



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 02:28 PM UTC

PDB ID : 8X22 / pdb_00008x22
Title : HIV-1 reverse transcriptase mutant Q151M/Y115F/F116Y/L74V:DNA:dGT
P ternary complex
Authors : Yasutake, Y.; Hattori, S.I.; Mitsuya, H.
Deposited on : 2023-11-09
Resolution : 2.31 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

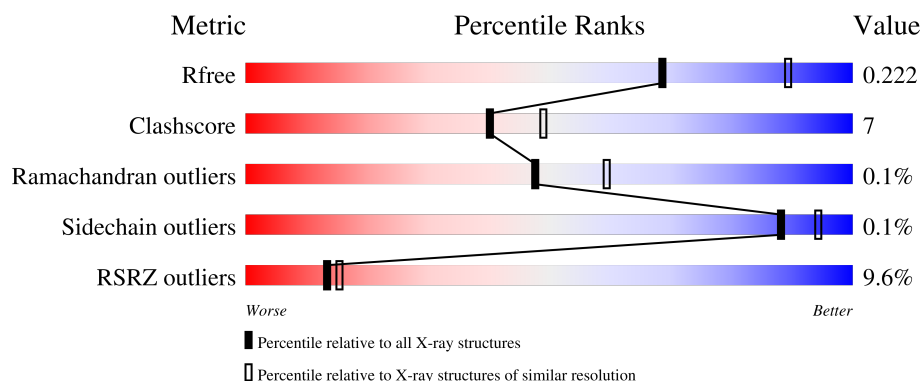
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	10% 81% 18% .
1	C	557	6% 83% 16% .
2	B	444	17% 77% 14% 9%
2	D	444	7% 81% 11% 9%
3	E	38	79% 8% 5% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	38	 76%18%5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17744 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 Pol protein (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4497	2910	750	829	8			
1	C	553	Total	C	N	O	S	0	1	0
			4505	2915	751	830	9			

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	74	VAL	LEU	engineered mutation	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	-	initiating methionine	UNP D3XFN5
C	0	VAL	-	expression tag	UNP D3XFN5
C	74	VAL	LEU	engineered mutation	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).

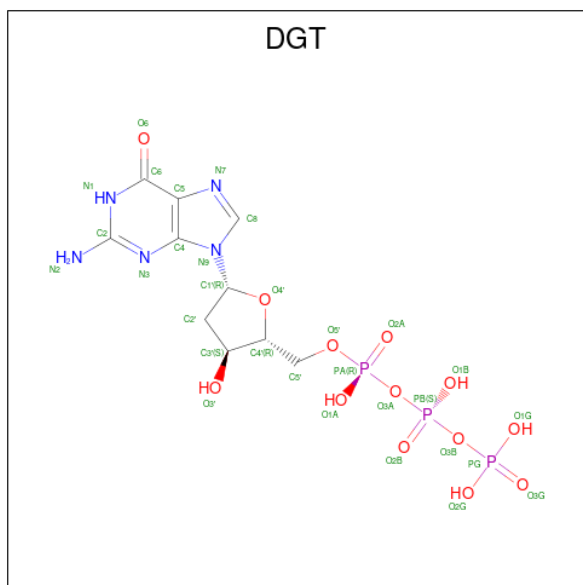
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			718	339	128	216	35			

Continued on next page...

Continued from previous page...

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

- 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
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

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

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



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

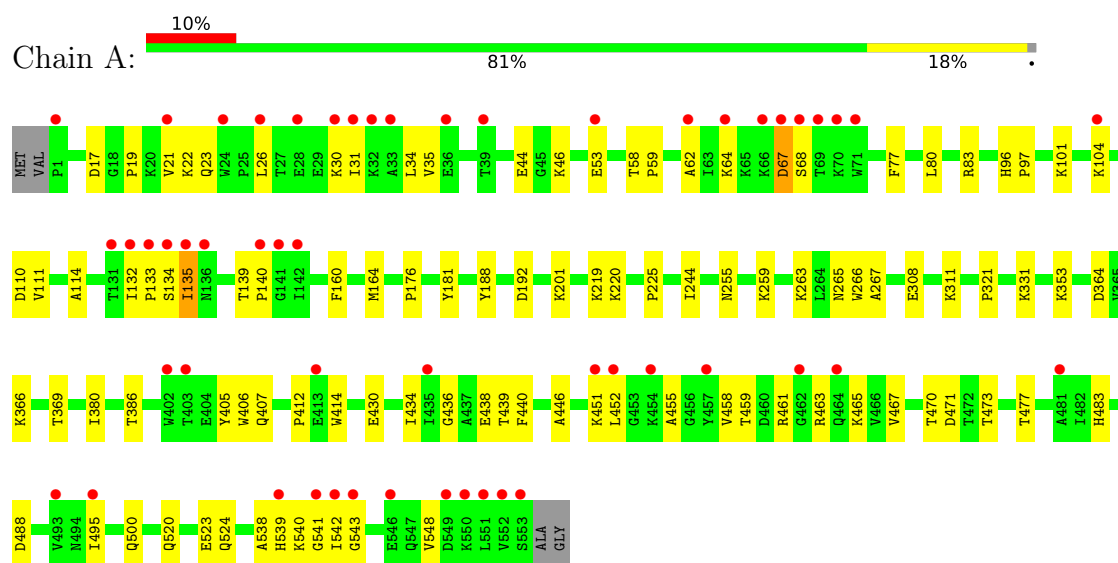
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	126	Total	O	0	0
			126	126		
7	B	52	Total	O	0	0
			52	52		
7	E	40	Total	O	0	0
			40	40		
7	C	115	Total	O	0	0
			115	115		
7	D	86	Total	O	0	0
			86	86		
7	F	34	Total	O	0	0
			34	34		

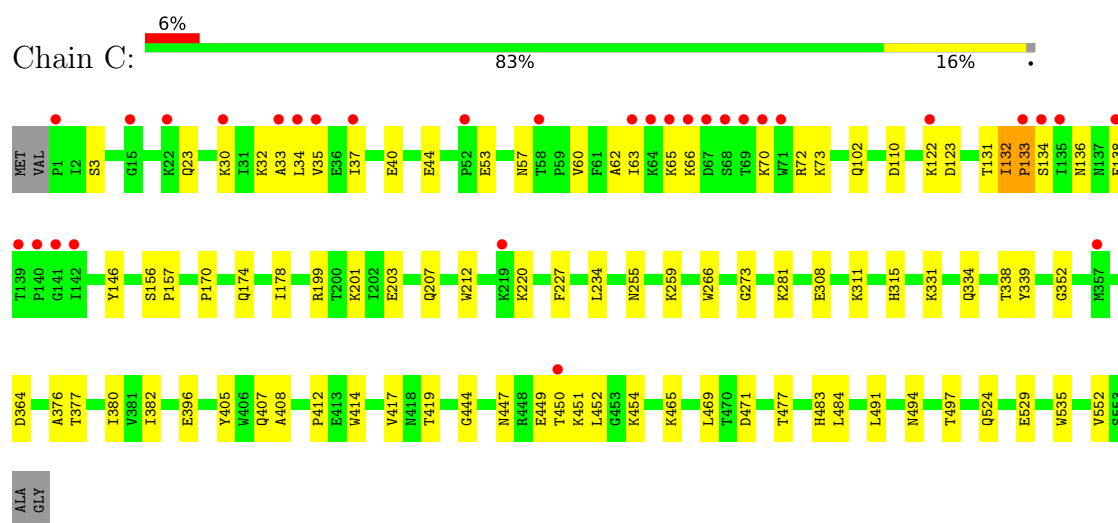
3 Residue-property plots [i](#)

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.

