



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:41 PM UTC

PDB ID : 6KDN / pdb_00006kdn
Title : HIV-1 reverse transcriptase with Q151M/Y115F/F116Y:DNA:dGTP ternary complex
Authors : Yasutake, Y.; Hattori, S.I.; Tamura, N.; Maeda, K.
Deposited on : 2019-07-02
Resolution : 2.30 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

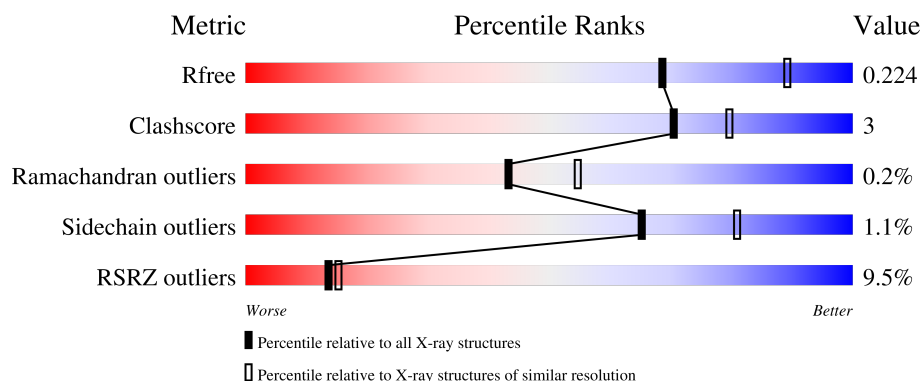
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	11% 88% 11% ..
1	C	557	4% 91% 8% .
2	B	444	16% 86% 5% . 9%
2	D	444	7% 84% 7% . 9%
3	E	38	3% 76% 11% 5% 8%

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17721 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
			718	339	128	216	35			

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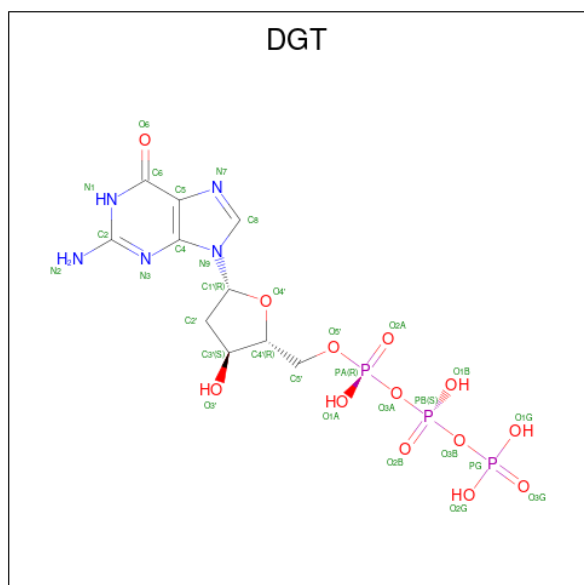
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	38	Total	C	N	O	P	0	0	0
			777	369	140	231	37			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

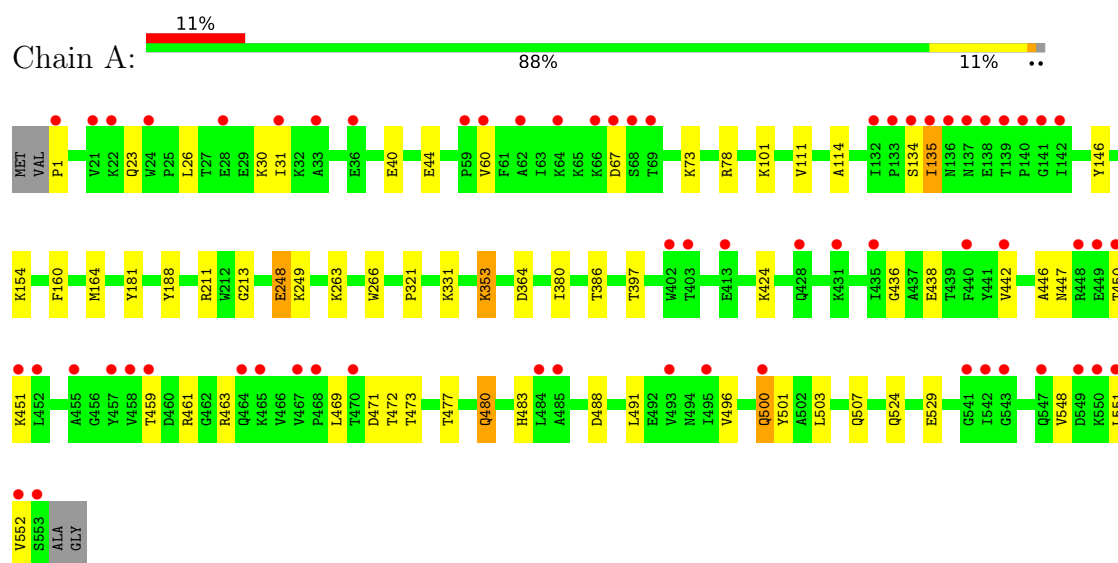
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	125	Total	O	0	0
			125	125		
7	B	49	Total	O	0	0
			49	49		
7	E	40	Total	O	0	0
			40	40		
7	C	107	Total	O	0	0
			107	107		
7	D	86	Total	O	0	0
			86	86		
7	F	35	Total	O	0	0
			35	35		

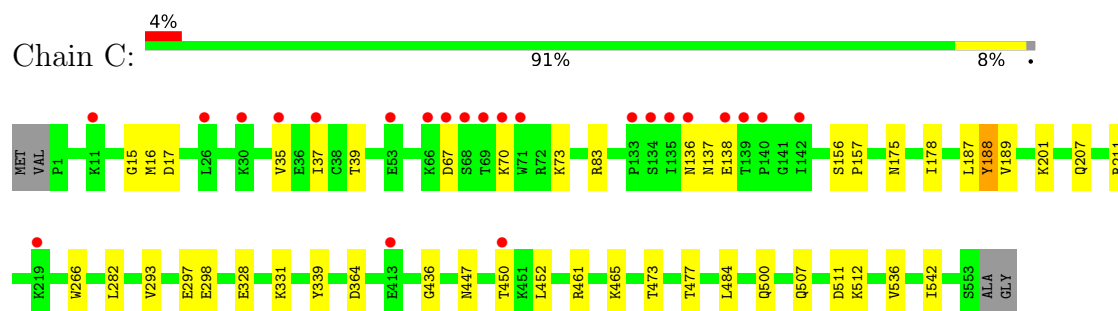
3 Residue-property plots

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.

