



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 11:56 AM EDT

PDB ID : 5BQP  
Title : Hypoxanthine-guanine-xanthine phosphoribosyltransferase (HGXPRT) from *Sulfolobus solfataricus* with xanthosine and phosphate bound in the nucleotide binding site and with sulfate bound in the pyrophosphate binding site  
Authors : Christoffersen, S.  
Deposited on : 2015-05-29  
Resolution : 1.70 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>.

---

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	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

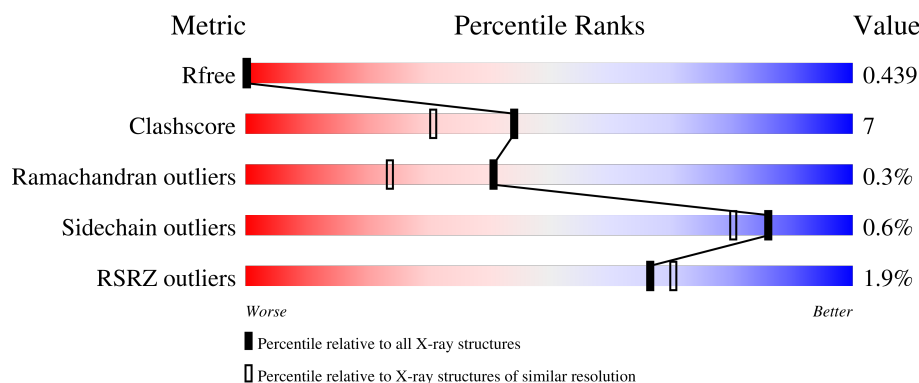
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 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	179	<div> <div>0%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	B	179	<div> <div>2%</div> <div>83%</div> <div>9%</div> <div>7%</div> </div>
1	C	179	<div> <div>3%</div> <div>82%</div> <div>13%</div> <div>5%</div> </div>
1	D	179	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>

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
4	SO4	A	204	-	-	X	-

## 2 Entry composition [i](#)

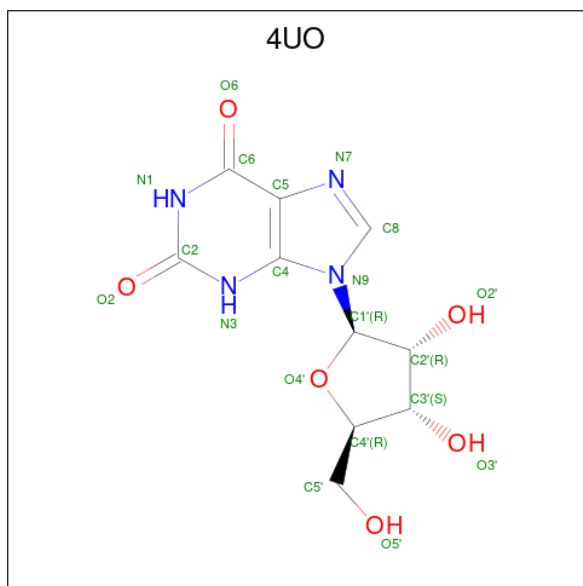
There are 8 unique types of molecules in this entry. The entry contains 6738 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Purine phosphoribosyltransferase (GpT-2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	3	0
			1396	921	221	252	2			
1	B	167	Total	C	N	O	S	0	2	0
			1370	905	213	249	3			
1	C	170	Total	C	N	O	S	0	2	0
			1396	920	220	253	3			
1	D	176	Total	C	N	O	S	0	2	0
			1446	950	230	264	2			

- Molecule 2 is 2,3-dihydroxanthosine (three-letter code: 4UO) (formula:  $C_{10}H_{12}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	10	4	6		
2	B	1	Total	C	N	O	0	0
			20	10	4	6		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			20	10	4	6		
2	D	1	Total	C	N	O	0	0
			20	10	4	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



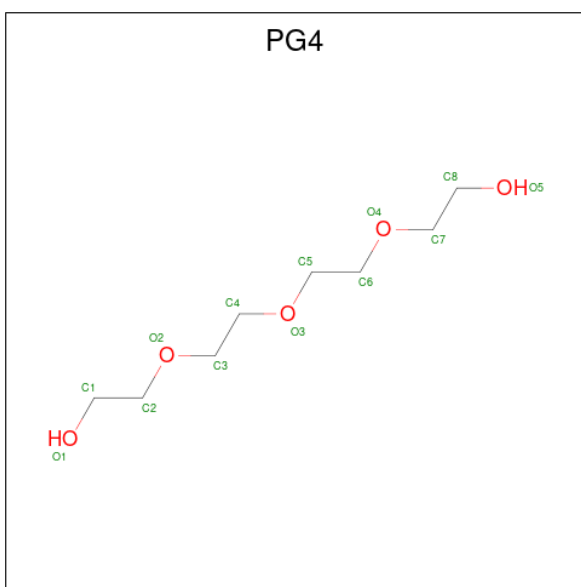
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

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



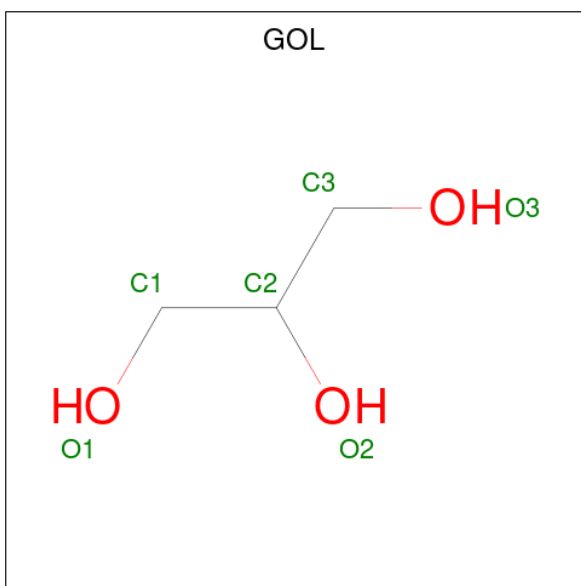
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



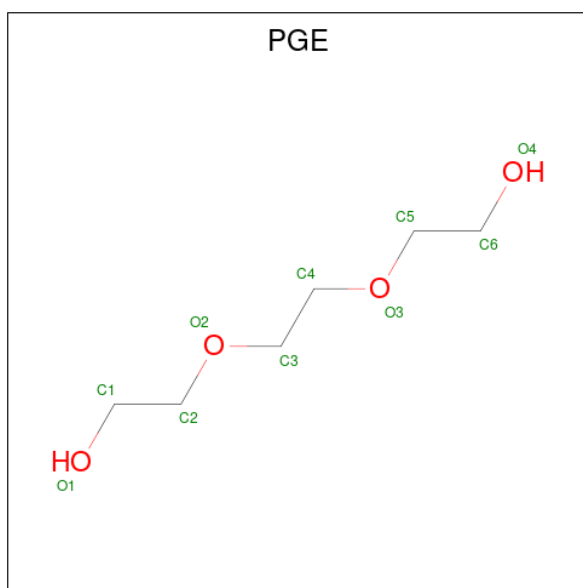
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0
5	D	1	Total C O 13 8 5	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



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

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is water.

