



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 27, 2021 – 12:14 PM JST

PDB ID : 7DBM
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.22
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.22

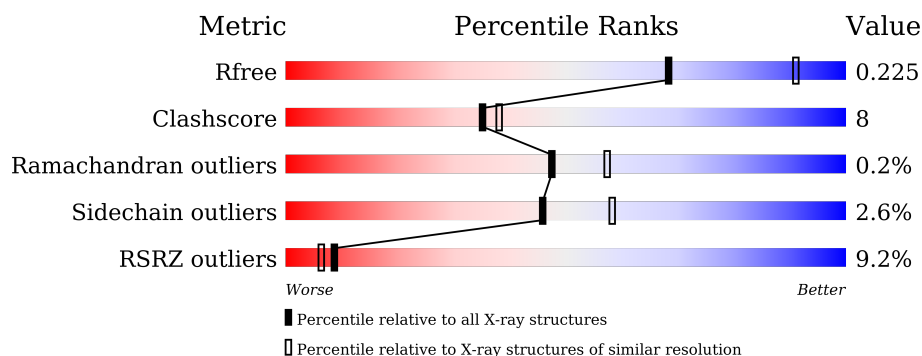
1 Overall quality at a glance

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}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	557	<div> <div>4%</div> <div>80%18%..</div> </div>
1	C	557	<div> <div>11%</div> <div>82%17%..</div> </div>
2	B	444	<div> <div>16%</div> <div>68%21%9%</div> </div>
2	D	444	<div> <div>7%</div> <div>78%12%9%</div> </div>
3	E	38	<div> <div>68%18%5%8%</div> </div>
3	F	38	<div> <div>3%</div> <div>79%13%8%</div> </div>

2 Entry composition

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
1	A	552	Total	C	N	O	S	0	0	0
			4490	2906	749	828	7			
1	C	552	Total	C	N	O	S	0	0	0
			4490	2906	749	828	7			

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
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).

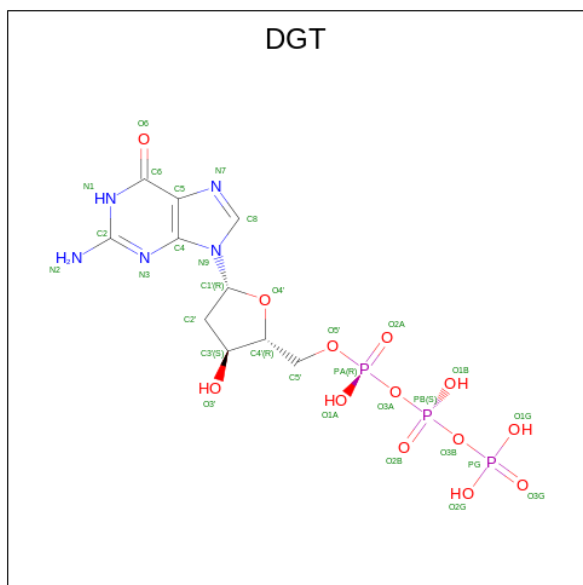
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			718	339	128	216	35			

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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 (three-letter code: 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 (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

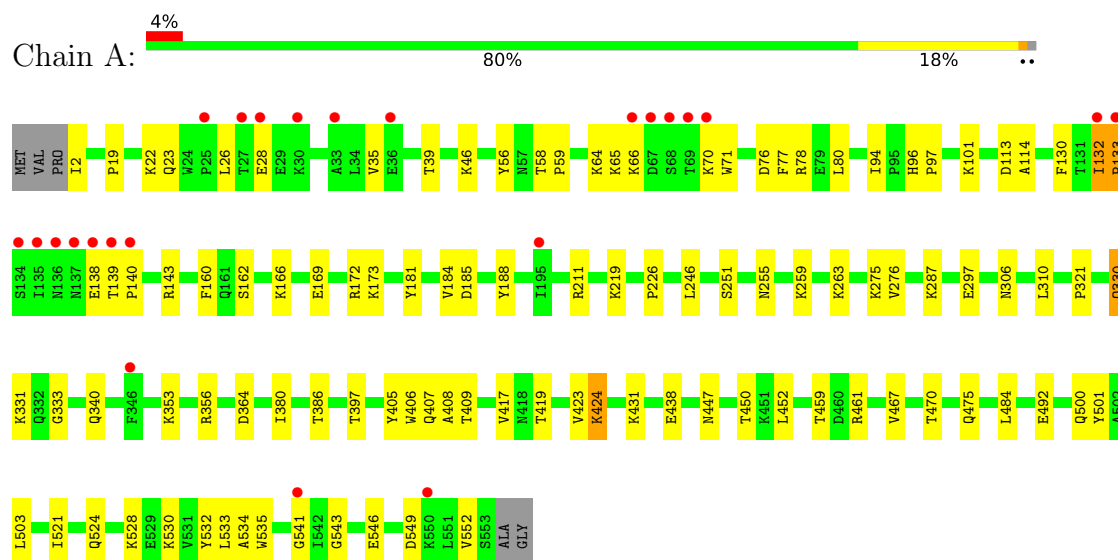
- Molecule 7 is water.

