



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 10:40 AM BST

PDB ID : 3TAB  
Title : 5-hydroxycytosine paired with dGMP in RB69 gp43  
Authors : Zahn, K.E.  
Deposited on : 2011-08-03  
Resolution : 2.80 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](mailto: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.

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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 : 2.13  
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) : 2.13

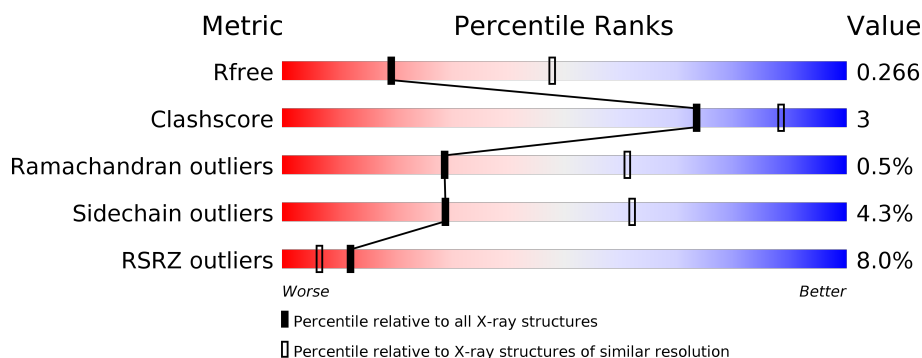
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	906	<div> <div>8%</div> <div>86% 13%</div> </div>
1	B	906	<div> <div>5%</div> <div>89% 9%</div> </div>
1	C	906	<div> <div>4%</div> <div>87% 12%</div> </div>
1	D	906	<div> <div>15%</div> <div>89% 10%</div> </div>
2	E	18	<div> <div>83% 11% 6%</div> </div>
2	G	18	<div> <div>61% 33% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	18	<div><div></div><div>83%17%</div></div>
2	K	18	<div><div></div><div>17%67%28%6%</div></div>
3	F	15	<div><div></div><div>7%80%20%</div></div>
3	H	15	<div><div></div><div>80%13%7%</div></div>
3	J	15	<div><div></div><div>73%27%</div></div>
3	L	15	<div><div></div><div>27%80%20%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32383 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 DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	904	Total	C	N	O	S	0	0	0
			7384	4743	1229	1379	33			
1	B	904	Total	C	N	O	S	0	0	0
			7384	4743	1229	1379	33			
1	C	903	Total	C	N	O	S	0	0	0
			7374	4737	1226	1378	33			
1	D	903	Total	C	N	O	S	0	0	0
			7374	4737	1226	1378	33			

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

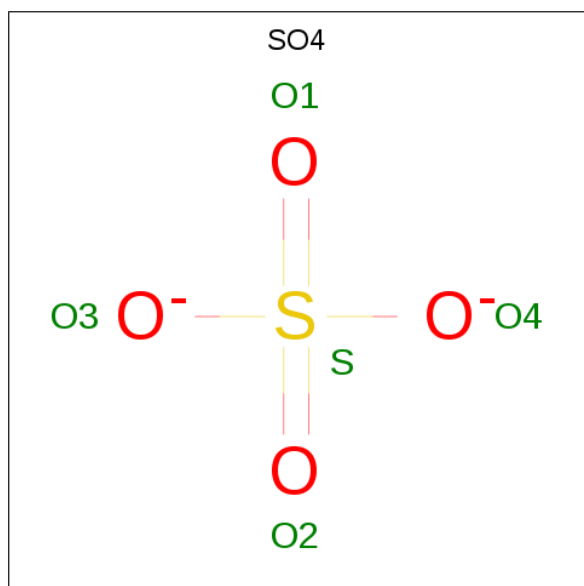
- Molecule 2 is a DNA chain called DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			366	173	70	106	17			
2	G	18	Total	C	N	O	P	0	0	0
			370	173	70	109	18			
2	I	18	Total	C	N	O	P	0	0	0
			366	173	70	106	17			
2	K	18	Total	C	N	O	P	0	0	0
			366	173	70	106	17			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			
3	H	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			
3	J	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			
3	L	15	Total	C	N	O	P	0	0	0
			304	145	56	89	14			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	25	Total O 25 25	0	0
5	E	1	Total O 1 1	0	0
5	B	71	Total O 71 71	0	0
5	G	6	Total O 6 6	0	0
5	H	6	Total O 6 6	0	0
5	C	39	Total O 39 39	0	0
5	I	4	Total O 4 4	0	0
5	D	10	Total O 10 10	0	0
5	K	1	Total O 1 1	0	0