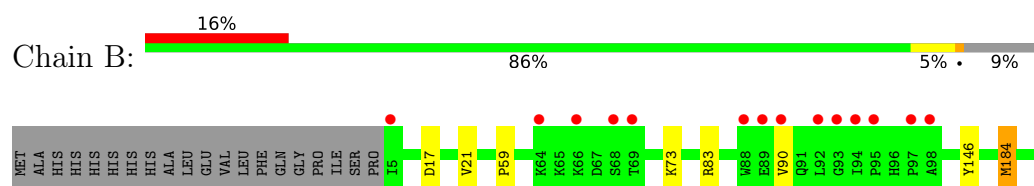
- Molecule 1: HIV-1 reverse transcriptase p66 subunit

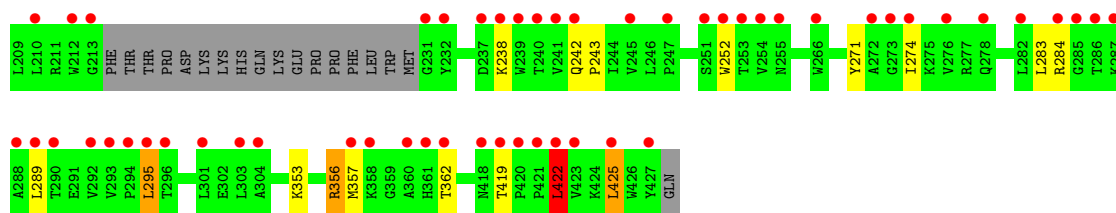


- Molecule 1: HIV-1 reverse transcriptase p66 subunit

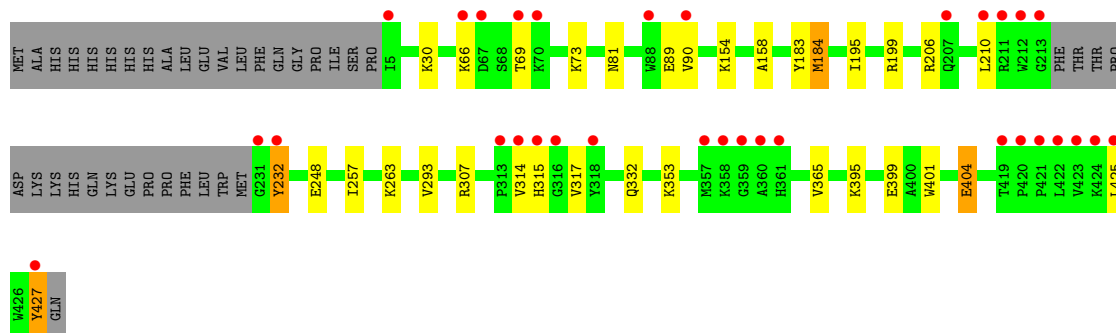
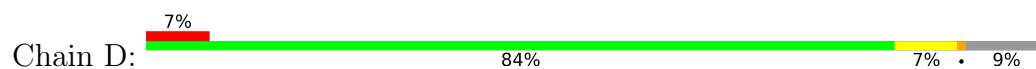


- Molecule 2: HIV-1 RT p51 subunit

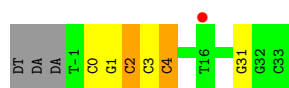
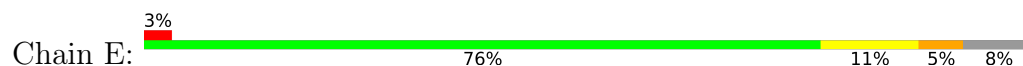




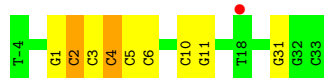
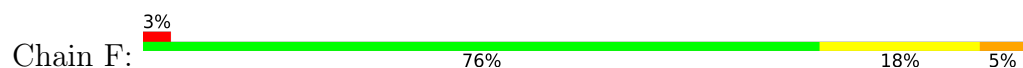
● Molecule 2: HIV-1 RT p51 subunit



● Molecule 3: DNA/RNA (38-MER)



● Molecule 3: DNA/RNA (38-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	284.17Å 284.17Å 95.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.60 – 2.30 48.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.60-2.30) 99.9 (48.60-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.186 , 0.221 0.189 , 0.224	Depositor DCC
R_{free} test set	6460 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17721	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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: GOL, DGT, 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	0.34	2/4616 (0.0%)	0.40	0/6268
1	C	0.31	2/4616 (0.0%)	0.40	0/6268
2	B	0.27	1/3441 (0.0%)	0.42	2/4673 (0.0%)
2	D	0.32	1/3441 (0.0%)	0.39	0/4673
3	E	0.20	0/756	0.41	0/1165
3	F	0.19	0/823	0.39	0/1269
All	All	0.30	6/17693 (0.0%)	0.40	2/24316 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	184	MET	C-O	-9.82	1.15	1.24
1	C	189	VAL	C-O	-6.24	1.17	1.24
1	A	353	LYS	C-O	-6.15	1.16	1.23
2	D	404	GLU	C-O	-5.50	1.17	1.24
1	C	187	LEU	C-O	-5.35	1.17	1.24
1	A	211	ARG	C-O	-5.07	1.17	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	422	LEU	N-CA-C	-7.13	101.77	112.04
2	B	362	THR	N-CA-C	6.52	120.86	112.26

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	4498	0	4553	47	0
1	C	4498	0	4553	26	0
2	B	3347	0	3379	19	0
2	D	3347	0	3379	19	0
3	E	718	0	397	4	0
3	F	777	0	432	5	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	31	0	12	1	0
5	C	31	0	12	0	0
6	A	6	0	8	0	0
6	B	12	0	16	0	0
6	D	12	0	16	0	0
7	A	125	0	0	2	0
7	B	49	0	0	0	0
7	C	107	0	0	2	0
7	D	86	0	0	0	0
7	E	40	0	0	0	0
7	F	35	0	0	0	0
All	All	17721	0	16757	117	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 3.

