



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:34 PM UTC

PDB ID : 3UO7 / pdb_00003uo7
Title : Crystal structure of Human Thymine DNA Glycosylase Bound to Substrate
5-carboxylcytosine
Authors : Zhang, L.; He, C.
Deposited on : 2011-11-16
Resolution : 3.00 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
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

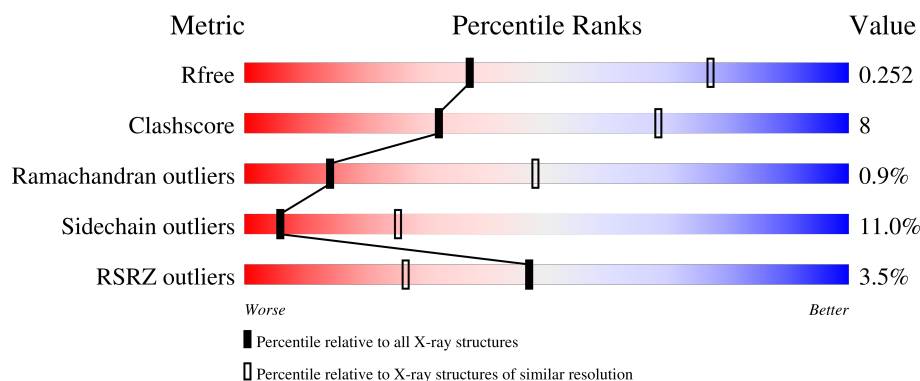
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	C	23	9% 61% 39%
2	D	23	9% 61% 35% .
3	A	201	2% 56% 28% 5% 10%
3	B	201	3% 59% 24% . 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3761 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 DNA chain called 5'-D(*CP*AP*GP*CP*TP*CP*TP*GP*TP*AP*CP*AP*TP*GP*AP*GP*CP*AP*GP*TP*GP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	23	Total	C	N	O	P	0	0	0
			471	224	90	135	22			

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*AP*CP*TP*GP*CP*TP*CP*AP*(1CC)P*GP*TP*AP*CP*AP*GP*AP*GP*CP*TP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	23	Total	C	N	O	P	0	0	0
			467	223	84	138	22			

- Molecule 3 is a protein called G/T mismatch-specific thymine DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	181	Total	C	N	O	S	0	0	0
			1444	932	247	256	9			
3	B	173	Total	C	N	O	S	0	0	0
			1379	892	232	247	8			

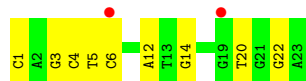
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	SER	-	expression tag	UNP Q13569
A	109	ASN	-	expression tag	UNP Q13569
A	110	ALA	-	expression tag	UNP Q13569
A	140	ALA	ASN	engineered mutation	UNP Q13569
B	108	SER	-	expression tag	UNP Q13569
B	109	ASN	-	expression tag	UNP Q13569
B	110	ALA	-	expression tag	UNP Q13569
B	140	ALA	ASN	engineered mutation	UNP Q13569

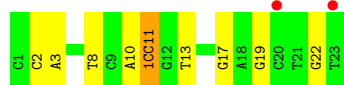
3 Residue-property plots

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.

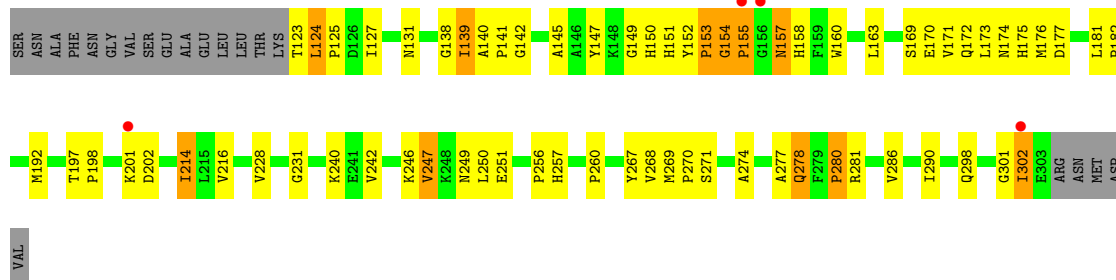
- Molecule 1: 5'-D(*CP*AP*GP*CP*TP*CP*TP*GP*TP*AP*CP*AP*TP*GP*AP*GP*CP*A P*GP*TP*GP*GP*A)-3'