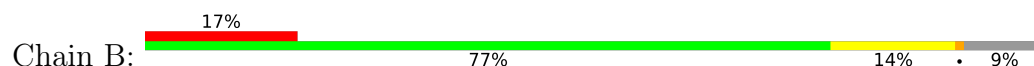
- Molecule 1: Pol protein (Fragment)

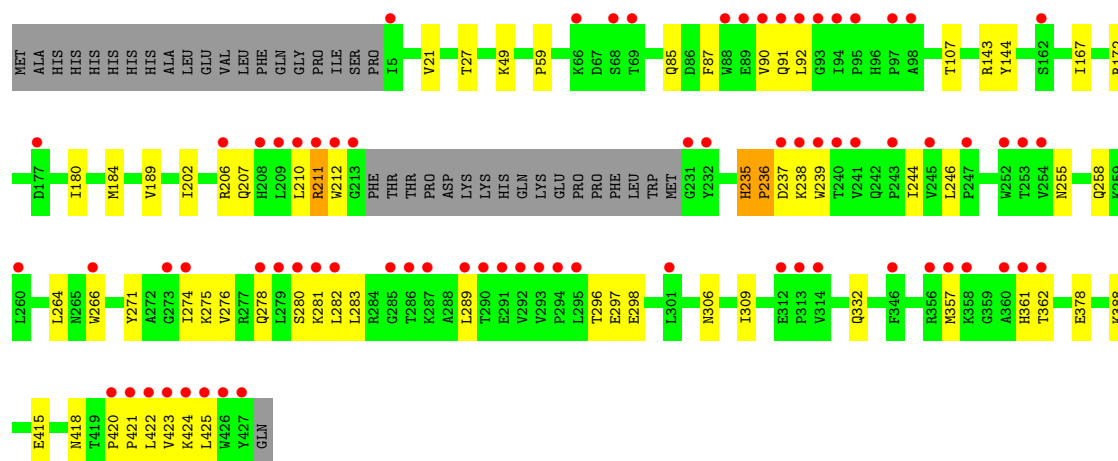


- Molecule 1: Pol protein (Fragment)

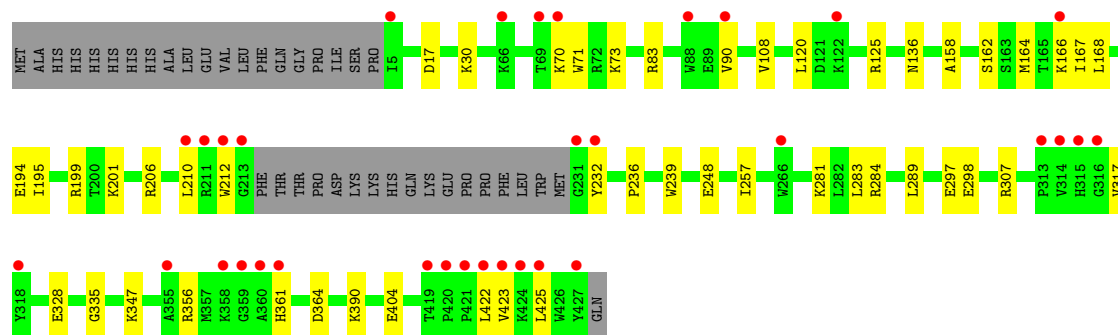
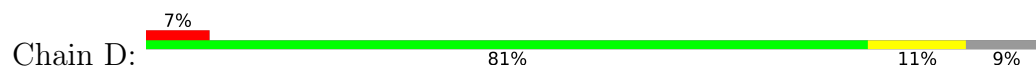