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

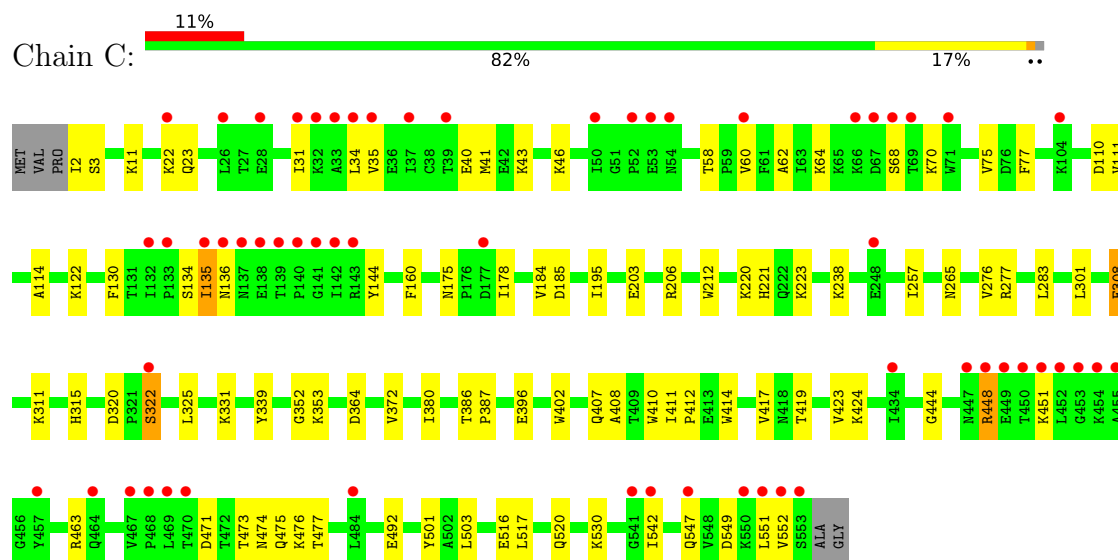
3 Residue-property plots [i](#)

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: Protease



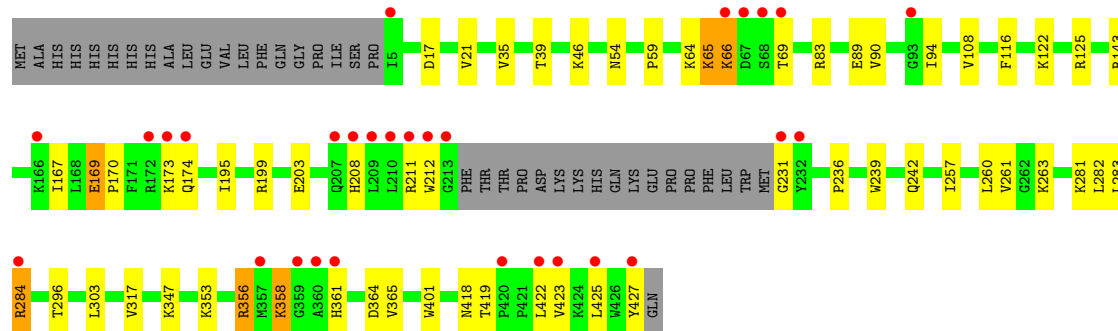
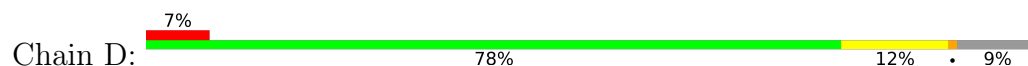
• Molecule 1: Protease



• Molecule 2: HIV-1 RT p51 subunit



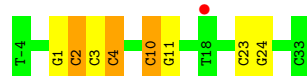
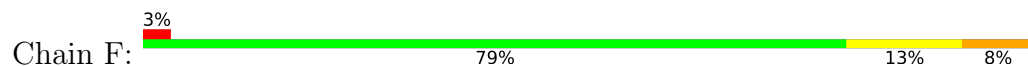
- Molecule 2: HIV-1 RT p51 subunit



- 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, α , β , γ	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) 100.0 (48.47-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.181 , 0.224 0.181 , 0.225	Depositor DCC
R_{free} test set	5472 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17702	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.41	2/4607 (0.0%)	0.52	1/6257 (0.0%)
1	C	0.32	0/4607	0.47	0/6257
2	B	0.35	0/3441	0.56	0/4673
2	D	0.34	0/3441	0.49	0/4673
3	E	0.60	0/756	0.91	1/1165 (0.1%)
3	F	0.74	1/823 (0.1%)	0.91	0/1269
All	All	0.40	3/17675 (0.0%)	0.56	2/24294 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	PRO	N-CA	12.93	1.69	1.47
1	A	132	ILE	C-N	5.79	1.45	1.34
3	F	10	DC	O3'-P	-5.08	1.55	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	PRO	CA-N-CD	-10.09	97.37	111.50
3	E	31	DG	O4'-C4'-C3'	-5.47	102.31	104.50