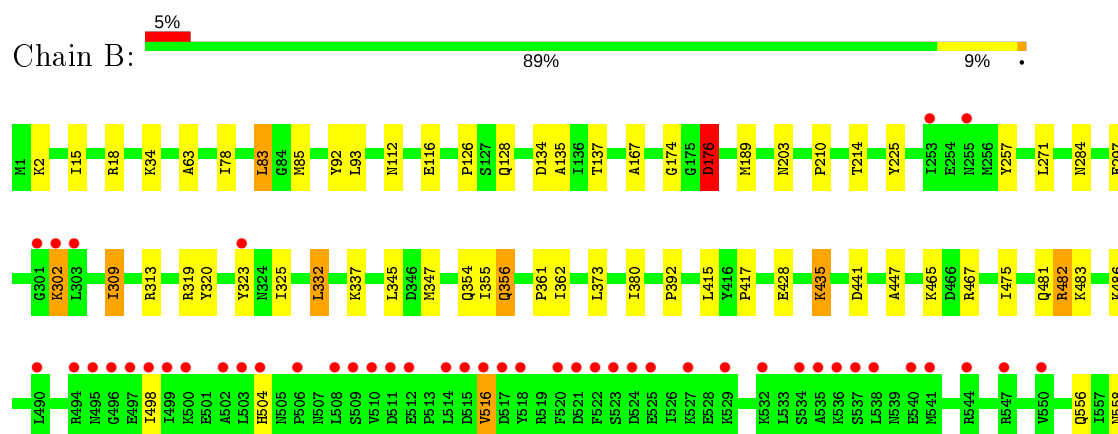
### 3 Residue-property plots

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: DNA polymerase

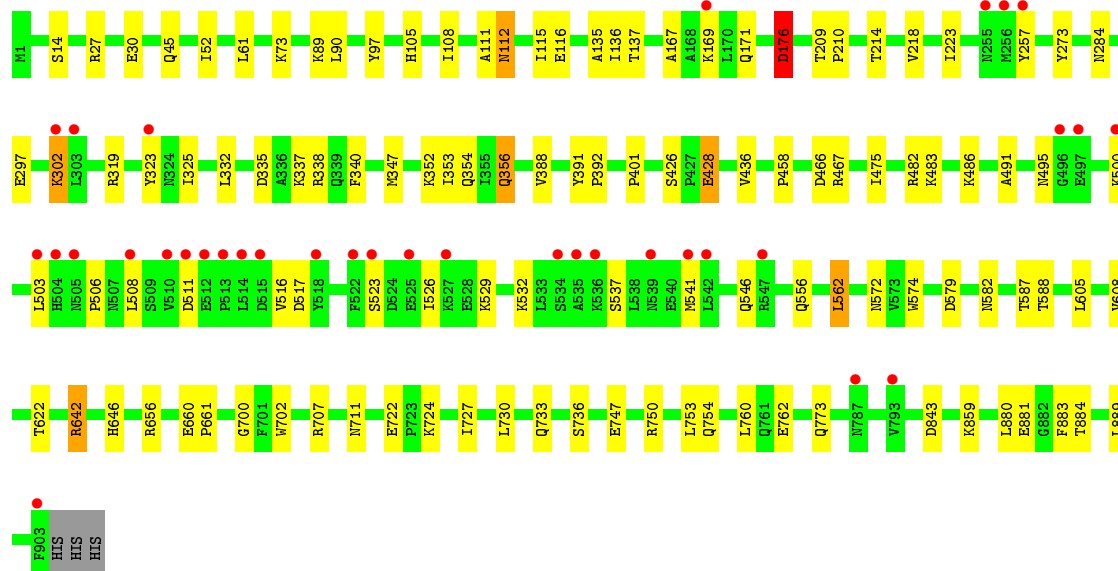
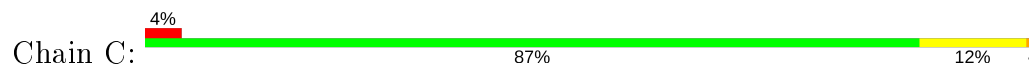