All (117) 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:31:ILE:HG21	1:A:134:SER:HA	1.62	0.80
1:A:473:THR:O	1:A:477:THR:HG23	1.84	0.76
2:B:271:TYR:HB2	2:B:274:ILE:HD11	1.69	0.75
1:A:500:GLN:H	1:A:500:GLN:CD	1.97	0.73
1:A:500:GLN:CD	1:A:500:GLN:N	2.50	0.69
1:C:15:GLY:O	1:C:16:MET:HE2	1.92	0.69
3:F:3:DC:H2'	3:F:4:OMC:C6	2.29	0.68
2:B:422:LEU:CD2	2:B:422:LEU:H	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:LYS:NZ	1:C:297:GLU:OE2	2.25	0.67
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.30	0.64
1:A:31:ILE:HD13	1:A:135:ILE:H	1.63	0.63
1:C:67:ASP:OD2	1:C:70:LYS:HE2	1.99	0.62
2:B:422:LEU:H	2:B:422:LEU:HD23	1.64	0.62
3:E:1:DG:H2'	3:E:2:OMC:C6	2.35	0.60
3:E:3:DC:H2'	3:E:4:OMC:C6	2.36	0.60
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.34	0.60
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.35	0.60
2:B:242:GLN:OE1	2:B:243:PRO:HD2	2.02	0.60
1:A:438:GLU:OE2	1:A:459:THR:HG21	2.03	0.59
1:A:463:ARG:NH2	1:A:488:ASP:O	2.36	0.58
1:A:436:GLY:O	1:A:461:ARG:NH2	2.36	0.58
2:B:271:TYR:HB2	2:B:274:ILE:CD1	2.34	0.57
2:B:425:LEU:H	2:B:425:LEU:HD22	1.69	0.57
1:C:511:ASP:OD1	1:C:512:LYS:NZ	2.39	0.56
3:F:1:DG:H2'	3:F:2:OMC:C6	2.41	0.56
1:C:136:ASN:O	1:C:138:GLU:N	2.37	0.55
1:A:380:ILE:HD11	1:A:386:THR:HG23	1.89	0.55
2:D:395:LYS:NZ	2:D:399:GLU:OE2	2.39	0.54
1:A:447:ASN:HB3	1:A:450:THR:HB	1.89	0.54
1:C:447:ASN:HB3	1:C:450:THR:HG22	1.88	0.54
1:A:459:THR:HB	1:A:463:ARG:H	1.72	0.54
1:A:500:GLN:NE2	1:A:501:TYR:H	2.06	0.54
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.90	0.53
1:A:483:HIS:ND1	1:A:524:GLN:OE1	2.42	0.53
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.91	0.53
2:B:422:LEU:CD2	2:B:422:LEU:N	2.71	0.53
2:D:89:GLU:HG2	2:D:90:VAL:HG13	1.91	0.53
1:C:331:LYS:NZ	1:C:364:ASP:OD1	2.42	0.52
2:D:263:LYS:HA	2:D:425:LEU:HD22	1.90	0.52
1:C:536:VAL:HB	1:C:542:ILE:HD12	1.92	0.52
1:A:248:GLU:O	1:A:249:LYS:HD2	2.10	0.51
1:C:298:GLU:OE2	1:C:298:GLU:N	2.37	0.51
2:D:90:VAL:HG11	2:D:158:ALA:HA	1.92	0.50
1:A:472:THR:HG21	1:A:477:THR:HG22	1.93	0.50
2:D:314:VAL:HG12	2:D:315:HIS:O	2.11	0.50
1:A:451:LYS:HG3	1:A:471:ASP:H	1.78	0.49
3:F:10:DC:H2''	3:F:11:DG:C8	2.48	0.49
1:A:40:GLU:O	1:A:44:GLU:HG3	2.13	0.49
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:263:LYS:HG3	2:D:425:LEU:HD13	1.96	0.47
1:A:266:TRP:CE2	3:E:31:DG:H4'	2.50	0.47
1:C:207:GLN:O	1:C:211:ARG:HG3	2.14	0.47
2:B:238:LYS:O	2:B:238:LYS:HG2	2.15	0.47
1:C:450:THR:HG23	1:C:452:LEU:H	1.79	0.47
1:A:459:THR:HG22	1:A:461:ARG:H	1.80	0.46
1:A:1:PRO:HB2	1:A:213:GLY:HA2	1.98	0.46
2:D:353:LYS:HE2	2:D:427:TYR:HE1	1.81	0.46
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.50	0.46
1:A:450:THR:O	1:A:451:LYS:HG2	2.16	0.46
2:D:317:VAL:HG23	2:D:317:VAL:O	2.15	0.46
2:B:90:VAL:HG12	2:B:90:VAL:O	2.16	0.46
1:C:266:TRP:CE2	3:F:31:DG:H4'	2.50	0.46
2:D:206:ARG:O	2:D:210:LEU:HG	2.16	0.45
1:C:188:TYR:CD1	1:C:188:TYR:C	2.93	0.45
2:D:332:GLN:CD	2:D:427:TYR:HB2	2.42	0.45
1:A:438:GLU:CG	1:A:459:THR:CG2	2.95	0.45
2:D:69:THR:HG22	2:D:69:THR:O	2.17	0.45
1:C:500:GLN:HG3	7:C:761:HOH:O	2.17	0.44
1:A:438:GLU:CD	1:A:459:THR:HG21	2.42	0.44
1:A:491:LEU:HB3	1:A:529:GLU:HB2	1.99	0.44
1:A:26:LEU:HD22	1:A:30:LYS:HD2	1.99	0.44
1:A:472:THR:HG23	1:A:473:THR:N	2.33	0.44
2:D:30:LYS:NZ	2:D:404:GLU:OE1	2.51	0.44
2:B:242:GLN:HE21	2:B:353:LYS:HE3	1.83	0.43
5:A:602:DGT:N2	3:E:0:DC:O2	2.40	0.43
2:B:252:TRP:CD1	2:B:295:LEU:HD21	2.53	0.43
2:B:17:ASP:O	2:B:83:ARG:NH1	2.45	0.43
1:A:101:LYS:HE3	1:A:321:PRO:HG3	1.99	0.43
1:A:181:TYR:HB2	1:A:188:TYR:HB3	2.00	0.43
1:A:548:VAL:O	1:A:552:VAL:HG23	2.17	0.43
2:B:283:LEU:O	2:B:284:ARG:C	2.60	0.43
1:C:175:ASN:HB3	1:C:178:ILE:HD12	1.99	0.43
1:A:111:VAL:HG21	1:A:164:MET:HE1	2.01	0.43
1:C:465:LYS:HD3	1:C:484:LEU:HD11	2.01	0.43
1:C:17:ASP:O	1:C:83:ARG:HD2	2.19	0.42
1:C:447:ASN:OD1	1:C:447:ASN:C	2.62	0.42
2:D:195:ILE:HG13	2:D:199:ARG:HE	1.84	0.42
2:D:81:ASN:O	2:D:154:LYS:NZ	2.51	0.42
1:A:397:THR:HG21	1:A:424:LYS:HA	2.02	0.42
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:NZ	7:A:710:HOH:O	2.52	0.42
1:C:436:GLY:O	1:C:461:ARG:NH2	2.53	0.42
2:D:66:LYS:HD2	2:D:232:TYR:HB3	2.02	0.42
1:C:37:ILE:HD11	1:C:73:LYS:HD2	2.01	0.41
2:B:425:LEU:H	2:B:425:LEU:CD2	2.33	0.41
3:F:5:DC:H2''	3:F:6:DC:H5'	2.01	0.41
1:A:331:LYS:HE2	7:C:736:HOH:O	2.20	0.41
2:B:356:ARG:HG2	2:B:357:MET:N	2.35	0.41
2:D:183:TYR:CE2	2:D:184:MET:HG3	2.56	0.41
2:D:257:ILE:HD12	2:D:293:VAL:CG2	2.51	0.41
1:A:23:GLN:OE1	1:A:60:VAL:HG12	2.21	0.41
1:A:31:ILE:CG2	1:A:134:SER:HA	2.41	0.41
1:C:473:THR:O	1:C:477:THR:HG23	2.20	0.41
1:A:101:LYS:CE	1:A:321:PRO:HG3	2.50	0.41
1:A:503:LEU:O	1:A:507:GLN:HB2	2.20	0.41
1:C:35:VAL:O	1:C:39:THR:HG23	2.21	0.41
1:A:263:LYS:NZ	7:A:713:HOH:O	2.52	0.41
1:A:442:VAL:HG22	1:A:496:VAL:O	2.21	0.41
2:B:197:GLN:HA	2:B:197:GLN:OE1	2.21	0.41
1:A:31:ILE:HD13	1:A:135:ILE:N	2.32	0.41
1:C:156:SER:HB2	1:C:157:PRO:HD3	2.03	0.41
1:C:282:LEU:HB3	1:C:293:VAL:HG11	2.03	0.41
2:B:419:THR:O	2:B:419:THR:HG23	2.21	0.40
1:C:328:GLU:O	1:C:339:TYR:HA	2.21	0.40
2:D:365:VAL:HG11	2:D:401:TRP:HB2	2.03	0.40
1:A:31:ILE:CD1	1:A:135:ILE:H	2.32	0.40
1:C:178:ILE:HD11	1:C:201:LYS:HG3	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%)	527 (96%)	22 (4%)	2 (0%)	30	38
1	C	551/557 (99%)	530 (96%)	20 (4%)	1 (0%)	43	55
2	B	402/444 (90%)	382 (95%)	20 (5%)	0	100	100
2	D	402/444 (90%)	388 (96%)	14 (4%)	0	100	100
All	All	1906/2002 (95%)	1827 (96%)	76 (4%)	3 (0%)	43	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	137	ASN
1	A	67	ASP
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%)	486 (99%)	6 (1%)	63	79
1	C	492/494 (100%)	490 (100%)	2 (0%)	84	92
2	B	365/400 (91%)	359 (98%)	6 (2%)	55	73
2	D	365/400 (91%)	361 (99%)	4 (1%)	65	81
All	All	1714/1788 (96%)	1696 (99%)	18 (1%)	65	81

