



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 PM UTC

PDB ID : 7DBM / pdb\_00007dbm  
Title : HIV-1 reverse transcriptase mutant Q151M/Y115F/F116Y/M184V:DNA:dG  
TP ternary complex  
Authors : Yasutake, Y.; Hattori, S.I.; Tamura, N.; Maeda, K.  
Deposited on : 2020-10-21  
Resolution : 2.43 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>.

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

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

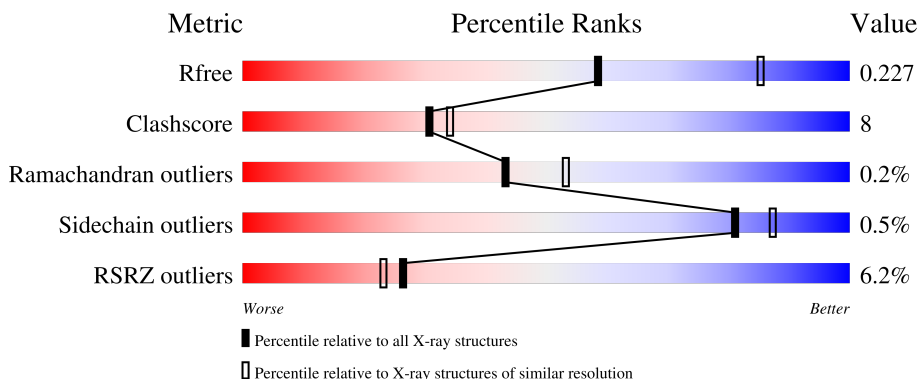
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.43 Å.

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




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	557	 4% 80% 19%
1	C	557	 3% 83% 16%
2	B	444	 12% 69% 22% 9%
2	D	444	 7% 78% 12% 9%
3	E	38	 71% 16% 5% 8%

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Mol	Chain	Length	Quality of chain
3	F	38	 79% 16% 5%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17702 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 Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	552	4490	2906	749	828	7	0	0	0
1	C	552	4490	2906	749	828	7	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	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	184	VAL	MET	engineered mutation	UNP D3XFN5
A	280	SER	CYS	engineered mutation	UNP D3XFN5
C	-1	MET	-	initiating methionine	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	184	VAL	MET	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
			Total	C	N	O	S			
2	B	406	3347	2178	557	606	6	0	0	0
2	D	406	3347	2178	557	606	6	0	0	0

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).

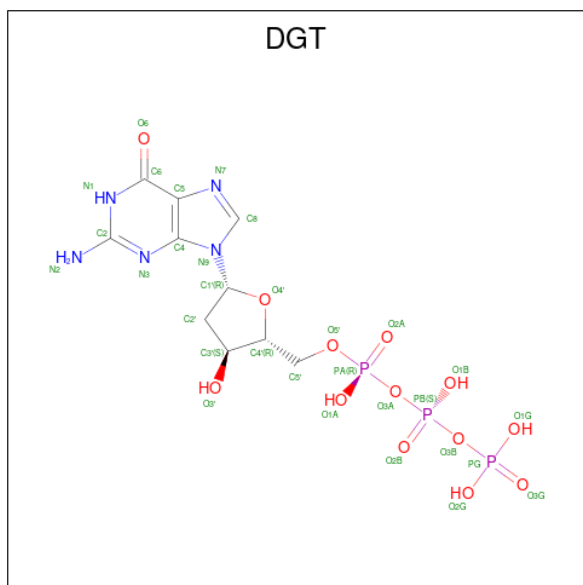
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	E	35	718	339	128	216	35	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	38	777	369	140	231	37	0	0	0

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	31	10	5	13	3	0	0
4	C	1	31	10	5	13	3	0	0

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

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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

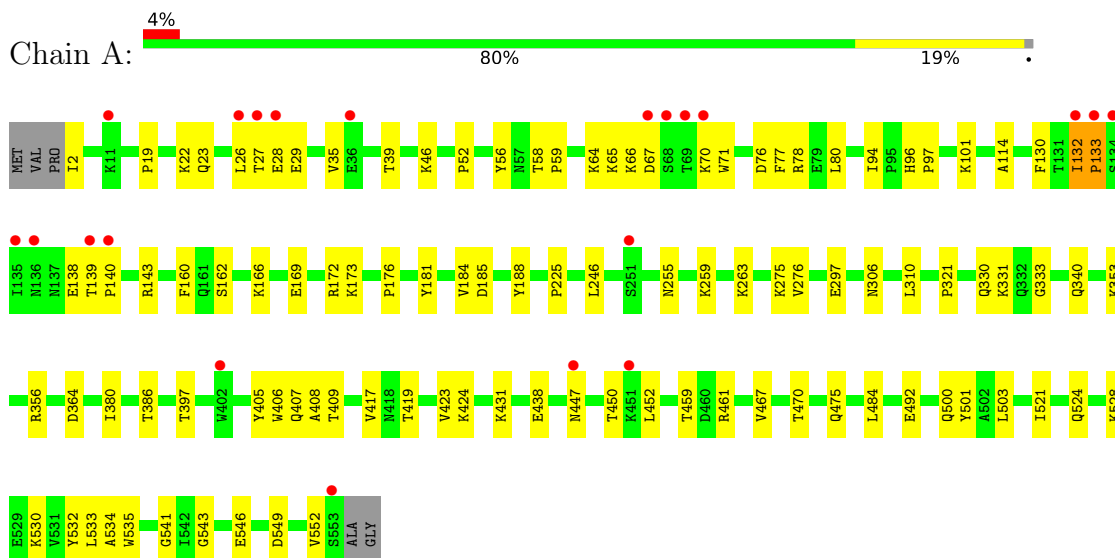
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	116	Total O 116 116	0	0
7	B	52	Total O 52 52	0	0
7	E	43	Total O 43 43	0	0
7	C	103	Total O 103 103	0	0
7	D	86	Total O 86 86	0	0
7	F	39	Total O 39 39	0	0

