GLY	5.3
2	D	212	TRP	5.3
2	B	67	ASP	5.3
1	C	50	ILE	5.3
2	B	297	GLU	5.2
1	C	34	LEU	5.2
1	C	452	LEU	5.2
2	D	232	TYR	5.2
1	C	132	ILE	5.1
1	A	134	SER	5.1
2	B	232	TYR	5.1
1	C	71	TRP	5.0
2	D	68	SER	5.0
2	B	90	VAL	5.0
1	A	141	GLY	5.0
1	C	449	GLU	4.9
2	B	423	VAL	4.8
2	B	299	ALA	4.8
2	B	295	LEU	4.7
1	A	135	ILE	4.7
1	A	138	GLU	4.6
2	B	231	GLY	4.6
2	D	67	ASP	4.6
1	A	66	LYS	4.6
1	A	24	TRP	4.5
1	A	67	ASP	4.5
2	B	362	THR	4.5
1	A	139	THR	4.4
1	A	33	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	136	ASN	4.4
1	C	28	GLU	4.3
1	C	68	SER	4.3
1	A	142	ILE	4.3
1	A	25	PRO	4.3
2	B	89	GLU	4.3
2	B	87	PHE	4.2
1	C	54	ASN	4.1
1	C	138	GLU	4.1
1	C	26	LEU	4.1
1	C	448	ARG	4.1
1	C	67	ASP	4.0
2	B	7	THR	3.9
1	A	541	GLY	3.9
1	A	68	SER	3.9
1	C	32	LYS	3.9
1	A	64	LYS	3.8
1	C	35	VAL	3.8
2	B	68	SER	3.8
1	C	52	PRO	3.8
2	B	252	TRP	3.8
1	C	33	ALA	3.7
2	B	211	ARG	3.7
2	D	69	THR	3.7
1	C	550	LYS	3.7
1	A	61	PHE	3.7
2	B	6	GLU	3.6
1	A	63	ILE	3.6
1	C	469	LEU	3.6
2	B	248	GLU	3.5
2	D	357	MET	3.5
2	D	5	ILE	3.5
2	B	209	LEU	3.5
2	B	66	LYS	3.4
2	D	166	LYS	3.4
2	B	10	VAL	3.3
1	C	142	ILE	3.3
2	B	95	PRO	3.3
2	D	358	LYS	3.2
1	C	552	VAL	3.2
2	B	251	SER	3.2
1	C	51	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	39	THR	3.1
1	A	413	GLU	3.1
1	C	104	LYS	3.1
2	B	5	ILE	3.1
2	B	422	LEU	3.1
2	D	425	LEU	3.0
1	C	66	LYS	3.0
2	D	174	GLN	3.0
1	C	551	LEU	3.0
2	B	178	ILE	3.0
2	B	195	ILE	2.9
1	C	49	LYS	2.9
2	B	168	LEU	2.9
2	D	283	LEU	2.9
2	D	211	ARG	2.9
2	B	177	ASP	2.9
2	D	421	PRO	2.9
1	A	132	ILE	2.9
1	A	36	GLU	2.8
2	D	66	LYS	2.8
1	A	30	LYS	2.8
2	B	279	LEU	2.8
1	C	144	TYR	2.8
2	D	172	ARG	2.8
2	B	250	ASP	2.8
2	B	161	GLN	2.8
1	C	37	ILE	2.7
1	C	143	ARG	2.7
1	A	29	GLU	2.7
1	C	131	THR	2.7
2	B	245	VAL	2.7
2	D	177	ASP	2.7
1	C	30	LYS	2.6
1	C	70	LYS	2.6
1	C	457	TYR	2.6
1	C	447	ASN	2.6
1	C	468	PRO	2.5
2	B	305	GLU	2.5
2	B	85	GLN	2.5
1	C	194	GLU	2.5
3	F	18	DT	2.5
2	B	9	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	70	LYS	2.5
1	C	55	PRO	2.5
2	B	196	GLY	2.4
1	A	346	PHE	2.4
1	C	450	THR	2.4
2	B	249	LYS	2.4
2	D	90	VAL	2.4
2	B	104	LYS	2.4
2	B	202	ILE	2.4
2	D	420	PRO	2.4
2	B	210	LEU	2.3
2	B	304	ALA	2.3
1	C	134	SER	2.3
2	D	93	GLY	2.3
1	C	128	THR	2.3
1	A	62	ALA	2.2
2	D	362	THR	2.2
2	D	95	PRO	2.2
1	C	177	ASP	2.2
1	C	470	THR	2.2
1	A	237	ASP	2.2
2	B	424	LYS	2.1
1	C	60	VAL	2.1
1	A	71	TRP	2.1
1	A	402	TRP	2.1
1	C	24	TRP	2.1
2	B	180	ILE	2.1
2	B	260	LEU	2.1
2	D	209	LEU	2.1
1	A	65	LYS	2.1
1	C	538	ALA	2.1
2	D	284	ARG	2.1
2	B	293	VAL	2.1
1	A	32	LYS	2.1
2	D	178	ILE	2.0
2	D	427	TYR	2.0
2	B	277	ARG	2.0
1	C	63	ILE	2.0
1	C	64	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

