



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:18 PM UTC

PDB ID : 9H0K / pdb\_00009h0k  
Title : Crystal structure of human CREBBP histone acetyltransferase domain in complex with Propionyl- Coenzyme A  
Authors : Mechaly, A.E.; Cui, G.; Green, M.R.; Rodrigues-Lima, F.  
Deposited on : 2024-10-08  
Resolution : 1.75 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](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

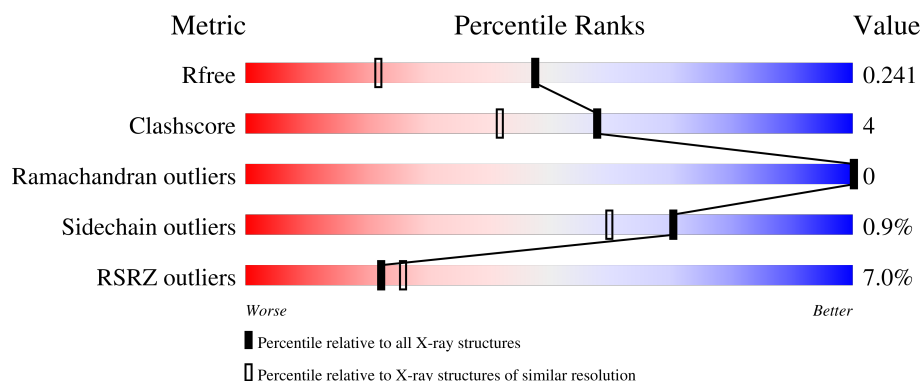
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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  $\geq 3$ , 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	348	<div> <div>5%</div> <div>80%</div> <div>11%</div> <div>9%</div> </div>
1	B	348	<div> <div>8%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5896 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 CREB-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	1	0
			2612	1679	449	469	15			
1	B	321	Total	C	N	O	S	0	2	0
			2634	1692	453	474	15			

There are 64 discrepancies between the modelled and reference sequences:

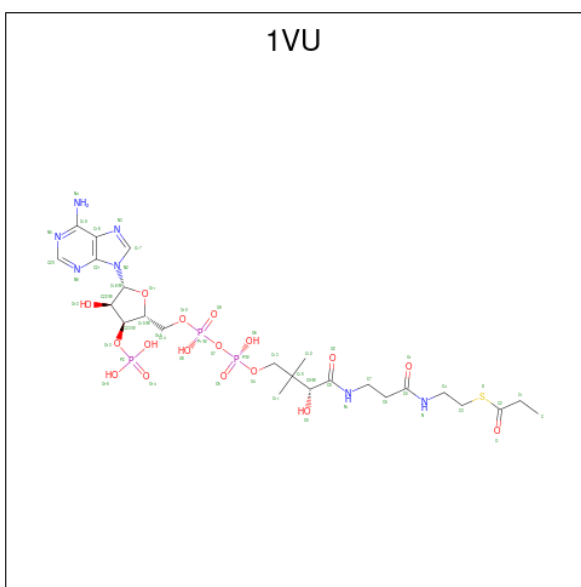
Chain	Residue	Modelled	Actual	Comment	Reference
A	1296	MET	-	initiating methionine	UNP Q92793
A	1297	GLY	-	expression tag	UNP Q92793
A	1298	SER	-	expression tag	UNP Q92793
A	1299	SER	-	expression tag	UNP Q92793
A	1300	HIS	-	expression tag	UNP Q92793
A	1301	HIS	-	expression tag	UNP Q92793
A	1302	HIS	-	expression tag	UNP Q92793
A	1303	HIS	-	expression tag	UNP Q92793
A	1304	HIS	-	expression tag	UNP Q92793
A	1305	HIS	-	expression tag	UNP Q92793
A	1306	ASP	-	expression tag	UNP Q92793
A	1307	TYR	-	expression tag	UNP Q92793
A	1308	ASP	-	expression tag	UNP Q92793
A	1309	ILE	-	expression tag	UNP Q92793
A	1310	PRO	-	expression tag	UNP Q92793
A	1311	THR	-	expression tag	UNP Q92793
A	1312	THR	-	expression tag	UNP Q92793
A	1313	GLU	-	expression tag	UNP Q92793
A	1314	ASN	-	expression tag	UNP Q92793
A	1315	LEU	-	expression tag	UNP Q92793
A	1316	TYR	-	expression tag	UNP Q92793
A	1317	PHE	-	expression tag	UNP Q92793
A	1318	GLN	-	expression tag	UNP Q92793
A	1319	GLY	-	expression tag	UNP Q92793
A	1320	HIS	-	expression tag	UNP Q92793

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1321	THR	-	expression tag	UNP Q92793
A	1503	PHE	TYR	engineered mutation	UNP Q92793
A	1556	SER	-	linker	UNP Q92793
A	1613	GLY	-	linker	UNP Q92793
A	1614	GLY	-	linker	UNP Q92793
A	1615	SER	-	linker	UNP Q92793
A	1616	GLY	-	linker	UNP Q92793
B	1296	MET	-	initiating methionine	UNP Q92793
B	1297	GLY	-	expression tag	UNP Q92793
B	1298	SER	-	expression tag	UNP Q92793
B	1299	SER	-	expression tag	UNP Q92793
B	1300	HIS	-	expression tag	UNP Q92793
B	1301	HIS	-	expression tag	UNP Q92793
B	1302	HIS	-	expression tag	UNP Q92793
B	1303	HIS	-	expression tag	UNP Q92793
B	1304	HIS	-	expression tag	UNP Q92793
B	1305	HIS	-	expression tag	UNP Q92793
B	1306	ASP	-	expression tag	UNP Q92793
B	1307	TYR	-	expression tag	UNP Q92793
B	1308	ASP	-	expression tag	UNP Q92793
B	1309	ILE	-	expression tag	UNP Q92793
B	1310	PRO	-	expression tag	UNP Q92793
B	1311	THR	-	expression tag	UNP Q92793
B	1312	THR	-	expression tag	UNP Q92793
B	1313	GLU	-	expression tag	UNP Q92793
B	1314	ASN	-	expression tag	UNP Q92793
B	1315	LEU	-	expression tag	UNP Q92793
B	1316	TYR	-	expression tag	UNP Q92793
B	1317	PHE	-	expression tag	UNP Q92793
B	1318	GLN	-	expression tag	UNP Q92793
B	1319	GLY	-	expression tag	UNP Q92793
B	1320	HIS	-	expression tag	UNP Q92793
B	1321	THR	-	expression tag	UNP Q92793
B	1503	PHE	TYR	engineered mutation	UNP Q92793
B	1556	SER	-	linker	UNP Q92793
B	1613	GLY	-	linker	UNP Q92793
B	1614	GLY	-	linker	UNP Q92793
B	1615	SER	-	linker	UNP Q92793
B	1616	GLY	-	linker	UNP Q92793