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	88	0
1	C	4490	0	4543	65	0
2	B	3347	0	3379	94	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	278	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 (278) 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
2:B:358:LYS:HE2	2:B:366:LYS:HZ1	1.29	0.96
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CB	2:B:312:GLU:OE1	2.26	0.84
1:A:500:GLN:HB3	2:B:422:LEU:HD11	1.59	0.83
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
2:B:311:LYS:HB3	2:B:312:GLU:CD	2.02	0.80
1:A:28:GLU:O	1:A:28:GLU:CD	2.22	0.79
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
1:A:65:LYS:HZ2	1:A:70:LYS:HE2	1.49	0.77
2:B:423:VAL:HB	2:B:425:LEU:HD13	1.68	0.76
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:358:LYS:HE2	2:B:366:LYS:HZ3	1.58	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
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
1:A:65:LYS:NZ	1:A:70:LYS:HE2	2.09	0.65
2:B:139:THR:HG22	2:B:140:PRO:O	1.96	0.65
1:C:175:ASN:HB3	1:C:178:ILE:HD12	1.80	0.63
2:B:301:LEU:HD13	2:B:301:LEU:C	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:65:LYS:HZ3	1:A:70:LYS:HD3	1.65	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
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
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:263:LYS:NZ	7:A:703:HOH:O	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.91	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:164:MET:HE3	2:B:187:LEU:HD21	1.90	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:396:GLU:CD	1:C:396:GLU:H	2.14	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
2:D:257:ILE:HB	2:D:283:LEU:HD21	1.92	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
2:D:208:HIS:CE1	2:D:212:TRP:HE1	2.29	0.50
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:A:65:LYS:HZ3	1:A:70:LYS:CE	2.25	0.49
1:A:65:LYS:HZ3	1:A:70:LYS:CD	2.25	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:B:87:PHE:C	2:B:90:VAL:HG12	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:402:TRP:HE1	2:D:364:ASP:CG	2.19	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: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:D:356:ARG:C	2:D:356:ARG:HD2	2.36	0.46
2:B:248:GLU:HB2	2:B:307:ARG:HH22	1.81	0.46
2:B:427:TYR:C	2:B:427:TYR:CD1	2.90	0.45
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
1:C:134:SER:C	1:C:136:ASN:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.52	0.45
2:B:73:LYS:HD3	2:B:75:VAL:HG23	1.97	0.45
1:A:185:ASP:OD1	3:E:33:DC:O3'	2.25	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
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
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: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
2:B:301:LEU:C	2:B:301:LEU:CD1	2.86	0.43
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:364:ASP:HB3	1:A:423:VAL:HG13	2.02	0.41
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
1:A:431:LYS:HE2	1:A:431:LYS:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:VAL:C	2:B:91:GLN:HG2	2.41	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:65:LYS:HZ2	1:A:70:LYS:CE	2.24	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	550/557 (99%)	535 (97%)	14 (2%)	1 (0%)	47	57
1	C	550/557 (99%)	534 (97%)	14 (2%)	2 (0%)	34	41
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%)	47	57

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 ⓘ

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%)	482 (98%)	9 (2%)	59	71
1	C	491/494 (99%)	482 (98%)	9 (2%)	59	71
2	B	365/400 (91%)	350 (96%)	15 (4%)	30	40
2	D	365/400 (91%)	354 (97%)	11 (3%)	41	53
All	All	1712/1788 (96%)	1668 (97%)	44 (3%)	46	58

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	138	GLU
1	A	211	ARG
1	A	219	LYS
1	A	226	PRO
1	A	251	SER
1	A	287	LYS
1	A	330	GLN
1	A	424	LYS
2	B	36	GLU
2	B	67	ASP
2	B	72	ARG
2	B	122	LYS
2	B	197	GLN
2	B	210	LEU
2	B	232	TYR
2	B	233	GLU

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Mol	Chain	Res	Type
2	B	280	SER
2	B	297	GLU
2	B	300	GLU
2	B	302	GLU
2	B	374	LYS
2	B	425	LEU
2	B	427	TYR
1	C	40	GLU
1	C	43	LYS
1	C	70	LYS
1	C	122	LYS
1	C	277	ARG
1	C	308	GLU
1	C	322	SER
1	C	448	ARG
1	C	463	ARG
2	D	64	LYS
2	D	65	LYS
2	D	66	LYS
2	D	69	THR
2	D	169	GLU
2	D	203	GLU
2	D	211	ARG
2	D	284	ARG
2	D	356	ARG
2	D	358	LYS
2	D	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	197	GLN
1	A	198	HIS
1	A	207	GLN
1	A	265	ASN
1	A	306	ASN
1	A	330	GLN
1	A	428	GLN
1	A	500	GLN
1	A	509	GLN
1	A	524	GLN