#### • Molecule 1: DNA polymerase

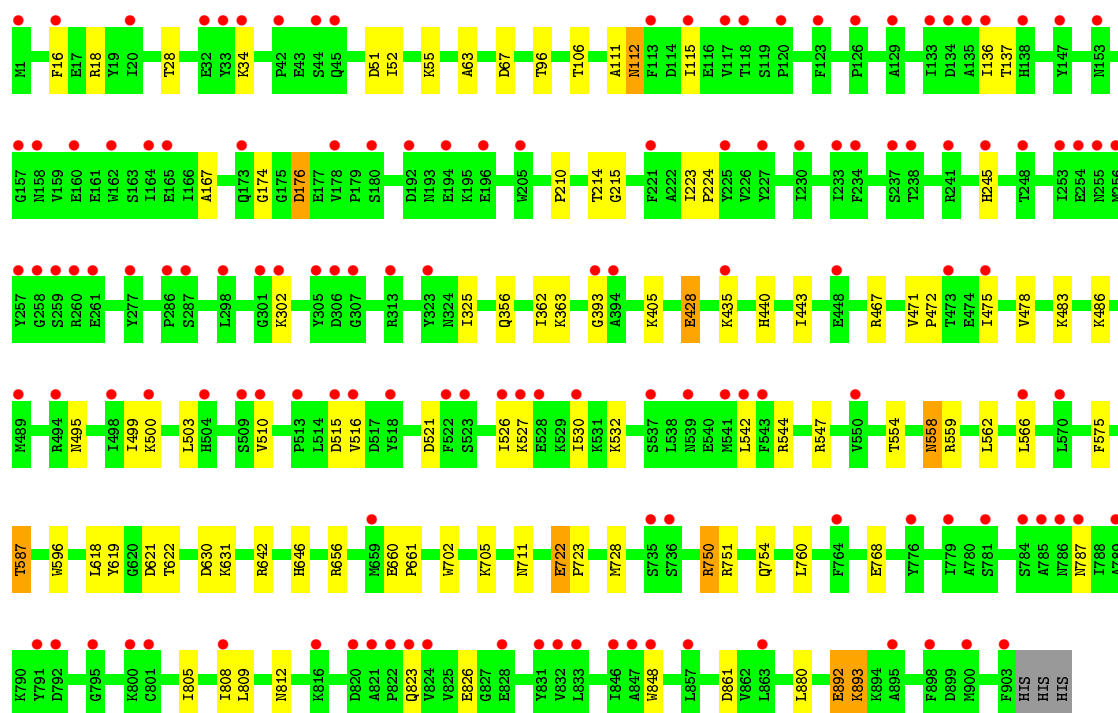
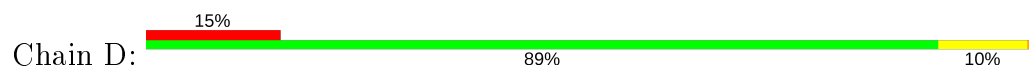




• Molecule 1: DNA polymerase




• Molecule 1: DNA polymerase





- Molecule 2: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain E: 




- Molecule 2: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain G: 



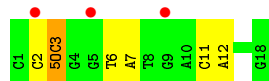
- Molecule 2: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain I: 




- Molecule 2: DNA (5'-D(\*CP\*CP\*(5OC)P\*GP\*GP\*TP\*AP\*TP\*GP\*AP\*CP\*AP\*GP\*CP\*CP\*GP\*CP\*G)-3')

Chain K: 




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

Chain F: 



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

Chain H: 




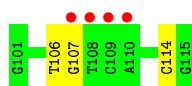
- Molecule 3: DNA (5'-D(\*GP\*CP\*GP\*GP\*CP\*TP\*GP\*TP\*CP\*AP\*TP\*AP\*CP\*CP\*G)-3')