- Molecule 2 is propionyl Coenzyme A (CCD ID: 1VU) (formula:  $C_{24}H_{40}N_7O_{17}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	1
			104	48	14	34	6	2		
2	B	1	Total	C	N	O	P	S	0	1
			104	48	14	34	6	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		

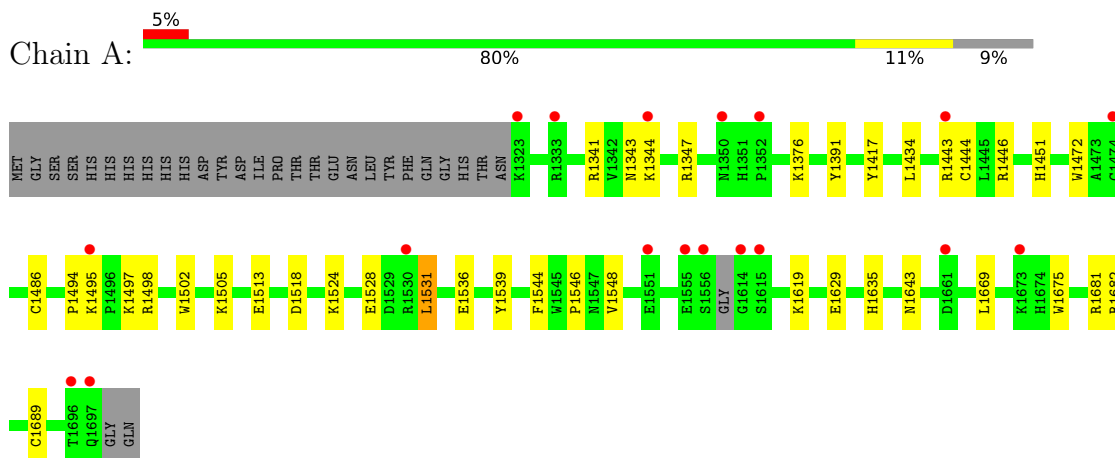
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	222	Total 222	O 222	0	0
4	B	215	Total 215	O 215	0	0

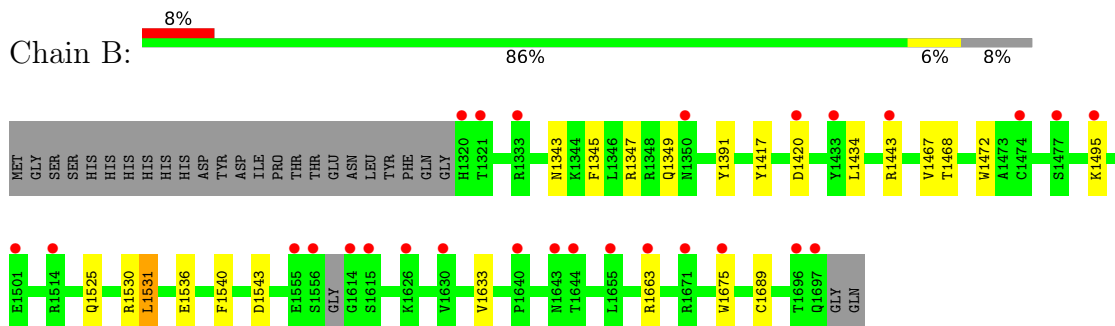
### 3 Residue-property plots [i](#)

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: CREB-binding protein



- Molecule 1: CREB-binding protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.41Å 88.51Å 112.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.55 – 1.75 69.55 – 1.75	Depositor EDS
% Data completeness (in resolution range)	69.3 (69.55-1.75) 69.3 (69.55-1.75)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, $R_{free}$	0.196 , 0.240 0.197 , 0.241	Depositor DCC
$R_{free}$ test set	3058 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.5666e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1VU, 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	0.31	0/2690	0.52	0/3635
1	B	0.31	0/2715	0.53	0/3670
All	All	0.31	0/5405	0.53	0/7305

There are no bond length outliers.

There are no bond angle outliers.

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	2612	0	2563	30	0
1	B	2634	0	2580	18	0
2	A	104	0	76	5	0
2	B	104	0	76	5	0
3	B	5	0	0	0	0
4	A	222	0	0	9	0
4	B	215	0	0	5	0
All	All	5896	0	5295	48	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.