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	248	GLU
1	A	353	LYS
1	A	480	GLN
1	A	500	GLN
1	A	551	LEU
2	B	184	MET
2	B	289	LEU

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Mol	Chain	Res	Type
2	B	295	LEU
2	B	356	ARG
2	B	422	LEU
2	B	425	LEU
1	C	188	TYR
1	C	507	GLN
2	D	73	LYS
2	D	184	MET
2	D	232	TYR
2	D	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	221	HIS
1	A	235	HIS
1	A	480	GLN
1	A	545	ASN
1	A	547	GLN
2	B	91	GLN
2	B	137	ASN
2	B	147	ASN
2	B	334	GLN
2	B	394	GLN
1	C	91	GLN
1	C	136	ASN
1	C	278	GLN
1	C	334	GLN
1	C	394	GLN
1	C	464	GLN
1	C	487	GLN
1	C	547	GLN
2	D	147	ASN
2	D	182	GLN
2	D	269	GLN
2	D	336	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	E	4	3	19,22,23	2.80	8 (42%)	25,31,34	0.74	0
3	OMC	F	4	3	19,22,23	2.82	8 (42%)	25,31,34	0.68	0
3	OMC	E	2	3	19,22,23	2.78	8 (42%)	25,31,34	0.80	0
3	OMC	F	2	3	19,22,23	2.81	8 (42%)	25,31,34	0.74	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	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
3	OMC	F	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	E	4	OMC	C2-N3	6.21	1.48	1.36
3	F	4	OMC	C2-N3	6.19	1.48	1.36
3	F	2	OMC	C6-C5	6.03	1.49	1.35
3	F	2	OMC	C2-N3	6.01	1.48	1.36
3	F	4	OMC	C6-C5	5.95	1.48	1.35
3	E	2	OMC	C6-C5	5.91	1.48	1.35
3	E	2	OMC	C2-N3	5.88	1.48	1.36
3	E	4	OMC	C6-C5	5.87	1.48	1.35
3	F	4	OMC	C4-N3	4.95	1.44	1.34
3	E	2	OMC	C2-N1	4.95	1.50	1.40
3	F	2	OMC	C4-N3	4.88	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	4	OMC	C4-N3	4.82	1.44	1.34
3	F	2	OMC	C2-N1	4.82	1.50	1.40
3	F	4	OMC	C2-N1	4.81	1.50	1.40
3	E	4	OMC	C2-N1	4.80	1.50	1.40
3	E	2	OMC	C4-N3	4.80	1.44	1.34
3	F	2	OMC	C6-N1	3.15	1.45	1.38
3	F	4	OMC	C6-N1	3.03	1.45	1.38
3	E	2	OMC	C6-N1	3.02	1.45	1.38
3	E	4	OMC	C6-N1	2.94	1.45	1.38
3	E	4	OMC	C4-N4	2.86	1.40	1.33
3	F	4	OMC	C4-N4	2.79	1.40	1.33
3	F	2	OMC	C4-N4	2.79	1.40	1.33
3	E	2	OMC	C4-N4	2.77	1.40	1.33
3	E	4	OMC	C5-C4	2.73	1.49	1.42
3	F	2	OMC	C5-C4	2.70	1.49	1.42
3	E	2	OMC	C5-C4	2.69	1.49	1.42
3	F	4	OMC	C5-C4	2.68	1.49	1.42
3	E	2	OMC	O2-C2	-2.29	1.19	1.23
3	E	4	OMC	O2-C2	-2.23	1.19	1.23
3	F	4	OMC	O2-C2	-2.20	1.19	1.23
3	F	2	OMC	O2-C2	-2.16	1.19	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 4 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
6	GOL	D	501	-	5,5,5	0.36	0	5,5,5	0.38	0
6	GOL	D	502	-	5,5,5	0.58	0	5,5,5	0.27	0
6	GOL	B	501	-	5,5,5	0.36	0	5,5,5	0.23	0
6	GOL	B	502	-	5,5,5	0.41	0	5,5,5	0.22	0
5	DGT	A	602	4	32,33,33	3.95	17 (53%)	48,52,52	1.59	11 (22%)
6	GOL	A	603	-	5,5,5	0.24	0	5,5,5	0.97	0
5	DGT	C	602	4	32,33,33	3.99	16 (50%)	48,52,52	1.57	9 (18%)