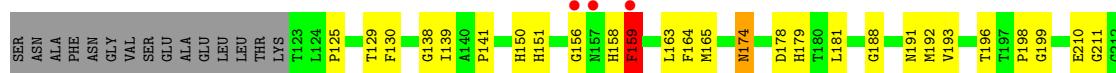
- Molecule 2: 5'-D(*CP*CP*AP*CP*TP*GP*CP*TP*CP*AP*(1CC)P*GP*TP*AP*CP*AP*G P*AP*GP*CP*TP*GP*T)-3'

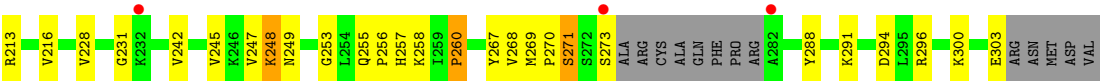


- Molecule 3: G/T mismatch-specific thymine DNA glycosylase



- Molecule 3: G/T mismatch-specific thymine DNA glycosylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	164.35Å 164.35Å 57.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.61 – 3.00 36.61 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.2 (36.61-3.00) 80.8 (36.61-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.227 , 0.280 0.235 , 0.252	Depositor DCC
R_{free} test set	735 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3761	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: 1CC

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	C	0.32	0/529	0.85	0/815
2	D	0.36	0/497	0.84	0/762
3	A	1.99	21/1481 (1.4%)	2.02	24/1997 (1.2%)
3	B	1.96	21/1413 (1.5%)	1.58	27/1904 (1.4%)
All	All	1.71	42/3920 (1.1%)	1.60	51/5478 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	4
3	B	0	4
All	All	0	8

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	138	GLY	CA-C	-10.88	1.44	1.52
3	A	231	GLY	CA-C	-8.14	1.42	1.52
3	A	268	VAL	CA-CB	-7.99	1.44	1.54
3	B	271	SER	C-N	7.78	1.44	1.33
3	B	268	VAL	CA-CB	-7.51	1.45	1.54
3	B	138	GLY	CA-C	-6.75	1.44	1.52
3	B	159	PHE	C-N	-6.61	1.24	1.33
3	B	193	VAL	CA-CB	-6.59	1.46	1.54
3	B	253	GLY	CA-C	-6.46	1.45	1.52
3	A	271	SER	CA-C	-6.39	1.44	1.52
3	B	188	GLY	CA-C	-5.96	1.45	1.52
3	B	199	GLY	N-CA	-5.88	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	141	PRO	CA-CB	-5.81	1.46	1.53
3	A	280	PRO	CA-CB	-5.80	1.45	1.53
3	B	231	GLY	CA-C	-5.77	1.46	1.52
3	A	228	VAL	CA-CB	-5.76	1.47	1.54
3	A	216	VAL	CA-CB	-5.75	1.47	1.54
3	A	290	ILE	CA-CB	-5.70	1.47	1.54
3	A	242	VAL	CA-CB	-5.68	1.48	1.54
3	B	269	MET	CG-SD	-5.68	1.66	1.80
3	B	211	GLY	CA-C	-5.66	1.45	1.52
3	A	256	PRO	CA-CB	-5.65	1.46	1.53
3	B	260	PRO	CA-CB	-5.63	1.46	1.53
3	A	160	TRP	NE1-CE2	-5.62	1.31	1.37
3	A	141	PRO	N-CD	-5.61	1.39	1.47
3	A	269	MET	CA-CB	-5.53	1.47	1.54
3	A	270	PRO	CA-CB	-5.52	1.46	1.53
3	A	182	PRO	CA-CB	-5.42	1.46	1.53
3	B	151	HIS	CE1-NE2	-5.36	1.27	1.32
3	A	267	TYR	C-O	-5.34	1.17	1.23
3	A	257	HIS	CB-CG	-5.33	1.42	1.50
3	B	256	PRO	CA-CB	-5.31	1.46	1.53
3	B	141	PRO	CA-CB	-5.28	1.47	1.53
3	A	256	PRO	N-CD	-5.28	1.40	1.47
3	B	228	VAL	CA-CB	-5.24	1.47	1.54
3	B	269	MET	CA-C	-5.19	1.47	1.52
3	B	141	PRO	N-CD	-5.16	1.40	1.47
3	B	125	PRO	N-CD	-5.14	1.40	1.47
3	B	198	PRO	N-CD	-5.11	1.40	1.47
3	B	256	PRO	N-CD	-5.06	1.40	1.47
3	A	260	PRO	CA-CB	-5.04	1.47	1.53
3	A	228	VAL	C-O	-5.00	1.18	1.24