All (48) 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:1681:ARG:NH2	4:A:1801:HOH:O	2.07	0.85
1:A:1486[A]:CYS:SG	4:A:2014:HOH:O	2.36	0.83
1:B:1531:LEU:HD22	1:B:1536:GLU:HB2	1.72	0.70
1:A:1444:CYS:SG	4:A:2007:HOH:O	2.49	0.70
1:A:1495:LYS:HE2	1:A:1497:LYS:HB3	1.72	0.70
1:A:1531:LEU:HD22	1:A:1536:GLU:HB2	1.73	0.68
1:A:1682:ARG:NH1	4:A:1801:HOH:O	2.27	0.67
1:A:1505:LYS:HD2	4:A:1949:HOH:O	2.00	0.60
1:A:1486[B]:CYS:SG	4:A:2014:HOH:O	2.57	0.58
1:A:1443:ARG:HH12	2:A:1701[A]:1VU:P2	2.28	0.56
1:A:1443:ARG:NH1	2:A:1701[B]:1VU:O15	2.26	0.54
1:A:1629:GLU:H	1:A:1629:GLU:CD	2.16	0.54
1:A:1675:TRP:CZ2	1:A:1689:CYS:HB3	2.44	0.53
1:B:1663:ARG:HG2	4:B:1809:HOH:O	2.09	0.53
1:B:1443:ARG:HH12	2:B:1701[B]:1VU:P2	2.34	0.50
1:B:1530:ARG:NH1	4:B:1810:HOH:O	2.45	0.49
1:A:1443:ARG:NH1	2:A:1701[A]:1VU:O15	2.31	0.49
1:B:1663:ARG:N	4:B:1809:HOH:O	2.44	0.48
1:B:1443:ARG:NH1	2:B:1701[B]:1VU:O15	2.39	0.48
1:A:1495:LYS:HZ2	1:A:1498:ARG:HB2	1.79	0.48
1:A:1539:TYR:CZ	1:A:1546:PRO:HB3	2.49	0.47
1:A:1391:TYR:HB3	1:A:1417:TYR:CE2	2.50	0.46
1:A:1518:ASP:OD2	1:A:1635:HIS:HD2	1.98	0.46
1:A:1376:LYS:NZ	4:A:1810:HOH:O	2.48	0.46
1:A:1619:LYS:NZ	4:A:1809:HOH:O	2.48	0.45
1:B:1675:TRP:CZ2	1:B:1689:CYS:HB3	2.51	0.45
1:A:1494:PRO:HB3	1:A:1498:ARG:HD2	1.98	0.45
1:A:1443:ARG:HH12	2:A:1701[B]:1VU:P2	2.32	0.44
1:B:1495:LYS:NZ	4:B:1807:HOH:O	2.40	0.44
1:A:1341:ARG:HH22	1:A:1513:GLU:CD	2.25	0.44
1:B:1467:VAL:HG12	1:B:1468[B]:THR:HG23	2.00	0.43
1:B:1391:TYR:HB3	1:B:1417:TYR:CE2	2.53	0.43
1:A:1451:HIS:HE1	1:A:1502:TRP:CE2	2.37	0.43
1:B:1420:ASP:HB2	4:B:1928:HOH:O	2.19	0.43
1:B:1540:PHE:HB2	1:B:1543:ASP:HB2	2.01	0.43
1:A:1343:ASN:O	1:A:1347:ARG:HG3	2.19	0.43
1:B:1525:GLN:HG2	1:B:1633:VAL:HG11	2.00	0.42
1:B:1472:TRP:H	2:B:1701[B]:1VU:C	2.32	0.42
1:B:1472:TRP:H	2:B:1701[B]:1VU:H38	1.84	0.42
1:A:1443:ARG:HG2	1:A:1446:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1544:PHE:CE2	1:A:1548:VAL:HG21	2.55	0.41
1:B:1345:PHE:O	1:B:1349:GLN:HG2	2.21	0.41
1:B:1343:ASN:O	1:B:1347:ARG:HG3	2.20	0.41
1:B:1472:TRP:H	2:B:1701[A]:1VU:C	2.32	0.41
1:A:1472:TRP:H	2:A:1701[B]:1VU:H38	1.86	0.41
1:A:1344:LYS:HD2	4:A:1859:HOH:O	2.21	0.41
1:A:1669:LEU:HD12	1:A:1669:LEU:HA	1.80	0.40
1:A:1524:LYS:O	1:A:1528:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/348 (90%)	309 (98%)	6 (2%)	0	100	100
1	B	319/348 (92%)	313 (98%)	6 (2%)	0	100	100
All	All	634/696 (91%)	622 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	288/313 (92%)	285 (99%)	3 (1%)	68	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	290/313 (93%)	288 (99%)	2 (1%)	76	67
All	All	578/626 (92%)	573 (99%)	5 (1%)	70	60

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1434	LEU
1	A	1531	LEU
1	A	1643	ASN
1	B	1434	LEU
1	B	1531	LEU

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

Mol	Chain	Res	Type
1	A	1330	GLN
1	A	1451	HIS
1	A	1643	ASN
1	B	1451	HIS
1	B	1643	ASN
1	B	1695	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

5 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$
2	1VU	B	1701[B]	-	52,54,54	2.65	16 (30%)	73,80,80	1.77	15 (20%)
2	1VU	A	1701[B]	-	52,54,54	2.70	18 (34%)	73,80,80	1.71	14 (19%)
2	1VU	B	1701[A]	-	52,54,54	2.72	19 (36%)	73,80,80	1.79	15 (20%)
3	SO4	B	1702	-	4,4,4	0.61	0	6,6,6	0.22	0
2	1VU	A	1701[A]	-	52,54,54	2.75	18 (34%)	73,80,80	1.77	15 (20%)

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	1VU	B	1701[B]	-	-	7/53/69/69	0/3/3/3
2	1VU	B	1701[A]	-	-	7/53/69/69	0/3/3/3
2	1VU	A	1701[B]	-	-	7/53/69/69	0/3/3/3
2	1VU	A	1701[A]	-	-	7/53/69/69	0/3/3/3

