



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 08:13 AM UTC

PDB ID : 3TAE / pdb_00003tae
Title : 5-hydroxycytosine paired with dAMP in RB69 gp43
Authors : Zahn, K.E.
Deposited on : 2011-08-04
Resolution : 2.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

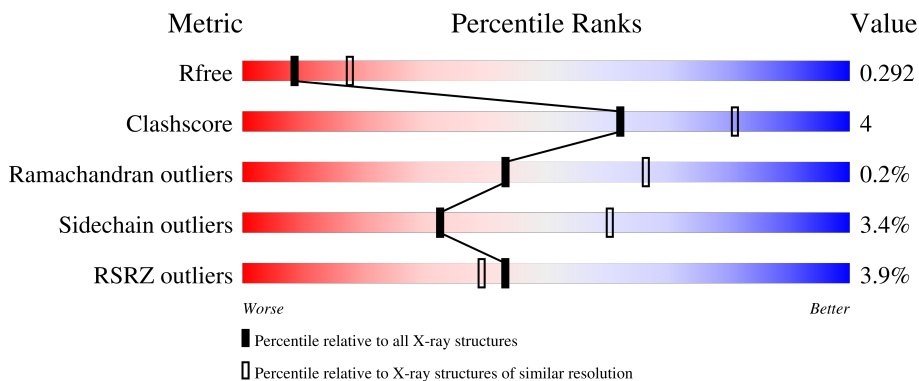
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	E	18	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 56%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">6% 56% 39% 6%</p>
1	G	18	<div style="display: flex; align-items: center;"> <div style="width: 44%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">44% 44% 6% 6%</p>
1	I	18	<div style="display: flex; align-items: center;"> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">72% 17% 6% 6%</p>
1	K	18	<div style="display: flex; align-items: center;"> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">72% 11% 17%</p>
2	F	15	<div style="display: flex; align-items: center;"> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange;"></div> </div> <p style="text-align: center;">60% 33% 7%</p>

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Mol	Chain	Length	Quality of chain
2	H	15	
2	J	15	
2	L	15	
3	A	906	
3	B	906	
3	C	906	
3	D	906	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	5OC	I	3	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 32066 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 DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			366	173	70	106	17			
1	I	17	Total	C	N	O	P	0	0	0
			350	164	67	102	17			
1	G	17	Total	C	N	O	P	0	0	1
			313	145	59	93	16			
1	K	15	Total	C	N	O	P	0	0	1
			271	125	52	80	14			

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			286	135	51	86	14			
2	J	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			
2	H	13	Total	C	N	O	P	0	0	0
			263	126	48	77	12			
2	L	11	Total	C	N	O	P	0	0	0
			223	107	40	66	10			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	903	Total	C	N	O	S	0	0	0
			7374	4737	1226	1378	33			
3	B	901	Total	C	N	O	S	0	0	0
			7355	4724	1224	1374	33			
3	C	903	Total	C	N	O	S	0	0	0
			7374	4737	1226	1378	33			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	898	7328	4706	1221	1369	32	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087
A	904	HIS	-	expression tag	UNP Q38087
A	905	HIS	-	expression tag	UNP Q38087
A	906	HIS	-	expression tag	UNP Q38087
B	222	ALA	ASP	engineered mutation	UNP Q38087
B	327	ALA	ASP	engineered mutation	UNP Q38087
B	904	HIS	-	expression tag	UNP Q38087
B	905	HIS	-	expression tag	UNP Q38087
B	906	HIS	-	expression tag	UNP Q38087
C	222	ALA	ASP	engineered mutation	UNP Q38087
C	327	ALA	ASP	engineered mutation	UNP Q38087
C	904	HIS	-	expression tag	UNP Q38087
C	905	HIS	-	expression tag	UNP Q38087
C	906	HIS	-	expression tag	UNP Q38087
D	222	ALA	ASP	engineered mutation	UNP Q38087
D	327	ALA	ASP	engineered mutation	UNP Q38087
D	904	HIS	-	expression tag	UNP Q38087
D	905	HIS	-	expression tag	UNP Q38087
D	906	HIS	-	expression tag	UNP Q38087

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	3	Total O 3 3	0	0
5	F	2	Total O 2 2	0	0
5	I	6	Total O 6 6	0	0
5	J	4	Total O 4 4	0	0
5	G	1	Total O 1 1	0	0
5	H	1	Total O 1 1	0	0
5	A	101	Total O 101 101	0	0
5	B	47	Total O 47 47	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	71	Total O 71 71	0	0
5	D	4	Total O 4 4	0	0

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.