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	D	501	-	-	2/4/4/4	-
6	GOL	D	502	-	-	0/4/4/4	-
6	GOL	B	501	-	-	2/4/4/4	-
6	GOL	B	502	-	-	2/4/4/4	-
5	DGT	A	602	4	-	5/22/34/34	0/3/3/3
6	GOL	A	603	-	-	4/4/4/4	-
5	DGT	C	602	4	-	3/22/34/34	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	602	DGT	O4'-C1'	8.93	1.62	1.42
5	A	602	DGT	O4'-C1'	8.77	1.61	1.42
5	A	602	DGT	O4'-C4'	-7.56	1.28	1.45
5	C	602	DGT	O4'-C4'	-7.55	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	602	DGT	PB-O3A	7.22	1.67	1.59
5	C	602	DGT	PB-O3A	7.20	1.67	1.59
5	C	602	DGT	PB-O3B	7.16	1.67	1.59
5	C	602	DGT	C2'-C1'	-6.98	1.33	1.52
5	A	602	DGT	PB-O3B	6.93	1.67	1.59
5	A	602	DGT	C2'-C1'	-6.89	1.33	1.52
5	A	602	DGT	C4-N3	6.86	1.49	1.34
5	C	602	DGT	C4-N3	6.83	1.49	1.34
5	C	602	DGT	C2-N3	5.94	1.47	1.33
5	A	602	DGT	C2-N3	5.83	1.47	1.33
5	A	602	DGT	C2-N2	5.53	1.47	1.34
5	C	602	DGT	C2-N2	5.52	1.47	1.34
5	C	602	DGT	O6-C6	-4.59	1.14	1.23
5	A	602	DGT	O6-C6	-4.55	1.14	1.23
5	C	602	DGT	PA-O3A	3.92	1.63	1.59
5	A	602	DGT	PA-O3A	3.84	1.63	1.59
5	C	602	DGT	C5-N7	-3.48	1.32	1.39
5	A	602	DGT	C5-N7	-3.39	1.32	1.39
5	C	602	DGT	C6-N1	3.03	1.44	1.38
5	C	602	DGT	O3'-C3'	-2.99	1.37	1.43
5	A	602	DGT	C6-N1	2.95	1.44	1.38
5	A	602	DGT	C2-N1	2.91	1.44	1.37
5	A	602	DGT	O3'-C3'	-2.90	1.37	1.43
5	C	602	DGT	C2-N1	2.88	1.44	1.37
5	A	602	DGT	C5-C6	2.70	1.54	1.44
5	C	602	DGT	C5-C6	2.70	1.54	1.44
5	C	602	DGT	PA-O5'	2.53	1.69	1.59
5	A	602	DGT	PA-O5'	2.44	1.69	1.59
5	A	602	DGT	C4-N9	-2.14	1.32	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	DGT	C5-C4-N3	-4.77	120.80	128.39
5	A	602	DGT	C5-C4-N3	-4.59	121.08	128.39
5	C	602	DGT	C2-N3-C4	4.29	119.69	112.30
5	A	602	DGT	C2-N3-C4	4.27	119.65	112.30
5	A	602	DGT	N9-C8-N7	-3.01	107.81	113.40
5	C	602	DGT	N9-C8-N7	-2.96	107.92	113.40
5	C	602	DGT	C2-N1-C6	-2.90	119.84	125.11
5	A	602	DGT	C2-N1-C6	-2.82	119.99	125.11
5	A	602	DGT	C5-C6-N1	2.59	119.85	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	DGT	C5-C6-N1	2.57	119.81	113.25
5	C	602	DGT	N9-C4-N3	2.54	131.02	125.95
5	A	602	DGT	O6-C6-C5	-2.45	120.07	126.53
5	C	602	DGT	O6-C6-C5	-2.41	120.17	126.53
5	A	602	DGT	C1'-N9-C4	-2.31	119.28	125.50
5	A	602	DGT	N9-C4-N3	2.30	130.54	125.95
5	A	602	DGT	C1'-N9-C8	2.10	132.63	127.91
5	C	602	DGT	C8-N7-C5	2.09	107.98	104.26
5	C	602	DGT	C1'-N9-C4	-2.06	119.94	125.50
5	A	602	DGT	C8-N7-C5	2.05	107.91	104.26
5	A	602	DGT	N2-C2-N1	2.01	121.00	116.76

There are no chirality outliers.