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	154	GLY	O-C-N	-56.44	100.75	121.07
3	A	154	GLY	CA-C-N	-10.76	108.68	119.76
3	A	154	GLY	C-N-CA	-10.76	108.68	119.76
3	A	247	VAL	N-CA-C	10.01	130.17	109.34
3	B	231	GLY	CA-C-O	-9.87	115.16	122.37
3	B	249	ASN	CA-CB-CG	-9.64	102.96	112.60
3	A	139	ILE	N-CA-C	9.47	129.04	109.34
3	B	271	SER	CB-CA-C	-9.41	94.83	109.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	249	ASN	CA-CB-CG	-8.15	104.45	112.60
3	A	140	ALA	O-C-N	-7.64	115.87	121.83
3	B	130	PHE	CA-CB-CG	-7.54	106.26	113.80
3	A	139	ILE	CB-CA-C	-7.30	99.32	111.29
3	B	300	LYS	CA-C-N	7.12	128.00	120.03
3	B	300	LYS	C-N-CA	7.12	128.00	120.03
3	A	153	PRO	CB-CA-C	6.85	117.67	110.00
3	A	124	LEU	CA-C-N	6.84	126.76	119.85
3	A	124	LEU	C-N-CA	6.84	126.76	119.85
3	B	158	HIS	CA-C-N	6.76	134.46	121.54
3	B	158	HIS	C-N-CA	6.76	134.46	121.54
3	B	294	ASP	CA-CB-CG	-6.64	105.96	112.60
3	B	188	GLY	CA-C-O	-6.52	114.20	121.31
3	A	201	LYS	N-CA-C	-6.46	105.43	113.38
3	A	247	VAL	CB-CA-C	-6.45	100.72	111.29
3	A	131	ASN	CA-CB-CG	-6.44	106.16	112.60
3	B	178	ASP	CA-CB-CG	6.13	118.73	112.60
3	A	181	LEU	O-C-N	-6.09	114.32	121.32
3	B	255	GLN	CA-C-N	6.08	125.76	119.56
3	B	255	GLN	C-N-CA	6.08	125.76	119.56
3	A	158	HIS	CA-CB-CG	-5.98	107.82	113.80
3	B	181	LEU	O-C-N	-5.75	115.37	120.48
3	A	214	ILE	CA-CB-CG1	5.68	120.06	110.40
3	A	298	GLN	CB-CG-CD	-5.62	103.05	112.60
3	A	197	THR	CA-C-N	5.59	126.83	119.84
3	A	197	THR	C-N-CA	5.59	126.83	119.84
3	B	158	HIS	N-CA-C	-5.58	106.46	113.72
3	B	271	SER	N-CA-C	5.54	118.27	109.96
3	A	301	GLY	N-CA-C	5.47	120.40	113.24
3	B	253	GLY	CA-C-O	-5.39	116.91	122.25
3	B	179	HIS	CE1-NE2-CD2	-5.29	103.71	109.00
3	B	288	TYR	CA-CB-CG	-5.28	104.40	113.90
3	B	231	GLY	N-CA-C	-5.27	106.76	112.08
3	B	174	ASN	CA-CB-CG	5.24	117.84	112.60
3	A	242	VAL	N-CA-C	5.13	115.24	110.42
3	B	198	PRO	CA-C-N	-5.13	116.63	122.42
3	B	198	PRO	C-N-CA	-5.13	116.63	122.42
3	B	150	HIS	CE1-NE2-CD2	-5.11	103.89	109.00
3	B	191	ASN	CA-CB-CG	-5.08	107.52	112.60
3	A	257	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
3	B	270	PRO	CA-C-O	-5.04	115.72	121.56
3	B	164	PHE	CA-CB-CG	5.02	118.82	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	177	ASP	CA-CB-CG	-5.01	107.59	112.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	147	TYR	Sidechain
3	A	154	GLY	Peptide
3	A	155	PRO	Peptide
3	A	281	ARG	Sidechain
3	B	156	GLY	Peptide
3	B	159	PHE	Mainchain
3	B	267	TYR	Sidechain
3	B	296	ARG	Sidechain