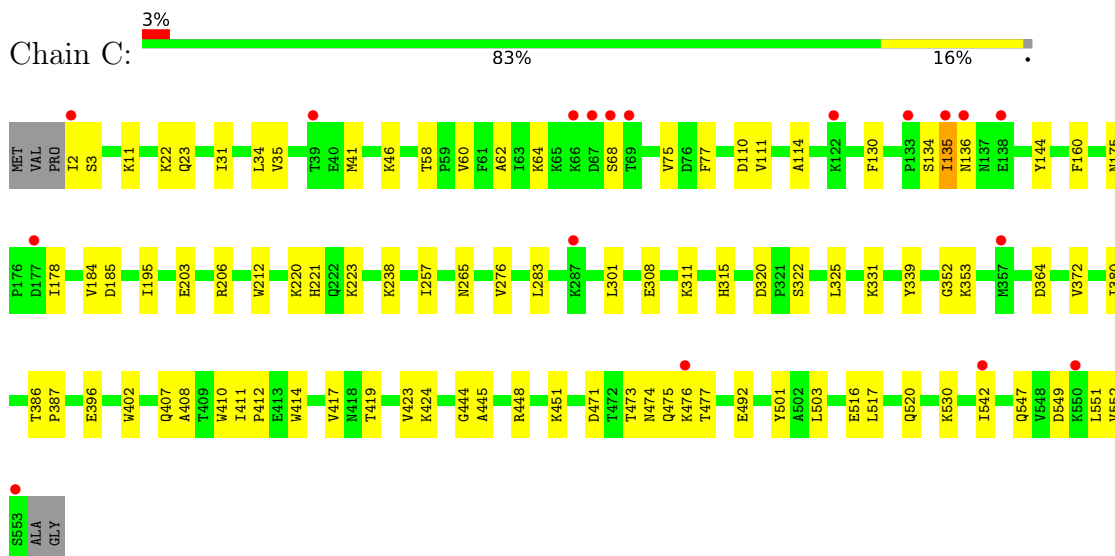
### 3 Residue-property plots

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: Protease

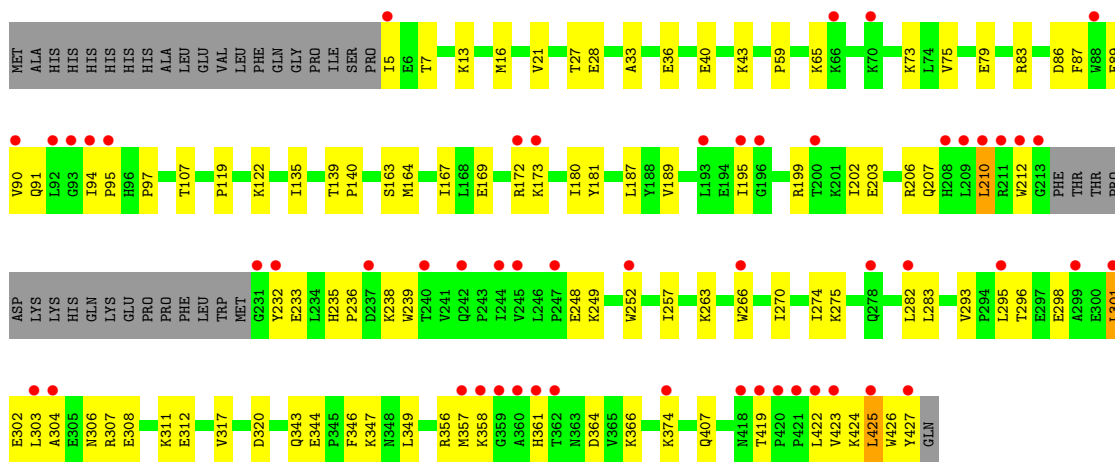


- Molecule 1: Protease

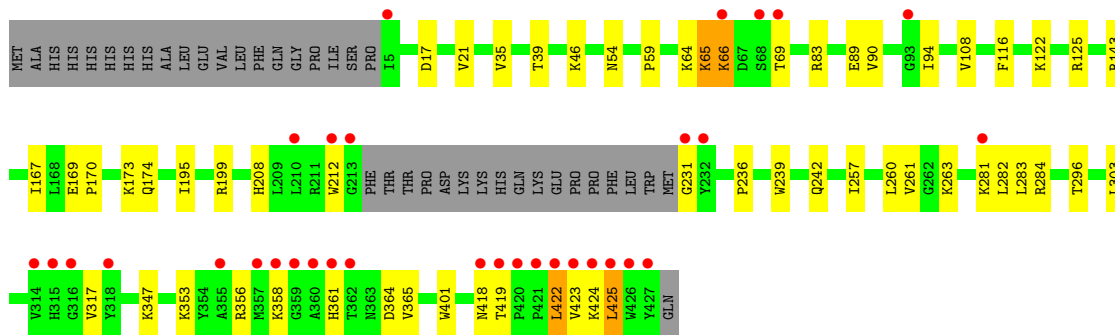
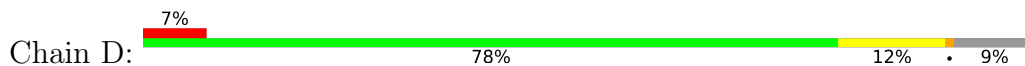


- Molecule 2: HIV-1 RT p51 subunit





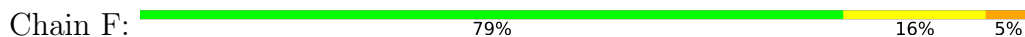
• Molecule 2: HIV-1 RT p51 subunit



• Molecule 3: DNA/RNA (38-MER)



• Molecule 3: DNA/RNA (38-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	283.51Å 283.51Å 95.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.47 – 2.43 48.47 – 2.43	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.47-2.43) 99.9 (48.47-2.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.19 (at 2.42Å)	Xtrriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, $R_{free}$	0.181 , 0.224 0.184 , 0.227	Depositor DCC
$R_{free}$ test set	5472 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: DGT, MG, OMC, GOL

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	0.51	5/4607 (0.1%)	0.62	5/6257 (0.1%)
1	C	0.30	0/4607	0.45	0/6257
2	B	0.38	0/3441	0.65	3/4673 (0.1%)
2	D	0.31	0/3441	0.48	4/4673 (0.1%)
3	E	0.25	0/756	0.44	0/1165
3	F	0.43	0/823	0.47	0/1269
All	All	0.39	5/17675 (0.0%)	0.55	12/24294 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	PRO	N-CA	19.52	1.69	1.47
1	A	132	ILE	C-N	9.59	1.45	1.33
1	A	225	PRO	C-O	-7.57	1.18	1.24
1	A	52	PRO	C-O	-5.09	1.17	1.24
1	A	176	PRO	C-O	-5.08	1.17	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ILE	CA-C-N	15.01	140.51	120.25
1	A	132	ILE	C-N-CA	15.01	140.51	120.25
1	A	133	PRO	CA-N-CD	-10.45	97.37	112.00
1	A	132	ILE	N-CA-C	-5.94	103.52	108.63
2	D	425	LEU	N-CA-C	-5.93	105.23	112.88
1	A	67	ASP	N-CA-C	-5.78	100.83	109.15
2	D	424	LYS	CA-C-N	5.57	131.29	122.60
2	D	424	LYS	C-N-CA	5.57	131.29	122.60
2	B	424	LYS	CA-C-N	5.38	127.49	120.28
2	B	424	LYS	C-N-CA	5.38	127.49	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	422	LEU	N-CA-C	-5.13	105.76	112.23
2	B	361	HIS	CB-CA-C	-5.07	102.76	110.06

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	4490	0	4543	87	0
1	C	4490	0	4543	67	0
2	B	3347	0	3379	98	0
2	D	3347	0	3379	43	0
3	E	718	0	397	7	0
3	F	777	0	432	5	0
4	A	31	0	12	0	0
4	C	31	0	12	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	12	0	16	1	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
6	E	6	0	8	0	0
7	A	116	0	0	3	0
7	B	52	0	0	0	0
7	C	103	0	0	0	0
7	D	86	0	0	0	0
7	E	43	0	0	0	0
7	F	39	0	0	0	0
All	All	17702	0	16737	283	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 8.