All (18) torsion outliers are listed below:

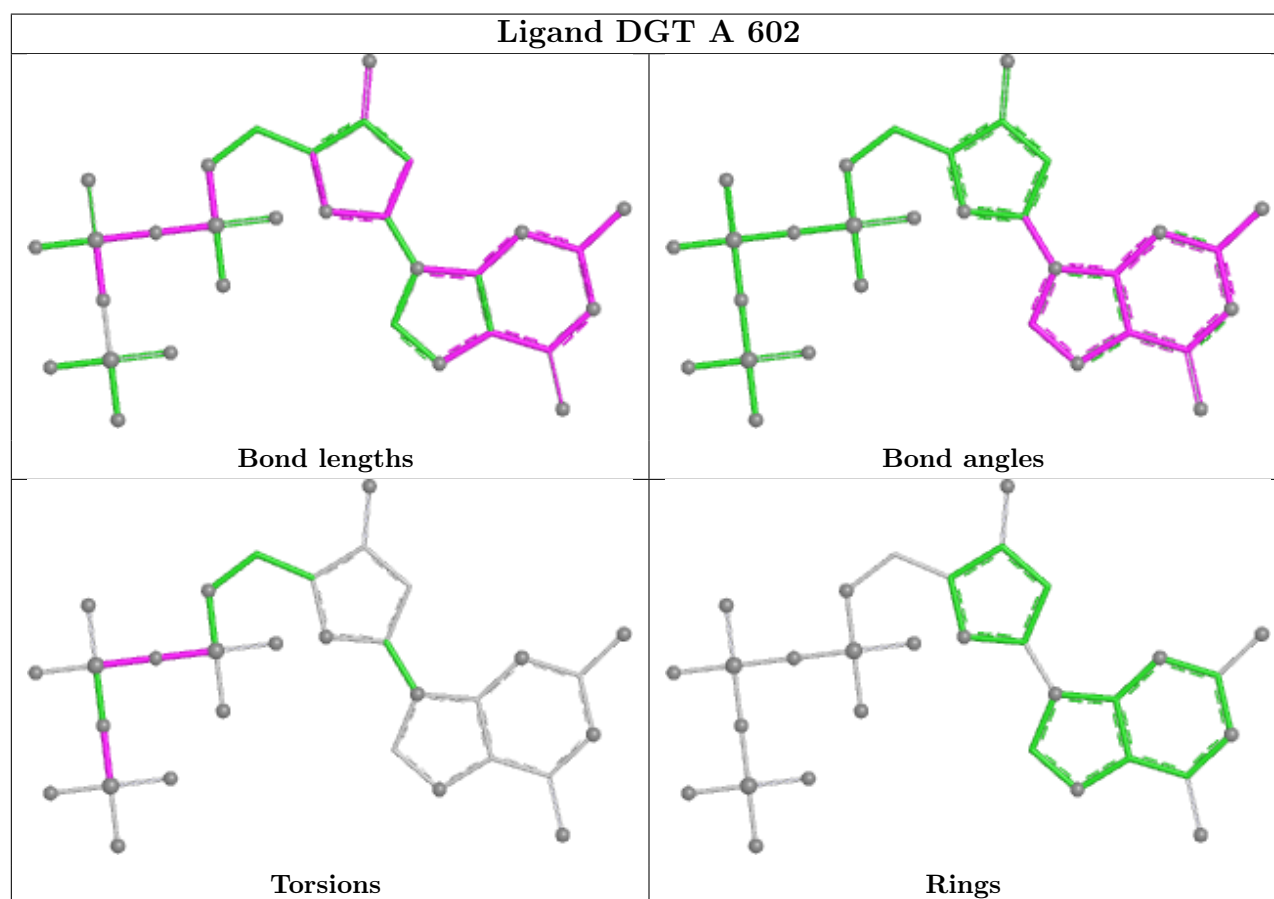
Mol	Chain	Res	Type	Atoms
5	A	602	DGT	PB-O3B-PG-O2G
5	C	602	DGT	PB-O3B-PG-O1G
6	A	603	GOL	O1-C1-C2-O2
6	A	603	GOL	O1-C1-C2-C3
6	B	501	GOL	C1-C2-C3-O3
6	D	501	GOL	O1-C1-C2-O2
6	A	603	GOL	C1-C2-C3-O3
6	B	502	GOL	O1-C1-C2-C3
6	D	501	GOL	O1-C1-C2-C3
6	A	603	GOL	O2-C2-C3-O3
5	A	602	DGT	PB-O3A-PA-O2A
6	B	501	GOL	O2-C2-C3-O3
5	C	602	DGT	PA-O3A-PB-O1B
6	B	502	GOL	O1-C1-C2-O2
5	A	602	DGT	PB-O3B-PG-O1G
5	C	602	DGT	PB-O3B-PG-O2G
5	A	602	DGT	PA-O3A-PB-O1B
5	A	602	DGT	PA-O3A-PB-O2B