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1701[A]	1VU	O11-C16	8.51	1.61	1.42
2	B	1701[A]	1VU	O11-C16	8.45	1.61	1.42
2	A	1701[B]	1VU	O11-C16	8.38	1.61	1.42
2	B	1701[B]	1VU	O11-C16	8.17	1.60	1.42
2	B	1701[B]	1VU	C8-N1	6.88	1.49	1.33
2	A	1701[A]	1VU	C8-N1	6.79	1.49	1.33
2	B	1701[A]	1VU	C8-N1	6.78	1.49	1.33
2	A	1701[B]	1VU	C8-N1	6.75	1.49	1.33
2	A	1701[A]	1VU	O11-C15	-6.27	1.31	1.45
2	A	1701[B]	1VU	O11-C15	-6.23	1.31	1.45
2	B	1701[A]	1VU	O11-C15	-6.22	1.31	1.45
2	A	1701[A]	1VU	C22-C16	-6.19	1.34	1.53
2	A	1701[B]	1VU	C22-C16	-6.16	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1701[B]	1VU	O11-C15	-6.14	1.31	1.45
2	B	1701[A]	1VU	C22-C16	-6.10	1.34	1.53
2	B	1701[B]	1VU	C22-C16	-5.90	1.34	1.53
2	A	1701[B]	1VU	C5-N	5.34	1.46	1.33
2	A	1701[A]	1VU	C5-N	5.20	1.45	1.33
2	A	1701[A]	1VU	P-O7	5.12	1.65	1.59
2	B	1701[A]	1VU	C5-N	5.09	1.45	1.33
2	B	1701[A]	1VU	P-O7	5.07	1.65	1.59
2	B	1701[B]	1VU	C5-N	5.01	1.45	1.33
2	A	1701[A]	1VU	P1-O7	4.69	1.64	1.59
2	B	1701[A]	1VU	P1-O7	4.62	1.64	1.59
2	A	1701[B]	1VU	P1-O7	4.30	1.64	1.59
2	A	1701[B]	1VU	P-O7	4.08	1.63	1.59
2	B	1701[B]	1VU	P1-O7	4.06	1.63	1.59
2	B	1701[B]	1VU	C19-N4	4.00	1.44	1.34
2	A	1701[B]	1VU	C19-N4	3.98	1.44	1.34
2	B	1701[A]	1VU	C19-N4	3.97	1.44	1.34
2	A	1701[A]	1VU	C19-N4	3.97	1.44	1.34
2	B	1701[B]	1VU	P-O7	3.94	1.63	1.59
2	B	1701[B]	1VU	C13-C10	3.74	1.58	1.52
2	A	1701[B]	1VU	C13-C10	3.57	1.58	1.52
2	A	1701[A]	1VU	C13-C10	3.52	1.58	1.52
2	B	1701[A]	1VU	C13-C10	3.50	1.58	1.52
2	A	1701[B]	1VU	P2-O13	3.48	1.65	1.59
2	B	1701[B]	1VU	P2-O13	3.40	1.65	1.59
2	A	1701[A]	1VU	P2-O13	3.00	1.64	1.59
2	B	1701[A]	1VU	P2-O13	2.97	1.64	1.59
2	B	1701[A]	1VU	C18-C21	-2.78	1.34	1.39
2	A	1701[B]	1VU	O12-C22	2.76	1.49	1.43
2	A	1701[A]	1VU	O12-C22	2.75	1.49	1.43
2	B	1701[B]	1VU	C18-C21	-2.74	1.34	1.39
2	B	1701[B]	1VU	O12-C22	2.73	1.49	1.43
2	A	1701[A]	1VU	C18-C21	-2.72	1.34	1.39
2	B	1701[A]	1VU	O12-C22	2.72	1.49	1.43
2	A	1701[A]	1VU	O13-C23	-2.70	1.34	1.44
2	B	1701[A]	1VU	O13-C23	-2.64	1.35	1.44
2	A	1701[B]	1VU	O13-C23	-2.62	1.35	1.44
2	B	1701[A]	1VU	P1-O10	2.60	1.69	1.59
2	A	1701[B]	1VU	C2-S	2.59	1.82	1.76
2	A	1701[B]	1VU	C18-C21	-2.58	1.34	1.39
2	A	1701[A]	1VU	P1-O10	2.57	1.69	1.59
2	B	1701[B]	1VU	O13-C23	-2.56	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1701[A]	1VU	C2-S	2.43	1.82	1.76
2	B	1701[B]	1VU	C2-S	2.41	1.81	1.76
2	A	1701[A]	1VU	C2-S	2.40	1.81	1.76
2	B	1701[B]	1VU	P1-O10	2.40	1.68	1.59
2	A	1701[B]	1VU	P1-O10	2.35	1.68	1.59
2	A	1701[B]	1VU	C17-N2	-2.19	1.33	1.37
2	B	1701[A]	1VU	C18-N3	-2.12	1.35	1.39
2	B	1701[B]	1VU	C18-N3	-2.11	1.35	1.39
2	A	1701[A]	1VU	C17-N2	-2.10	1.34	1.37
2	A	1701[A]	1VU	C23-C15	2.09	1.58	1.52
2	B	1701[A]	1VU	C23-C15	2.08	1.58	1.52
2	A	1701[A]	1VU	C18-N3	-2.06	1.35	1.39
2	A	1701[B]	1VU	C23-C15	2.05	1.58	1.52
2	B	1701[A]	1VU	C7-C6	2.03	1.58	1.51
2	B	1701[A]	1VU	C17-N2	-2.03	1.34	1.37
2	A	1701[B]	1VU	C18-N3	-2.02	1.35	1.39