All (283) 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)
1:A:133:PRO:CA	1:A:133:PRO:N	1.69	1.47
1:A:500:GLN:CB	2:B:422:LEU:HD11	1.81	1.11
1:A:500:GLN:HB2	2:B:422:LEU:HD11	1.32	1.05
2:B:87:PHE:HA	2:B:90:VAL:HG12	1.33	1.04
2:B:358:LYS:HE2	2:B:366:LYS:NZ	1.74	1.03
1:A:65:LYS:HZ2	1:A:70:LYS:HE2	1.26	0.99
2:B:311:LYS:HB3	2:B:312:GLU:OE1	1.67	0.95
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.10	0.93
2:B:358:LYS:HE2	2:B:366:LYS:HZ1	1.36	0.90
2:B:308:GLU:HA	2:B:311:LYS:HG3	1.53	0.90
1:A:543:GLY:HA3	2:B:283:LEU:O	1.72	0.90
1:A:503:LEU:HD23	2:B:422:LEU:HD23	1.52	0.88
2:B:320:ASP:H	2:B:343:GLN:HE22	1.18	0.88
2:B:87:PHE:CA	2:B:90:VAL:HG12	2.05	0.85
2:D:419:THR:HG21	2:D:423:VAL:HG21	1.57	0.85
2:B:311:LYS:HB3	2:B:312:GLU:CD	2.02	0.84
2:B:311:LYS:CB	2:B:312:GLU:OE1	2.26	0.84
1:A:28:GLU:O	1:A:28:GLU:CD	2.22	0.83
1:A:500:GLN:HB3	2:B:422:LEU:HD11	1.59	0.83
1:A:65:LYS:HZ2	1:A:70:LYS:CE	1.91	0.82
1:A:28:GLU:O	1:A:28:GLU:OE1	1.99	0.81
2:B:87:PHE:HA	2:B:90:VAL:CG1	2.10	0.81
1:A:139:THR:HG23	1:A:140:PRO:HD2	1.65	0.79
1:A:64:LYS:HE2	1:A:71:TRP:CZ2	2.18	0.78
1:A:447:ASN:HB2	1:A:450:THR:HB	1.63	0.78
2:B:263:LYS:HE3	2:B:425:LEU:HA	1.64	0.78
2:B:423:VAL:HB	2:B:425:LEU:HD13	1.68	0.76
2:B:358:LYS:HE2	2:B:366:LYS:HZ3	1.51	0.75
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.17	0.74
1:C:2:ILE:HD11	1:C:46:LYS:HD3	1.71	0.73
1:C:407:GLN:NE2	2:D:418:ASN:HA	2.04	0.73
1:A:503:LEU:HD23	2:B:422:LEU:CD2	2.20	0.72
2:B:425:LEU:HD22	2:B:425:LEU:H	1.53	0.72
2:B:87:PHE:CD2	2:B:90:VAL:HG11	2.25	0.71
1:C:503:LEU:CD2	2:D:422:LEU:HD21	2.21	0.71
1:A:500:GLN:HB3	2:B:422:LEU:CD1	2.20	0.70
2:B:296:THR:HG22	2:B:298:GLU:H	1.58	0.69
2:D:195:ILE:HG13	2:D:199:ARG:HE	1.58	0.69
1:A:459:THR:HG22	1:A:461:ARG:H	1.58	0.68
2:B:301:LEU:HD13	2:B:301:LEU:C	2.18	0.68
1:A:521:ILE:HA	1:A:524:GLN:HE21	1.59	0.67
2:D:356:ARG:HD3	2:D:361:HIS:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:LEU:HD11	2:B:293:VAL:CG1	2.25	0.67
1:C:195:ILE:HD12	1:C:195:ILE:H	1.60	0.67
2:D:169:GLU:HG3	2:D:170:PRO:HD3	1.77	0.67
1:A:500:GLN:CB	2:B:422:LEU:CD1	2.67	0.66
2:B:139:THR:HG22	2:B:140:PRO:O	1.96	0.65
1:A:65:LYS:NZ	1:A:70:LYS:HE2	2.09	0.64
1:C:175:ASN:HB3	1:C:178:ILE:HD12	1.80	0.63
2:B:296:THR:HG22	2:B:298:GLU:N	2.13	0.63
1:A:65:LYS:NZ	1:A:70:LYS:CE	2.62	0.62
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.79	0.62
2:B:320:ASP:H	2:B:343:GLN:NE2	1.95	0.62
3:F:3:DC:H2'	3:F:4:OMC:C6	2.35	0.62
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.81	0.62
2:B:122:LYS:H	2:B:122:LYS:HD3	1.64	0.61
1:C:473:THR:O	1:C:477:THR:HG23	2.00	0.61
1:C:22:LYS:HD3	1:C:23:GLN:H	1.66	0.60
1:C:135:ILE:HG22	1:C:135:ILE:O	2.01	0.60
1:A:447:ASN:HB2	1:A:450:THR:CB	2.31	0.59
1:C:448:ARG:H	1:C:448:ARG:HD2	1.67	0.59
2:B:195:ILE:O	2:B:199:ARG:HG3	2.03	0.59
1:A:276:VAL:HG22	1:A:353:LYS:HE2	1.84	0.59
1:C:22:LYS:HA	1:C:22:LYS:HE2	1.85	0.59
2:D:170:PRO:O	2:D:174:GLN:HG3	2.04	0.58
2:D:419:THR:HG21	2:D:423:VAL:CG2	2.32	0.58
1:A:275:LYS:H	1:A:306:ASN:HD21	1.50	0.58
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.33	0.58
3:E:3:DC:H2'	3:E:4:OMC:C6	2.39	0.58
1:A:172:ARG:NH1	7:A:702:HOH:O	2.36	0.57
2:D:90:VAL:HA	2:D:94:ILE:HG13	1.87	0.57
2:B:282:LEU:HD11	2:B:293:VAL:HG12	1.86	0.57
2:B:311:LYS:HB2	2:B:312:GLU:OE1	2.04	0.56
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.87	0.56
2:B:235:HIS:HB2	2:B:238:LYS:HE2	1.87	0.56
1:C:407:GLN:HE22	2:D:418:ASN:HA	1.69	0.56
1:C:372:VAL:HG11	1:C:411:ILE:HG23	1.87	0.56
1:C:396:GLU:CD	1:C:396:GLU:H	2.14	0.56
2:B:374:LYS:HD3	2:B:374:LYS:N	2.21	0.55
2:D:260:LEU:HD21	2:D:303:LEU:HD11	1.88	0.55
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.87	0.55
1:C:474:ASN:O	1:C:477:THR:OG1	2.23	0.55
2:D:89:GLU:HG2	2:D:90:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:LEU:N	2:B:425:LEU:CD2	2.70	0.55
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.88	0.55
2:B:425:LEU:H	2:B:425:LEU:CD2	2.18	0.54
2:B:87:PHE:HD2	2:B:90:VAL:HG11	1.71	0.54
1:C:135:ILE:O	1:C:135:ILE:CG2	2.56	0.54
1:C:417:VAL:HG22	1:C:419:THR:HG23	1.89	0.54
1:A:185:ASP:OD1	3:E:33:DC:O3'	2.25	0.53
2:B:252:TRP:CD1	2:B:295:LEU:HD21	2.44	0.53
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.44	0.53
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.90	0.53
2:B:425:LEU:HD22	2:B:425:LEU:N	2.23	0.53
3:F:1:DG:H2'	3:F:2:OMC:C6	2.43	0.53
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.91	0.53
2:B:87:PHE:C	2:B:90:VAL:HG12	2.33	0.53