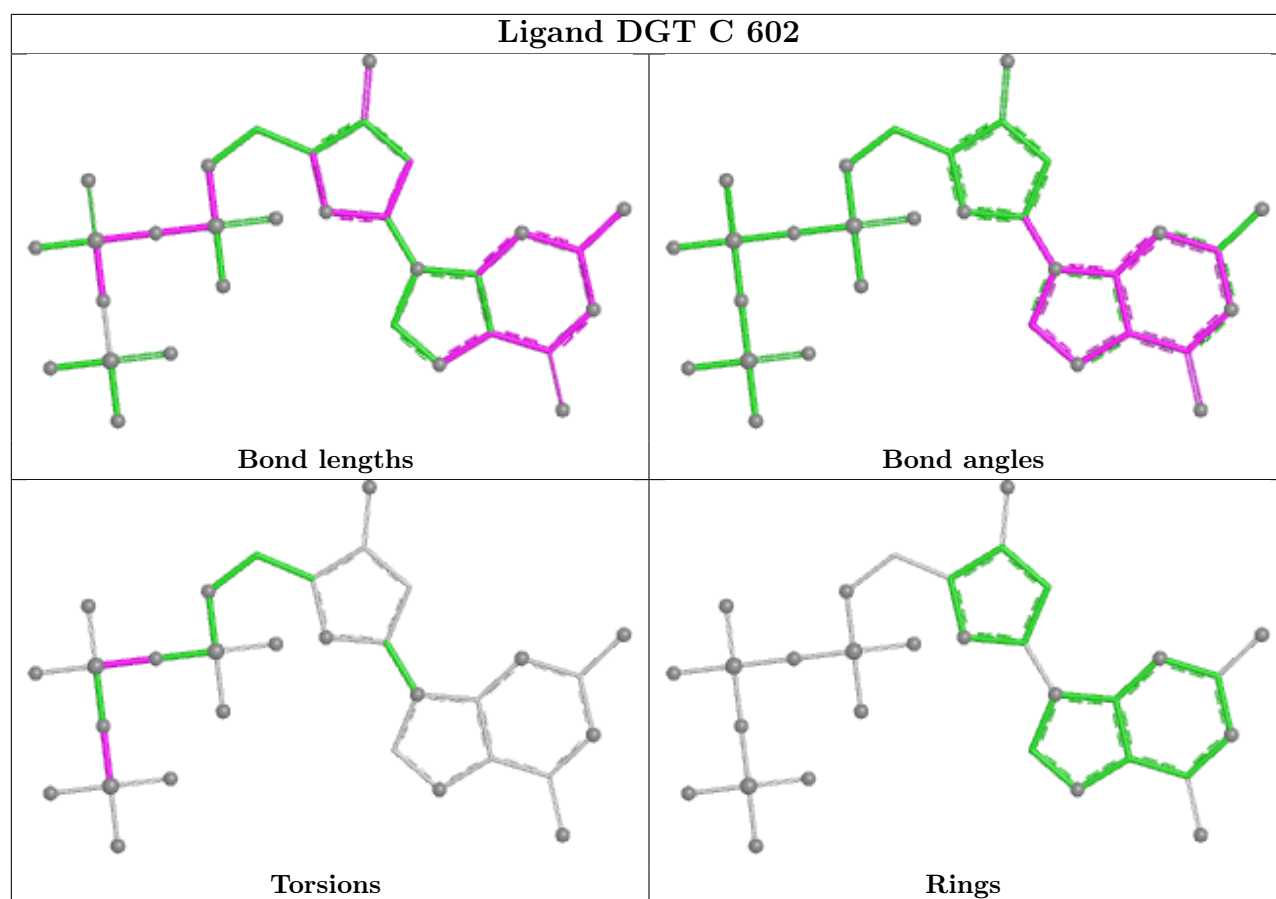
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	DGT	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%)	0.47	63 (11%) 10 11	27, 52, 98, 152	0
1	C	553/557 (99%)	0.23	23 (4%) 40 42	27, 52, 93, 173	0
2	B	406/444 (91%)	0.78	69 (16%) 4 5	30, 64, 130, 172	0
2	D	406/444 (91%)	0.26	32 (7%) 18 20	27, 49, 94, 189	0
3	E	33/38 (86%)	-0.48	1 (3%) 52 54	31, 50, 80, 129	0
3	F	36/38 (94%)	-0.17	1 (2%) 55 57	34, 60, 108, 145	0
All	All	1987/2078 (95%)	0.40	189 (9%) 14 15	27, 53, 110, 189	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	425	LEU	7.9
1	C	135	ILE	6.9
2	B	95	PRO	6.6
2	B	360	ALA	6.2
2	B	301	LEU	6.0
2	D	232	TYR	5.9
2	B	88	TRP	5.7
2	B	423	VAL	5.7
1	A	135	ILE	5.6
2	B	92	LEU	5.5
2	B	94	ILE	5.5
2	D	360	ALA	5.4
2	D	212	TRP	5.4
1	A	140	PRO	5.3
2	D	424	LYS	5.0
2	B	213	GLY	4.9
2	D	427	TYR	4.8
2	B	425	LEU	4.8
2	D	213	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	90	VAL	4.7
2	D	5	ILE	4.6
2	B	212	TRP	4.4
2	B	210	LEU	4.4
2	B	232	TYR	4.3
2	B	93	GLY	4.3
2	B	290	THR	4.2
2	D	422	LEU	4.2
2	B	294	PRO	4.1
2	B	5	ILE	4.1
2	D	361	HIS	4.1
2	B	241	VAL	4.1
1	A	551	LEU	4.0
1	A	67	ASP	4.0
1	A	133	PRO	4.0
2	B	422	LEU	4.0
2	D	231	GLY	4.0
1	A	132	ILE	4.0
2	B	293	VAL	3.9
1	A	464	GLN	3.8
2	D	359	GLY	3.8
2	B	231	GLY	3.7
2	B	266	TRP	3.6
1	C	68	SER	3.6
1	A	141	GLY	3.6
2	B	285	GLY	3.6
2	B	195	ILE	3.6
1	C	69	THR	3.5
2	B	420	PRO	3.5
2	B	286	THR	3.5
2	B	66	LYS	3.5
1	C	133	PRO	3.5
2	B	292	VAL	3.4
2	B	361	HIS	3.4
2	D	423	VAL	3.3
2	B	237	ASP	3.3
1	A	451	LYS	3.3
2	B	247	PRO	3.3
2	D	210	LEU	3.3
1	C	138	GLU	3.2
2	D	315	HIS	3.2
1	A	431	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	274	ILE	3.2
2	B	421	PRO	3.2
2	B	98	ALA	3.1
1	A	22	LYS	3.1
2	D	357	MET	3.1
1	A	403	THR	3.1
2	D	313	PRO	3.1
1	A	457	TYR	3.0
1	A	31	ILE	3.0
1	A	28	GLU	3.0
1	A	136	ASN	3.0
2	D	67	ASP	3.0
2	B	295	LEU	3.0
1	A	549	ASP	3.0
1	A	484	LEU	2.9
2	B	278	GLN	2.9
1	A	62	ALA	2.9
2	B	362	THR	2.9
1	A	458	VAL	2.9
1	A	552	VAL	2.9
1	A	495	ILE	2.9
1	C	37	ILE	2.9
1	C	70	LYS	2.8
1	C	66	LYS	2.8
1	C	219	LYS	2.8
2	B	287	LYS	2.8
1	C	136	ASN	2.8
2	B	245	VAL	2.8
2	D	314	VAL	2.8
2	B	238	LYS	2.8
2	B	419	THR	2.8
1	A	543	GLY	2.8
2	B	97	PRO	2.8
2	B	427	TYR	2.8
1	A	64	LYS	2.8
1	A	142	ILE	2.7
1	C	139	THR	2.7
1	A	1	PRO	2.7
1	C	140	PRO	2.7
2	B	276	VAL	2.7
1	A	435	ILE	2.7
1	C	142	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	421	PRO	2.7
1	C	134	SER	2.7
2	B	288	ALA	2.6
1	A	459	THR	2.6
1	C	26	LEU	2.6
1	C	67	ASP	2.6
2	B	253	THR	2.6
2	D	419	THR	2.6
2	B	358	LYS	2.6
1	A	402	TRP	2.6
2	B	282	LEU	2.6
2	D	69	THR	2.6
1	A	485	ALA	2.5
2	B	239	TRP	2.5
1	C	450	THR	2.5
1	A	550	LYS	2.5
2	B	303	LEU	2.5
2	B	252	TRP	2.5
1	A	449	GLU	2.5
2	D	211	ARG	2.5
2	B	357	MET	2.5
1	A	541	GLY	2.5
2	B	273	GLY	2.5
1	A	36	GLU	2.4
1	C	53	GLU	2.4
2	B	69	THR	2.4
1	A	134	SER	2.4
2	D	88	TRP	2.4
1	C	11	LYS	2.4
2	D	66	LYS	2.4
2	D	207	GLN	2.4
1	A	33	ALA	2.4
1	A	452	LEU	2.4
1	C	413	GLU	2.4
2	B	272	ALA	2.4
2	B	68	SER	2.4
2	B	289	LEU	2.4
1	A	60	VAL	2.3
1	C	71	TRP	2.3
1	A	553	SER	2.3
1	A	500	GLN	2.3
2	B	418	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	240	THR	2.3
2	B	89	GLU	2.3
1	A	440	PHE	2.3
2	D	420	PRO	2.3
1	A	139	THR	2.3
2	D	70	LYS	2.3
2	B	208	HIS	2.2
1	A	428	GLN	2.2
2	B	242	GLN	2.2
1	A	137	ASN	2.2
2	B	284	ARG	2.2
1	A	138	GLU	2.2
1	A	413	GLU	2.2
1	A	69	THR	2.2
2	B	296	THR	2.2
1	A	442	VAL	2.2
2	D	90	VAL	2.2
1	A	465	LYS	2.2
2	B	251	SER	2.2
1	A	68	SER	2.2
1	A	455	ALA	2.2
2	D	318	TYR	2.1
1	A	542	ILE	2.1
1	A	24	TRP	2.1
3	F	18	DT	2.1
2	D	358	LYS	2.1
1	A	21	VAL	2.1
1	A	547	GLN	2.1
1	A	467	VAL	2.1
1	A	468	PRO	2.1
1	A	493	VAL	2.1
1	A	448	ARG	2.1
1	A	59	PRO	2.1
1	C	35	VAL	2.1
1	A	66	LYS	2.0
1	A	450	THR	2.0
1	A	470	THR	2.0
3	E	16	DT	2.0
2	B	304	ALA	2.0
2	B	255	ASN	2.0
2	B	254	VAL	2.0
2	D	316	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	30	LYS	2.0
2	B	64	LYS	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	E	2	21/22	0.97	0.06	30,34,39,43	0
3	OMC	F	2	21/22	0.97	0.08	37,42,47,51	0
3	OMC	E	4	21/22	0.98	0.07	26,30,37,43	0
3	OMC	F	4	21/22	0.98	0.06	26,36,40,41	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.