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1701[B]	1VU	N5-C20-N6	-5.65	120.03	128.58
2	B	1701[A]	1VU	N5-C20-N6	-5.64	120.04	128.58
2	B	1701[A]	1VU	C1-C2-S	5.60	120.62	113.56
2	A	1701[A]	1VU	N5-C20-N6	-5.51	120.25	128.58
2	A	1701[B]	1VU	C1-C2-S	5.50	120.50	113.56
2	A	1701[A]	1VU	C1-C2-S	5.45	120.43	113.56
2	A	1701[B]	1VU	N5-C20-N6	-5.30	120.55	128.58
2	B	1701[B]	1VU	C1-C2-S	5.03	119.90	113.56
2	A	1701[B]	1VU	C18-C21-N6	-4.91	119.96	126.72
2	A	1701[A]	1VU	C18-C21-N6	-4.89	119.99	126.72
2	B	1701[A]	1VU	C18-C21-N6	-4.86	120.03	126.72
2	B	1701[B]	1VU	C18-C21-N6	-4.79	120.12	126.72
2	B	1701[A]	1VU	N2-C17-N3	-4.26	107.89	113.94
2	A	1701[A]	1VU	N2-C17-N3	-4.22	107.94	113.94
2	B	1701[B]	1VU	N2-C17-N3	-4.13	108.07	113.94
2	A	1701[B]	1VU	N2-C17-N3	-4.05	108.19	113.94
2	B	1701[B]	1VU	O-C2-S	-3.85	117.78	122.68
2	B	1701[A]	1VU	C20-N6-C21	3.31	119.92	111.83
2	B	1701[B]	1VU	C20-N6-C21	3.31	119.91	111.83
2	A	1701[A]	1VU	C20-N6-C21	3.24	119.75	111.83
2	B	1701[A]	1VU	C21-N2-C16	-3.17	119.22	126.63
2	A	1701[A]	1VU	C21-N2-C16	-3.14	119.29	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1701[B]	1VU	C20-N6-C21	3.13	119.48	111.83
2	B	1701[B]	1VU	N6-C21-N2	3.04	132.34	127.17
2	B	1701[A]	1VU	N6-C21-N2	3.01	132.29	127.17
2	A	1701[A]	1VU	N6-C21-N2	2.97	132.22	127.17
2	A	1701[B]	1VU	N6-C21-N2	2.97	132.22	127.17
2	B	1701[B]	1VU	C21-N2-C16	-2.97	119.69	126.63
2	A	1701[A]	1VU	C18-N3-C17	2.93	108.06	103.45
2	A	1701[B]	1VU	C18-N3-C17	2.91	108.02	103.45
2	B	1701[A]	1VU	C18-N3-C17	2.87	107.97	103.45
2	A	1701[B]	1VU	C21-N2-C16	-2.85	119.96	126.63
2	B	1701[A]	1VU	O-C2-S	-2.83	119.09	122.68
2	B	1701[B]	1VU	C3-S-C2	2.75	109.97	101.84
2	B	1701[B]	1VU	C18-N3-C17	2.66	107.64	103.45
2	A	1701[B]	1VU	O-C2-S	-2.66	119.30	122.68
2	A	1701[A]	1VU	O-C2-C1	-2.62	119.80	123.72
2	A	1701[A]	1VU	C3-S-C2	2.57	109.45	101.84
2	B	1701[B]	1VU	C21-N2-C17	2.47	108.33	105.74
2	B	1701[A]	1VU	C21-N2-C17	2.43	108.29	105.74
2	B	1701[A]	1VU	C16-N2-C17	2.43	132.49	127.09
2	A	1701[A]	1VU	C16-N2-C17	2.43	132.48	127.09
2	B	1701[B]	1VU	C4-N-C5	-2.38	118.39	122.82
2	A	1701[B]	1VU	C21-C18-N3	-2.38	107.86	110.58
2	A	1701[A]	1VU	C21-N2-C17	2.37	108.23	105.74
2	B	1701[B]	1VU	C22-C16-N2	-2.36	107.45	113.30
2	A	1701[B]	1VU	O-C2-C1	-2.35	120.19	123.72
2	B	1701[A]	1VU	O-C2-C1	-2.30	120.28	123.72
2	A	1701[A]	1VU	O-C2-S	-2.30	119.76	122.68
2	A	1701[A]	1VU	C21-C18-N3	-2.27	107.98	110.58
2	B	1701[A]	1VU	C4-N-C5	-2.26	118.61	122.82
2	A	1701[B]	1VU	C21-N2-C17	2.25	108.10	105.74
2	B	1701[B]	1VU	C16-N2-C17	2.18	131.94	127.09
2	A	1701[B]	1VU	C16-N2-C17	2.18	131.93	127.09
2	A	1701[B]	1VU	C19-C18-C21	2.15	120.12	117.18
2	B	1701[A]	1VU	C21-C18-N3	-2.11	108.17	110.58
2	B	1701[B]	1VU	C23-C22-C16	2.08	104.47	99.89
2	A	1701[A]	1VU	C23-C22-C16	2.02	104.34	99.89
2	B	1701[A]	1VU	O4-C13-C10	-2.01	107.32	110.55

There are no chirality outliers.

All (28) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	A	1701[A]	1VU	C13-O4-P-O5
2	A	1701[A]	1VU	O-C2-S-C3
2	A	1701[A]	1VU	C1-C2-S-C3
2	A	1701[B]	1VU	O-C2-S-C3
2	A	1701[B]	1VU	C1-C2-S-C3
2	B	1701[A]	1VU	C13-O4-P-O5
2	B	1701[A]	1VU	S-C3-C4-N
2	B	1701[A]	1VU	C4-C3-S-C2
2	B	1701[B]	1VU	O-C2-S-C3
2	B	1701[B]	1VU	C1-C2-S-C3
2	B	1701[A]	1VU	C15-C23-O13-P2
2	B	1701[B]	1VU	C15-C23-O13-P2
2	B	1701[A]	1VU	C22-C23-O13-P2
2	B	1701[B]	1VU	C22-C23-O13-P2
2	A	1701[A]	1VU	C15-C23-O13-P2
2	A	1701[B]	1VU	C13-O4-P-O5
2	B	1701[A]	1VU	C13-O4-P-O7
2	B	1701[B]	1VU	C13-O4-P-O5
2	A	1701[A]	1VU	C22-C23-O13-P2
2	A	1701[A]	1VU	S-C3-C4-N
2	A	1701[A]	1VU	C23-O13-P2-O14
2	B	1701[A]	1VU	C23-O13-P2-O14
2	B	1701[B]	1VU	C23-O13-P2-O14
2	A	1701[B]	1VU	C5-C6-C7-N1
2	B	1701[B]	1VU	C23-O13-P2-O15
2	A	1701[B]	1VU	C11-C10-C13-O4
2	A	1701[B]	1VU	C12-C10-C13-O4
2	A	1701[B]	1VU	C23-O13-P2-O14