2:B:169:GLU:HG3	2:B:173:LYS:HD3	1.90	0.52
1:A:255:ASN:O	1:A:259:LYS:HG3	2.09	0.52
1:C:451:LYS:HB3	1:C:471:ASP:HA	1.91	0.52
1:A:333:GLY:HA3	1:C:301:LEU:HD11	1.90	0.52
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.09	0.52
2:B:425:LEU:HD23	2:B:426:TRP:H	1.75	0.52
2:D:263:LYS:HA	2:D:425:LEU:HD22	1.91	0.52
2:D:35:VAL:O	2:D:39:THR:HG23	2.10	0.52
1:C:221:HIS:CE1	1:C:223:LYS:HE2	2.45	0.52
1:A:56:TYR:O	1:A:143:ARG:NH2	2.42	0.52
2:B:33:ALA:O	2:B:36:GLU:HG3	2.10	0.51
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.93	0.51
1:C:412:PRO:O	1:C:414:TRP:HD1	1.93	0.51
2:B:311:LYS:HD3	2:B:312:GLU:OE2	2.10	0.51
1:C:402:TRP:HE1	2:D:364:ASP:CG	2.19	0.51
2:B:303:LEU:O	2:B:307:ARG:HG3	2.10	0.51
3:E:23:DC:H2''	3:E:24:DG:C8	2.46	0.51
1:A:169:GLU:HG3	1:A:173:LYS:HD2	1.93	0.51
1:A:263:LYS:NZ	7:A:703:HOH:O	2.40	0.51
2:B:164:MET:HE3	2:B:187:LEU:HD11	1.92	0.50
2:D:257:ILE:HB	2:D:283:LEU:HD21	1.92	0.50
2:D:356:ARG:C	2:D:356:ARG:HD2	2.36	0.50
1:C:130:PHE:CZ	1:C:144:TYR:HB2	2.47	0.50
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.38	0.50
2:B:172:ARG:NH2	2:B:180:ILE:HB	2.27	0.50
1:C:320:ASP:OD2	1:C:322:SER:HB3	2.12	0.50
2:B:303:LEU:HD21	2:B:307:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:HIS:CE1	2:D:212:TRP:HE1	2.29	0.50
2:B:427:TYR:CD1	2:B:427:TYR:C	2.90	0.49
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.94	0.49
1:C:60:VAL:HG12	1:C:75:VAL:HG22	1.94	0.49
2:D:356:ARG:HE	2:D:361:HIS:CG	2.31	0.49
1:C:134:SER:C	1:C:136:ASN:H	2.20	0.49
2:B:249:LYS:HG3	2:B:252:TRP:CE2	2.47	0.49
2:D:282:LEU:HD21	2:D:296:THR:HG23	1.94	0.49
1:C:448:ARG:HD2	1:C:448:ARG:N	2.27	0.49
1:A:541:GLY:HA2	1:A:546:GLU:HG3	1.94	0.49
2:B:163:SER:O	2:B:167:ILE:HG13	2.13	0.48
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.47	0.48
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.94	0.48
2:B:303:LEU:HD21	2:B:307:ARG:HH11	1.78	0.48
2:D:423:VAL:O	2:D:425:LEU:N	2.43	0.48
1:A:22:LYS:HD3	1:A:23:GLN:O	2.13	0.48
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.96	0.48
1:A:409:THR:HB	6:B:501:GOL:H11	1.95	0.48
1:C:3:SER:HB2	1:C:212:TRP:O	2.14	0.48
1:A:467:VAL:HG22	1:A:484:LEU:HD11	1.96	0.47
1:A:549:ASP:HA	1:A:552:VAL:HG22	1.96	0.47
2:D:108:VAL:O	2:D:231:GLY:HA3	2.13	0.47
1:C:448:ARG:H	1:C:448:ARG:CD	2.26	0.47
1:A:66:LYS:HD3	1:A:66:LYS:HA	1.53	0.47
1:A:380:ILE:HD11	1:A:386:THR:HG23	1.95	0.47
3:E:1:DG:H2'	3:E:2:OMC:C6	2.49	0.47
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.97	0.47
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.80	0.47
2:B:90:VAL:HG22	2:B:90:VAL:O	2.15	0.47
2:B:344:GLU:HB2	2:B:347:LYS:HD3	1.97	0.47
1:A:76:ASP:OD1	1:A:78:ARG:NH2	2.48	0.46
2:B:87:PHE:CA	2:B:90:VAL:CG1	2.84	0.46
2:B:356:ARG:NE	2:B:357:MET:H	2.14	0.46
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.96	0.46
2:D:66:LYS:HB3	2:D:66:LYS:HE2	1.58	0.46
2:D:122:LYS:HG2	2:D:125:ARG:CZ	2.45	0.46
3:F:23:DC:H2''	3:F:24:DG:C8	2.50	0.46
1:A:447:ASN:CB	1:A:450:THR:HB	2.39	0.46
1:C:22:LYS:HD3	1:C:23:GLN:N	2.30	0.46
1:C:238:LYS:HG2	1:C:315:HIS:CD2	2.51	0.46
2:B:90:VAL:C	2:B:91:GLN:HG2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:423:VAL:CB	2:B:425:LEU:HD13	2.43	0.46
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.98	0.46
1:C:220:LYS:NZ	4:C:601:DGT:O1G	2.44	0.46
2:D:17:ASP:O	2:D:83:ARG:HD3	2.16	0.46
2:B:248:GLU:HB2	2:B:307:ARG:HH22	1.81	0.46
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.51	0.45
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.99	0.45
2:B:301:LEU:C	2:B:301:LEU:CD1	2.86	0.45
2:D:358:LYS:HB2	2:D:358:LYS:HE2	1.68	0.45
1:C:503:LEU:HD22	2:D:422:LEU:HD21	1.97	0.45
2:D:46:LYS:HD2	2:D:116:PHE:HB3	1.98	0.45
3:F:10:DC:H2''	3:F:11:DG:C8	2.52	0.45
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.52	0.45
2:B:73:LYS:HD3	2:B:75:VAL:HG23	1.97	0.45
2:D:242:GLN:HG2	2:D:353:LYS:HE2	1.98	0.45
3:E:4:OMC:HM23	3:E:4:OMC:H1'	1.84	0.45
1:C:325:LEU:HB3	1:C:387:PRO:HB3	1.99	0.45
2:B:65:LYS:HA	2:B:407:GLN:OE1	2.17	0.44
1:C:11:LYS:HA	1:C:11:LYS:HD2	1.88	0.44
1:C:476:LYS:HG3	1:C:517:LEU:HD23	1.99	0.44
3:F:4:OMC:HM23	3:F:4:OMC:H1'	1.87	0.44
2:B:427:TYR:C	2:B:427:TYR:HD1	2.26	0.44
1:C:444:GLY:HA3	1:C:477:THR:HB	1.99	0.44
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.00	0.44
1:A:492:GLU:HG2	1:A:530:LYS:HB2	2.00	0.44
1:A:503:LEU:HD12	1:A:533:LEU:HG	1.99	0.44
2:B:5:ILE:HG23	2:B:119:PRO:HG3	1.99	0.44
1:C:503:LEU:HD21	2:D:422:LEU:HD21	1.99	0.44
1:A:130:PHE:HE2	1:A:132:ILE:HG12	1.82	0.44
