



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2021 – 10:16 AM EST

PDB ID : 7LJE  
Title : Discovery of Spirohydantoin as Selective, Orally Bioavailable Inhibitors of p300/CBP Histone Acetyltransferases  
Authors : Jakob, C.G.  
Deposited on : 2021-01-29  
Resolution : 2.61 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.

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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 : 2.17.1  
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) : 2.17.1

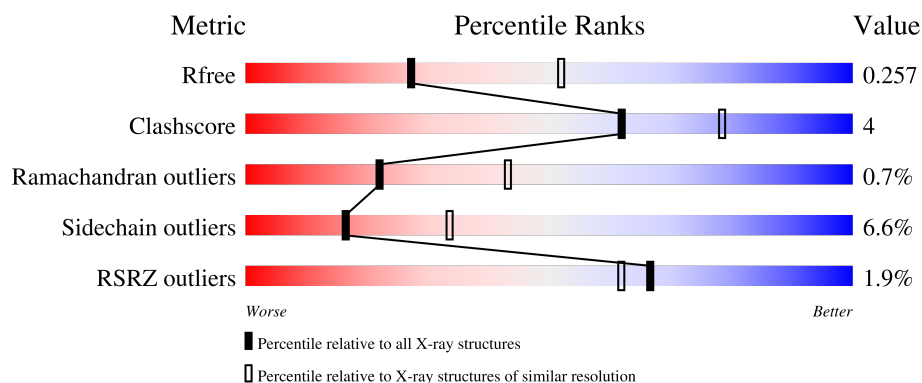
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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> <div></div> <div>80%</div> <div>11%</div> <div>• 8%</div> </div> </div>
1	B	348	<div> <div> <div>2%</div> <div>77%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	C	348	<div> <div> <div></div> <div>77%</div> <div>13%</div> <div>• 8%</div> </div> </div>
1	D	348	<div> <div> <div>3%</div> <div>79%</div> <div>13%</div> <div>• 7%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11200 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 Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	1	0
			2611	1674	448	474	15			
1	B	324	Total	C	N	O	S	0	0	0
			2653	1699	457	483	14			
1	C	319	Total	C	N	O	S	0	1	0
			2611	1674	448	474	15			
1	D	324	Total	C	N	O	S	0	1	0
			2656	1701	457	483	15			

There are 136 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q09472
A	?	-	GLU	deletion	UNP Q09472
A	?	-	GLU	deletion	UNP Q09472
A	?	-	GLU	deletion	UNP Q09472
A	?	-	ARG	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	ARG	deletion	UNP Q09472
A	?	-	GLU	deletion	UNP Q09472
A	?	-	GLU	deletion	UNP Q09472
A	?	-	ASN	deletion	UNP Q09472
A	?	-	THR	deletion	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	ASN	deletion	UNP Q09472
A	?	-	GLU	deletion	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	THR	deletion	UNP Q09472
A	?	-	ASP	deletion	UNP Q09472
A	?	-	VAL	deletion	UNP Q09472
A	?	-	THR	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	GLY	deletion	UNP Q09472

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q09472
A	?	-	SER	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	ASN	deletion	UNP Q09472
A	?	-	ALA	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	?	-	ASN	deletion	UNP Q09472
A	?	-	ASN	deletion	UNP Q09472
A	?	-	LYS	deletion	UNP Q09472
A	1637	ARG	LYS	conflict	UNP Q09472
A	1652	GLY	MET	conflict	UNP Q09472
B	?	-	GLU	deletion	UNP Q09472
B	?	-	GLU	deletion	UNP Q09472
B	?	-	GLU	deletion	UNP Q09472
B	?	-	GLU	deletion	UNP Q09472
B	?	-	ARG	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	ARG	deletion	UNP Q09472
B	?	-	GLU	deletion	UNP Q09472
B	?	-	GLU	deletion	UNP Q09472
B	?	-	ASN	deletion	UNP Q09472
B	?	-	THR	deletion	UNP Q09472
B	?	-	SER	deletion	UNP Q09472
B	?	-	ASN	deletion	UNP Q09472
B	?	-	GLU	deletion	UNP Q09472
B	?	-	SER	deletion	UNP Q09472
B	?	-	THR	deletion	UNP Q09472
B	?	-	ASP	deletion	UNP Q09472
B	?	-	VAL	deletion	UNP Q09472
B	?	-	THR	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	GLY	deletion	UNP Q09472
B	?	-	ASP	deletion	UNP Q09472
B	?	-	SER	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	ASN	deletion	UNP Q09472
B	?	-	ALA	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472