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Mol	Chain	Res	Type
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	306	ASN
2	B	343	GLN
1	C	265	ASN
1	C	315	HIS
1	C	336	GLN
1	C	428	GLN
1	C	509	GLN
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	258	GLN
2	D	334	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	2	3	15,22,23	3.94	6 (40%)	17,31,34	1.28	1 (5%)
3	OMC	F	4	3	15,22,23	3.83	6 (40%)	17,31,34	1.27	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	F	2	3	15,22,23	3.84	6 (40%)	17,31,34	1.35	1 (5%)
3	OMC	E	4	3	15,22,23	3.80	6 (40%)	17,31,34	1.31	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	E	2	3	-	0/7/27/28	0/2/2/2
3	OMC	F	4	3	-	0/7/27/28	0/2/2/2
3	OMC	F	2	3	-	0/7/27/28	0/2/2/2
3	OMC	E	4	3	-	0/7/27/28	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	OMC	C6-N1	9.55	1.47	1.35
3	F	2	OMC	C6-N1	9.51	1.47	1.35
3	E	4	OMC	C6-N1	9.30	1.47	1.35
3	F	4	OMC	C6-N1	9.18	1.47	1.35
3	E	2	OMC	C4-N3	7.17	1.47	1.35
3	F	4	OMC	C4-N3	6.92	1.46	1.35
3	E	4	OMC	C4-N3	6.80	1.46	1.35
3	F	2	OMC	C4-N3	6.74	1.46	1.35
3	F	4	OMC	C2-N3	5.59	1.49	1.38
3	E	2	OMC	C6-C5	5.44	1.50	1.38
3	E	4	OMC	C2-N3	5.40	1.48	1.38
3	F	2	OMC	C6-C5	5.32	1.49	1.38
3	E	2	OMC	C2-N3	5.28	1.48	1.38
3	F	4	OMC	C6-C5	5.26	1.49	1.38
3	F	2	OMC	C2-N3	5.15	1.48	1.38
3	E	4	OMC	C6-C5	5.13	1.49	1.38
3	E	2	OMC	C4-N4	4.30	1.47	1.35
3	F	2	OMC	C4-N4	4.21	1.47	1.35
3	F	4	OMC	C4-N4	4.15	1.47	1.35
3	E	4	OMC	C4-N4	4.08	1.47	1.35
3	E	2	OMC	C5-C4	3.50	1.49	1.41
3	F	2	OMC	C5-C4	3.28	1.49	1.41
3	F	4	OMC	C5-C4	3.25	1.49	1.41
3	E	4	OMC	C5-C4	3.21	1.48	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2	OMC	C2-N3-C4	4.61	121.02	116.34
3	E	4	OMC	C2-N3-C4	4.40	120.80	116.34
3	E	2	OMC	C2-N3-C4	4.09	120.48	116.34
3	F	4	OMC	C2-N3-C4	4.00	120.39	116.34
3	F	4	OMC	N4-C4-N3	2.23	120.02	116.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	$\# Z > 2$
6	GOL	B	501	-	5,5,5	0.96	0	5,5,5	1.00	0
4	DGT	A	601	5	26,33,33	3.94	12 (46%)	32,52,52	1.80	7 (21%)
6	GOL	D	501	-	5,5,5	1.01	0	5,5,5	0.92	0
6	GOL	E	101	-	5,5,5	0.86	0	5,5,5	1.04	0
6	GOL	C	603	-	5,5,5	1.08	0	5,5,5	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	B	502	-	5,5,5	1.05	0	5,5,5	0.95	0
4	DGT	C	601	5	26,33,33	3.93	12 (46%)	32,52,52	1.74	6 (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	B	501	-	-	0/4/4/4	-
4	DGT	A	601	5	-	3/18/34/34	0/3/3/3
6	GOL	D	501	-	-	2/4/4/4	-
6	GOL	E	101	-	-	4/4/4/4	-
6	GOL	C	603	-	-	0/4/4/4	-
6	GOL	B	502	-	-	0/4/4/4	-
4	DGT	C	601	5	-	3/18/34/34	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	601	DGT	C4-N3	8.58	1.49	1.35
4	A	601	DGT	C4-N3	8.52	1.49	1.35
4	A	601	DGT	C3'-C4'	-7.29	1.33	1.53
4	C	601	DGT	C3'-C4'	-7.18	1.33	1.53
4	A	601	DGT	C6-C5	7.03	1.53	1.41
4	C	601	DGT	C6-C5	6.88	1.53	1.41
4	C	601	DGT	O4'-C4'	6.60	1.59	1.45
4	A	601	DGT	O4'-C4'	6.56	1.59	1.45
4	A	601	DGT	C6-N1	5.92	1.43	1.33
4	C	601	DGT	C6-N1	5.87	1.43	1.33
4	C	601	DGT	C2-N2	5.73	1.45	1.33
4	A	601	DGT	C2-N2	5.69	1.45	1.33
4	C	601	DGT	C2'-C1'	-5.61	1.36	1.52
4	A	601	DGT	O4'-C1'	5.33	1.54	1.42
4	A	601	DGT	C2'-C1'	-5.33	1.37	1.52
4	C	601	DGT	O4'-C1'	5.11	1.53	1.42
4	A	601	DGT	C2-N1	4.83	1.44	1.35
4	C	601	DGT	C2-N1	4.73	1.43	1.35
4	A	601	DGT	C2'-C3'	3.87	1.63	1.52
4	C	601	DGT	C2'-C3'	3.75	1.62	1.52
4	C	601	DGT	C2-N3	2.50	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	DGT	C2-N3	2.33	1.45	1.34
4	C	601	DGT	O6-C6	-2.32	1.18	1.24
4	A	601	DGT	O6-C6	-2.21	1.19	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	DGT	N3-C2-N1	-5.69	119.64	127.22
4	A	601	DGT	N3-C2-N1	-5.52	119.86	127.22
4	A	601	DGT	C2-N3-C4	4.54	120.55	115.36
4	C	601	DGT	C2-N3-C4	4.14	120.08	115.36
4	A	601	DGT	PB-O3B-PG	-2.95	122.72	132.83
4	A	601	DGT	C5-C6-N1	-2.65	119.81	123.43
4	C	601	DGT	C6-N1-C2	2.63	120.11	115.93
4	C	601	DGT	C5-C6-N1	-2.57	119.92	123.43
4	A	601	DGT	C6-N1-C2	2.42	119.77	115.93
4	A	601	DGT	C2'-C1'-N9	-2.32	108.93	114.27
4	A	601	DGT	N2-C2-N1	2.23	120.72	117.25
4	C	601	DGT	PA-O3A-PB	-2.17	125.37	132.83
4	C	601	DGT	PB-O3B-PG	-2.02	125.91	132.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