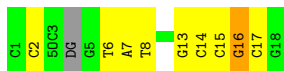
- Molecule 1: DNA (5'-D(*CP*CP*(5OC)P*GP*GP*TP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')



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



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



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

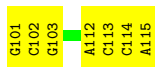


- Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')

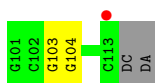
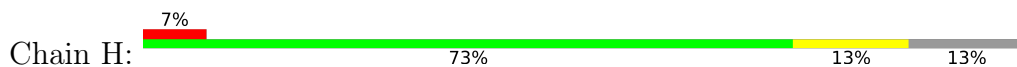




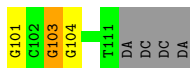
- Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')



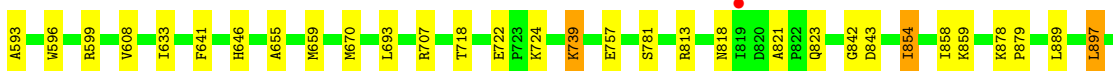
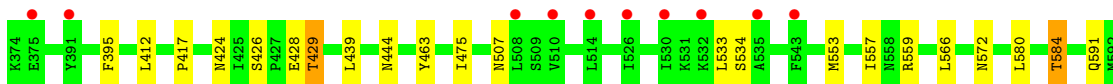
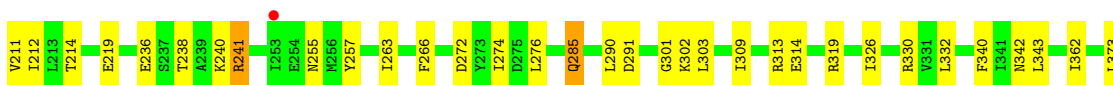
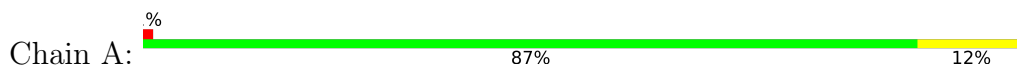
- Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')



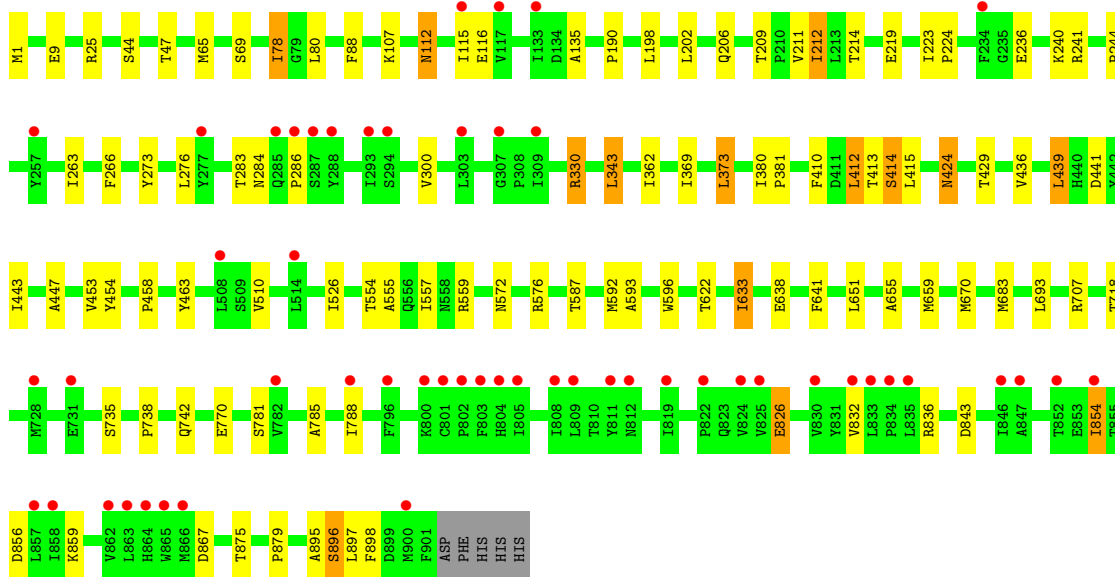
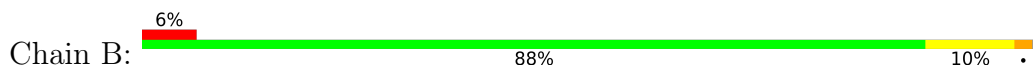
- Molecule 2: DNA (5'-D(*GP*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*AP*CP*CP*A)-3')