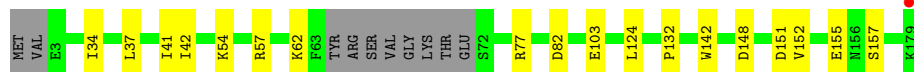
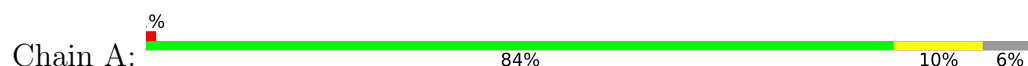
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	274	Total	O	0	0
			274	274		
8	B	202	Total	O	0	0
			202	202		
8	C	212	Total	O	0	0
			212	212		
8	D	264	Total	O	0	0
			264	264		



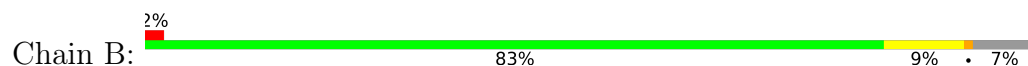
### 3 Residue-property plots

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.

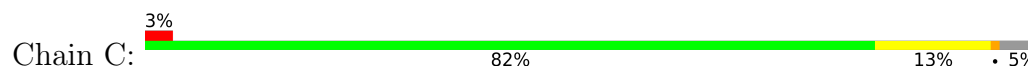
- Molecule 1: Purine phosphoribosyltransferase (GpT-2)



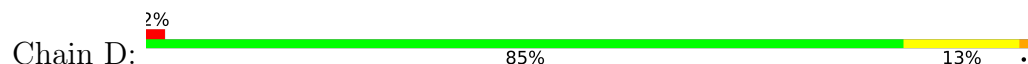
- Molecule 1: Purine phosphoribosyltransferase (GpT-2)



- Molecule 1: Purine phosphoribosyltransferase (GpT-2)



- Molecule 1: Purine phosphoribosyltransferase (GpT-2)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.22Å 132.22Å 103.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.01 – 1.70 47.01 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.01-1.70) 99.5 (47.01-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.9	Depositor
R, $R_{free}$	0.162 , 0.190 0.437 , 0.439	Depositor DCC
$R_{free}$ test set	5678 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6738	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PGE, GOL, PG4, 4UO, PO4

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	0.66	0/1437	0.73	3/1952 (0.2%)
1	B	0.57	0/1408	0.67	3/1916 (0.2%)
1	C	0.56	0/1434	0.65	1/1950 (0.1%)
1	D	0.65	0/1486	0.70	0/2021
All	All	0.61	0/5765	0.69	7/7839 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	82[A]	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	82[B]	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	94	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	82[A]	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	82[B]	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	93	ASP	CB-CG-OD1	5.00	122.80	118.30

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	1396	0	1449	14	0
1	B	1370	0	1414	14	0
1	C	1396	0	1444	22	0
1	D	1446	0	1489	21	0
2	A	20	0	12	1	0
2	B	20	0	12	0	0
2	C	20	0	12	1	0
2	D	20	0	12	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	10	0	0	2	0
4	B	5	0	0	0	0
4	C	5	0	0	1	0
4	D	10	0	0	0	0
5	A	13	0	18	3	0
5	D	13	0	18	1	0
6	B	6	0	8	1	0
6	C	6	0	8	3	0
7	C	10	0	14	2	0
8	A	274	0	0	4	2
8	B	202	0	0	2	2
8	C	212	0	0	7	1
8	D	264	0	0	10	6
All	All	6738	0	5910	77	10

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 7.

All (77) 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:178:ARG:NH2	8:D:301:HOH:O	1.90	1.03
1:C:157:SER:H	7:C:205:PGE:H5	1.40	0.85
1:A:54:LYS:NZ	8:A:303:HOH:O	2.16	0.79
1:D:82[A]:ASP:OD1	8:D:302:HOH:O	2.06	0.74
4:A:204:SO4:O3	8:A:301:HOH:O	2.06	0.72
1:C:178:ARG:NH1	8:C:303:HOH:O	2.24	0.71
1:D:178:ARG:NH1	8:D:304:HOH:O	2.20	0.70
1:D:3:GLU:OE2	8:D:303:HOH:O	2.11	0.69
1:C:62:LYS:HG3	1:C:77:ARG:HH21	1.59	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ASP:OD2	8:B:301:HOH:O	2.13	0.66
1:C:173:GLN:NE2	8:C:305:HOH:O	2.31	0.63
1:D:66:SER:O	1:D:70:THR:OG1	2.18	0.62
4:A:204:SO4:O4	8:A:302:HOH:O	2.14	0.62
1:D:174:LEU:HD13	1:D:178:ARG:HH12	1.66	0.60
1:D:174:LEU:HD13	1:D:178:ARG:NH1	2.16	0.60
2:C:201:4UO:H2	2:C:201:4UO:H9	1.67	0.59
1:C:163:LYS:H	6:C:204:GOL:H2	1.69	0.58
1:A:152:VAL:HG22	5:A:205:PG4:H41	1.86	0.57
1:D:114:PRO:HG3	1:D:117:VAL:HG22	1.87	0.56
1:C:174:LEU:HD23	1:C:177:ILE:HD11	1.88	0.56
1:A:103:GLU:OE2	1:C:116:LYS:NZ	2.36	0.55
1:D:70:THR:HG23	8:D:318:HOH:O	2.07	0.55
1:B:131:ILE:H	1:D:70:THR:HG21	1.73	0.54
1:B:41[A]:ILE:HG22	1:B:42:ILE:HG13	1.90	0.54
2:A:201:4UO:H2	2:A:201:4UO:H9	1.73	0.53
2:D:201:4UO:H4	8:D:325:HOH:O	2.08	0.53
1:A:157:SER:O	8:A:304:HOH:O	2.19	0.53
1:B:163:LYS:HA	6:B:204:GOL:H2	1.90	0.52
1:C:62:LYS:NZ	4:C:203:SO4:O1	2.40	0.52
1:B:133:ASP:HA	1:D:67:VAL:HG13	1.92	0.52
1:C:73:LYS:O	8:C:301:HOH:O	2.19	0.52
1:D:174:LEU:HD22	1:D:178:ARG:CZ	2.40	0.52
1:A:62[A]:LYS:NZ	1:A:77:ARG:HH11	2.09	0.51
1:C:157:SER:HB3	7:C:205:PGE:H32	1.92	0.51
1:C:129:LYS:HG3	1:C:130:ARG:HG2	1.91	0.51
1:A:142:TRP:CE2	5:A:205:PG4:H52	2.46	0.51
1:A:124:LEU:HD13	1:A:132:PRO:HD3	1.93	0.51
1:D:106:SER:HB3	8:D:514:HOH:O	2.11	0.51
6:C:204:GOL:H12	8:C:375:HOH:O	2.11	0.51
1:A:37:LEU:CD2	1:A:41[B]:ILE:HD12	2.42	0.49
1:B:34:ILE:HD13	1:B:57:ARG:HB2	1.93	0.49
1:A:155:GLU:HG3	5:A:205:PG4:H31	1.94	0.49
1:B:62:LYS:HD3	1:B:77:ARG:NH1	2.27	0.49
1:C:114:PRO:HG3	1:C:117:VAL:HG22	1.94	0.49
1:A:62[A]:LYS:HE2	1:A:77:ARG:HE	1.78	0.49
6:C:204:GOL:H11	8:C:390:HOH:O	2.12	0.48
1:D:137:LYS:NZ	8:D:306:HOH:O	2.36	0.48
1:A:62[A]:LYS:HD3	1:A:77:ARG:NH1	2.30	0.47
1:C:28:TYR:CZ	1:C:118:MET:HG3	2.50	0.46
1:A:34:ILE:HD13	1:A:57:ARG:HB2	1.96	0.46