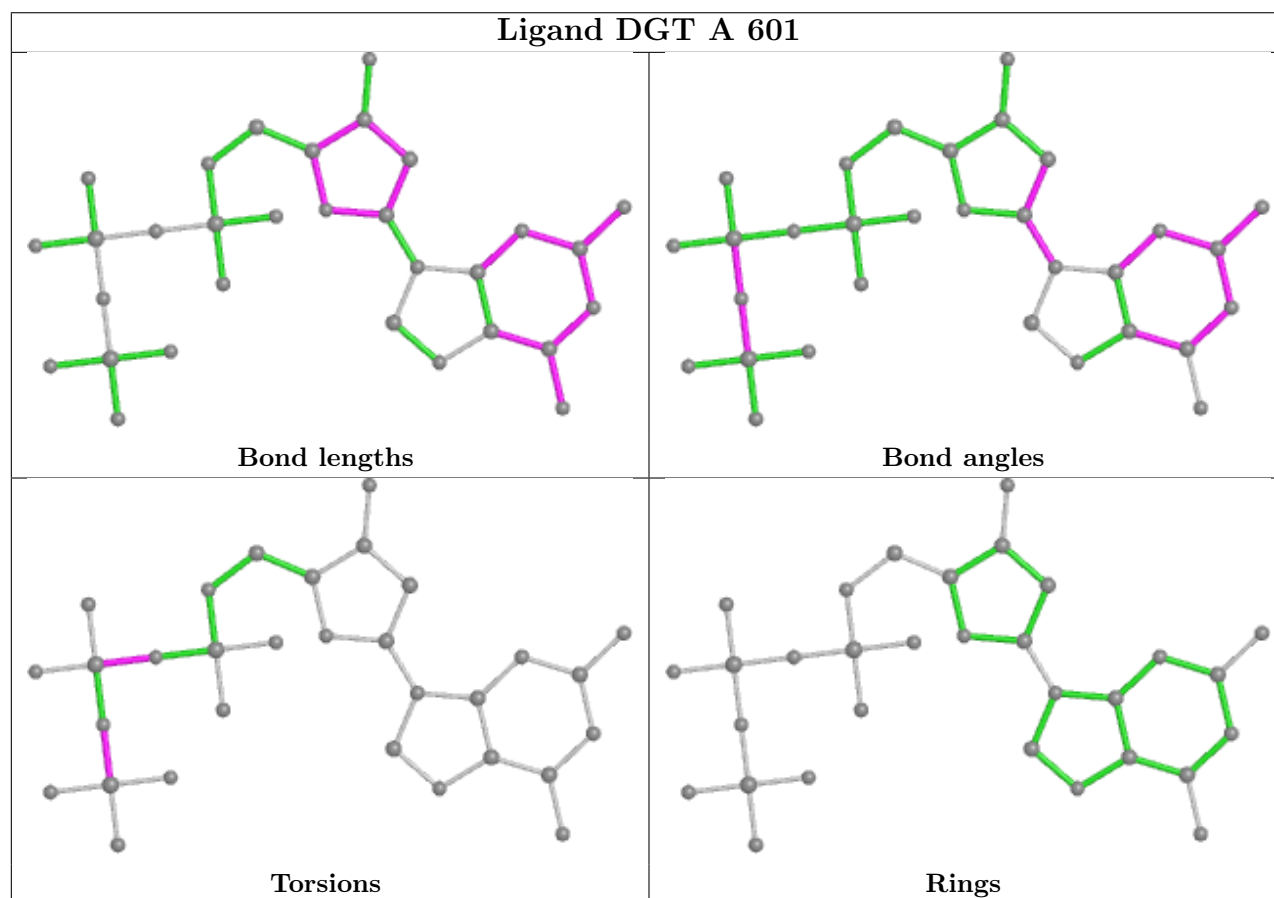
Mol	Chain	Res	Type	Atoms
4	A	601	DGT	PB-O3B-PG-O1G
4	C	601	DGT	PB-O3B-PG-O1G
6	E	101	GOL	C1-C2-C3-O3
6	D	501	GOL	O1-C1-C2-C3
6	D	501	GOL	O1-C1-C2-O2
6	E	101	GOL	O1-C1-C2-C3
6	E	101	GOL	O2-C2-C3-O3
4	A	601	DGT	PA-O3A-PB-O2B
6	E	101	GOL	O1-C1-C2-O2
4	A	601	DGT	PB-O3B-PG-O2G
4	C	601	DGT	PB-O3B-PG-O2G
4	C	601	DGT	PA-O3A-PB-O1B