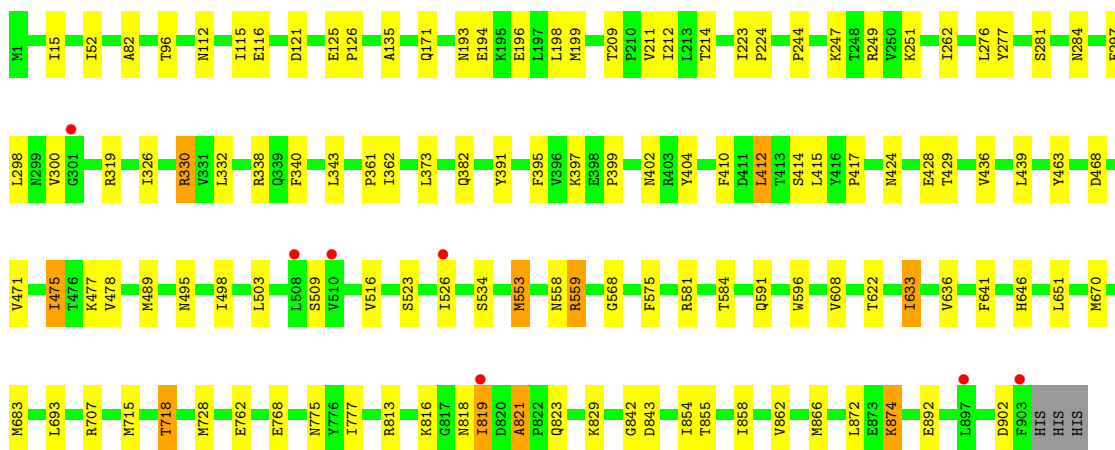
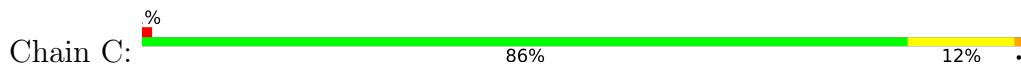
- Molecule 3: DNA polymerase



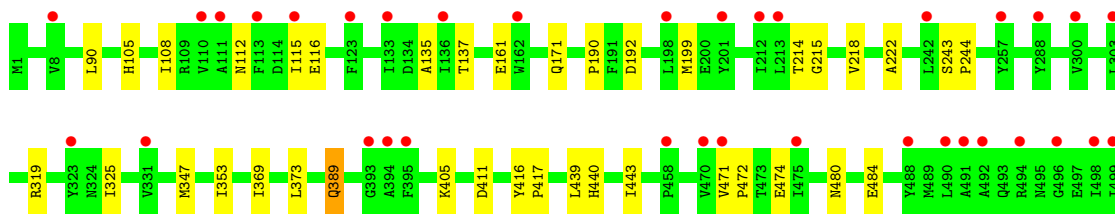
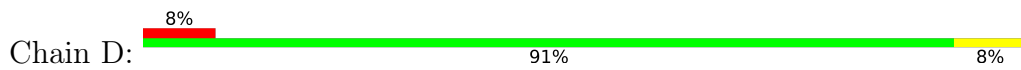
- Molecule 3: DNA polymerase