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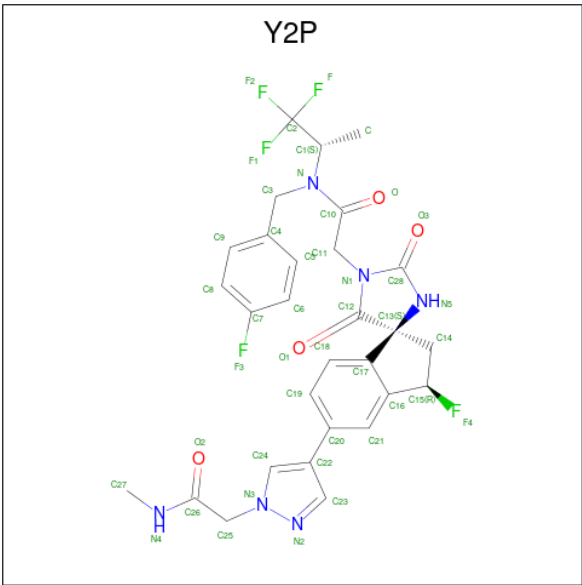
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP Q09472
B	?	-	ASN	deletion	UNP Q09472
B	?	-	LYS	deletion	UNP Q09472
B	1637	ARG	LYS	conflict	UNP Q09472
B	1652	GLY	MET	conflict	UNP Q09472
C	?	-	GLU	deletion	UNP Q09472
C	?	-	GLU	deletion	UNP Q09472
C	?	-	GLU	deletion	UNP Q09472
C	?	-	GLU	deletion	UNP Q09472
C	?	-	ARG	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	ARG	deletion	UNP Q09472
C	?	-	GLU	deletion	UNP Q09472
C	?	-	GLU	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	THR	deletion	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	GLU	deletion	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	THR	deletion	UNP Q09472
C	?	-	ASP	deletion	UNP Q09472
C	?	-	VAL	deletion	UNP Q09472
C	?	-	THR	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	GLY	deletion	UNP Q09472
C	?	-	ASP	deletion	UNP Q09472
C	?	-	SER	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	ALA	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	ASN	deletion	UNP Q09472
C	?	-	LYS	deletion	UNP Q09472
C	1637	ARG	LYS	conflict	UNP Q09472
C	1652	GLY	MET	conflict	UNP Q09472
D	?	-	GLU	deletion	UNP Q09472
D	?	-	GLU	deletion	UNP Q09472
D	?	-	GLU	deletion	UNP Q09472

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP Q09472
D	?	-	ARG	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	ARG	deletion	UNP Q09472
D	?	-	GLU	deletion	UNP Q09472
D	?	-	GLU	deletion	UNP Q09472
D	?	-	ASN	deletion	UNP Q09472
D	?	-	THR	deletion	UNP Q09472
D	?	-	SER	deletion	UNP Q09472
D	?	-	ASN	deletion	UNP Q09472
D	?	-	GLU	deletion	UNP Q09472
D	?	-	SER	deletion	UNP Q09472
D	?	-	THR	deletion	UNP Q09472
D	?	-	ASP	deletion	UNP Q09472
D	?	-	VAL	deletion	UNP Q09472
D	?	-	THR	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	GLY	deletion	UNP Q09472
D	?	-	ASP	deletion	UNP Q09472
D	?	-	SER	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	ASN	deletion	UNP Q09472
D	?	-	ALA	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	?	-	ASN	deletion	UNP Q09472
D	?	-	ASN	deletion	UNP Q09472
D	?	-	LYS	deletion	UNP Q09472
D	1637	ARG	LYS	conflict	UNP Q09472
D	1652	GLY	MET	conflict	UNP Q09472

- Molecule 2 is 2-[4-[(3'R,4S)-3'-fluoro-1-[2-[(4-fluorophenyl)methyl-[(1S)-2,2,2-trifluoro-1-methyl-ethyl]amino]-2-oxo-ethyl]-2,5-dioxo-spiro[imidazolidine-4,1'-indane]-5'-yl]pyrazol-1-yl]-N-methyl-acetamide (three-letter code: Y2P) (formula: C<sub>29</sub>H<sub>27</sub>F<sub>5</sub>N<sub>6</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			44	29	5	6	4		
2	B	1	Total	C	F	N	O	0	0
			44	29	5	6	4		
2	C	1	Total	C	F	N	O	0	0
			44	29	5	6	4		
2	D	1	Total	C	F	N	O	0	0
			44	29	5	6	4		