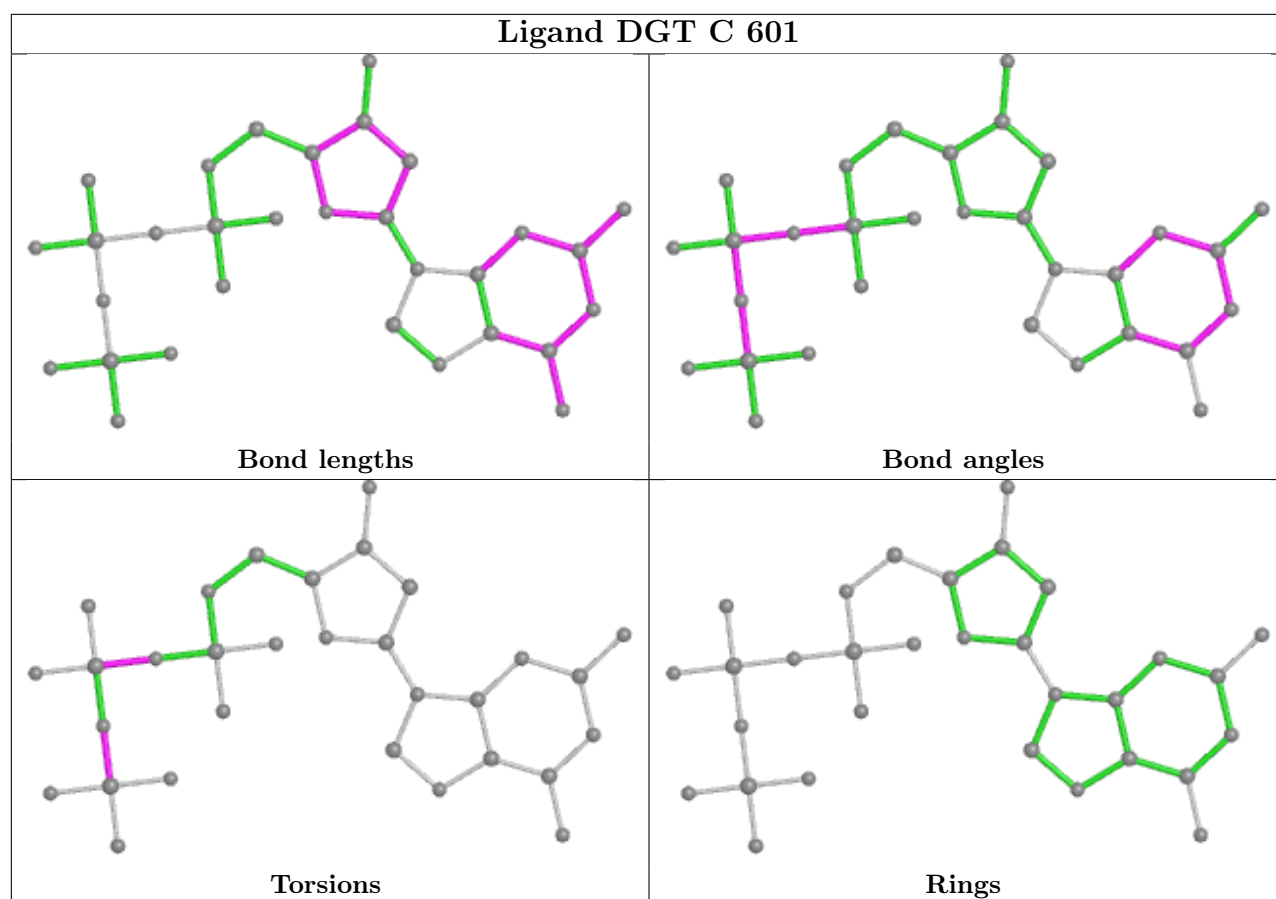
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	501	GOL	1	0
4	C	601	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	552/557 (99%)	0.28	24 (4%) 35 32	33, 56, 97, 156	0
1	C	552/557 (99%)	0.54	59 (10%) 6 4	34, 62, 104, 148	0
2	B	406/444 (91%)	0.92	70 (17%) 1 1	35, 74, 130, 159	0
2	D	406/444 (91%)	0.43	29 (7%) 16 12	34, 60, 104, 168	0
3	E	33/38 (86%)	-0.07	0 100 100	36, 57, 86, 132	0
3	F	36/38 (94%)	0.08	1 (2%) 53 49	38, 65, 120, 160	0
All	All	1985/2078 (95%)	0.50	183 (9%) 9 6	33, 61, 115, 168	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	136	ASN	8.4
2	D	360	ALA	8.3
1	A	139	THR	8.2
2	B	361	HIS	7.4
2	B	357	MET	7.3
2	B	90	VAL	7.0
2	B	301	LEU	7.0
2	B	212	TRP	6.8
1	C	69	THR	6.7
1	C	68	SER	6.7
2	D	67	ASP	6.7
2	D	68	SER	6.5
2	B	88	TRP	6.2
1	C	452	LEU	6.1
1	C	448	ARG	5.9
1	A	140	PRO	5.9
2	D	212	TRP	5.8
2	B	296	THR	5.6
1	A	134	SER	5.6