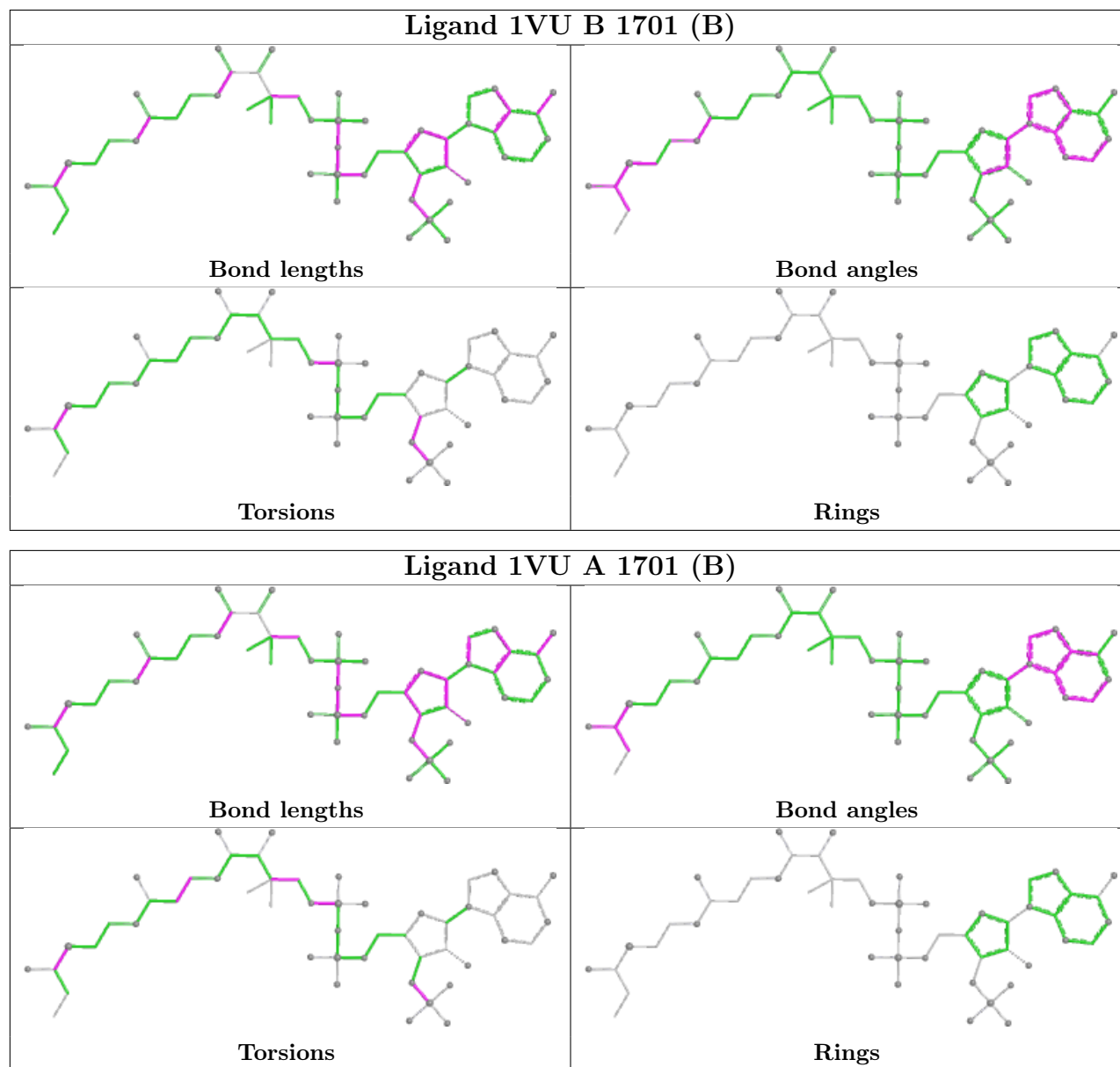
There are no ring outliers.