- Molecule 2: HIV-1 RT p51 subunit

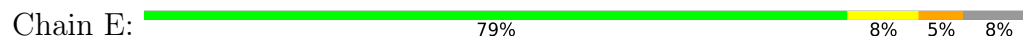




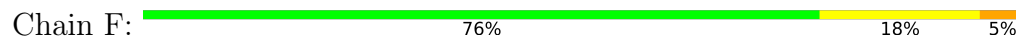
• Molecule 2: HIV-1 RT p51 subunit



• 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, α , β , γ	285.23Å 285.23Å 96.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.81 – 2.31 48.81 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.81-2.31) 100.0 (48.81-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.182 , 0.219 0.185 , 0.222	Depositor DCC
R_{free} test set	6481 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17744	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.42	2/4615 (0.0%)	0.60	2/6267 (0.0%)
1	C	0.47	5/4623 (0.1%)	0.60	6/6277 (0.1%)
2	B	0.52	3/3441 (0.1%)	0.72	6/4673 (0.1%)
2	D	0.33	0/3441	0.50	0/4673
3	E	0.32	0/756	0.51	0/1165
3	F	0.46	0/823	0.52	0/1269
All	All	0.44	10/17699 (0.1%)	0.60	14/24324 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	133	PRO	N-CA	19.41	1.69	1.46
2	B	236	PRO	N-CA	16.61	1.69	1.47
1	C	132	ILE	C-N	8.84	1.44	1.33
1	C	199	ARG	CZ-NH2	7.80	1.43	1.33
2	B	235	HIS	C-N	7.09	1.44	1.33
1	C	199	ARG	NE-CZ	-6.31	1.26	1.33
1	A	176	PRO	C-O	-5.67	1.16	1.24
2	B	211	ARG	CB-CG	-5.36	1.36	1.52
1	A	225	PRO	CA-C	-5.17	1.49	1.51
1	C	315	HIS	C-O	-5.13	1.17	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	ILE	CA-C-N	17.23	138.40	120.14
1	C	132	ILE	C-N-CA	17.23	138.40	120.14
2	B	235	HIS	CA-C-N	15.04	136.91	119.47
2	B	235	HIS	C-N-CA	15.04	136.91	119.47
1	C	133	PRO	CA-N-CD	-8.24	100.46	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	236	PRO	N-CA-C	-7.24	103.31	113.81
1	A	67	ASP	N-CA-C	-6.91	99.21	109.15
1	A	133	PRO	N-CA-C	6.26	122.24	113.53
2	B	236	PRO	CA-N-CD	-6.19	103.33	112.00
2	B	211	ARG	CB-CG-CD	-5.68	98.22	111.30
2	B	235	HIS	O-C-N	-5.35	116.99	121.27
1	C	134	SER	CA-C-N	-5.21	115.86	122.37
1	C	134	SER	C-N-CA	-5.21	115.86	122.37
1	C	199	ARG	NE-CZ-NH1	-5.10	116.40	121.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4497	0	4551	77	0
1	C	4505	0	4559	61	0
2	B	3347	0	3379	58	0
2	D	3347	0	3379	33	0
3	E	718	0	397	3	0
3	F	777	0	432	6	0
4	A	31	0	12	0	0
4	C	31	0	12	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	12	0	16	3	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
6	D	12	0	16	1	0
7	A	126	0	0	1	0
7	B	52	0	0	0	0
7	C	115	0	0	1	0
7	D	86	0	0	1	0
7	E	40	0	0	0	0
7	F	34	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17744	0	16769	226	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 (226) 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:236:PRO:N	2:B:236:PRO:CA	1.69	1.45
1:C:133:PRO:N	1:C:133:PRO:CA	1.69	1.44
1:C:450:THR:HG23	1:C:452:LEU:H	1.37	0.88
2:D:356:ARG:HE	2:D:361:HIS:HB3	1.41	0.83
2:D:356:ARG:NE	2:D:361:HIS:HB3	1.95	0.81
2:B:246:LEU:HD21	2:B:264:LEU:HD21	1.63	0.80
1:C:66:LYS:HD2	1:C:66:LYS:O	1.83	0.77
2:D:164:MET:HE2	2:D:168:LEU:HG	1.67	0.76
2:D:70:LYS:HD3	2:D:71:TRP:H	1.49	0.76
2:B:237:ASP:OD1	2:B:237:ASP:O	2.04	0.76
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.70	0.74
1:A:31:ILE:HD13	1:A:135:ILE:H	1.52	0.74
1:A:459:THR:HG22	1:A:461:ARG:H	1.55	0.72
1:C:203:GLU:O	1:C:207:GLN:HG2	1.88	0.72
1:A:451:LYS:HD2	1:A:471:ASP:HA	1.72	0.71
1:A:67:ASP:OD2	1:A:219:LYS:HE2	1.90	0.71
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.23	0.71
1:C:32:LYS:HA	1:C:35:VAL:HG22	1.73	0.70
2:B:207:GLN:HA	2:B:210:LEU:HD12	1.74	0.70
1:C:33:ALA:O	1:C:37:ILE:HG13	1.94	0.67
2:D:422:LEU:O	2:D:425:LEU:HG	1.93	0.67
2:B:266:TRP:CD1	2:B:425:LEU:HD22	2.30	0.66
1:A:440:PHE:HB2	1:A:495:ILE:HD13	1.76	0.66
1:A:406:TRP:HE1	2:B:418:ASN:ND2	1.94	0.65
2:B:236:PRO:N	2:B:236:PRO:C	2.53	0.65
2:B:422:LEU:HG	2:B:423:VAL:H	1.60	0.65
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.77	0.65
2:B:244:ILE:HD13	2:B:425:LEU:HD11	1.78	0.64
1:A:31:ILE:O	1:A:35:VAL:HG23	1.98	0.64
2:B:180:ILE:HG12	2:B:189:VAL:HG12	1.80	0.64
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.98	0.63
2:B:91:GLN:OE1	2:B:91:GLN:HA	1.98	0.63
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:GLN:HE22	2:B:90:VAL:HG21	1.63	0.63
6:D:502:GOL:H32	7:D:603:HOH:O	1.99	0.63
2:B:274:ILE:HG23	2:B:306:ASN:ND2	2.14	0.62
2:B:332:GLN:OE1	2:B:424:LYS:HD2	1.99	0.62
1:A:31:ILE:HG21	1:A:134:SER:HA	1.81	0.62
2:B:90:VAL:HG12	2:B:92:LEU:HG	1.80	0.62
1:C:331:LYS:NZ	1:C:364:ASP:OD1	2.32	0.61
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.32	0.60
1:A:459:THR:HG22	1:A:461:ARG:N	2.16	0.60
2:B:235:HIS:HB2	2:B:238:LYS:HE2	1.81	0.60
1:A:436:GLY:O	1:A:461:ARG:NH2	2.35	0.60
2:B:87:PHE:HB3	2:B:92:LEU:HB2	1.84	0.59
2:B:278:GLN:OE1	2:B:298:GLU:HB2	2.03	0.58
1:A:263:LYS:NZ	7:A:704:HOH:O	2.37	0.58
1:A:64:LYS:HE3	1:A:68:SER:O	2.03	0.58
1:A:17:ASP:O	1:A:83:ARG:HD3	2.03	0.58
1:A:540:LYS:HB2	1:A:542:ILE:HD11	1.85	0.58
1:A:459:THR:CG2	1:A:461:ARG:H	2.17	0.57
2:B:357:MET:HE1	2:B:361:HIS:CD2	2.40	0.57
1:A:366:LYS:HA	6:A:604:GOL:H31	1.86	0.56
2:B:297:GLU:HG3	2:B:298:GLU:OE1	2.04	0.56
1:A:308:GLU:O	1:A:311:LYS:HG2	2.05	0.56
3:F:3:DC:H2'	3:F:4:OMC:C6	2.41	0.56
1:A:255:ASN:O	1:A:259:LYS:HG3	2.07	0.55
3:E:3:DC:H2'	3:E:4:OMC:C6	2.41	0.55
1:C:417:VAL:HG22	1:C:419:THR:HG23	1.88	0.55
2:D:195:ILE:O	2:D:199:ARG:HG3	2.05	0.55
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.89	0.55
2:B:424:LYS:HA	2:B:424:LYS:CE	2.35	0.55
3:F:1:DG:H2'	3:F:2:OMC:C6	2.42	0.55
1:A:135:ILE:HG22	1:A:135:ILE:O	2.06	0.55
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.88	0.55
1:C:23:GLN:NE2	1:C:60:VAL:H	2.05	0.55
1:C:110:ASP:HB3	1:C:220:LYS:HD3	1.88	0.55
2:B:388:LYS:NZ	2:B:415:GLU:OE1	2.40	0.55
1:A:543:GLY:HA3	2:B:283:LEU:O	2.07	0.54
1:C:447:ASN:HB3	1:C:450:THR:HG22	1.89	0.54
1:A:369:THR:HG21	6:A:604:GOL:H32	1.90	0.54
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.38	0.54
1:C:170:PRO:O	1:C:174:GLN:HG3	2.08	0.54
1:C:255:ASN:O	1:C:259:LYS:HG3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:LEU:HG	2:B:423:VAL:N	2.24	0.53
2:D:162:SER:O	2:D:166:LYS:HD2	2.07	0.53
1:A:446:ALA:HB2	1:A:477:THR:CG2	2.38	0.53
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.89	0.53
1:A:520:GLN:O	1:A:524:GLN:HG3	2.08	0.53
2:B:278:GLN:CD	2:B:298:GLU:HB2	2.34	0.52
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.90	0.52
2:B:422:LEU:HD23	2:B:422:LEU:H	1.74	0.52
1:C:30:LYS:O	1:C:34:LEU:HG	2.09	0.52
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.92	0.52
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.74	0.52
1:A:135:ILE:HD13	1:A:135:ILE:N	2.25	0.51
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.45	0.51
1:C:3:SER:HB2	1:C:212:TRP:O	2.11	0.51
1:A:139:THR:HG22	1:A:140:PRO:O	2.10	0.51
1:C:133:PRO:N	1:C:133:PRO:C	2.59	0.51
1:C:138:GLU:HA	1:C:138:GLU:OE2	2.11	0.51
1:A:380:ILE:HD11	1:A:386:THR:HG23	1.91	0.51
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.45	0.51
3:E:1:DG:H2'	3:E:2:OMC:C6	2.46	0.51
1:C:465:LYS:HD3	1:C:484:LEU:HD11	1.92	0.51
2:B:167:ILE:HG23	2:B:212:TRP:HD1	1.76	0.51
2:D:90:VAL:HG11	2:D:158:ALA:HA	1.93	0.51
2:B:207:GLN:O	2:B:211:ARG:HG3	2.11	0.50
1:C:405:TYR:CE2	1:C:407:GLN:HB2	2.46	0.50
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.45	0.50
2:D:281:LYS:HG2	2:D:284:ARG:HH21	1.75	0.50
2:B:282:LEU:HD13	2:B:296:THR:HG23	1.93	0.50
1:A:22:LYS:HD2	1:A:23:GLN:H	1.76	0.50
2:B:274:ILE:HG23	2:B:306:ASN:HD22	1.76	0.49
2:B:276:VAL:O	2:B:280:SER:N	2.38	0.49
2:D:70:LYS:HE2	2:D:70:LYS:HA	1.94	0.49
2:D:328:GLU:HG2	2:D:390:LYS:HD3	1.93	0.49
2:D:361:HIS:CD2	2:D:361:HIS:O	2.65	0.49
2:B:236:PRO:N	2:B:237:ASP:N	2.61	0.49
1:C:73:LYS:HE3	1:C:146:TYR:OH	2.12	0.49
1:C:136:ASN:N	1:C:136:ASN:HD22	2.11	0.49
2:D:361:HIS:O	2:D:361:HIS:CG	2.64	0.49
1:A:440:PHE:HB2	1:A:495:ILE:CD1	2.42	0.49
2:B:255:ASN:HD22	2:B:258:GLN:HE21	1.61	0.49
2:D:236:PRO:HA	2:D:239:TRP:CD2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:ARG:HE	2:D:361:HIS:CB	2.19	0.49
1:C:122:LYS:HG2	1:C:123:ASP:N	2.28	0.49
2:B:424:LYS:HA	2:B:424:LYS:HE2	1.95	0.48
1:C:34:LEU:HB3	1:C:132:ILE:HD13	1.94	0.48
1:C:454:LYS:HB2	1:C:552:VAL:HG13	1.95	0.48
1:A:26:LEU:HD22	1:A:30:LYS:HE3	1.95	0.48
2:D:335:GLY:HA3	2:D:356:ARG:HG2	1.95	0.48
2:B:235:HIS:CB	2:B:238:LYS:HE2	2.43	0.48
1:C:447:ASN:CG	1:C:450:THR:HG22	2.38	0.48
2:D:167:ILE:HD12	2:D:212:TRP:CD1	2.49	0.48
2:B:207:GLN:HG2	2:B:210:LEU:HD12	1.96	0.48
1:C:308:GLU:OE1	1:C:311:LYS:NZ	2.35	0.47
1:A:31:ILE:HD13	1:A:135:ILE:HD13	1.96	0.47
1:C:444:GLY:HA2	1:C:552:VAL:HG11	1.97	0.47
1:C:447:ASN:OD1	1:C:450:THR:N	2.32	0.47
2:B:90:VAL:HG12	2:B:90:VAL:O	2.15	0.47
2:B:296:THR:OG1	2:B:298:GLU:HG2	2.13	0.47
2:D:194:GLU:OE2	2:D:194:GLU:HA	2.14	0.47
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.95	0.47
2:B:202:ILE:O	2:B:206:ARG:HG3	2.15	0.47
1:C:412:PRO:O	1:C:414:TRP:HD1	1.97	0.47
2:D:108:VAL:HG21	2:D:232:TYR:CE1	2.50	0.46
1:A:473:THR:O	1:A:477:THR:HG23	2.14	0.46
2:D:317:VAL:HG22	2:D:347:LYS:HB3	1.96	0.46
1:C:65:LYS:H	1:C:65:LYS:HG2	1.51	0.46
1:C:227:PHE:HB2	1:C:234:LEU:HB2	1.97	0.46
1:A:483:HIS:ND1	1:A:524:GLN:OE1	2.44	0.46
1:C:23:GLN:NE2	1:C:60:VAL:O	2.48	0.46
2:D:206:ARG:O	2:D:210:LEU:HD13	2.16	0.46
2:B:274:ILE:N	2:B:275:LYS:HZ3	2.14	0.46
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.96	0.46
1:C:110:ASP:HB3	1:C:220:LYS:HB3	1.97	0.45
1:A:430:GLU:HG3	1:A:434:ILE:HD11	1.97	0.45
1:A:458:VAL:HG22	1:A:548:VAL:HB	1.99	0.45
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.52	0.45
1:A:412:PRO:O	1:A:414:TRP:HD1	1.99	0.45
2:B:361:HIS:C	2:B:362:THR:HG23	2.41	0.45
1:C:40:GLU:O	1:C:44:GLU:HG3	2.17	0.45
1:A:53:GLU:O	1:A:53:GLU:CD	2.60	0.45
1:A:406:TRP:HE1	2:B:418:ASN:HD21	1.61	0.45
1:C:497:THR:O	1:C:535:TRP:HA	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LYS:HG2	6:A:604:GOL:H2	1.98	0.45
1:C:377:THR:OG1	7:C:701:HOH:O	2.21	0.45
1:A:266:TRP:CE2	3:E:31:DG:H4'	2.52	0.44
1:A:520:GLN:O	1:A:523:GLU:HG2	2.17	0.44
1:A:67:ASP:OD2	1:A:219:LYS:CE	2.63	0.44
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.99	0.44
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.52	0.44
1:A:500:GLN:CD	1:A:500:GLN:H	2.24	0.44
2:B:49:LYS:HG2	2:B:144:TYR:CE2	2.52	0.44
2:D:423:VAL:C	2:D:425:LEU:H	2.25	0.44
1:C:376:ALA:O	1:C:380:ILE:HG12	2.18	0.44
3:F:23:DC:H2''	3:F:24:DG:C8	2.52	0.44
2:B:85:GLN:NE2	2:B:90:VAL:HG21	2.29	0.44
1:C:156:SER:HB2	1:C:157:PRO:HD3	2.00	0.44
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.53	0.44
1:C:63:ILE:O	1:C:72:ARG:N	2.44	0.44
1:A:30:LYS:HG2	1:A:62:ALA:HB3	1.99	0.44
1:A:459:THR:HB	1:A:463:ARG:H	1.83	0.44
1:A:406:TRP:CZ2	2:B:420:PRO:HG3	2.53	0.43
1:C:178:ILE:HD11	1:C:201:LYS:HG3	1.99	0.43
1:C:266:TRP:CE2	3:F:31:DG:H4'	2.53	0.43
1:C:451:LYS:HB3	1:C:471:ASP:HA	2.00	0.43
1:C:382:ILE:O	2:D:136:ASN:HB2	2.18	0.43
3:F:4:OMC:HM23	3:F:4:OMC:H1'	1.88	0.43
2:B:236:PRO:N	2:B:237:ASP:H	2.17	0.43
1:A:500:GLN:CD	1:A:500:GLN:N	2.77	0.43
1:C:281:LYS:HB3	1:C:281:LYS:HE3	1.83	0.43
1:C:447:ASN:OD1	1:C:449:GLU:N	2.51	0.43
1:A:34:LEU:HB2	1:A:132:ILE:HD11	1.99	0.43
1:A:452:LEU:HD21	1:A:470:THR:HG22	2.00	0.43
2:B:309:ILE:O	2:B:309:ILE:HG22	2.17	0.43
2:D:70:LYS:HD3	2:D:71:TRP:N	2.27	0.43
1:A:44:GLU:HB3	1:A:46:LYS:HE3	2.02	0.42
1:C:483:HIS:ND1	1:C:524:GLN:OE1	2.52	0.42
1:C:273:GLY:HA2	1:C:338:THR:HG21	2.00	0.42
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.48	0.42
1:C:65:LYS:HE2	1:C:72:ARG:HB2	2.01	0.42
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.84	0.42
1:A:22:LYS:HD2	1:A:23:GLN:N	2.34	0.42
1:C:491:LEU:HB3	1:C:529:GLU:HB2	2.01	0.42
1:A:110:ASP:HB3	1:A:220:LYS:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:10:DC:H2"	3:F:11:DG:C8	2.56	0.41
1:A:465:LYS:NZ	1:A:488:ASP:OD2	2.46	0.41
2:D:201:LYS:HD3	2:D:201:LYS:HA	1.83	0.41
1:A:541:GLY:O	2:B:281:LYS:HE3	2.20	0.41
1:C:408:ALA:HB1	2:D:364:ASP:HB3	2.02	0.41
2:D:30:LYS:NZ	2:D:404:GLU:OE1	2.53	0.41
2:B:172:ARG:HH11	2:B:180:ILE:HB	1.86	0.41
1:A:31:ILE:CD1	1:A:135:ILE:H	2.27	0.41
1:C:396:GLU:CD	1:C:396:GLU:H	2.29	0.41
1:C:447:ASN:CB	1:C:450:THR:HG22	2.50	0.41
2:B:239:TRP:CE3	2:B:378:GLU:HG2	2.55	0.41
1:C:57:ASN:ND2	1:C:131:THR:OG1	2.54	0.41
1:C:469:LEU:HD12	1:C:477:THR:HG22	2.03	0.41
2:D:257:ILE:HB	2:D:283:LEU:HD21	2.02	0.41
1:A:104:LYS:NZ	1:A:192:ASP:OD1	2.51	0.41
2:D:297:GLU:HG2	2:D:298:GLU:OE1	2.21	0.41
1:A:244:ILE:HD13	1:A:267:ALA:HB2	2.02	0.40
2:B:107:THR:O	2:B:189:VAL:HG22	2.21	0.40
2:B:244:ILE:HD12	2:B:271:TYR:HE1	1.86	0.40
1:C:494:ASN:HB3	2:D:289:LEU:HD12	2.04	0.40
2:D:17:ASP:O	2:D:83:ARG:HD3	2.20	0.40
1:A:538:ALA:HB1	1:A:539:HIS:CD2	2.56	0.40
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.93	0.40
1:C:334:GLN:HE21	1:C:334:GLN:HB2	1.65	0.40
1:A:265:ASN:OD1	1:A:353:LYS:HE3	2.21	0.40
1:C:70:LYS:HZ2	1:C:70:LYS:HG2	1.69	0.40
1:A:455:ALA:O	1:A:467:VAL:HG12	2.22	0.40
1:C:53:GLU:H	1:C:53:GLU:CD	2.29	0.40
1:C:102:GLN:HE21	1:C:102:GLN:HB2	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	535 (97%)	15 (3%)	1 (0%)	43	53
1	C	552/557 (99%)	535 (97%)	17 (3%)	0	100	100
2	B	402/444 (90%)	385 (96%)	17 (4%)	0	100	100
2	D	402/444 (90%)	390 (97%)	12 (3%)	0	100	100
All	All	1907/2002 (95%)	1845 (97%)	61 (3%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	492 (100%)	0	100	100
1	C	493/494 (100%)	493 (100%)	0	100	100
2	B	365/400 (91%)	364 (100%)	1 (0%)	86	92
2	D	365/400 (91%)	364 (100%)	1 (0%)	86	92
All	All	1715/1788 (96%)	1713 (100%)	2 (0%)	88	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	184	MET
2	D	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	197	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	207	GLN
1	A	235	HIS
1	A	394	GLN
1	A	500	GLN
1	A	539	HIS
1	A	545	ASN
2	B	96	HIS
2	B	137	ASN
2	B	147	ASN
2	B	182	GLN
2	B	208	HIS
2	B	255	ASN
2	B	361	HIS
2	B	394	GLN
2	B	418	ASN
1	C	23	GLN
1	C	57	ASN
1	C	102	GLN
1	C	136	ASN
1	C	137	ASN
1	C	278	GLN
1	C	315	HIS
1	C	330	GLN
1	C	340	GLN
1	C	407	GLN
1	C	507	GLN
1	C	539	HIS
2	D	91	GLN
2	D	147	ASN
2	D	182	GLN
2	D	197	GLN
2	D	258	GLN
2	D	269	GLN
2	D	394	GLN
2	D	407	GLN