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Mol	Chain	Res	Type	RSRZ
1	C	553	SER	5.6
1	C	141	GLY	5.5
2	D	231	GLY	5.4
1	A	28	GLU	5.3
2	B	297	GLU	5.2
1	C	449	GLU	5.2
2	B	196	GLY	5.1
1	A	138	GLU	5.0
2	B	312	GLU	5.0
2	B	91	GLN	5.0
1	A	135	ILE	5.0
2	B	168	LEU	5.0
2	D	361	HIS	4.9
2	B	362	THR	4.8
2	D	66	LYS	4.8
2	B	89	GLU	4.7
2	B	359	GLY	4.6
2	B	360	ALA	4.6
2	B	5	ILE	4.6
2	B	7	THR	4.5
2	B	281	LYS	4.5
2	B	92	LEU	4.5
1	C	133	PRO	4.4
2	B	278	GLN	4.4
2	B	252	TRP	4.4
1	C	140	PRO	4.4
2	B	422	LEU	4.4
2	B	195	ILE	4.3
1	C	137	ASN	4.3
2	B	248	GLU	4.3
2	B	250	ASP	4.3
1	C	50	ILE	4.3
2	B	249	LYS	4.3
1	C	469	LEU	4.2
1	C	138	GLU	4.2
2	B	427	TYR	4.2
1	C	136	ASN	4.2
2	D	359	GLY	4.1
1	C	550	LYS	4.1
2	B	303	LEU	4.1
2	D	232	TYR	4.1
1	A	27	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	94	ILE	4.0
2	B	245	VAL	3.9
1	A	69	THR	3.9
1	C	39	THR	3.9
2	B	172	ARG	3.9
2	D	420	PRO	3.7
1	C	450	THR	3.7
2	B	251	SER	3.7
1	C	66	LYS	3.7
2	B	93	GLY	3.6
1	A	67	ASP	3.6
1	A	137	ASN	3.6
1	A	133	PRO	3.6
1	C	457	TYR	3.6
2	B	295	LEU	3.6
2	D	357	MET	3.6
2	D	69	THR	3.5
2	B	87	PHE	3.5
2	B	423	VAL	3.5
1	C	67	ASP	3.5
1	A	66	LYS	3.4
2	B	213	GLY	3.3
1	C	52	PRO	3.3
1	C	552	VAL	3.2
1	C	132	ILE	3.2
2	B	6	GLU	3.2
3	F	18	DT	3.2
2	B	231	GLY	3.2
1	C	33	ALA	3.1
2	B	85	GLN	3.1
1	C	468	PRO	3.1
1	C	139	THR	3.1
1	C	32	LYS	3.1
1	C	542	ILE	3.1
2	D	210	LEU	3.1
1	C	451	LYS	3.1
2	B	424	LYS	3.1
1	C	547	GLN	3.1
1	C	551	LEU	3.1
2	B	95	PRO	3.0
1	A	70	LYS	3.0
2	B	66	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	67	ASP	2.9
1	C	467	VAL	2.9
2	D	208	HIS	2.9
2	B	202	ILE	2.9
2	B	299	ALA	2.9
2	B	279	LEU	2.9
2	D	423	VAL	2.9
2	D	207	GLN	2.8
2	D	209	LEU	2.8
1	C	54	ASN	2.8
1	C	35	VAL	2.8
2	D	427	TYR	2.8
1	A	132	ILE	2.8
2	B	274	ILE	2.8
2	D	166	LYS	2.8
1	C	447	ASN	2.7
1	A	33	ALA	2.7
2	D	174	GLN	2.7
1	C	135	ILE	2.7
2	B	244	ILE	2.7
2	D	213	GLY	2.7
2	B	237	ASP	2.7
2	B	419	THR	2.6
1	C	28	GLU	2.6
1	C	484	LEU	2.6
2	B	209	LEU	2.6
1	C	26	LEU	2.6
1	C	60	VAL	2.6
2	B	418	ASN	2.6
1	C	34	LEU	2.5
2	B	358	LYS	2.5
2	B	238	LYS	2.5
2	B	280	SER	2.5
2	B	305	GLU	2.4
1	A	195	ILE	2.4
2	B	356	ARG	2.4
2	D	173	LYS	2.3
2	D	5	ILE	2.3
2	D	425	LEU	2.3
1	C	71	TRP	2.3
2	B	200	THR	2.3
1	A	36	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	434	ILE	2.3
1	A	25	PRO	2.3
2	B	10	VAL	2.3
1	A	30	LYS	2.3
1	C	142	ILE	2.3
1	C	454	LYS	2.2
1	C	248	GLU	2.2
2	D	172	ARG	2.2
2	D	284	ARG	2.2
2	D	93	GLY	2.2
1	C	53	GLU	2.2
1	C	31	ILE	2.2
1	A	346	PHE	2.2
1	C	22	LYS	2.2
1	C	104	LYS	2.2
1	C	464	GLN	2.2
2	B	68	SER	2.2
1	C	37	ILE	2.2
2	D	211	ARG	2.2
1	A	541	GLY	2.2
2	D	422	LEU	2.2
1	C	470	THR	2.1
2	B	294	PRO	2.1
1	A	68	SER	2.1
2	B	162	SER	2.1
1	C	453	GLY	2.1
1	C	455	ALA	2.1
2	B	275	LYS	2.1
2	B	211	ARG	2.1
2	B	273	GLY	2.1
2	B	282	LEU	2.1
1	C	541	GLY	2.1
1	C	143	ARG	2.1
2	B	118	VAL	2.0
1	C	322	SER	2.0
2	B	334	GLN	2.0
1	C	177	ASP	2.0
1	A	550	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(\AA^2)	Q<0.9
3	OMC	F	2	21/22	0.96	0.18	39,47,54,59	0
3	OMC	E	2	21/22	0.97	0.21	28,43,47,49	0
3	OMC	F	4	21/22	0.97	0.21	33,39,47,52	0
3	OMC	E	4	21/22	0.98	0.20	27,38,44,48	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