1:A:459:THR:HG22	1:A:461:ARG:N	2.31	0.44
1:C:31:ILE:O	1:C:35:VAL:HG13	2.18	0.44
1:C:331:LYS:NZ	1:C:364:ASP:OD1	2.45	0.44
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.53	0.43
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.00	0.43
2:B:94:ILE:HA	2:B:95:PRO:HD3	1.88	0.43
1:A:162:SER:O	1:A:166:LYS:HG3	2.18	0.43
2:B:207:GLN:HA	2:B:210:LEU:HB2	1.99	0.43
1:C:110:ASP:HB3	1:C:220:LYS:HB3	1.99	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.43
2:B:28:GLU:HA	2:B:135:ILE:HD11	2.00	0.43
2:B:308:GLU:O	2:B:311:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ASP:HB2	2:B:89:GLU:OE1	2.19	0.43
1:C:408:ALA:HB1	2:D:364:ASP:HB3	1.99	0.43
2:D:65:LYS:HB3	2:D:65:LYS:HE3	1.68	0.43
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.94	0.43
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.43	0.43
1:A:500:GLN:CD	1:A:500:GLN:H	2.26	0.43
2:B:257:ILE:HD13	2:B:282:LEU:HD23	2.01	0.43
2:B:301:LEU:HD13	2:B:301:LEU:O	2.18	0.43
1:C:547:GLN:O	1:C:551:LEU:HG	2.18	0.43
2:D:422:LEU:O	2:D:425:LEU:HG	2.18	0.43
1:A:22:LYS:O	1:A:59:PRO:HG3	2.18	0.43
1:A:452:LEU:HD21	1:A:470:THR:HG22	1.98	0.43
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.54	0.43
1:A:406:TRP:HD1	2:B:419:THR:HG23	1.84	0.43
1:C:364:ASP:HB3	1:C:423:VAL:HG13	2.01	0.42
1:A:166:LYS:HE2	7:A:813:HOH:O	2.19	0.42
1:A:330:GLN:NE2	1:A:340:GLN:HE22	1.94	0.42
1:C:34:LEU:HD21	1:C:62:ALA:HB2	2.01	0.42
1:C:549:ASP:O	1:C:552:VAL:HG22	2.19	0.42
1:A:2:ILE:HD11	1:A:46:LYS:HD3	2.01	0.42
1:A:438:GLU:CG	1:A:461:ARG:HD2	2.49	0.42
2:B:40:GLU:OE1	2:B:43:LYS:NZ	2.44	0.42
2:B:304:ALA:O	2:B:308:GLU:HG2	2.19	0.42
1:C:308:GLU:O	1:C:311:LYS:HG2	2.20	0.42
1:A:397:THR:HG21	1:A:424:LYS:HA	2.02	0.42
2:B:423:VAL:HG12	2:B:425:LEU:HB3	2.02	0.42
3:E:16:DT:O2	3:E:16:DT:H2'	2.19	0.42
2:D:195:ILE:HG12	2:D:199:ARG:HH21	1.85	0.42
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.02	0.42
1:C:276:VAL:HG22	1:C:353:LYS:HE3	2.02	0.42
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.49	0.42
1:C:64:LYS:HD2	1:C:68:SER:O	2.20	0.42
2:D:167:ILE:O	2:D:208:HIS:NE2	2.49	0.42
1:A:452:LEU:HD23	1:A:470:THR:HA	2.01	0.41
2:B:169:GLU:HA	2:B:172:ARG:HG2	2.02	0.41
1:C:424:LYS:HB2	1:C:424:LYS:HE3	1.80	0.41
1:C:542:ILE:HD11	2:D:261:VAL:HG11	2.02	0.41
1:C:41:MET:HB3	1:C:46:LYS:HB2	2.01	0.41
1:C:257:ILE:HB	1:C:283:LEU:HD21	2.03	0.41
1:C:445:ALA:C	1:C:477:THR:HG21	2.44	0.41
1:A:364:ASP:HB3	1:A:423:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:OE1	2:B:43:LYS:HD2	2.20	0.41
1:C:203:GLU:HA	1:C:206:ARG:HB2	2.02	0.41
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.55	0.41
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.54	0.41
2:B:167:ILE:HG23	2:B:212:TRP:HD1	1.85	0.41
2:B:275:LYS:HB2	2:B:302:GLU:OE1	2.20	0.41
1:C:451:LYS:HA	1:C:451:LYS:HD3	1.87	0.41
2:D:281:LYS:HD2	2:D:284:ARG:HD2	2.03	0.41
1:A:35:VAL:O	1:A:39:THR:OG1	2.27	0.41
1:C:410:TRP:CZ2	1:C:412:PRO:HA	2.56	0.41
1:C:492:GLU:HA	1:C:530:LYS:O	2.20	0.41
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.85	0.41
2:D:236:PRO:HA	2:D:239:TRP:CD2	2.55	0.41
1:A:94:ILE:HG12	3:E:4:OMC:H1'	2.02	0.41
2:B:164:MET:HE3	2:B:187:LEU:HD21	2.03	0.41
1:C:134:SER:C	1:C:136:ASN:N	2.77	0.41
1:A:431:LYS:HE2	1:A:431:LYS:HB2	1.83	0.41
1:A:524:GLN:O	1:A:528:LYS:HG2	2.21	0.41
2:B:107:THR:HA	2:B:232:TYR:O	2.21	0.41
2:D:173:LYS:HG3	2:D:174:GLN:N	2.35	0.41
2:D:317:VAL:CG1	2:D:347:LYS:HB3	2.51	0.41
1:A:26:LEU:HD12	1:A:133:PRO:HG2	2.03	0.41
1:C:265:ASN:HD22	1:C:265:ASN:HA	1.73	0.41
1:A:356:ARG:HE	1:A:356:ARG:HB3	1.69	0.41
2:B:97:PRO:HD3	2:B:181:TYR:CD1	2.56	0.41
2:B:202:ILE:O	2:B:206:ARG:HG3	2.20	0.41
1:C:380:ILE:HD11	1:C:386:THR:HG23	2.02	0.41
1:A:297:GLU:OE2	1:C:331:LYS:NZ	2.39	0.41
1:A:406:TRP:CD1	2:B:419:THR:HG23	2.56	0.41
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.56	0.40
2:B:266:TRP:CD1	2:B:425:LEU:HD12	2.56	0.40
1:A:503:LEU:HD22	1:A:535:TRP:HB2	2.03	0.40
2:B:203:GLU:HA	2:B:206:ARG:HD3	2.04	0.40
1:C:58:THR:HG21	1:C:77:PHE:CD1	2.57	0.40
1:C:516:GLU:OE2	1:C:520:GLN:NE2	2.54	0.40
1:A:27:THR:C	1:A:29:GLU:H	2.29	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	550/557 (99%)	535 (97%)	14 (2%)	1 (0%)	43	53
1	C	550/557 (99%)	534 (97%)	14 (2%)	2 (0%)	30	36
2	B	402/444 (90%)	383 (95%)	19 (5%)	0	100	100
2	D	402/444 (90%)	387 (96%)	15 (4%)	0	100	100
All	All	1904/2002 (95%)	1839 (97%)	62 (3%)	3 (0%)	43	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	135	ILE
1	A	184	VAL
1	C	184	VAL