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	2	3	19,22,23	2.78	8 (42%)	25,31,34	0.76	0
3	OMC	F	4	3	19,22,23	2.68	8 (42%)	25,31,34	0.65	0
3	OMC	E	4	3	19,22,23	2.73	8 (42%)	25,31,34	0.74	0
3	OMC	E	2	3	19,22,23	2.68	8 (42%)	25,31,34	0.72	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	F	4	3	-	0/9/27/28	0/2/2/2
3	OMC	E	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	2	OMC	C6-C5	6.02	1.49	1.35
3	F	4	OMC	C6-C5	5.89	1.48	1.35
3	E	4	OMC	C6-C5	5.84	1.48	1.35
3	E	4	OMC	C2-N3	5.81	1.47	1.36
3	F	2	OMC	C2-N3	5.76	1.47	1.36
3	F	4	OMC	C2-N3	5.61	1.47	1.36
3	E	2	OMC	C6-C5	5.59	1.48	1.35
3	E	2	OMC	C2-N3	5.19	1.46	1.36
3	F	2	OMC	C4-N3	4.82	1.44	1.34
3	F	2	OMC	C2-N1	4.78	1.50	1.40
3	E	2	OMC	C4-N3	4.77	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	C2-N1	4.72	1.50	1.40
3	E	4	OMC	C2-N1	4.64	1.49	1.40
3	F	4	OMC	C2-N1	4.57	1.49	1.40
3	F	4	OMC	C4-N3	4.49	1.43	1.34
3	E	4	OMC	C4-N3	4.40	1.43	1.34
3	F	2	OMC	C6-N1	3.20	1.45	1.38
3	E	2	OMC	C6-N1	3.15	1.45	1.38
3	E	4	OMC	C6-N1	3.13	1.45	1.38
3	E	4	OMC	C4-N4	3.09	1.41	1.33
3	F	2	OMC	C4-N4	3.00	1.41	1.33
3	F	4	OMC	C6-N1	3.00	1.45	1.38
3	E	2	OMC	C5-C4	2.85	1.49	1.42
3	F	4	OMC	C4-N4	2.82	1.40	1.33
3	E	2	OMC	C4-N4	2.78	1.40	1.33
3	E	4	OMC	C5-C4	2.73	1.49	1.42
3	F	2	OMC	C5-C4	2.73	1.49	1.42
3	E	2	OMC	O2-C2	-2.60	1.18	1.23
3	F	4	OMC	C5-C4	2.50	1.48	1.42
3	F	4	OMC	O2-C2	-2.09	1.19	1.23
3	E	4	OMC	O2-C2	-2.03	1.19	1.23
3	F	2	OMC	O2-C2	-2.02	1.20	1.23