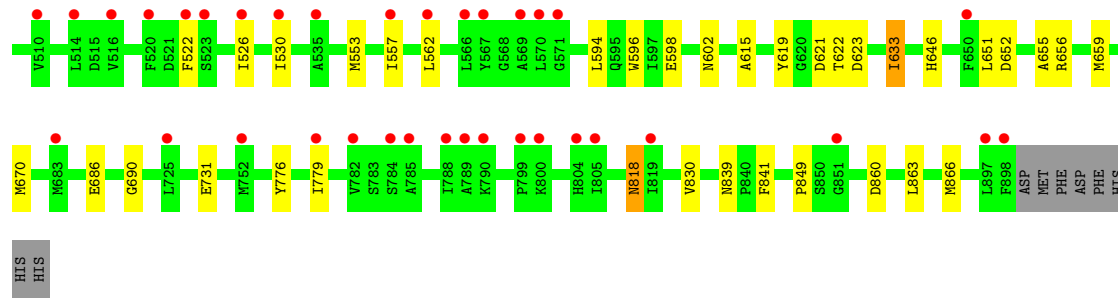


• Molecule 3: DNA polymerase



• Molecule 3: DNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	133.27Å 123.71Å 165.90Å 90.00° 95.97° 90.00°	Depositor
Resolution (Å)	30.00 – 2.71 30.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-2.71) 98.0 (30.00-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.72Å)	Xtrriage
Refinement program	REFMAC 5.6.0116, CNS	Depositor
R, R_{free}	0.224 , 0.268 (Not available) , 0.292	Depositor DCC
R_{free} test set	13797 reflections (9.48%)	wwPDB-VP
Wilson B-factor (Å ²)	67.1	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32066	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: SO4, 5OC

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	E	0.28	0/387	0.68	0/593
1	G	0.28	0/345	0.63	1/529 (0.2%)
1	I	0.31	0/369	0.70	0/565
1	K	0.28	0/298	0.56	0/456
2	F	0.28	0/319	0.74	1/491 (0.2%)
2	H	0.28	0/294	0.66	0/452
2	J	0.30	0/339	0.72	0/521
2	L	0.28	0/249	0.81	2/383 (0.5%)
3	A	0.53	0/7555	0.80	2/10209 (0.0%)
3	B	0.52	0/7535	0.77	0/10182
3	C	0.53	0/7555	0.79	2/10209 (0.0%)
3	D	0.51	0/7507	0.76	0/10145
All	All	0.51	0/32752	0.77	8/44735 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	103	DG	P-O3'-C3'	6.03	129.25	120.20
3	C	821	ALA	N-CA-C	-5.58	102.75	109.83
3	A	189	MET	CA-C-N	5.47	125.67	120.31
3	A	189	MET	C-N-CA	5.47	125.67	120.31
2	L	101	DG	P-O3'-C3'	5.18	127.97	120.20

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	E	366	0	201	5	0
1	G	313	0	168	7	0
1	I	350	0	189	11	0
1	K	271	0	145	2	0
2	F	286	0	158	6	0
2	H	263	0	148	1	0
2	J	303	0	170	8	0
2	L	223	0	126	1	0
3	A	7374	0	7267	67	0
3	B	7355	0	7254	60	0
3	C	7374	0	7267	61	0
3	D	7328	0	7232	36	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	F	5	0	0	0	0
4	H	5	0	0	0	0
5	A	101	0	0	3	0
5	B	47	0	0	0	0
5	C	71	0	0	0	0
5	D	4	0	0	0	0
5	E	3	0	0	0	0
5	F	2	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	6	0	0	0	0
5	J	4	0	0	0	0
All	All	32066	0	30325	252	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 4.

The worst 5 of 252 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:I:2:DC:H4'	1:I:3:5OC:H5'A	1.23	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3:5OC:O2	3:C:568:GLY:HA3	1.47	1.13
1:I:2:DC:H4'	1:I:3:5OC:C5'	1.91	0.99
2:F:112:DA:H2''	2:F:113:DC:H5''	1.49	0.94
1:G:2:DC:H2'	1:G:2:DC:O2	1.73	0.87

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
3	A	901/906 (99%)	875 (97%)	25 (3%)	1 (0%)	48 72
3	B	899/906 (99%)	858 (95%)	38 (4%)	3 (0%)	36 59
3	C	901/906 (99%)	873 (97%)	27 (3%)	1 (0%)	48 72
3	D	896/906 (99%)	855 (95%)	39 (4%)	2 (0%)	43 66
All	All	3597/3624 (99%)	3461 (96%)	129 (4%)	7 (0%)	43 66