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	C	471	0	257	15	0
2	D	467	0	260	21	0
3	A	1444	0	1455	38	1
3	B	1379	0	1389	5	1
All	All	3761	0	3361	54	1

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 (54) 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)
3:A:246:LYS:O	3:A:247:VAL:HG12	1.52	1.07
3:A:247:VAL:HG22	3:A:247:VAL:O	1.62	0.97
2:D:11:1CC:H10	2:D:11:1CC:H3	1.57	0.87
2:D:13:DT:H1'	3:A:278:GLN:NE2	1.89	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:246:LYS:O	3:A:247:VAL:CG1	2.24	0.85
3:A:153:PRO:HB3	3:A:175:HIS:CG	2.13	0.84
2:D:13:DT:C1'	3:A:278:GLN:NE2	2.45	0.80
3:A:155:PRO:HA	3:A:157:ASN:H	1.47	0.79
2:D:11:1CC:OP1	3:A:157:ASN:ND2	2.17	0.77
3:A:246:LYS:C	3:A:247:VAL:HG12	2.16	0.71
1:C:6:DC:H42	2:D:17:DG:H1	1.40	0.68
2:D:10:DA:N3	3:A:274:ALA:HB3	2.08	0.68
2:D:13:DT:O2	3:A:278:GLN:NE2	2.22	0.63
3:B:271:SER:C	3:B:273:SER:H	2.06	0.62
3:A:152:TYR:N	3:A:153:PRO:HD3	2.13	0.61
1:C:12:DA:C4	3:A:277:ALA:CB	2.83	0.61
1:C:5:DT:OP2	3:A:246:LYS:NZ	2.33	0.61
2:D:13:DT:H1'	3:A:278:GLN:HE22	1.65	0.59
3:B:139:ILE:H	3:B:139:ILE:HD12	1.68	0.58
2:D:11:1CC:H4	3:A:142:GLY:HA3	1.86	0.57
3:A:149:GLY:O	3:A:150:HIS:CD2	2.58	0.56
3:A:124:LEU:HD12	3:A:125:PRO:HD2	1.86	0.56
1:C:22:DG:N2	2:D:2:DC:O2	2.40	0.55
3:A:155:PRO:HA	3:A:157:ASN:N	2.20	0.54
2:D:10:DA:C2	3:A:274:ALA:HB1	2.43	0.53
1:C:4:DC:H42	2:D:19:DG:H1	1.56	0.53
2:D:10:DA:N3	3:A:274:ALA:CB	2.76	0.49
1:C:12:DA:C4	3:A:277:ALA:HB2	2.47	0.49
3:A:247:VAL:O	3:A:247:VAL:HG13	2.12	0.49
1:C:1:DC:N4	2:D:22:DG:O6	2.46	0.49
2:D:13:DT:O4'	3:A:278:GLN:NE2	2.46	0.48
1:C:12:DA:N3	3:A:277:ALA:HA	2.29	0.48
3:A:152:TYR:N	3:A:153:PRO:CD	2.78	0.47
2:D:8:DT:H5''	2:D:8:DT:H6	1.79	0.47
2:D:2:DC:H2''	2:D:3:DA:C8	2.49	0.46
3:A:153:PRO:HB3	3:A:175:HIS:CB	2.45	0.46
3:A:174:ASN:ND2	3:A:174:ASN:H	2.13	0.46
1:C:3:DG:H2'	1:C:4:DC:H6	1.81	0.46
1:C:12:DA:C4	3:A:277:ALA:HB1	2.50	0.45
2:D:10:DA:C2	3:A:274:ALA:CB	3.00	0.45
2:D:11:1CC:C21	3:A:145:ALA:HB2	2.48	0.43
3:A:151:HIS:C	3:A:153:PRO:HD3	2.43	0.43
1:C:12:DA:C5	3:A:277:ALA:HB2	2.54	0.43
1:C:20:DT:C6	1:C:20:DT:H5'	2.53	0.43
3:A:127:ILE:HG22	3:A:127:ILE:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:153:PRO:HB3	3:A:175:HIS:CD2	2.53	0.42
1:C:14:DG:C2	2:D:10:DA:C2	3.08	0.42
3:A:151:HIS:HB3	3:A:152:TYR:HD2	1.84	0.42
3:B:271:SER:C	3:B:273:SER:N	2.76	0.42
3:B:248:LYS:CB	3:B:248:LYS:NZ	2.83	0.42
1:C:12:DA:H2	3:A:274:ALA:O	2.04	0.41
1:C:1:DC:H42	2:D:22:DG:H1	1.68	0.40
3:A:247:VAL:HG21	3:A:250:LEU:HD13	2.04	0.40
3:B:163:LEU:HD12	3:B:163:LEU:HA	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:302:ILE:CD1	3:B:257:HIS:NE2[6_554]	2.01	0.19