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 5 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
6	GOL	B	501	-	5,5,5	1.29	1 (20%)	5,5,5	0.83	0
6	GOL	A	604	-	5,5,5	0.99	0	5,5,5	0.81	0
6	GOL	D	501	-	5,5,5	1.22	0	5,5,5	1.27	1 (20%)
6	GOL	D	502	-	5,5,5	0.23	0	5,5,5	0.39	0
4	DGT	A	601	5	32,33,33	3.80	17 (53%)	48,52,52	1.74	12 (25%)
4	DGT	C	601	5	32,33,33	3.94	17 (53%)	48,52,52	1.62	9 (18%)
6	GOL	A	603	-	5,5,5	0.86	0	5,5,5	1.17	1 (20%)
6	GOL	C	603	-	5,5,5	1.15	0	5,5,5	0.92	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	B	501	-	-	2/4/4/4	-
6	GOL	A	604	-	-	0/4/4/4	-
6	GOL	D	501	-	-	3/4/4/4	-
6	GOL	D	502	-	-	2/4/4/4	-
4	DGT	A	601	5	-	5/22/34/34	0/3/3/3
4	DGT	C	601	5	-	4/22/34/34	0/3/3/3
6	GOL	A	603	-	-	4/4/4/4	-
6	GOL	C	603	-	-	0/4/4/4	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	DGT	O4'-C1'	8.97	1.62	1.42
4	A	601	DGT	O4'-C1'	8.47	1.61	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	DGT	O4'-C4'	-7.47	1.28	1.45
4	C	601	DGT	PB-O3A	7.40	1.67	1.59
4	C	601	DGT	O4'-C4'	-7.37	1.28	1.45
4	C	601	DGT	PB-O3B	6.91	1.67	1.59
4	A	601	DGT	C2'-C1'	-6.86	1.33	1.52
4	C	601	DGT	C2'-C1'	-6.78	1.34	1.52
4	C	601	DGT	C4-N3	6.70	1.49	1.34
4	A	601	DGT	C4-N3	6.56	1.49	1.34
4	A	601	DGT	PB-O3A	6.40	1.66	1.59
4	A	601	DGT	PB-O3B	6.16	1.66	1.59
4	C	601	DGT	C2-N3	5.87	1.47	1.33
4	A	601	DGT	C2-N3	5.70	1.47	1.33
4	C	601	DGT	C2-N2	5.63	1.47	1.34
4	A	601	DGT	C2-N2	5.36	1.46	1.34
4	A	601	DGT	O6-C6	-4.95	1.14	1.23
4	C	601	DGT	O6-C6	-4.42	1.15	1.23
4	C	601	DGT	C5-N7	-3.70	1.31	1.39
4	C	601	DGT	PA-O3A	3.63	1.63	1.59
4	A	601	DGT	PA-O3A	3.61	1.63	1.59
4	A	601	DGT	C5-N7	-3.47	1.32	1.39
4	C	601	DGT	C6-N1	2.92	1.44	1.38
4	C	601	DGT	C2-N1	2.86	1.44	1.37
4	A	601	DGT	C6-N1	2.77	1.44	1.38
4	C	601	DGT	O3'-C3'	-2.73	1.37	1.43
4	A	601	DGT	C2-N1	2.73	1.44	1.37
4	A	601	DGT	O3'-C3'	-2.72	1.37	1.43
4	C	601	DGT	C5-C6	2.64	1.54	1.44
4	A	601	DGT	C5-C6	2.60	1.54	1.44
4	C	601	DGT	PA-O5'	2.33	1.68	1.59
4	A	601	DGT	PA-O5'	2.30	1.68	1.59
4	A	601	DGT	C4-N9	-2.20	1.32	1.38
6	B	501	GOL	O2-C2	-2.03	1.37	1.43
4	C	601	DGT	C4-N9	-2.01	1.32	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	-4.86	120.65	128.39
4	C	601	DGT	C5-C4-N3	-4.85	120.67	128.39
4	A	601	DGT	C2-N3-C4	4.50	120.05	112.30
4	C	601	DGT	C2-N3-C4	4.17	119.48	112.30
4	A	601	DGT	N9-C8-N7	-3.42	107.07	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	DGT	C2-N1-C6	-3.25	119.22	125.11
4	C	601	DGT	N9-C8-N7	-3.09	107.67	113.40
4	C	601	DGT	C2-N1-C6	-2.94	119.79	125.11
4	A	601	DGT	C5-C6-N1	2.81	120.42	113.25
4	A	601	DGT	O1A-PA-O3A	2.69	114.54	107.27
4	A	601	DGT	N9-C4-N3	2.69	131.33	125.95
4	A	601	DGT	O6-C6-C5	-2.67	119.48	126.53
4	C	601	DGT	N9-C4-N3	2.53	131.01	125.95
4	C	601	DGT	C5-C6-N1	2.44	119.47	113.25
6	D	501	GOL	C3-C2-C1	-2.41	102.96	111.80
4	C	601	DGT	O6-C6-C5	-2.41	120.18	126.53
4	A	601	DGT	C8-N7-C5	2.30	108.36	104.26
4	C	601	DGT	C8-N7-C5	2.29	108.33	104.26
4	A	601	DGT	O2G-PG-O3B	2.22	112.09	104.64
6	A	603	GOL	C3-C2-C1	-2.16	103.88	111.80
4	A	601	DGT	N2-C2-N1	2.07	121.14	116.76
4	A	601	DGT	C1'-N9-C4	-2.07	119.91	125.50
4	C	601	DGT	O1G-PG-O3B	2.06	111.54	104.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	DGT	PB-O3B-PG-O2G
4	C	601	DGT	PB-O3B-PG-O1G
6	A	603	GOL	O1-C1-C2-C3
6	D	501	GOL	C1-C2-C3-O3
6	A	603	GOL	C1-C2-C3-O3
6	B	501	GOL	O1-C1-C2-C3
6	D	502	GOL	O1-C1-C2-C3
6	A	603	GOL	O1-C1-C2-O2
6	D	501	GOL	O2-C2-C3-O3
6	D	502	GOL	O1-C1-C2-O2
6	A	603	GOL	O2-C2-C3-O3
6	D	501	GOL	O1-C1-C2-O2
4	C	601	DGT	PA-O3A-PB-O1B
6	B	501	GOL	O1-C1-C2-O2
4	A	601	DGT	PA-O3A-PB-O2B
4	A	601	DGT	PB-O3A-PA-O2A
4	A	601	DGT	PB-O3B-PG-O1G
4	C	601	DGT	PB-O3B-PG-O2G
4	A	601	DGT	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