Chain J:  73% 27%



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

Chain L:  27% 80% 20%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.76Å 121.93Å 168.91Å 90.00° 96.63° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 49.48 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.80) 100.0 (49.48-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0116, CNS	Depositor
R, $R_{free}$	0.232 , 0.281 0.220 , 0.266	Depositor DCC
$R_{free}$ test set	12706 reflections (9.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 5OC, SO4

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	2/7566 (0.0%)	0.48	0/10224
1	B	0.41	1/7566 (0.0%)	0.50	0/10224
1	C	0.41	1/7555 (0.0%)	0.49	0/10209
1	D	0.41	3/7555 (0.0%)	0.46	0/10209
2	E	0.22	0/387	0.75	0/593
2	G	0.54	1/391 (0.3%)	0.77	0/597
2	I	0.23	0/387	0.78	0/593
2	K	0.21	0/387	0.78	0/593
3	F	0.21	0/340	0.77	0/523
3	H	0.24	0/340	0.83	1/523 (0.2%)
3	J	0.28	0/340	0.82	1/523 (0.2%)
3	L	0.20	0/340	0.83	0/523
All	All	0.40	8/33154 (0.0%)	0.52	2/45334 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	DC	OP3-P	-9.49	1.49	1.61
1	C	702	TRP	CD2-CE2	5.15	1.47	1.41
1	B	848	TRP	CD2-CE2	5.07	1.47	1.41
1	A	702	TRP	CD2-CE2	5.07	1.47	1.41
1	D	596	TRP	CD2-CE2	5.04	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	101	DG	P-O3'-C3'	5.70	126.54	119.70
3	H	101	DG	P-O3'-C3'	5.23	125.97	119.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7384	0	7274	59	0
1	B	7384	0	7274	50	0
1	C	7374	0	7267	46	0
1	D	7374	0	7267	39	0
2	E	366	0	201	3	0
2	G	370	0	200	6	0
2	I	366	0	201	2	0
2	K	366	0	201	4	0
3	F	304	0	170	3	0
3	H	304	0	170	2	0
3	J	304	0	170	2	0
3	L	304	0	170	3	0
4	E	5	0	0	0	0
4	G	5	0	0	0	0
4	I	5	0	0	0	0
4	K	5	0	0	0	0
5	A	25	0	0	4	0
5	B	71	0	0	0	0
5	C	39	0	0	0	0
5	D	10	0	0	1	0
5	E	1	0	0	0	0
5	G	6	0	0	0	0
5	H	6	0	0	0	0
5	I	4	0	0	0	0
5	K	1	0	0	0	0
All	All	32383	0	30565	207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 207 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:D:112:ASN:HB3	1:D:214:THR:HG23	1.45	0.94
1:A:112:ASN:HB3	1:A:214:THR:HG23	1.53	0.91
1:B:112:ASN:HB3	1:B:214:THR:HG23	1.54	0.90
1:B:361:PRO:HG2	2:G:2:DC:H5"	1.62	0.82
1:A:392:PRO:O	1:A:587:THR:HG21	1.88	0.73

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	902/906 (100%)	858 (95%)	41 (4%)	3 (0%)	41	72
1	B	902/906 (100%)	859 (95%)	39 (4%)	4 (0%)	34	66
1	C	901/906 (99%)	864 (96%)	32 (4%)	5 (1%)	25	56
1	D	901/906 (99%)	855 (95%)	41 (5%)	5 (1%)	25	56
All	All	3606/3624 (100%)	3436 (95%)	153 (4%)	17 (0%)	29	61

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	893	LYS
1	B	176	ASP
1	C	622	THR
1	D	622	THR
1	B	893	LYS

### 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	
1	A	801/803 (100%)	763 (95%)	38 (5%)	26	59
1	B	801/803 (100%)	773 (96%)	28 (4%)	36	70
1	C	800/803 (100%)	760 (95%)	40 (5%)	24	56
1	D	800/803 (100%)	767 (96%)	33 (4%)	30	64
All	All	3202/3212 (100%)	3063 (96%)	139 (4%)	29	62