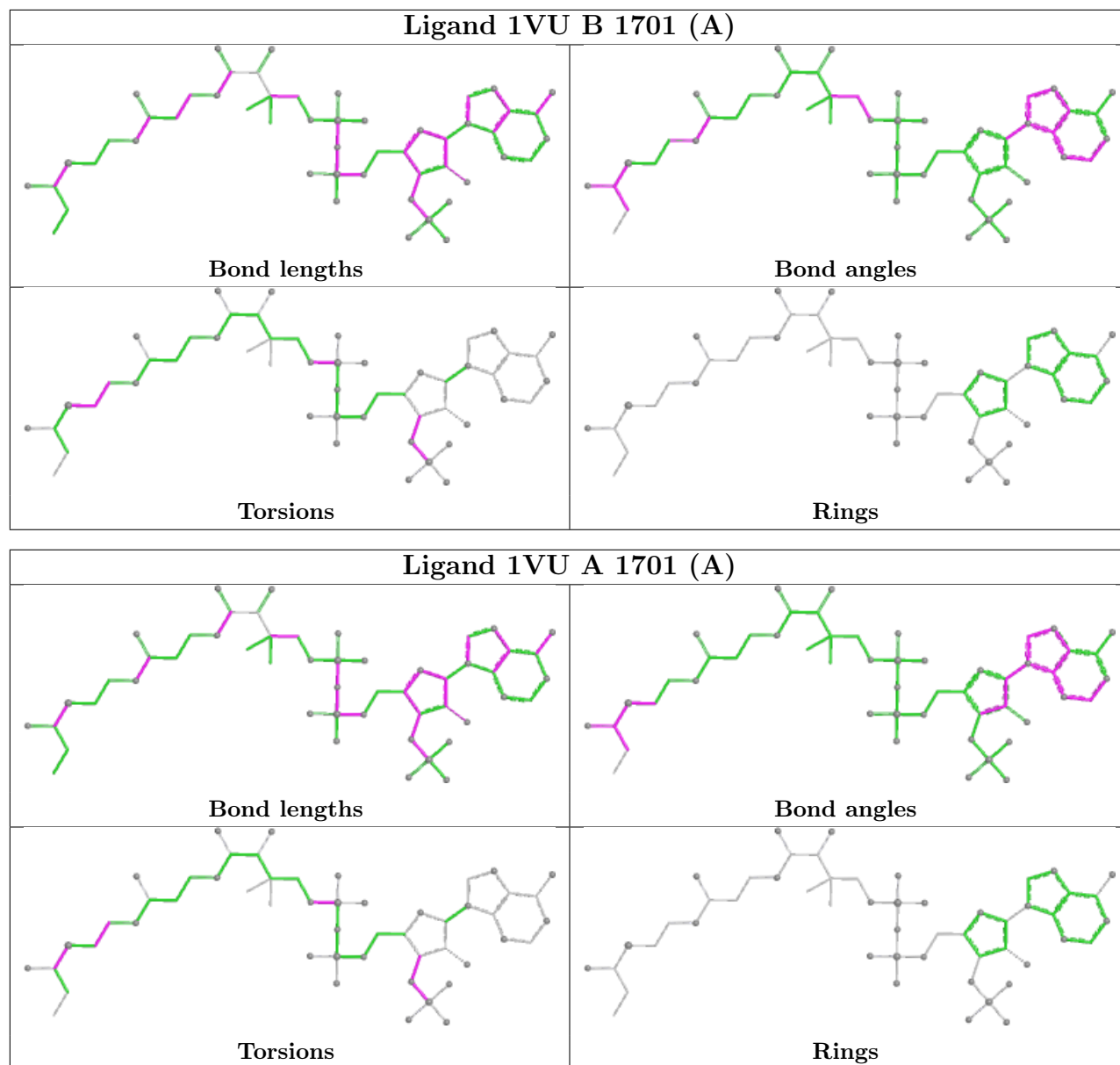
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1701[B]	1VU	4	0
2	A	1701[B]	1VU	3	0
2	B	1701[A]	1VU	1	0
2	A	1701[A]	1VU	2	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, 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	318/348 (91%)	0.18	18 (5%) 29 33	9, 24, 54, 90	1 (0%)
1	B	321/348 (92%)	0.13	27 (8%) 17 20	10, 22, 52, 90	2 (0%)
All	All	639/696 (91%)	0.15	45 (7%) 22 26	9, 23, 53, 90	3 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1614	GLY	6.5
1	B	1321	THR	5.0
1	B	1433	TYR	4.7
1	A	1555	GLU	4.3
1	A	1697	GLN	3.9
1	B	1555	GLU	3.4
1	B	1556	SER	3.4
1	B	1350	ASN	3.4
1	B	1614	GLY	3.3
1	A	1495	LYS	3.2
1	B	1697	GLN	3.2
1	A	1696	THR	3.1
1	A	1551	GLU	3.0
1	A	1344	LYS	3.0
1	A	1323	LYS	3.0
1	A	1661	ASP	2.9
1	A	1556	SER	2.9
1	B	1420	ASP	2.7
1	B	1320	HIS	2.7
1	B	1671	ARG	2.7
1	A	1673	LYS	2.7
1	B	1615	SER	2.7
1	B	1643	ASN	2.6
1	B	1626	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1350	ASN	2.6
1	B	1474	CYS	2.4
1	A	1615	SER	2.4
1	B	1495	LYS	2.4
1	B	1501	GLU	2.3
1	B	1696	THR	2.2
1	A	1443	ARG	2.2
1	A	1352	PRO	2.2
1	B	1644	THR	2.2
1	B	1675	TRP	2.2
1	B	1663	ARG	2.2
1	B	1443	ARG	2.2
1	B	1477	SER	2.2
1	A	1474	CYS	2.1
1	A	1530	ARG	2.1
1	B	1514	ARG	2.1
1	A	1333	ARG	2.1
1	B	1333	ARG	2.1
1	B	1640	PRO	2.1
1	B	1655	LEU	2.1
1	B	1630	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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, 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( $\text{\AA}^2$ )	Q<0.9
2	1VU	A	1701[A]	52/52	0.92	0.10	20,28,41,41	52
2	1VU	A	1701[B]	52/52	0.92	0.10	17,24,44,45	52

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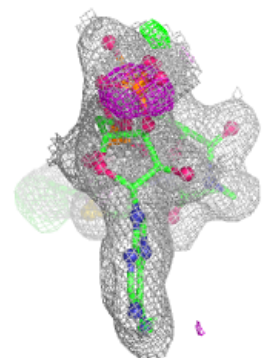
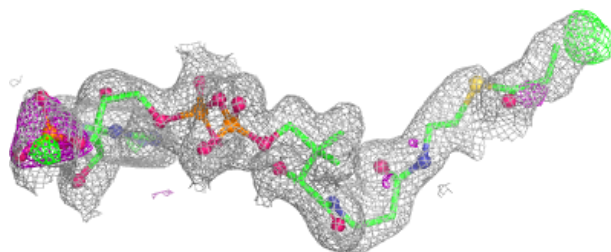
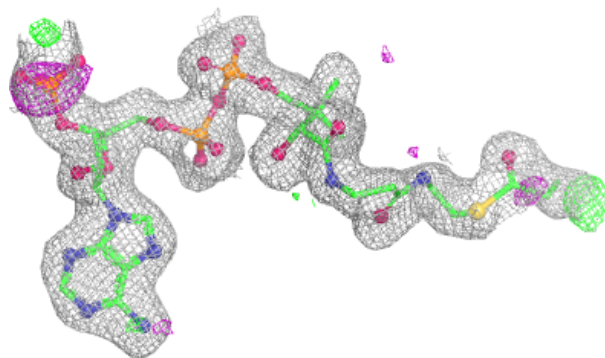
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	1VU	B	1701[A]	52/52	0.92	0.10	14,25,39,40	52
2	1VU	B	1701[B]	52/52	0.92	0.10	12,20,42,43	52
3	SO4	B	1702	5/5	0.97	0.08	31,32,32,33	0