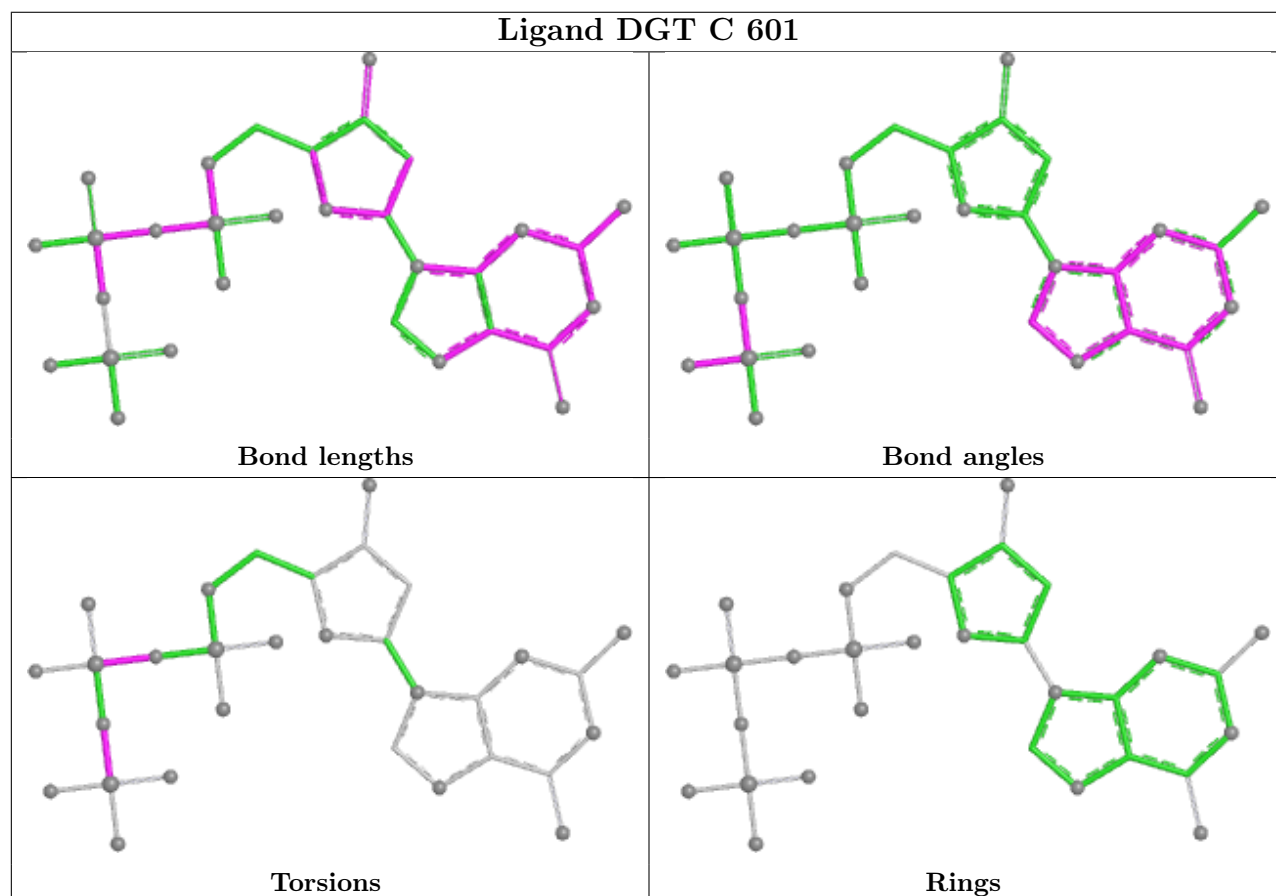
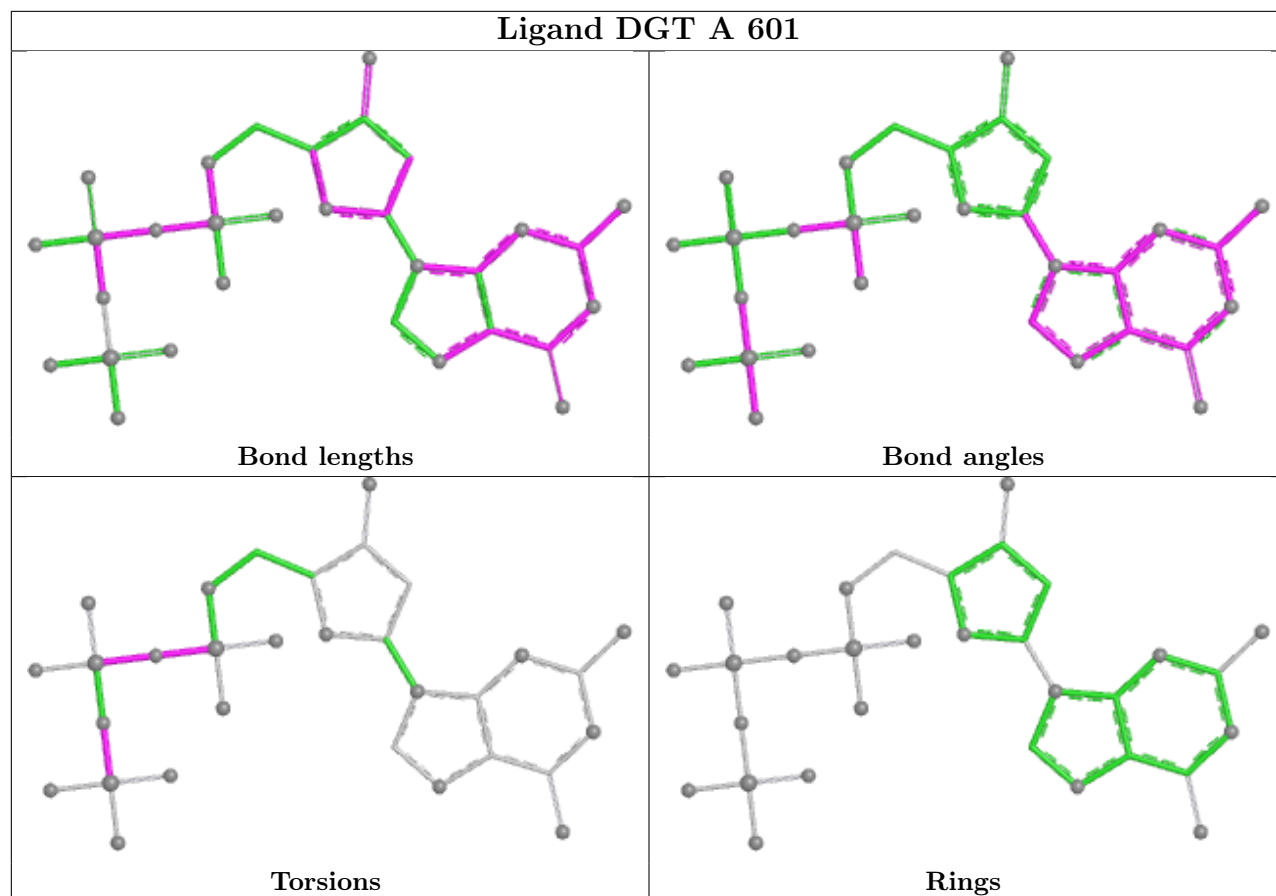
Mol	Chain	Res	Type	Atoms
4	C	601	DGT	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	604	GOL	3	0
6	D	502	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	553/557 (99%)	0.43	53 (9%) 13 15	33, 59, 104, 180	0
1	C	553/557 (99%)	0.25	31 (5%) 30 32	23, 58, 109, 156	1 (0%)
2	B	406/444 (91%)	0.79	74 (18%) 3 4	35, 69, 141, 176	0
2	D	406/444 (91%)	0.25	33 (8%) 18 20	32, 55, 100, 164	0
3	E	33/38 (86%)	-0.52	0 100 100	35, 55, 88, 138	0
3	F	36/38 (94%)	-0.20	0 100 100	39, 65, 112, 157	0
All	All	1987/2078 (95%)	0.39	191 (9%) 13 15	23, 59, 119, 180	1 (0%)