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LEU:HD22	1:B:41[B]:ILE:HD12	1.97	0.46
1:B:77:ARG:NH1	8:B:305:HOH:O	2.39	0.45
1:D:37:LEU:HA	1:D:38:THR:HA	1.73	0.45
1:C:73:LYS:HB3	1:C:73:LYS:HE2	1.83	0.45
1:D:7:PRO:HD2	1:D:144:ILE:O	2.17	0.44
1:C:25:LYS:NZ	8:C:319:HOH:O	2.51	0.44
5:D:205:PG4:H31	5:D:205:PG4:H11	1.60	0.44
1:C:107:ASN:OD1	8:C:302:HOH:O	2.21	0.43
1:C:125:LYS:HE2	1:C:141:LYS:O	2.19	0.43
2:D:201:4UO:H2	2:D:201:4UO:H9	1.82	0.43
1:B:37:LEU:CD2	1:B:41[B]:ILE:HD12	2.48	0.43
1:D:41[A]:ILE:HG22	1:D:42:ILE:N	2.33	0.43
1:C:62:LYS:HG3	1:C:77:ARG:HE	1.83	0.42
1:D:70:THR:N	8:D:312:HOH:O	2.52	0.42
1:D:88:LYS:HE2	8:D:320:HOH:O	2.20	0.42
1:C:176:LYS:O	1:C:178:ARG:N	2.45	0.42
1:B:136:TYR:CE2	1:B:137:LYS:HE2	2.54	0.42
1:C:103:GLU:OE2	1:C:130:ARG:NH2	2.53	0.41
1:A:41[A]:ILE:HG22	1:A:42:ILE:N	2.33	0.41
1:D:122:LEU:O	1:D:136:TYR:HB3	2.20	0.41
1:A:37:LEU:HD22	1:A:41[B]:ILE:HD12	2.02	0.41
1:C:125:LYS:HA	1:C:126:PRO:HD3	1.92	0.41
1:D:123:TYR:CD1	1:D:139:ILE:HG13	2.55	0.41
1:C:103:GLU:HB2	1:C:130:ARG:HG3	2.03	0.41
1:B:169:ASN:O	1:B:173:GLN:HG3	2.21	0.40
1:B:37:LEU:HA	1:B:38:THR:HA	1.69	0.40
1:B:41[A]:ILE:HG22	1:B:42:ILE:N	2.36	0.40

All (10) 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)
8:D:394:HOH:O	8:D:512:HOH:O[6_554]	1.90	0.30
8:B:499:HOH:O	8:B:499:HOH:O[6_555]	1.95	0.25
8:D:347:HOH:O	8:D:512:HOH:O[6_554]	1.97	0.23
8:A:491:HOH:O	8:D:460:HOH:O[5_665]	2.03	0.17
8:B:323:HOH:O	8:B:478:HOH:O[6_555]	2.03	0.17
8:D:519:HOH:O	8:D:520:HOH:O[6_554]	2.07	0.13
8:C:359:HOH:O	8:C:502:HOH:O[6_554]	2.11	0.09
8:D:301:HOH:O	8:D:424:HOH:O[6_554]	2.12	0.08

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:539:HOH:O	8:D:539:HOH:O[6_554]	2.15	0.05
8:A:438:HOH:O	8:A:490:HOH:O[6_555]	2.16	0.04

## 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	168/179 (94%)	165 (98%)	3 (2%)	0	100	100
1	B	165/179 (92%)	161 (98%)	4 (2%)	0	100	100
1	C	168/179 (94%)	164 (98%)	3 (2%)	1 (1%)	25	11
1	D	176/179 (98%)	173 (98%)	2 (1%)	1 (1%)	25	11
All	All	677/716 (95%)	663 (98%)	12 (2%)	2 (0%)	41	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	177	ILE
1	D	160	PRO

### 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	158/164 (96%)	157 (99%)	1 (1%)	86	80
1	B	155/164 (94%)	153 (99%)	2 (1%)	69	56

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	158/164 (96%)	158 (100%)	0	100	100
1	D	163/164 (99%)	161 (99%)	2 (1%)	71	59
All	All	634/656 (97%)	629 (99%)	5 (1%)	86	74

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

Mol	Chain	Res	Type
1	A	151	ASP
1	B	82[A]	ASP
1	B	82[B]	ASP
1	D	3	GLU
1	D	151	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