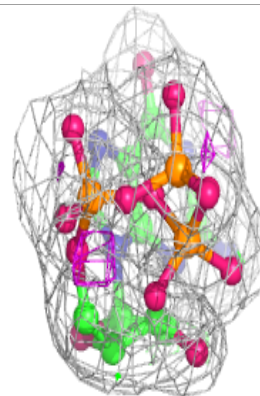
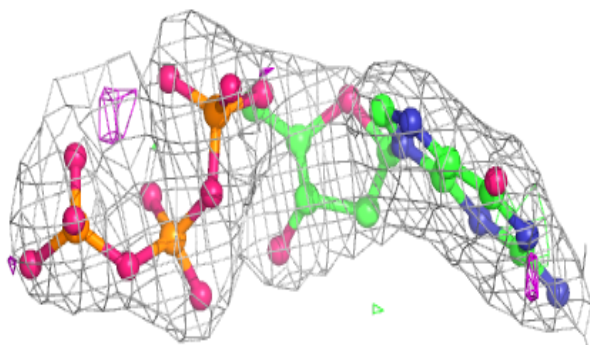
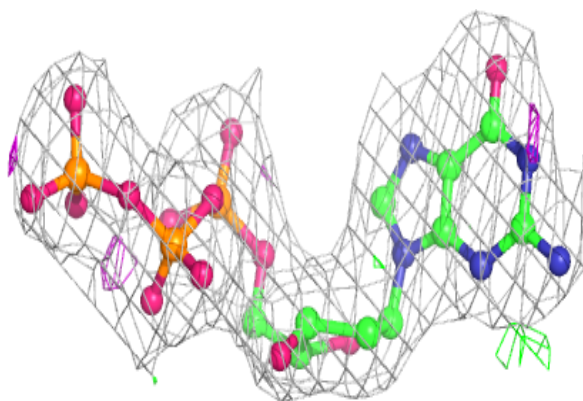
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	MG	C	602	1/1	0.79	0.15	48,48,48,48	0
6	GOL	B	501	6/6	0.91	0.25	69,77,81,90	0
6	GOL	C	603	6/6	0.91	0.22	56,65,69,70	0
6	GOL	D	501	6/6	0.91	0.31	49,52,57,60	0
5	MG	A	602	1/1	0.92	0.06	47,47,47,47	0
4	DGT	C	601	31/31	0.94	0.15	39,52,65,69	0
4	DGT	A	601	31/31	0.95	0.18	32,41,67,75	0
6	GOL	E	101	6/6	0.96	0.29	67,67,68,71	0
6	GOL	B	502	6/6	0.97	0.27	44,47,52,55	0

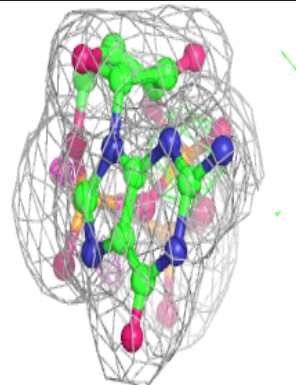
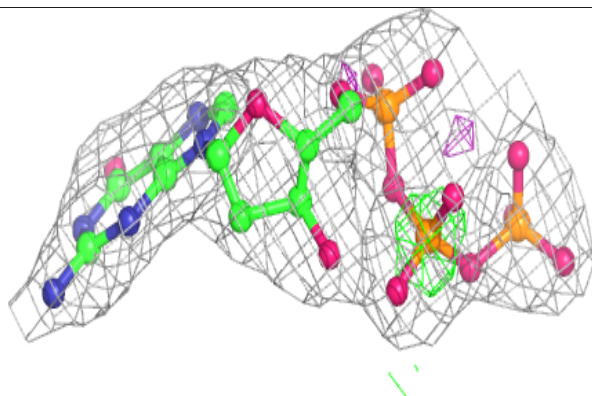
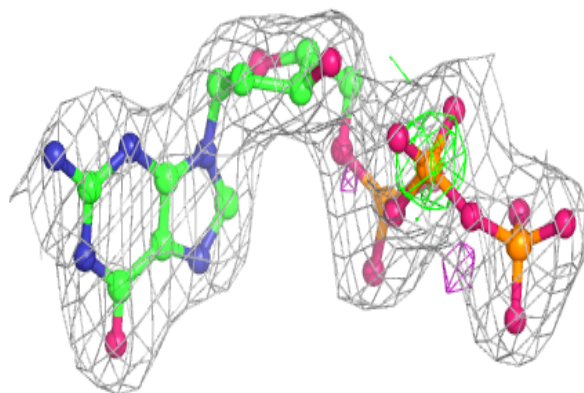
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGT C 601:

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

**Electron density around DGT A 601:**

$2mF_o-DF_c$ (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.