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	LEU	8.0
2	D	232	TYR	7.3
2	D	425	LEU	6.8
1	A	135	ILE	6.6
2	B	425	LEU	6.4
1	C	135	ILE	6.3
2	B	94	ILE	6.0
2	D	360	ALA	5.7
2	B	92	LEU	5.6
2	B	301	LEU	5.6
1	A	132	ILE	5.6
2	D	213	GLY	5.4
2	B	423	VAL	5.3
1	A	140	PRO	5.2
1	C	133	PRO	5.2
2	B	95	PRO	5.1
2	B	213	GLY	4.9
2	D	427	TYR	4.9
2	B	88	TRP	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	361	HIS	4.5
2	B	232	TYR	4.4
2	B	360	ALA	4.3
1	A	136	ASN	4.3
2	B	210	LEU	4.3
2	D	424	LYS	4.3
1	A	141	GLY	4.3
2	D	212	TRP	4.2
1	A	69	THR	4.2
1	A	133	PRO	4.1
2	D	5	ILE	4.1
2	B	93	GLY	4.1
2	B	212	TRP	4.0
2	B	90	VAL	4.0
2	B	358	LYS	4.0
1	C	64	LYS	3.9
1	A	67	ASP	3.9
2	B	231	GLY	3.8
1	A	62	ALA	3.8
2	D	231	GLY	3.7
1	C	70	LYS	3.7
2	D	359	GLY	3.6
1	A	66	LYS	3.6
1	A	28	GLU	3.6
2	B	281	LYS	3.6
2	B	5	ILE	3.6
2	B	241	VAL	3.6
1	C	139	THR	3.5
2	B	247	PRO	3.5
1	C	357[A]	MET	3.5
2	B	290	THR	3.4
1	A	493	VAL	3.4
2	B	420	PRO	3.4
2	B	421	PRO	3.4
2	D	423	VAL	3.3
2	B	260	LEU	3.3
2	B	362	THR	3.3
1	C	71	TRP	3.3
2	B	245	VAL	3.3
1	A	142	ILE	3.2
2	B	361	HIS	3.2
1	A	553	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	285	GLY	3.2
2	B	66	LYS	3.2
2	B	357	MET	3.2
2	B	287	LYS	3.2
2	D	420	PRO	3.2
1	A	68	SER	3.1
2	B	280	SER	3.1
2	B	266	TRP	3.1
1	C	69	THR	3.1
1	A	495	ILE	3.0
1	C	63	ILE	3.0
1	A	39	THR	3.0
1	C	134	SER	3.0
2	D	422	LEU	3.0
2	B	238	LYS	3.0
1	A	402	TRP	3.0
1	A	31	ILE	3.0
1	A	403	THR	3.0
1	A	24	TRP	3.0
1	C	35	VAL	2.9
2	B	427	TYR	2.9
1	C	68	SER	2.9
2	B	294	PRO	2.9
1	A	104	LYS	2.9
1	A	454	LYS	2.9
2	B	98	ALA	2.9
2	B	177	ASP	2.9
1	C	52	PRO	2.9
2	D	90	VAL	2.8
2	D	421	PRO	2.8
1	A	70	LYS	2.8
1	A	21	VAL	2.8
2	B	237	ASP	2.8
1	C	15	GLY	2.8
1	A	462	GLY	2.7
2	B	240	THR	2.7
1	A	542	ILE	2.7
1	A	53	GLU	2.7
2	B	89	GLU	2.7
1	A	551	LEU	2.7
1	C	67	ASP	2.7
1	A	550	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	286	THR	2.7
2	B	282	LEU	2.7
1	C	65	LYS	2.6
2	B	313	PRO	2.6
2	D	211	ARG	2.6
2	B	68	SER	2.6
1	A	552	VAL	2.6
2	D	315	HIS	2.6
2	B	278	GLN	2.6
1	A	451	LYS	2.6
2	D	66	LYS	2.6
1	A	541	GLY	2.6
1	C	140	PRO	2.6
2	B	293	VAL	2.6
2	B	356	ARG	2.6
1	A	33	ALA	2.6
2	B	426	TRP	2.5
2	B	243	PRO	2.5
1	A	71	TRP	2.5
2	B	291	GLU	2.5
2	B	97	PRO	2.5
2	B	295	LEU	2.5
2	D	419	THR	2.4
1	C	66	LYS	2.4
2	D	358	LYS	2.4
2	D	88	TRP	2.4
2	B	69	THR	2.4
2	B	279	LEU	2.4
1	A	64	LYS	2.4
1	C	142	ILE	2.4
2	B	346	PHE	2.4
2	D	314	VAL	2.4
2	B	91	GLN	2.4
1	C	1	PRO	2.3
1	C	450	THR	2.3
2	B	274	ILE	2.3
1	A	546	GLU	2.3
2	B	239	TRP	2.3
2	D	318	TYR	2.3
2	D	316	GLY	2.3
2	D	69	THR	2.3
1	A	134	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	413	GLU	2.3
2	B	314	VAL	2.3
2	D	122	LYS	2.3
2	D	166	LYS	2.3
2	B	211	ARG	2.3
1	A	539	HIS	2.3
1	A	36	GLU	2.3
1	A	543	GLY	2.3
2	B	253	THR	2.3
1	A	30	LYS	2.3
1	C	30	LYS	2.3
1	C	122	LYS	2.3
1	A	26	LEU	2.2
2	D	210	LEU	2.2
1	C	141	GLY	2.2
1	A	435	ILE	2.2
2	D	313	PRO	2.2
1	C	138	GLU	2.2
2	B	252	TRP	2.2
1	A	464	GLN	2.2
2	B	208	HIS	2.2
2	D	70	LYS	2.2
2	D	266	TRP	2.2
1	C	219	LYS	2.2
1	A	481	ALA	2.2
1	C	33	ALA	2.2
2	D	355	ALA	2.2
1	C	37	ILE	2.1
1	A	1	PRO	2.1
1	A	32	LYS	2.1
1	C	22	LYS	2.1
2	B	289	LEU	2.1
2	B	254	VAL	2.1
2	B	206	ARG	2.1
2	B	424	LYS	2.1
1	C	34	LEU	2.1
2	B	209	LEU	2.1
1	A	549	ASP	2.1
1	C	58	THR	2.0
2	B	162	SER	2.0
2	B	312	GLU	2.0
1	A	457	TYR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	292	VAL	2.0
2	B	273	GLY	2.0
1	A	131	THR	2.0
1	A	452	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	OMC	F	2	21/22	0.97	0.07	45,51,53,57	0
3	OMC	F	4	21/22	0.97	0.07	33,38,44,46	0
3	OMC	E	4	21/22	0.98	0.06	32,35,41,44	0
3	OMC	E	2	21/22	0.98	0.06	33,40,44,47	0