19 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	4UO	B	201	-	16,22,22	3.33	4 (25%)	20,33,33	3.55	5 (25%)
4	SO4	D	204	-	4,4,4	0.38	0	6,6,6	0.70	0
2	4UO	A	201	-	16,22,22	3.18	6 (37%)	20,33,33	3.48	5 (25%)
5	PG4	A	205	-	12,12,12	0.81	0	11,11,11	0.55	0
4	SO4	C	203	-	4,4,4	0.13	0	6,6,6	0.21	0
3	PO4	A	202	-	4,4,4	1.86	2 (50%)	6,6,6	0.38	0
4	SO4	B	203	-	4,4,4	0.20	0	6,6,6	0.16	0
3	PO4	C	202	-	4,4,4	1.32	0	6,6,6	0.56	0
6	GOL	C	204	-	5,5,5	0.34	0	5,5,5	0.36	0
7	PGE	C	205	-	9,9,9	0.29	0	8,8,8	0.31	0
5	PG4	D	205	-	12,12,12	0.85	0	11,11,11	0.49	0
2	4UO	D	201	-	16,22,22	3.24	3 (18%)	20,33,33	3.14	6 (30%)
2	4UO	C	201	-	16,22,22	3.31	5 (31%)	20,33,33	3.01	4 (20%)
3	PO4	D	202	-	4,4,4	2.12	2 (50%)	6,6,6	0.60	0
4	SO4	A	203	-	4,4,4	0.22	0	6,6,6	0.15	0
3	PO4	B	202	-	4,4,4	1.55	0	6,6,6	0.72	0
4	SO4	A	204	-	4,4,4	0.11	0	6,6,6	0.18	0
4	SO4	D	203	-	4,4,4	0.10	0	6,6,6	0.32	0
6	GOL	B	204	-	5,5,5	0.35	0	5,5,5	0.80	0

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
5	PG4	D	205	-	-	6/10/10/10	-
2	4UO	D	201	-	-	0/2/22/22	0/3/3/3
2	4UO	A	201	-	-	0/2/22/22	0/3/3/3
2	4UO	C	201	-	-	0/2/22/22	0/3/3/3
2	4UO	B	201	-	-	0/2/22/22	0/3/3/3
6	GOL	C	204	-	-	0/4/4/4	-
5	PG4	A	205	-	-	7/10/10/10	-
7	PGE	C	205	-	-	3/7/7/7	-
6	GOL	B	204	-	-	2/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	201	4UO	O6-C6	9.58	1.42	1.23

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	4UO	O6-C6	9.56	1.42	1.23
2	D	201	4UO	O6-C6	9.11	1.41	1.23
2	A	201	4UO	O6-C6	8.55	1.40	1.23
2	D	201	4UO	O2-C2	8.19	1.40	1.23
2	C	201	4UO	O2-C2	7.80	1.39	1.23
2	B	201	4UO	O2-C2	7.77	1.39	1.23
2	A	201	4UO	O2-C2	7.16	1.38	1.23
2	A	201	4UO	C6-N1	-4.30	1.31	1.37
2	B	201	4UO	C6-N1	-3.58	1.32	1.37
2	C	201	4UO	C6-N1	-2.97	1.33	1.37
3	D	202	PO4	P-O4	-2.88	1.45	1.54
2	D	201	4UO	C6-N1	-2.86	1.33	1.37
2	A	201	4UO	C2-N1	-2.53	1.33	1.37
2	A	201	4UO	C2-N3	-2.46	1.32	1.36
2	B	201	4UO	C2-N1	-2.43	1.33	1.37
2	C	201	4UO	C2-N3	-2.40	1.32	1.36
3	D	202	PO4	P-O2	-2.36	1.47	1.54
3	A	202	PO4	P-O2	-2.31	1.47	1.54
2	A	201	4UO	C5-C6	-2.19	1.43	1.47
3	A	202	PO4	P-O4	-2.13	1.48	1.54
2	C	201	4UO	C2-N1	-2.12	1.33	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	4UO	N3-C2-N1	12.02	122.89	115.90
2	B	201	4UO	N3-C2-N1	11.82	122.77	115.90
2	D	201	4UO	N3-C2-N1	10.06	121.75	115.90
2	C	201	4UO	N3-C2-N1	9.49	121.41	115.90
2	B	201	4UO	C6-N1-C2	-7.17	121.22	126.88
2	C	201	4UO	C6-N1-C2	-6.61	121.67	126.88
2	D	201	4UO	C6-N1-C2	-6.41	121.82	126.88
2	A	201	4UO	C4-N3-C2	-6.19	118.44	128.11
2	A	201	4UO	C6-N1-C2	-5.58	122.48	126.88
2	D	201	4UO	C4-N3-C2	-5.22	119.94	128.11
2	B	201	4UO	C4-N3-C2	-5.01	120.28	128.11
2	C	201	4UO	C4-N3-C2	-4.51	121.06	128.11
2	B	201	4UO	O2-C2-N1	-3.88	114.51	121.82
2	C	201	4UO	C5-C6-N1	3.25	119.70	113.95
2	B	201	4UO	C5-C6-N1	3.00	119.24	113.95
2	D	201	4UO	C5-C6-N1	2.97	119.19	113.95
2	A	201	4UO	O2-C2-N1	-2.96	116.23	121.82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	4UO	C5-C6-N1	2.57	118.49	113.95
2	D	201	4UO	O6-C6-C5	-2.07	120.34	124.37
2	D	201	4UO	O2-C2-N1	-2.04	117.96	121.82

There are no chirality outliers.

All (18) torsion outliers are listed below:

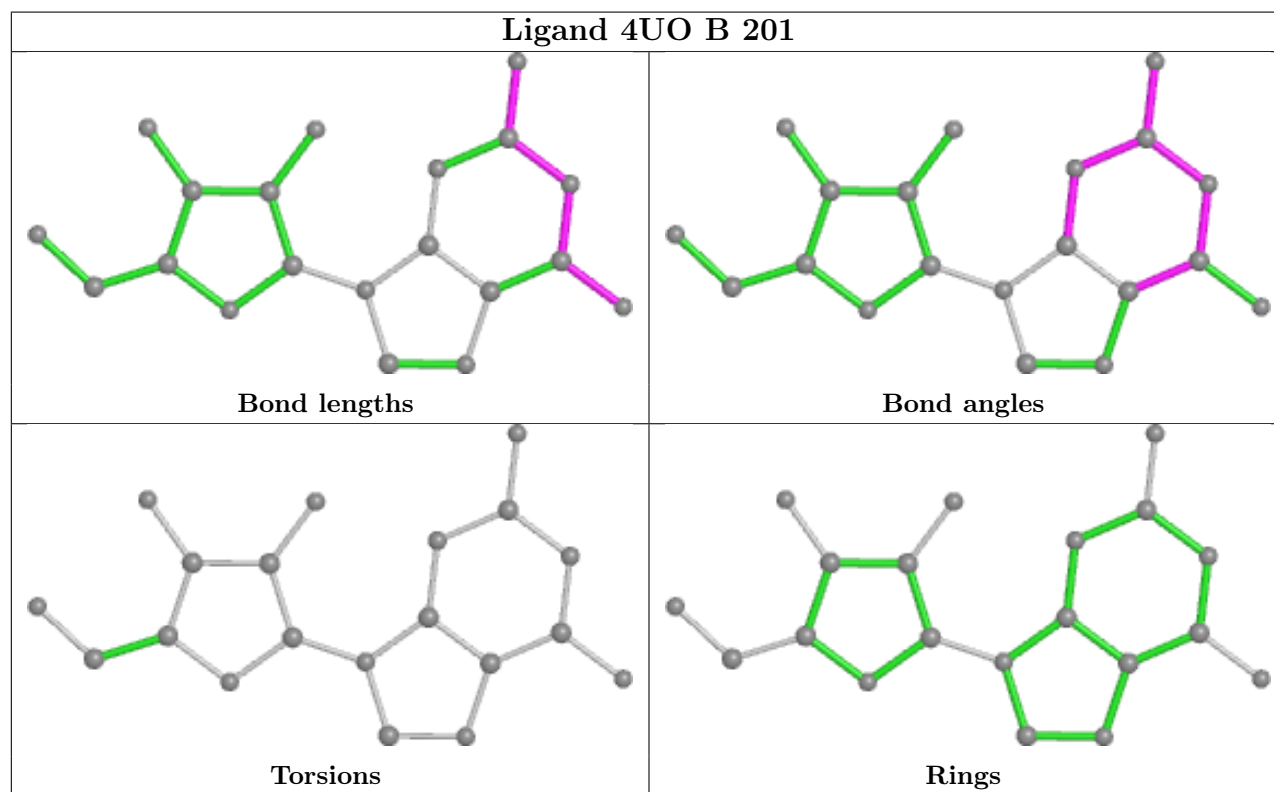
Mol	Chain	Res	Type	Atoms
5	D	205	PG4	C1-C2-O2-C3
5	A	205	PG4	C4-C3-O2-C2
5	D	205	PG4	O2-C3-C4-O3
5	A	205	PG4	O2-C3-C4-O3
7	C	205	PGE	C3-C4-O3-C5
5	A	205	PG4	O3-C5-C6-O4
5	A	205	PG4	O1-C1-C2-O2
5	A	205	PG4	O4-C7-C8-O5
5	D	205	PG4	C6-C5-O3-C4
5	D	205	PG4	C3-C4-O3-C5
5	A	205	PG4	C8-C7-O4-C6
7	C	205	PGE	O2-C3-C4-O3
6	B	204	GOL	O1-C1-C2-O2
5	D	205	PG4	C5-C6-O4-C7
5	A	205	PG4	C6-C5-O3-C4
7	C	205	PGE	C1-C2-O2-C3
5	D	205	PG4	C4-C3-O2-C2
6	B	204	GOL	O1-C1-C2-C3

There are no ring outliers.

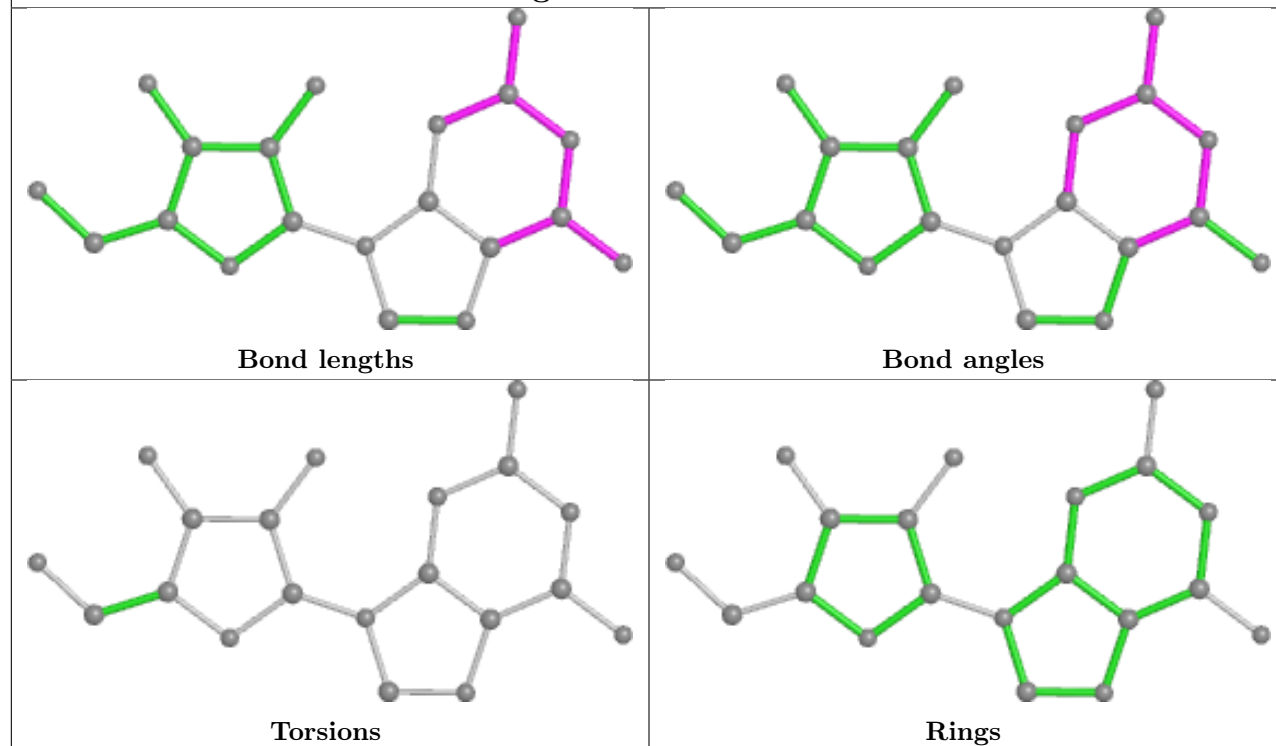
10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	4UO	1	0
5	A	205	PG4	3	0
4	C	203	SO4	1	0
6	C	204	GOL	3	0
7	C	205	PGE	2	0
5	D	205	PG4	1	0
2	D	201	4UO	2	0
2	C	201	4UO	1	0
4	A	204	SO4	2	0
6	B	204	GOL	1	0