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	
3	A	179/201 (89%)	170 (95%)	7 (4%)	2 (1%)	11	43
3	B	169/201 (84%)	156 (92%)	12 (7%)	1 (1%)	21	56
All	All	348/402 (87%)	326 (94%)	19 (6%)	3 (1%)	14	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	240	LYS
3	B	159	PHE
3	A	139	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	
3	A	158/175 (90%)	140 (89%)	18 (11%)	5	24
3	B	152/175 (87%)	136 (90%)	16 (10%)	6	27
All	All	310/350 (89%)	276 (89%)	34 (11%)	6	25

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	123	THR
3	A	157	ASN
3	A	163	LEU
3	A	169	SER
3	A	170	GLU
3	A	171	VAL
3	A	172	GLN
3	A	173	LEU
3	A	176	MET
3	A	192	MET
3	A	198	PRO
3	A	202	ASP
3	A	214	ILE
3	A	251	GLU
3	A	278	GLN
3	A	280	PRO
3	A	286	VAL
3	A	302	ILE
3	B	129	THR
3	B	165	MET
3	B	174	ASN
3	B	192	MET
3	B	196	THR
3	B	210	GLU
3	B	213	ARG
3	B	216	VAL
3	B	242	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	245	VAL
3	B	247	VAL
3	B	248	LYS
3	B	258	LYS
3	B	260	PRO
3	B	291	LYS
3	B	303	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	150	HIS
3	A	151	HIS
3	A	157	ASN
3	A	174	ASN
3	A	191	ASN
3	A	257	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	1CC	D	11	2	20,23,24	1.09	1 (5%)	25,33,36	0.85	1 (4%)

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
2	1CC	D	11	2	-	1/11/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	11	1CC	C5-C4	-2.40	1.39	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	11	1CC	C1'-N1-C6	2.06	124.20	120.74

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	11	1CC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	11	1CC	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	C	23/23 (100%)	1.08	2 (8%) 16 8	87, 109, 147, 152	0
2	D	22/23 (95%)	0.97	2 (9%) 15 8	72, 119, 145, 153	0
3	A	181/201 (90%)	0.03	4 (2%) 62 39	45, 67, 84, 116	0
3	B	173/201 (86%)	0.10	6 (3%) 47 27	47, 67, 90, 106	0
All	All	399/448 (89%)	0.17	14 (3%) 47 27	45, 69, 120, 153	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	155	PRO	3.6
2	D	23	DT	3.2
3	B	232	LYS	3.1
3	B	273	SER	3.1
3	A	302	ILE	2.6
3	B	282	ALA	2.6
3	B	159	PHE	2.5
3	A	201	LYS	2.5
3	B	156	GLY	2.3
1	C	19	DG	2.3
3	B	157	ASN	2.2
2	D	20	DC	2.2
3	A	156	GLY	2.1
1	C	6	DC	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($\text{\AA}^2$)	Q<0.9
2	1CC	D	11	22/23	0.96	0.10	57,64,68,69	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.