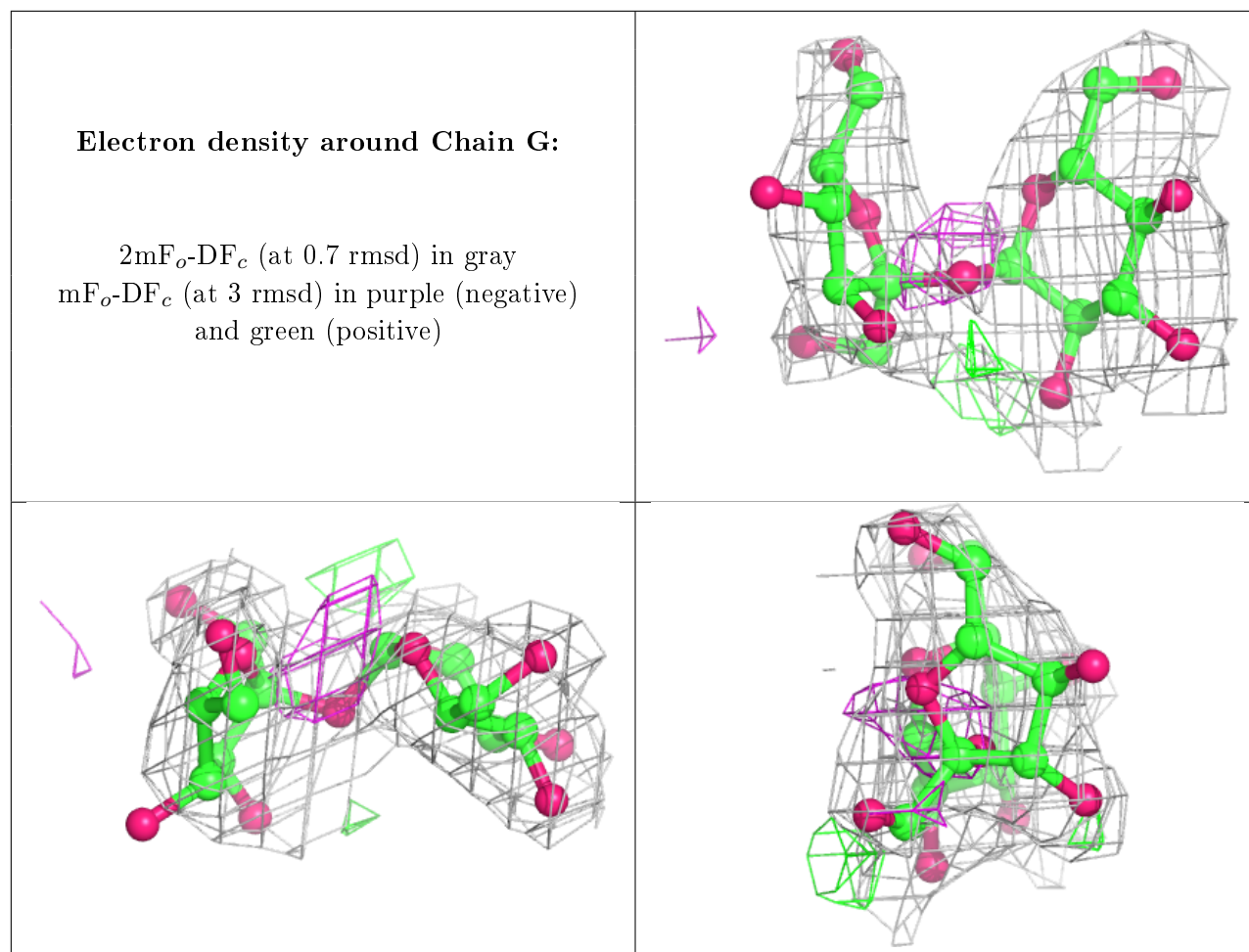
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	OMC	F	4	21/22	0.97	0.22	39,49,54,57	0
3	OMC	E	4	21/22	0.98	0.21	31,43,49,51	0
3	OMC	E	2	21/22	0.98	0.21	40,45,57,61	0
3	OMC	F	2	21/22	0.98	0.18	49,61,68,75	0