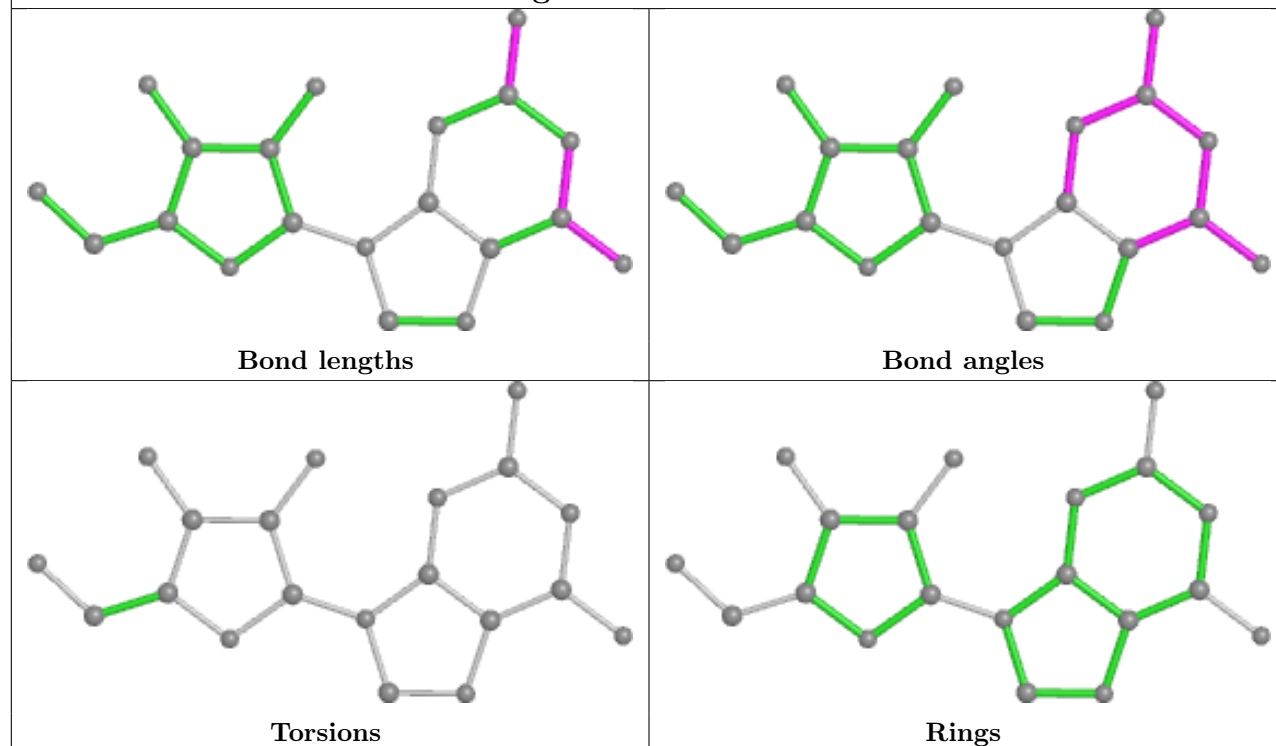
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

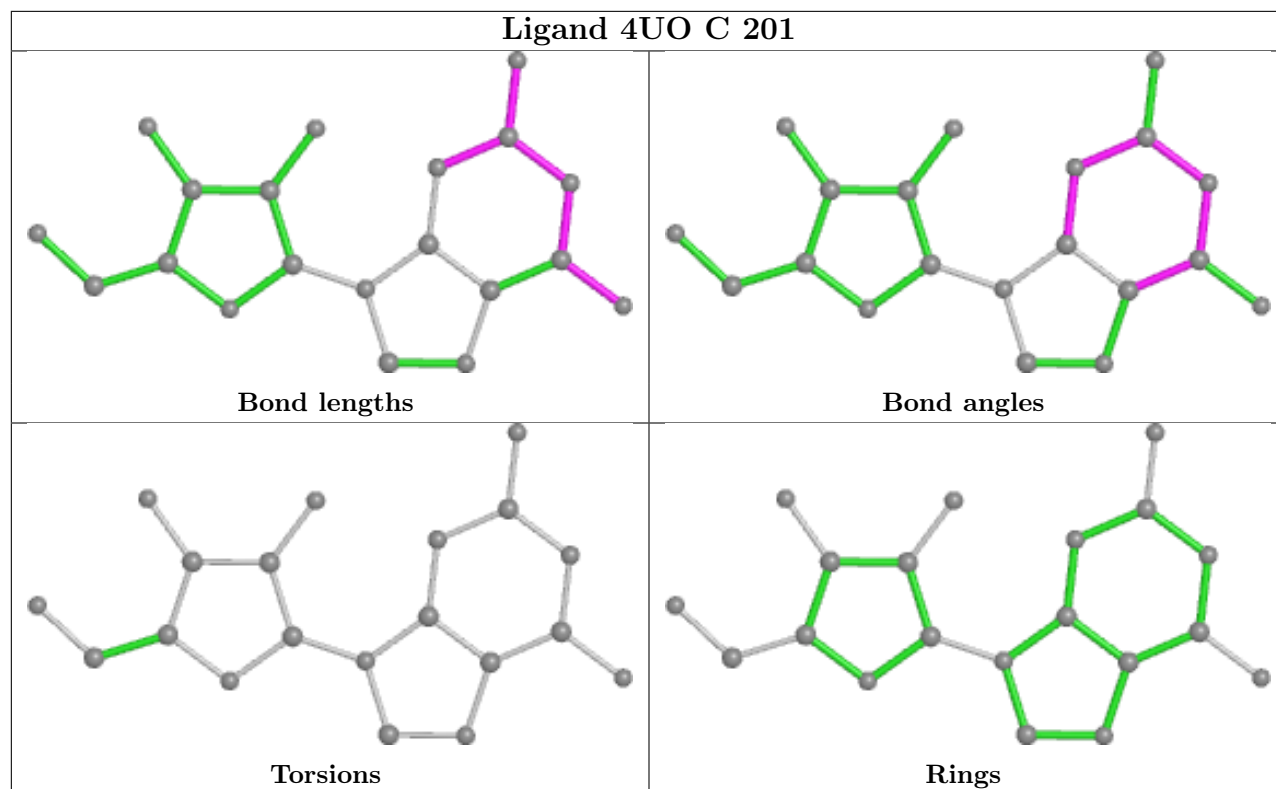


## Ligand 4UO A 201



## Ligand 4UO D 201





## 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 [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	169/179 (94%)	-0.55	1 (0%) 89 91	12, 18, 34, 76	0
1	B	167/179 (93%)	-0.41	3 (1%) 68 72	14, 23, 46, 66	0
1	C	170/179 (94%)	-0.29	5 (2%) 51 56	13, 22, 47, 81	0
1	D	176/179 (98%)	-0.46	4 (2%) 60 65	12, 18, 47, 78	0
All	All	682/716 (95%)	-0.43	13 (1%) 66 70	12, 20, 46, 81	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	178	ARG	6.5
1	B	177	ILE	5.4
1	A	179	LYS	5.3
1	C	72	SER	5.1
1	D	67	VAL	4.4
1	C	1	MET	3.9
1	B	175	LEU	3.8
1	C	177	ILE	3.7
1	C	178	ARG	3.0
1	C	2	VAL	2.8
1	D	177	ILE	2.5
1	D	68	GLY	2.3
1	B	2	VAL	2.1