6.3 Carbohydrates [i](#)

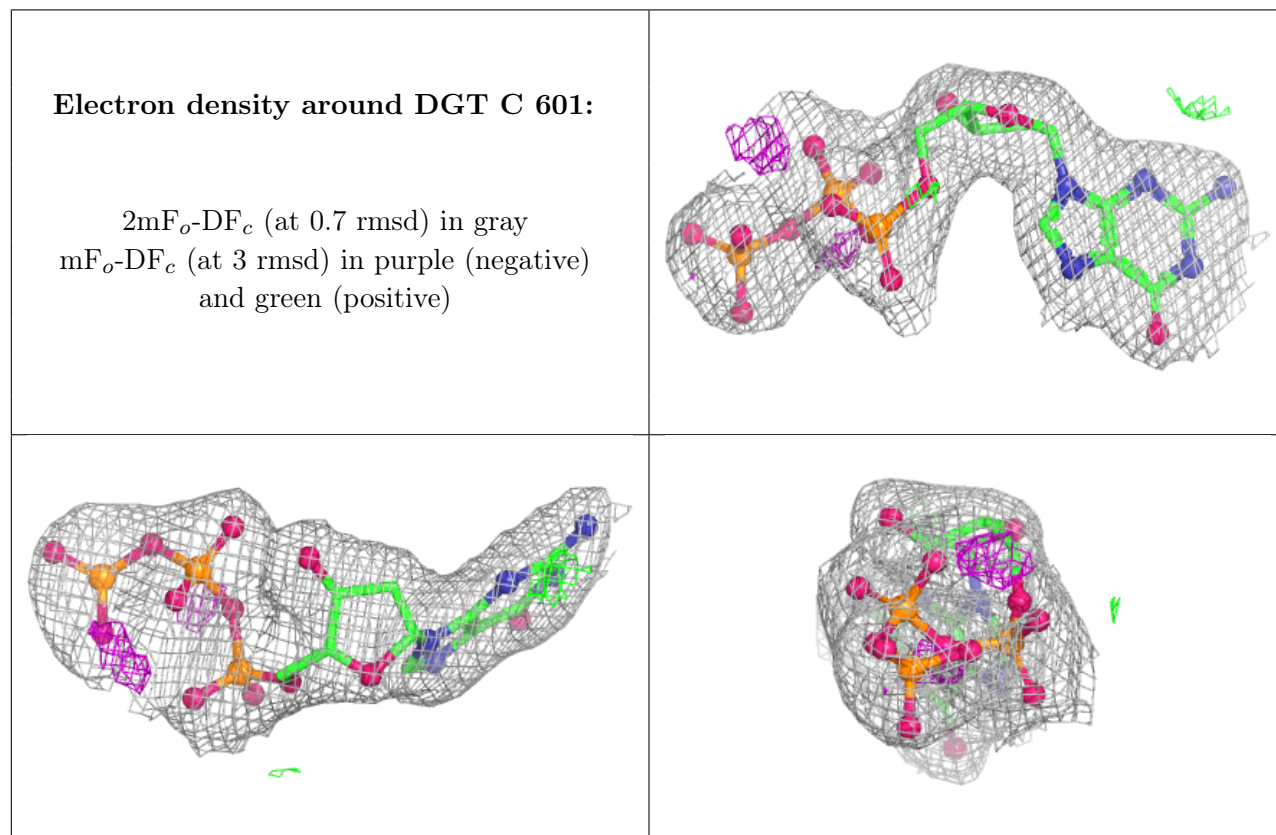
There are no oligosaccharides in this entry.

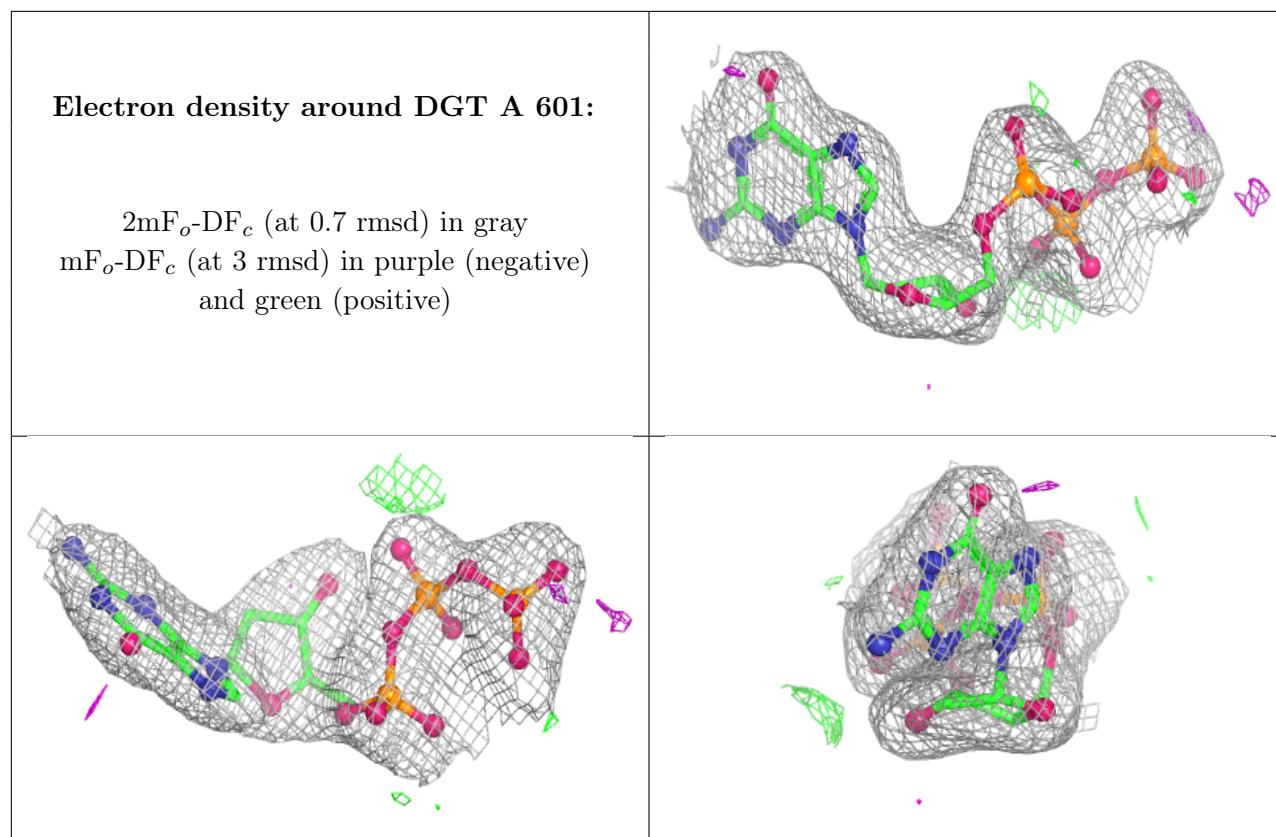
6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	A	604	6/6	0.81	0.22	57,64,70,70	0
6	GOL	A	603	6/6	0.93	0.17	65,71,72,72	0
6	GOL	D	502	6/6	0.93	0.11	60,64,64,65	0
5	MG	C	602	1/1	0.94	0.13	55,55,55,55	0
6	GOL	D	501	6/6	0.94	0.15	46,50,52,53	0
4	DGT	C	601	31/31	0.94	0.09	45,59,80,84	0
4	DGT	A	601	31/31	0.96	0.07	42,50,64,67	0
6	GOL	B	501	6/6	0.96	0.10	44,46,47,50	0
6	GOL	C	603	6/6	0.97	0.09	42,45,50,53	0
5	MG	A	602	1/1	0.98	0.07	51,51,51,51	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.