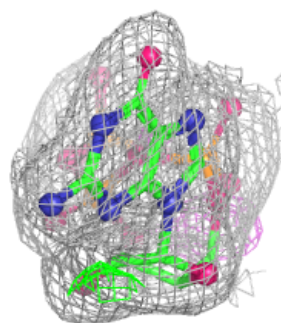
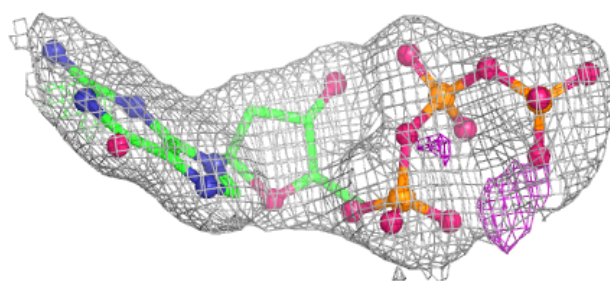
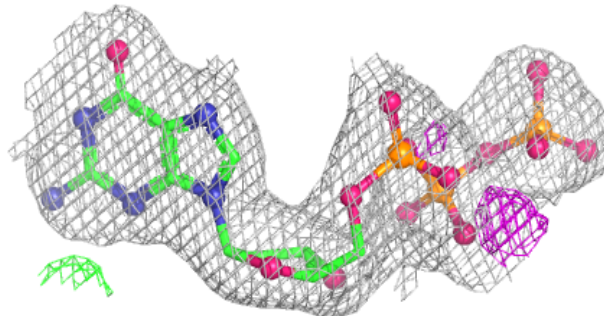
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	GOL	B	501	6/6	0.80	0.23	53,67,68,71	0
4	MG	C	601	1/1	0.90	0.16	56,56,56,56	0
6	GOL	D	502	6/6	0.90	0.19	46,51,55,56	0
6	GOL	A	603	6/6	0.91	0.17	60,67,68,72	0
5	DGT	C	602	31/31	0.94	0.09	43,54,75,81	0
6	GOL	B	502	6/6	0.95	0.10	38,49,50,54	0
6	GOL	D	501	6/6	0.95	0.11	38,50,50,50	0
4	MG	A	601	1/1	0.95	0.10	49,49,49,49	0
5	DGT	A	602	31/31	0.96	0.08	40,50,58,64	0

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

orientation to approximate a three-dimensional view.

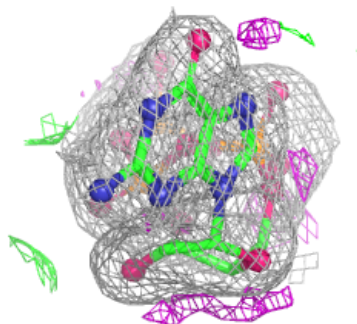
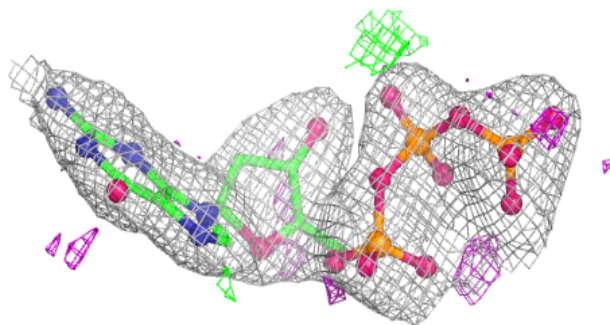
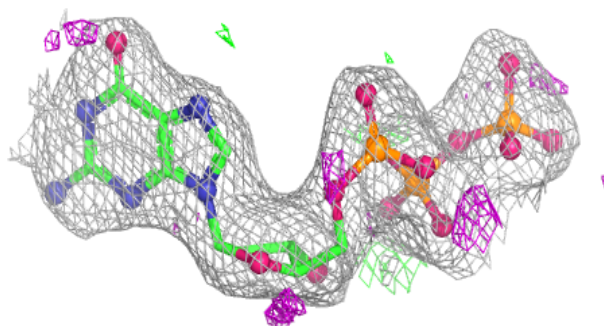
Electron density around DGT C 602:

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



Electron density around DGT A 602:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.