### 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 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.

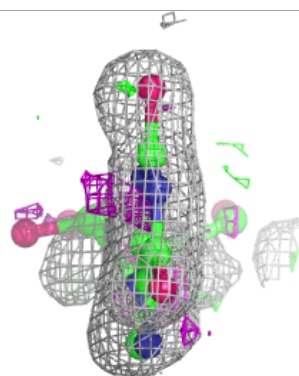
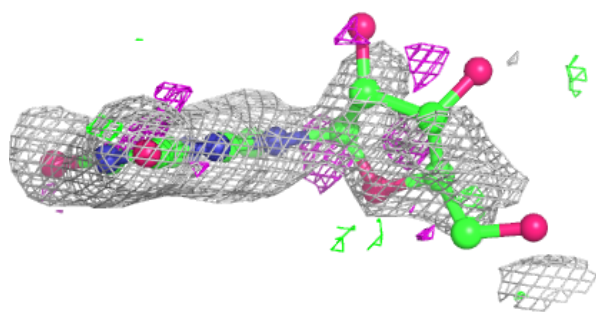
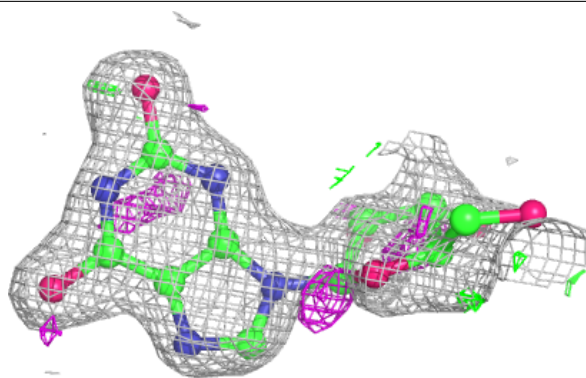
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	B	204	6/6	0.77	0.25	54,64,65,73	0
5	PG4	A	205	13/13	0.78	0.22	32,51,67,69	0
6	GOL	C	204	6/6	0.84	0.20	44,49,67,72	0
5	PG4	D	205	13/13	0.85	0.22	41,54,63,69	0
4	SO4	D	204	5/5	0.89	0.18	18,27,61,63	0
2	4UO	B	201	20/20	0.90	0.24	31,53,90,93	0
7	PGE	C	205	10/10	0.91	0.12	45,50,60,73	0
2	4UO	C	201	20/20	0.92	0.14	22,36,58,68	0
2	4UO	A	201	20/20	0.95	0.09	19,26,51,52	0
2	4UO	D	201	20/20	0.95	0.09	17,23,49,57	0
4	SO4	A	204	5/5	0.95	0.17	44,48,55,78	0
4	SO4	B	203	5/5	0.96	0.21	48,61,66,68	0
4	SO4	C	203	5/5	0.97	0.12	45,52,58,61	0
4	SO4	A	203	5/5	0.98	0.07	42,45,49,49	0
3	PO4	B	202	5/5	0.99	0.08	20,22,26,31	0
3	PO4	C	202	5/5	0.99	0.07	21,23,27,29	0
3	PO4	D	202	5/5	0.99	0.10	15,17,25,35	0
4	SO4	D	203	5/5	0.99	0.05	33,35,46,58	0
3	PO4	A	202	5/5	0.99	0.08	18,20,21,23	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.



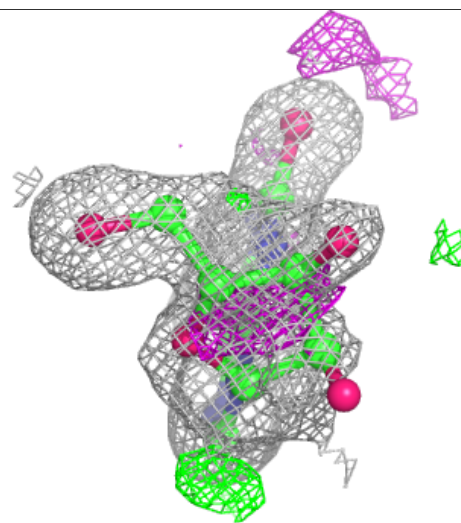
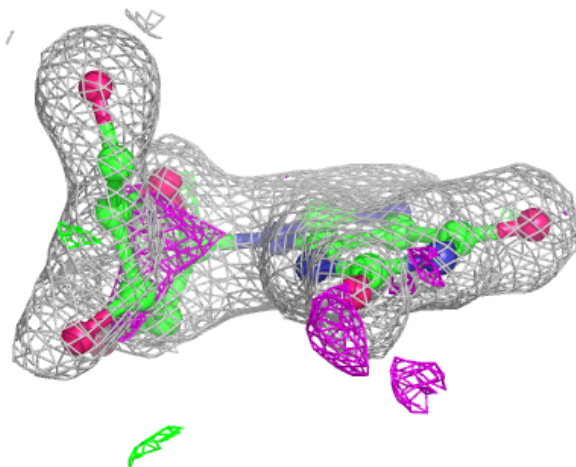
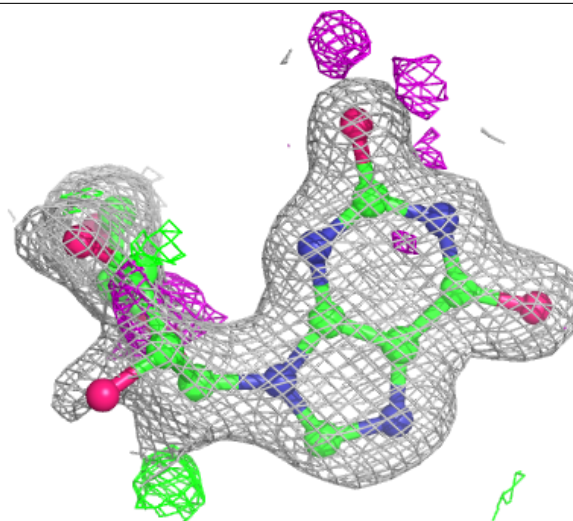
**Electron density around 4UO B 201:**