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	760	LEU
1	C	332	LEU
1	D	630	ASP
1	B	880	LEU
1	C	89	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	572	ASN
1	C	45	GLN
1	D	481	GLN
1	B	646	HIS
1	B	711	ASN

### 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	$\# Z  > 2$
2	5OC	G	3	2	15,21,22	1.15	1 (6%)	15,30,33	0.98	1 (6%)
2	5OC	E	3	2	15,21,22	1.14	1 (6%)	15,30,33	0.96	1 (6%)
2	5OC	K	3	2	15,21,22	1.16	1 (6%)	15,30,33	0.95	1 (6%)
2	5OC	I	3	2	15,21,22	1.17	1 (6%)	15,30,33	0.97	1 (6%)

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	5OC	G	3	2	-	0/4/21/22	0/2/2/2
2	5OC	E	3	2	-	0/4/21/22	0/2/2/2
2	5OC	K	3	2	-	0/4/21/22	0/2/2/2
2	5OC	I	3	2	-	0/4/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	5OC	C6-C5	-3.64	1.34	1.39
2	K	3	5OC	C6-C5	-3.58	1.34	1.39
2	G	3	5OC	C6-C5	-3.54	1.34	1.39
2	E	3	5OC	C6-C5	-3.54	1.34	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	3	5OC	C2-N3-C4	3.30	120.00	116.02
2	E	3	5OC	C2-N3-C4	3.28	119.98	116.02
2	K	3	5OC	C2-N3-C4	3.28	119.97	116.02
2	I	3	5OC	C2-N3-C4	3.26	119.95	116.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3	5OC	1	0
2	E	3	5OC	3	0
2	K	3	5OC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	I	19	-	4,4,4	0.35	0	6,6,6	0.06	0
4	SO4	K	19	-	4,4,4	0.34	0	6,6,6	0.04	0
4	SO4	E	19	-	4,4,4	0.35	0	6,6,6	0.10	0
4	SO4	G	19	-	4,4,4	0.36	0	6,6,6	0.08	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	904/906 (99%)	0.53	73 (8%) 12 6	48, 84, 166, 266	0
1	B	904/906 (99%)	0.32	48 (5%) 26 17	35, 63, 156, 343	0
1	C	903/906 (99%)	0.28	35 (3%) 39 29	38, 68, 137, 233	0
1	D	903/906 (99%)	0.89	136 (15%) 2 1	69, 115, 201, 249	0
2	E	17/18 (94%)	-0.04	0 100 100	69, 88, 133, 141	0
2	G	17/18 (94%)	-0.43	0 100 100	37, 52, 71, 72	0
2	I	17/18 (94%)	-0.31	0 100 100	50, 57, 78, 81	0
2	K	17/18 (94%)	1.19	3 (17%) 1 1	87, 123, 145, 148	0
3	F	15/15 (100%)	0.09	1 (6%) 17 10	65, 97, 160, 162	0
3	H	15/15 (100%)	-0.44	0 100 100	40, 53, 77, 82	0
3	J	15/15 (100%)	-0.31	0 100 100	45, 66, 99, 100	0
3	L	15/15 (100%)	1.73	4 (26%) 0 0	104, 145, 162, 163	0
All	All	3742/3756 (99%)	0.49	300 (8%) 12 6	35, 82, 181, 343	0

The worst 5 of 300 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	MET	12.6
1	D	135	ALA	12.4
1	B	510	VAL	10.1
1	D	847	ALA	9.5
1	D	789	ALA	9.1

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	5OC	K	3	20/21	0.82	0.47	112,114,118,119	0
2	5OC	E	3	20/21	0.92	0.17	69,76,81,82	0
2	5OC	I	3	20/21	0.95	0.15	56,60,62,64	0
2	5OC	G	3	20/21	0.97	0.18	38,40,43,44	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	E	19	5/5	0.87	0.21	99,101,101,104	0
4	SO4	K	19	5/5	0.88	0.15	126,126,126,128	0
4	SO4	G	19	5/5	0.92	0.18	77,78,81,85	0
4	SO4	I	19	5/5	0.97	0.13	84,86,87,90	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.