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.

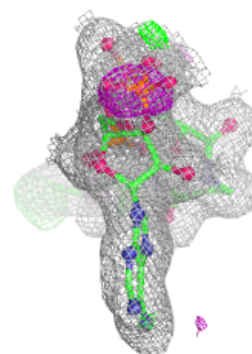
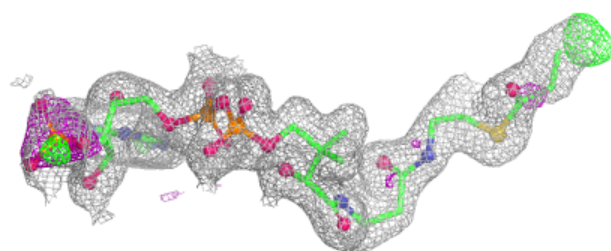
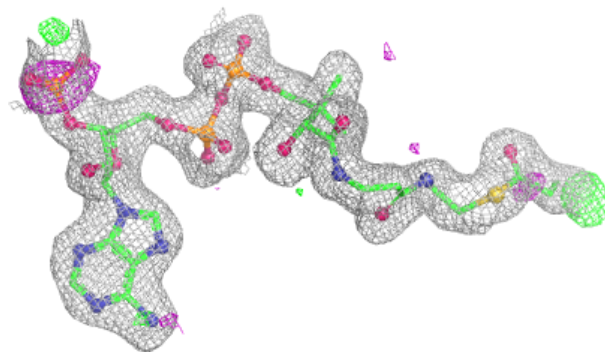
**Electron density around 1VU A 1701 (A):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

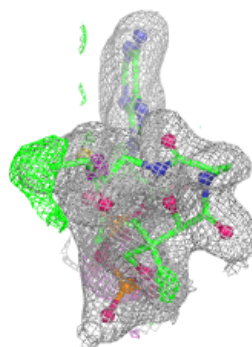
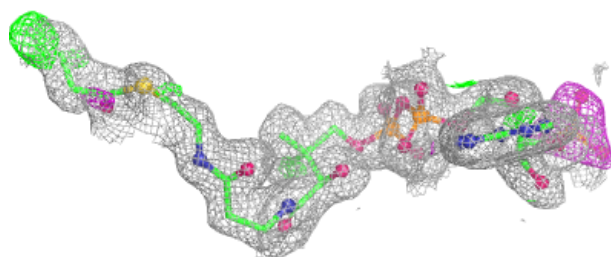
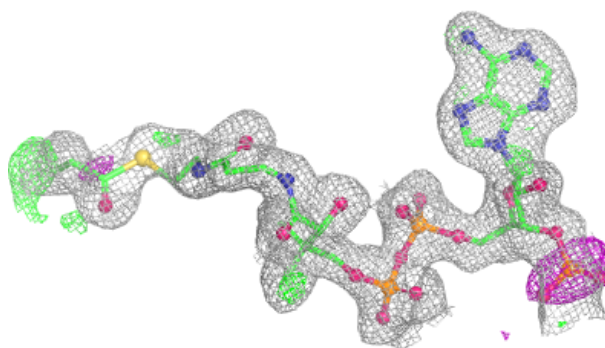


**Electron density around 1VU A 1701 (B):**

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

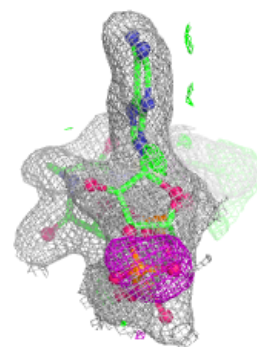
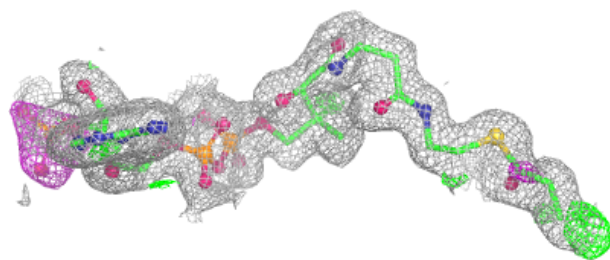
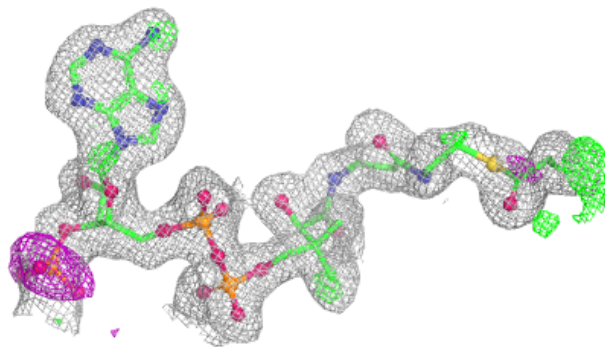
**Electron density around 1VU B 1701 (A):**

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



**Electron density around 1VU B 1701 (B):**

$2mF_o-DF_c$  (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.