### 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	491/494 (99%)	490 (100%)	1 (0%)	87	92
1	C	491/494 (99%)	491 (100%)	0	100	100
2	B	365/400 (91%)	361 (99%)	4 (1%)	65	75
2	D	365/400 (91%)	361 (99%)	4 (1%)	65	75
All	All	1712/1788 (96%)	1703 (100%)	9 (0%)	81	87

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
2	B	210	LEU
2	B	233	GLU
2	B	301	LEU
2	B	425	LEU
2	D	64	LYS
2	D	65	LYS
2	D	66	LYS
2	D	69	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	198	HIS
1	A	207	GLN
1	A	265	ASN
1	A	278	GLN
1	A	306	ASN
1	A	330	GLN
1	A	407	GLN
1	A	428	GLN
1	A	487	GLN
1	A	500	GLN
1	A	509	GLN
1	A	524	GLN
1	A	545	ASN
2	B	137	ASN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	174	GLN
2	B	208	HIS
2	B	255	ASN
2	B	258	GLN
2	B	343	GLN
2	B	394	GLN
1	C	54	ASN
1	C	221	HIS
1	C	222	GLN
1	C	265	ASN
1	C	315	HIS
1	C	330	GLN

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Mol	Chain	Res	Type
1	C	336	GLN
1	C	340	GLN
1	C	407	GLN
1	C	428	GLN
1	C	509	GLN
1	C	545	ASN
2	D	137	ASN
2	D	145	GLN
2	D	151	GLN
2	D	175	ASN
2	D	182	GLN
2	D	197	GLN
2	D	207	GLN
2	D	269	GLN
2	D	334	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	3.26	8 (42%)	25,31,34	0.73	0
3	OMC	E	4	3	19,22,23	3.24	8 (42%)	25,31,34	0.56	0
3	OMC	F	4	3	19,22,23	3.30	8 (42%)	25,31,34	0.60	0
3	OMC	E	2	3	19,22,23	3.36	8 (42%)	25,31,34	0.73	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	-	0/9/27/28	0/2/2/2
3	OMC	E	4	3	-	0/9/27/28	0/2/2/2
3	OMC	F	4	3	-	0/9/27/28	0/2/2/2
3	OMC	E	2	3	-	0/9/27/28	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	4	OMC	C2-N3	6.50	1.49	1.36
3	E	2	OMC	C6-C5	6.47	1.50	1.35
3	E	2	OMC	C4-N3	6.39	1.47	1.34
3	F	2	OMC	C6-C5	6.36	1.49	1.35
3	E	4	OMC	C2-N3	6.31	1.48	1.36
3	F	4	OMC	C6-C5	6.30	1.49	1.35
3	E	2	OMC	C2-N3	6.19	1.48	1.36
3	F	4	OMC	C4-N3	6.18	1.46	1.34
3	E	4	OMC	C6-C5	6.17	1.49	1.35
3	E	4	OMC	C4-N3	6.08	1.46	1.34
3	F	2	OMC	C2-N3	6.06	1.48	1.36
3	F	2	OMC	C4-N3	6.03	1.46	1.34
3	E	2	OMC	C4-N4	5.76	1.47	1.33
3	F	2	OMC	C4-N4	5.66	1.47	1.33
3	F	4	OMC	C4-N4	5.57	1.47	1.33
3	E	4	OMC	C4-N4	5.49	1.47	1.33
3	E	2	OMC	C2-N1	5.07	1.50	1.40
3	E	4	OMC	C2-N1	4.90	1.50	1.40
3	F	4	OMC	C2-N1	4.90	1.50	1.40
3	F	2	OMC	C2-N1	4.79	1.50	1.40
3	E	2	OMC	C6-N1	4.00	1.47	1.38
3	F	2	OMC	C6-N1	3.98	1.47	1.38
3	E	4	OMC	C6-N1	3.87	1.47	1.38
3	F	4	OMC	C6-N1	3.81	1.47	1.38
3	E	2	OMC	O2-C2	-3.11	1.17	1.23
3	F	2	OMC	O2-C2	-3.09	1.18	1.23
3	F	4	OMC	O2-C2	-2.98	1.18	1.23
3	E	4	OMC	O2-C2	-2.94	1.18	1.23
3	E	2	OMC	C5-C4	2.88	1.49	1.42
3	F	2	OMC	C5-C4	2.66	1.49	1.42
3	F	4	OMC	C5-C4	2.64	1.49	1.42
3	E	4	OMC	C5-C4	2.59	1.48	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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
4	DGT	A	601	5	32,33,33	3.44	16 (50%)	48,52,52	1.73	10 (20%)
4	DGT	C	601	5	32,33,33	3.54	16 (50%)	48,52,52	1.67	11 (22%)
6	GOL	B	501	-	5,5,5	1.00	0	5,5,5	1.08	0
6	GOL	B	502	-	5,5,5	1.09	0	5,5,5	1.03	0
6	GOL	E	101	-	5,5,5	0.88	0	5,5,5	1.12	1 (20%)
6	GOL	C	603	-	5,5,5	1.13	0	5,5,5	1.10	1 (20%)
6	GOL	D	501	-	5,5,5	1.04	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
4	DGT	A	601	5	-	4/22/34/34	0/3/3/3
4	DGT	C	601	5	-	4/22/34/34	0/3/3/3
6	GOL	B	501	-	-	0/4/4/4	-
6	GOL	B	502	-	-	0/4/4/4	-
6	GOL	E	101	-	-	4/4/4/4	-
6	GOL	C	603	-	-	0/4/4/4	-
6	GOL	D	501	-	-	2/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	DGT	C3'-C4'	-7.62	1.33	1.53
4	C	601	DGT	C3'-C4'	-7.50	1.33	1.53
4	C	601	DGT	O4'-C4'	6.64	1.59	1.45
4	A	601	DGT	O4'-C4'	6.59	1.59	1.45
4	C	601	DGT	C4-N3	6.49	1.49	1.34
4	A	601	DGT	C4-N3	6.45	1.49	1.34
4	C	601	DGT	C2'-C1'	-5.78	1.36	1.52
4	A	601	DGT	C2'-C1'	-5.49	1.37	1.52
4	C	601	DGT	PA-O3A	5.47	1.65	1.59
4	C	601	DGT	C2-N3	5.44	1.46	1.33
4	C	601	DGT	PB-O3B	5.38	1.65	1.59
4	A	601	DGT	O4'-C1'	5.35	1.54	1.42
4	C	601	DGT	O4'-C1'	5.13	1.53	1.42
4	A	601	DGT	C2-N3	5.12	1.45	1.33
4	C	601	DGT	PB-O3A	5.06	1.65	1.59
4	C	601	DGT	C2-N2	4.78	1.45	1.34
4	A	601	DGT	PB-O3B	4.78	1.64	1.59
4	A	601	DGT	C2-N2	4.74	1.45	1.34
4	A	601	DGT	PB-O3A	4.57	1.64	1.59
4	A	601	DGT	PA-O3A	4.47	1.64	1.59
4	A	601	DGT	C2'-C3'	4.03	1.63	1.52
4	C	601	DGT	C2'-C3'	3.90	1.62	1.52
4	A	601	DGT	C5-N7	-2.89	1.33	1.39
4	C	601	DGT	C5-N7	-2.75	1.33	1.39
4	A	601	DGT	C2-N1	2.62	1.44	1.37
4	C	601	DGT	O6-C6	-2.55	1.18	1.23
4	C	601	DGT	C2-N1	2.54	1.43	1.37
4	A	601	DGT	C5-C6	2.43	1.53	1.44
4	A	601	DGT	O6-C6	-2.40	1.19	1.23
4	A	601	DGT	C6-N1	2.40	1.43	1.38
4	C	601	DGT	C5-C6	2.36	1.53	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	DGT	C6-N1	2.35	1.43	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	DGT	C5-C4-N3	-5.28	119.99	128.39
4	C	601	DGT	C5-C4-N3	-4.92	120.55	128.39
4	A	601	DGT	C2-N3-C4	4.79	120.55	112.30
4	C	601	DGT	C2-N3-C4	4.52	120.08	112.30
4	C	601	DGT	N9-C8-N7	-3.11	107.63	113.40
4	A	601	DGT	N9-C8-N7	-3.11	107.63	113.40
4	A	601	DGT	N9-C4-N3	2.98	131.92	125.95
4	C	601	DGT	N9-C4-N3	2.96	131.87	125.95
4	A	601	DGT	C2-N1-C6	-2.94	119.77	125.11
4	C	601	DGT	C2-N1-C6	-2.76	120.11	125.11
4	C	601	DGT	C1'-N9-C4	-2.72	118.17	125.50
4	C	601	DGT	C5-C6-N1	2.62	119.92	113.25
4	C	601	DGT	O6-C6-C5	-2.60	119.67	126.53
4	A	601	DGT	C5-C6-N1	2.58	119.81	113.25
4	A	601	DGT	O6-C6-C5	-2.47	120.02	126.53
4	C	601	DGT	C1'-N9-C8	2.40	133.30	127.91
4	A	601	DGT	C1'-N9-C4	-2.38	119.07	125.50
4	A	601	DGT	C8-N7-C5	2.28	108.33	104.26
4	A	601	DGT	C1'-N9-C8	2.15	132.74	127.91
6	C	603	GOL	C3-C2-C1	-2.12	104.03	111.80
6	E	101	GOL	C3-C2-C1	-2.08	104.16	111.80
4	C	601	DGT	C8-N7-C5	2.08	107.96	104.26
4	C	601	DGT	N1-C2-N3	-2.01	119.64	123.32