## 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	G	2	12/12	0.81	0.22	86,103,105,110	0
4	GLC	G	1	11/12	0.92	0.19	61,70,82,88	0

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



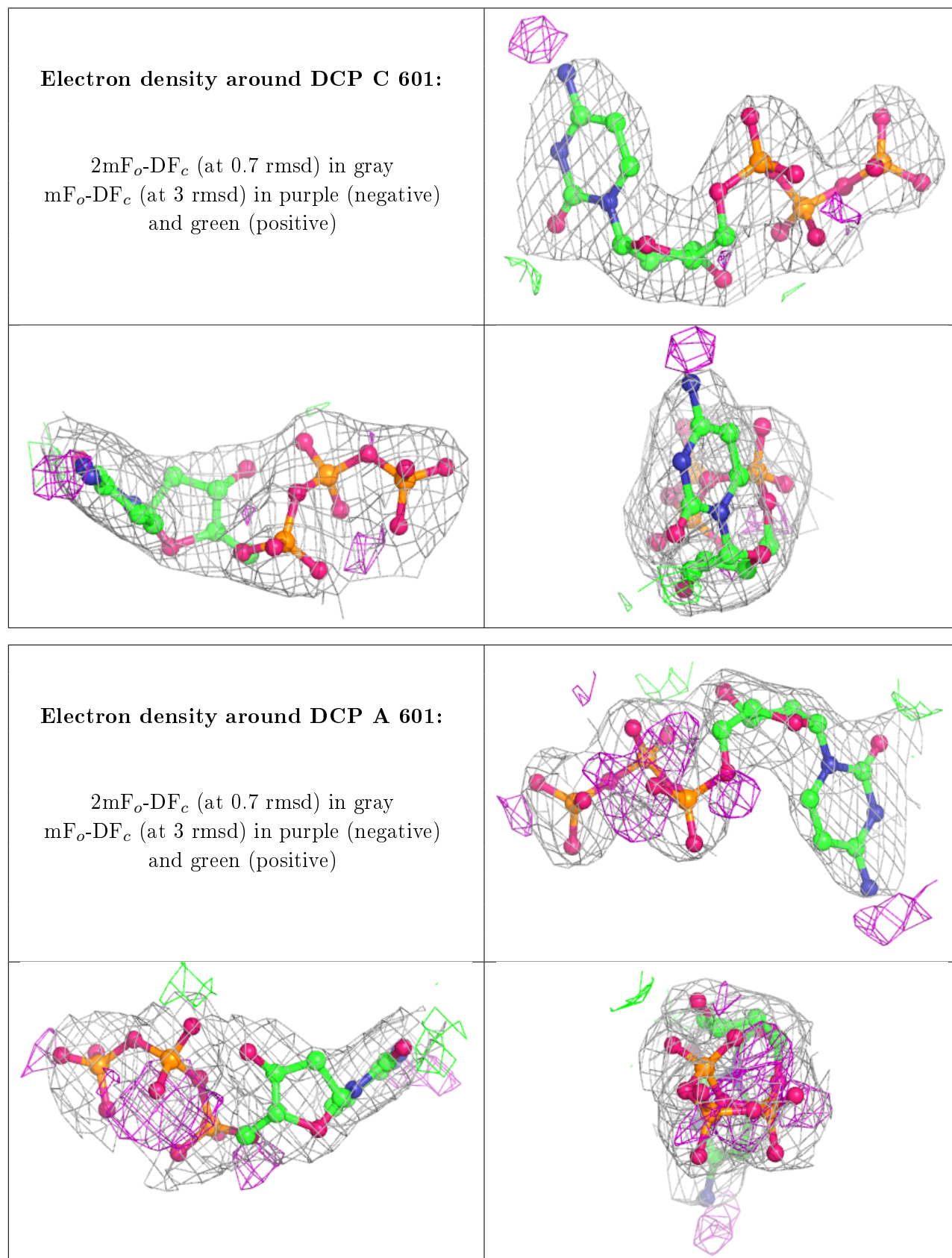
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	GOL	B	701	6/6	0.79	0.26	72,74,78,79	0
6	MG	A	602	1/1	0.81	0.12	63,63,63,63	0
6	MG	C	603	1/1	0.84	0.08	58,58,58,58	0
7	GOL	C	602	6/6	0.93	0.20	58,60,64,66	0
5	DCP	C	601	28/28	0.94	0.15	49,62,81,85	0
5	DCP	A	601	28/28	0.94	0.16	53,60,72,83	0
7	GOL	D	501	6/6	0.95	0.26	54,55,56,57	0
7	GOL	B	702	6/6	0.95	0.31	52,57,61,69	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

There are no such residues in this entry.