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



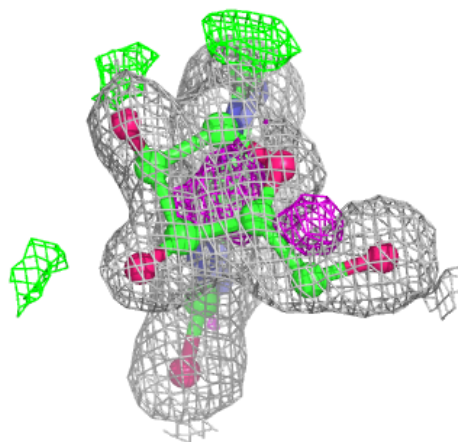
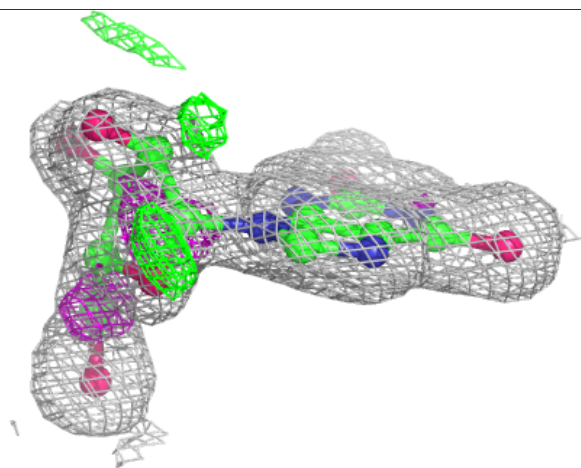
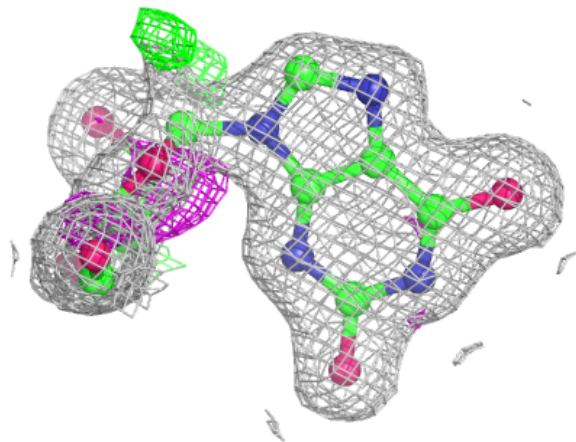
**Electron density around 4UO C 201:**

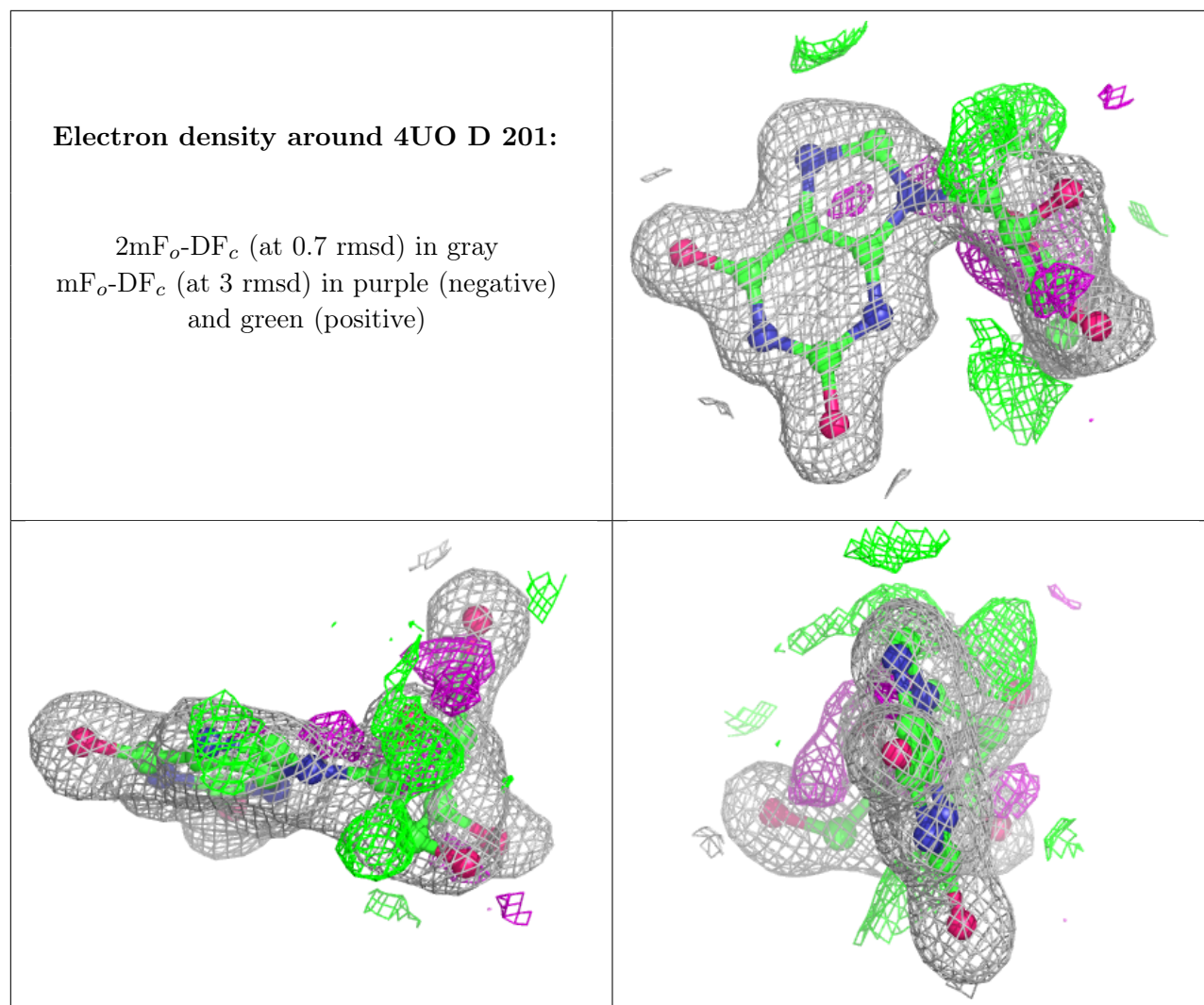
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 4UO A 201:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.