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	DGT	PB-O3B-PG-O1G
4	C	601	DGT	PB-O3B-PG-O1G
6	E	101	GOL	C1-C2-C3-O3
6	D	501	GOL	O1-C1-C2-C3
6	D	501	GOL	O1-C1-C2-O2
6	E	101	GOL	O1-C1-C2-C3
6	E	101	GOL	O2-C2-C3-O3
4	A	601	DGT	PA-O3A-PB-O2B
6	E	101	GOL	O1-C1-C2-O2

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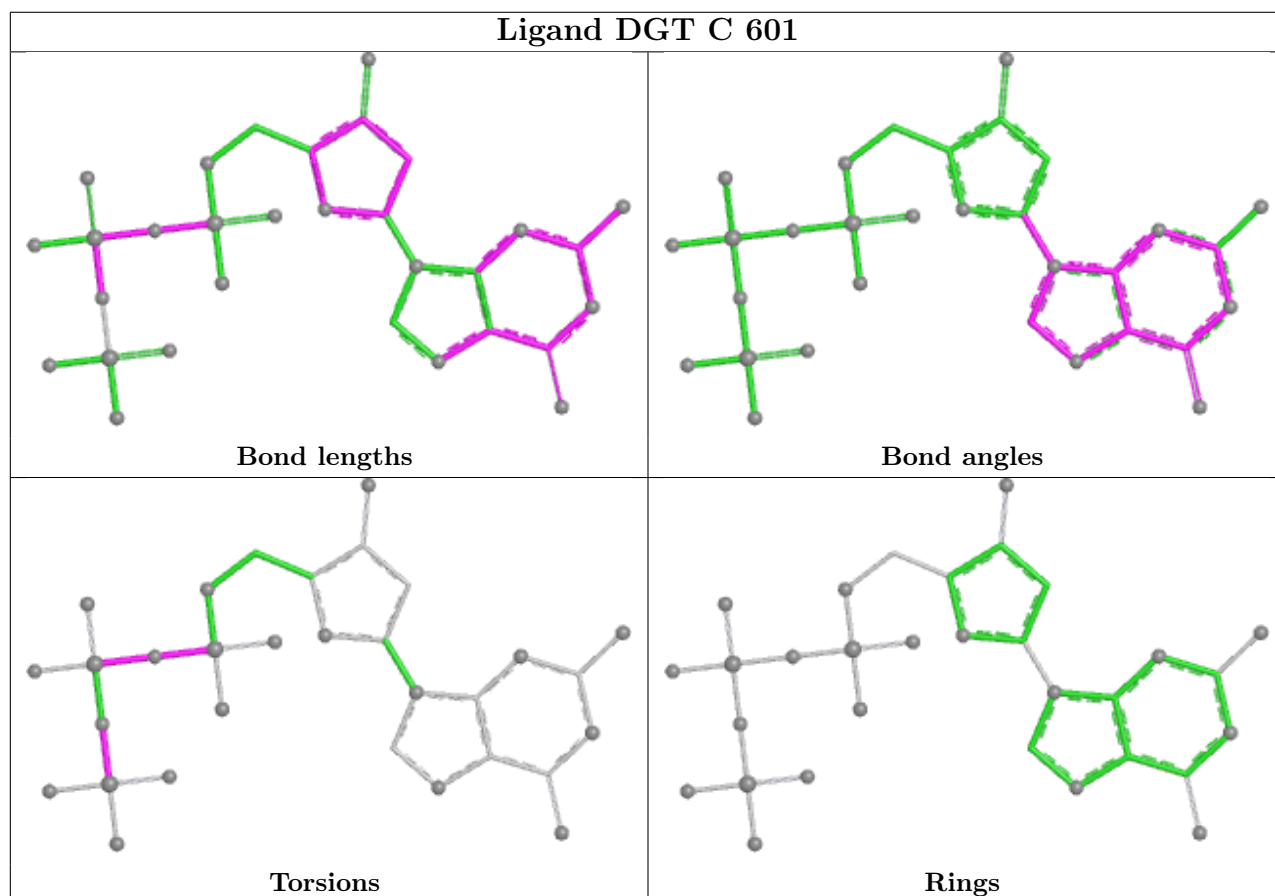
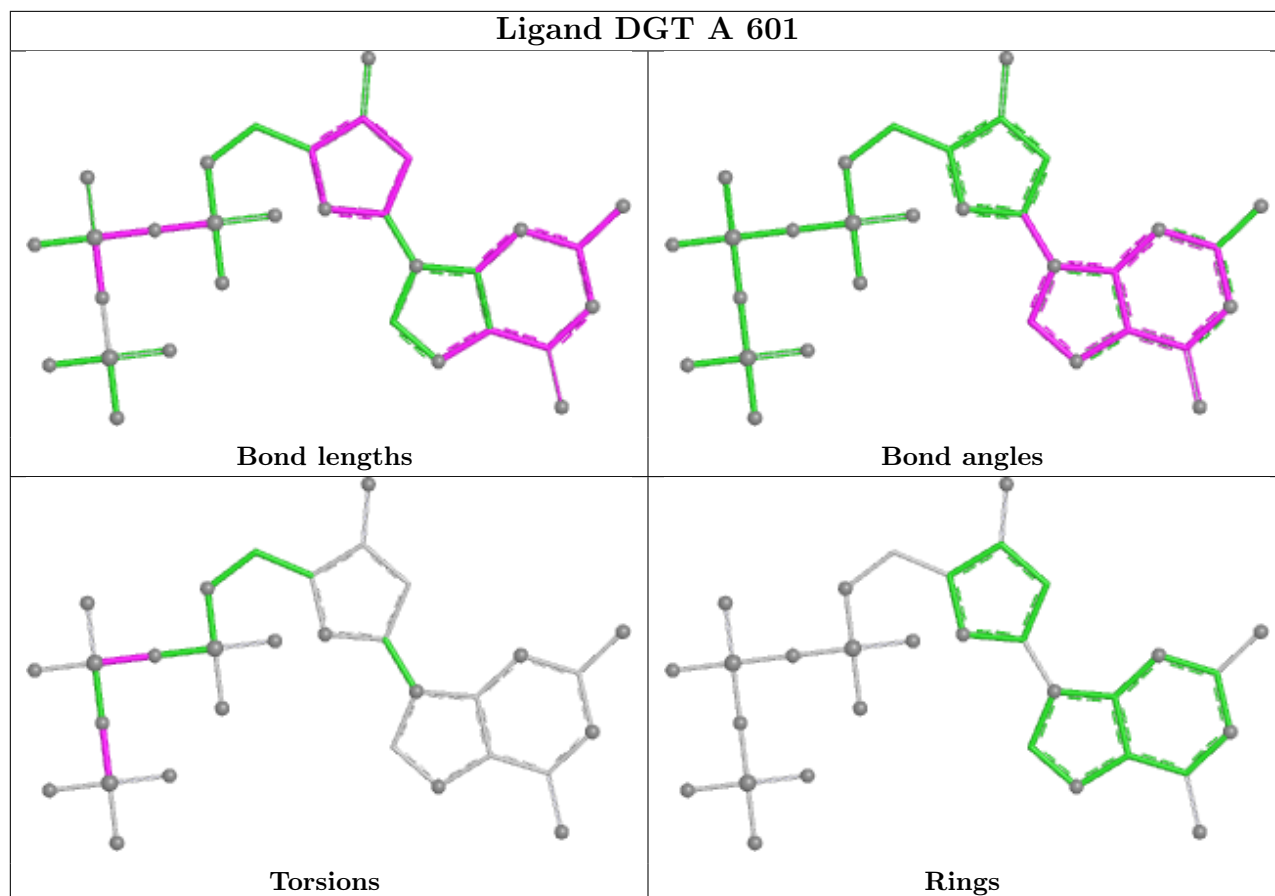
Mol	Chain	Res	Type	Atoms
4	A	601	DGT	PB-O3B-PG-O2G
4	C	601	DGT	PB-O3B-PG-O2G
4	C	601	DGT	PA-O3A-PB-O1B
4	A	601	DGT	PA-O3A-PB-O1B
4	C	601	DGT	PB-O3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	DGT	1	0
6	B	501	GOL	1	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	552/557 (99%)	0.05	21 (3%) 44 42	33, 56, 97, 156	0
1	C	552/557 (99%)	0.17	18 (3%) 49 48	34, 62, 104, 148	0
2	B	406/444 (91%)	0.57	53 (13%) 7 5	35, 74, 130, 159	0
2	D	406/444 (91%)	0.18	32 (7%) 18 16	34, 60, 104, 168	0
3	E	33/38 (86%)	-0.49	0 100 100	36, 57, 86, 132	0
3	F	36/38 (94%)	-0.26	0 100 100	38, 65, 120, 160	0
All	All	1985/2078 (95%)	0.20	124 (6%) 26 23	33, 61, 115, 168	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	232	TYR	6.3
2	B	301	LEU	5.4
2	D	212	TRP	5.1
2	B	422	LEU	5.1
2	B	195	ILE	4.9
2	D	360	ALA	4.9
2	D	425	LEU	4.9
1	C	135	ILE	4.8
2	B	360	ALA	4.8
2	D	427	TYR	4.7
2	B	423	VAL	4.4
1	A	135	ILE	4.3
2	D	213	GLY	4.2
2	D	423	VAL	4.1
1	A	132	ILE	4.0
2	B	362	THR	4.0
2	B	5	ILE	4.0
2	D	420	PRO	3.8
2	B	420	PRO	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	88	TRP	3.7
1	A	140	PRO	3.7
2	D	357	MET	3.5
1	A	70	LYS	3.5
2	B	232	TYR	3.5
2	B	92	LEU	3.5
1	C	66	LYS	3.5
2	D	422	LEU	3.4
2	B	419	THR	3.4
2	B	427	TYR	3.3
1	A	28	GLU	3.3
1	A	134	SER	3.3
2	D	68	SER	3.3
2	B	212	TRP	3.3
1	A	67	ASP	3.2
2	B	358	LYS	3.2
2	B	357	MET	3.2
2	B	299	ALA	3.2
1	A	133	PRO	3.2
1	A	451	LYS	3.2
2	B	361	HIS	3.2
2	D	66	LYS	3.1
2	D	69	THR	3.1
1	A	553	SER	3.1
1	A	69	THR	2.9
2	D	362	THR	2.9
2	B	425	LEU	2.9
2	D	424	LYS	2.9
2	B	304	ALA	2.9
2	B	200	THR	2.9
2	D	231	GLY	2.9
2	D	361	HIS	2.8
2	D	355	ALA	2.8
2	D	316	GLY	2.8
1	C	553	SER	2.8
2	B	278	GLN	2.8
2	B	90	VAL	2.8
2	D	421	PRO	2.7
1	A	139	THR	2.7
2	B	211	ARG	2.7
2	B	213	GLY	2.7
2	B	247	PRO	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	282	LEU	2.7
2	D	358	LYS	2.6
2	B	266	TRP	2.6
2	D	418	ASN	2.6
2	B	418	ASN	2.6
2	B	231	GLY	2.6
2	B	237	ASP	2.6
1	A	68	SER	2.6
2	B	295	LEU	2.5
2	B	95	PRO	2.4
2	B	359	GLY	2.4
1	C	476	LYS	2.4
2	B	209	LEU	2.4
1	C	39	THR	2.4
2	D	419	THR	2.4
2	B	421	PRO	2.4
1	C	2	ILE	2.4
2	B	94	ILE	2.4
1	A	11	LYS	2.4
2	B	245	VAL	2.4
2	B	172	ARG	2.4
2	B	242	GLN	2.4
1	A	136	ASN	2.4
1	A	402	TRP	2.4
1	C	138	GLU	2.4
2	B	66	LYS	2.3
2	D	426	TRP	2.3
2	D	318	TYR	2.3
2	B	240	THR	2.3
1	C	357	MET	2.3
2	B	70	LYS	2.3
1	A	27	THR	2.2
2	D	315	HIS	2.2
1	C	287	LYS	2.2
1	A	26	LEU	2.2
2	B	244	ILE	2.2
2	D	93	GLY	2.2
1	A	251	SER	2.2
1	A	447	ASN	2.2
1	C	69	THR	2.2
2	D	210	LEU	2.2
2	D	359	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	177	ASP	2.2
1	C	550	LYS	2.2
1	C	542	ILE	2.1
1	C	122	LYS	2.1
2	B	173	LYS	2.1
2	B	252	TRP	2.1
2	B	208	HIS	2.1
1	C	67	ASP	2.1
1	C	136	ASN	2.1
2	B	193	LEU	2.1
2	D	314	VAL	2.1
2	B	303	LEU	2.1
2	B	93	GLY	2.1
2	B	196	GLY	2.1
2	D	5	ILE	2.1
2	D	281	LYS	2.1
1	A	36	GLU	2.0
2	B	210	LEU	2.0
2	B	374	LYS	2.0
1	C	133	PRO	2.0
1	C	68	SER	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(Å <sup>2</sup> )	Q<0.9
3	OMC	E	2	21/22	0.97	0.07	28,43,47,49	0
3	OMC	F	2	21/22	0.97	0.07	39,47,54,59	0
3	OMC	E	4	21/22	0.97	0.06	27,38,44,48	0
3	OMC	F	4	21/22	0.97	0.07	33,39,47,52	0