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	819	ILE
3	D	192	ASP
3	D	622	THR
3	B	896	SER
3	B	424	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	800/803 (100%)	764 (96%)	36 (4%)	24	50
3	B	798/803 (99%)	767 (96%)	31 (4%)	28	56
3	C	800/803 (100%)	768 (96%)	32 (4%)	28	55
3	D	795/803 (99%)	784 (99%)	11 (1%)	59	80
All	All	3193/3212 (99%)	3083 (97%)	110 (3%)	32	60

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	587	THR
3	C	199	MET
3	D	860	ASP
3	D	115	ILE
3	B	693	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	504	HIS
3	D	602	ASN
3	C	285	GLN
3	D	485	HIS
3	D	786	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	5OC	I	3	1	18,21,22	0.41	0	24,30,33	0.93	1 (4%)
1	5OC	K	3	1	0,3,22	-	-	0,3,33	-	-
1	5OC	G	3	1	0,3,22	-	-	0,3,33	-	-
1	5OC	E	3	1	18,21,22	0.39	0	24,30,33	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
1	5OC	I	3	1	-	0/7/21/22	0/2/2/2
1	5OC	E	3	1	-	2/7/21/22	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	3	5OC	O5-C5-C4	3.74	122.60	114.82
1	E	3	5OC	O5-C5-C4	3.69	122.51	114.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	3	5OC	C3'-C4'-C5'-O5'
1	E	3	5OC	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	3	5OC	7	0
1	E	3	5OC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z > 2$
4	SO4	F	3	-	4,4,4	0.44	0	6,6,6	0.06	0
4	SO4	C	907	-	4,4,4	0.44	0	6,6,6	0.10	0
4	SO4	H	2	-	4,4,4	0.44	0	6,6,6	0.07	0
4	SO4	B	907	-	4,4,4	0.45	0	6,6,6	0.14	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3:5OC	OP2	4:DG	P	7.44
1	E	3:5OC	OP2	4:DG	P	6.90

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	E	17/18 (94%)	-0.00	1 (5%) 28 25	57, 89, 126, 143	0
1	G	16/18 (88%)	0.61	0 100 100	62, 114, 138, 155	0
1	I	16/18 (88%)	-0.65	0 100 100	37, 50, 70, 94	0
1	K	14/18 (77%)	0.59	0 100 100	53, 162, 197, 200	0
2	F	15/15 (100%)	0.07	0 100 100	72, 87, 138, 141	0
2	H	13/15 (86%)	0.79	1 (7%) 19 17	94, 116, 140, 141	0
2	J	15/15 (100%)	-0.53	0 100 100	36, 61, 87, 87	0
2	L	11/15 (73%)	0.68	0 100 100	158, 169, 173, 174	0
3	A	903/906 (99%)	-0.20	13 (1%) 73 71	30, 54, 146, 263	0
3	B	901/906 (99%)	0.37	53 (5%) 28 25	34, 80, 218, 286	0
3	C	903/906 (99%)	-0.14	7 (0%) 82 81	28, 62, 135, 197	0
3	D	898/906 (99%)	0.73	70 (7%) 19 17	84, 135, 213, 253	0
All	All	3722/3756 (99%)	0.19	145 (3%) 43 39	28, 78, 201, 286	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	862	VAL	6.8
3	B	286	PRO	5.4
3	A	508	LEU	5.2
3	B	802	PRO	4.9
3	B	805	ILE	4.8

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
1	5OC	E	3	20/21	0.31	0.14	148,155,160,160	0
1	5OC	K	3	4/21	0.50	0.14	123,130,134,136	0
1	5OC	G	3	4/21	0.82	0.10	108,111,111,113	0
1	5OC	I	3	20/21	0.86	0.13	78,91,100,100	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
4	SO4	F	3	5/5	0.75	0.09	121,121,123,124	0
4	SO4	H	2	5/5	0.79	0.10	126,128,128,130	0
4	SO4	B	907	5/5	0.86	0.20	83,85,88,88	0
4	SO4	C	907	5/5	0.88	0.15	112,115,116,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.