## 6.3 Carbohydrates [i](#)

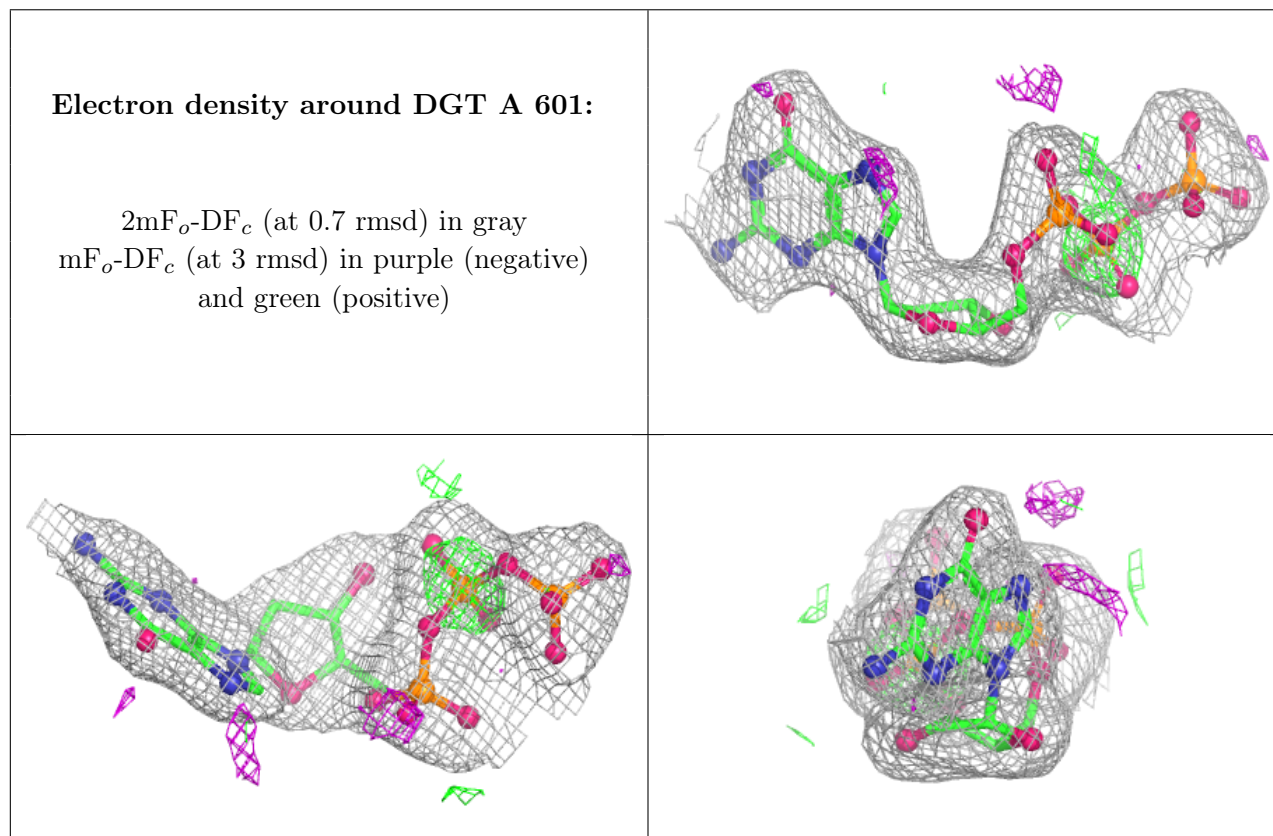
There are no oligosaccharides in this entry.

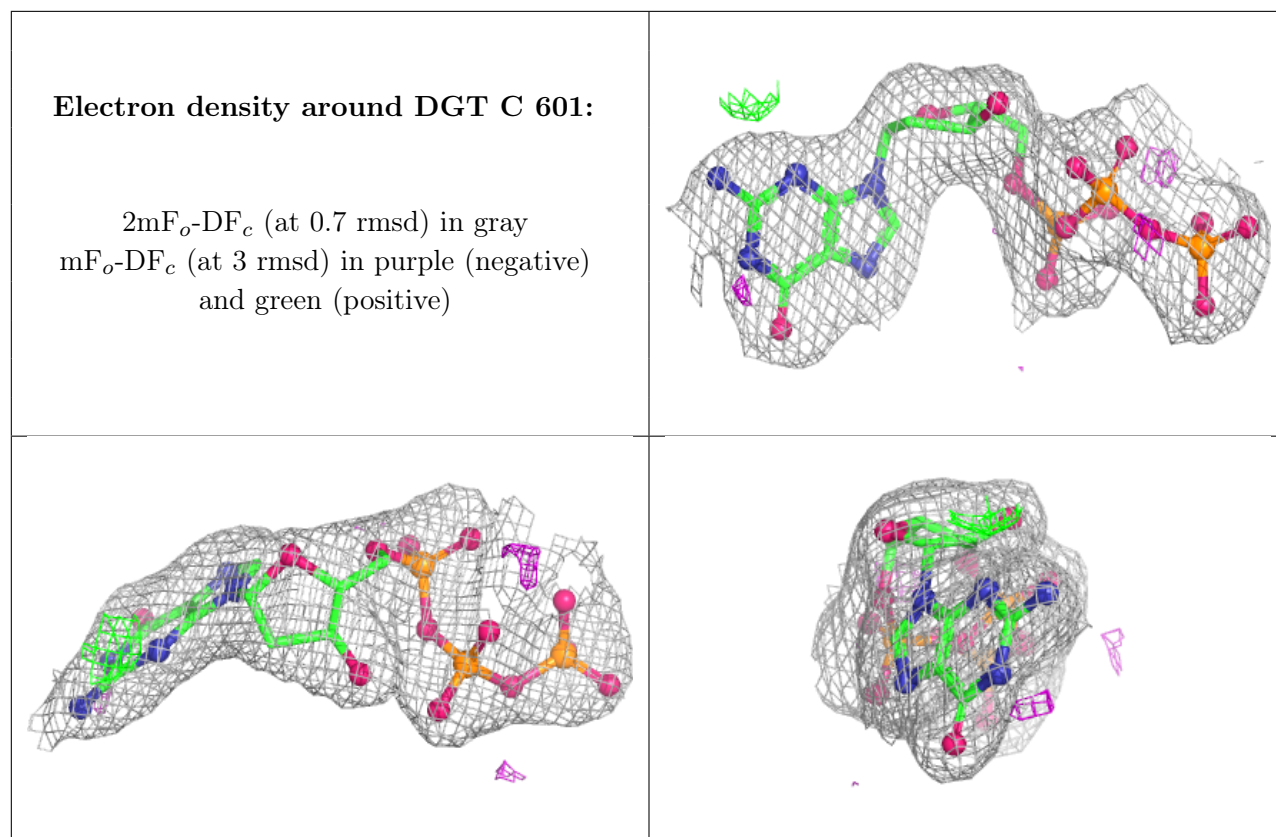
## 6.4 Ligands [i](#)

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
6	GOL	B	501	6/6	0.92	0.16	69,77,81,90	0
6	GOL	E	101	6/6	0.92	0.14	67,67,68,71	0
6	GOL	D	501	6/6	0.93	0.11	49,52,57,60	0
6	GOL	C	603	6/6	0.95	0.12	56,65,69,70	0
4	DGT	A	601	31/31	0.96	0.08	32,41,67,75	0
4	DGT	C	601	31/31	0.96	0.07	39,52,65,69	0
6	GOL	B	502	6/6	0.97	0.07	44,47,52,55	0
5	MG	C	602	1/1	0.98	0.09	48,48,48,48	0
5	MG	A	602	1/1	0.99	0.04	47,47,47,47	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.