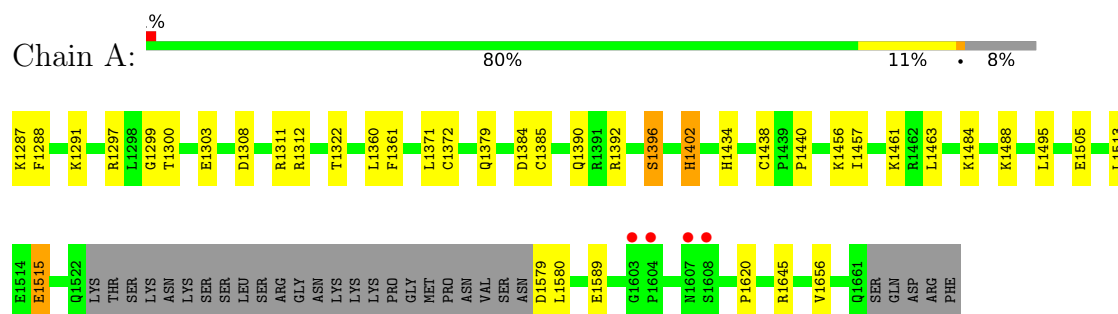
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	137	Total	O	0	0
			137	137		
3	C	135	Total	O	0	0
			135	135		
3	D	99	Total	O	0	0
			99	99		

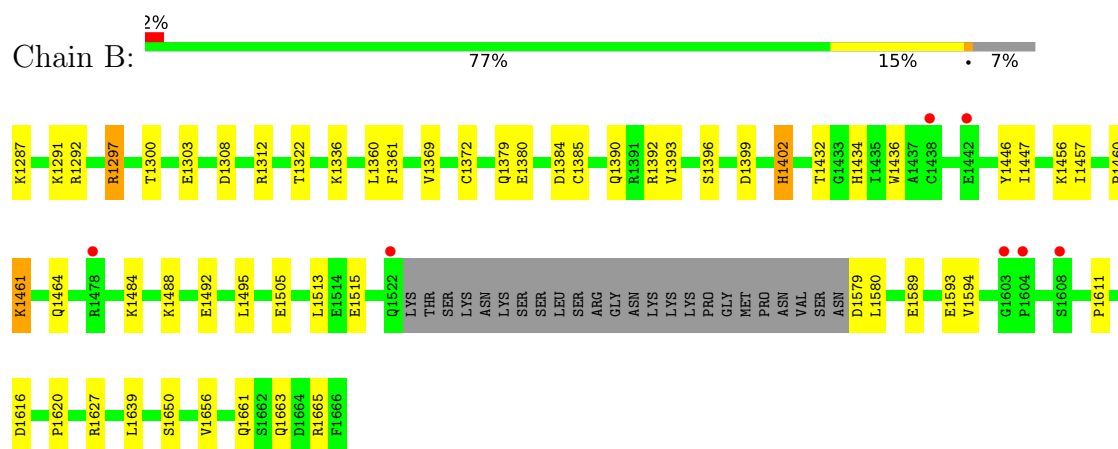
### 3 Residue-property plots [i](#)

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.

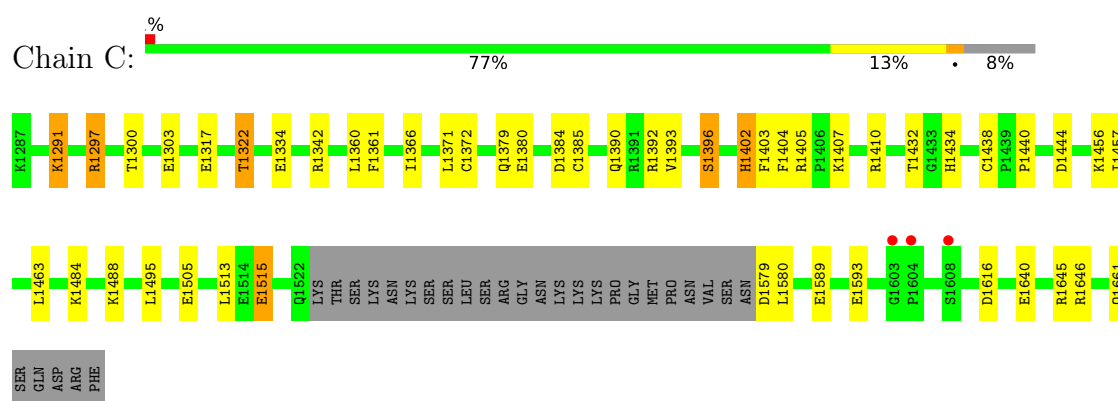
#### • Molecule 1: Histone acetyltransferase p300



#### • Molecule 1: Histone acetyltransferase p300

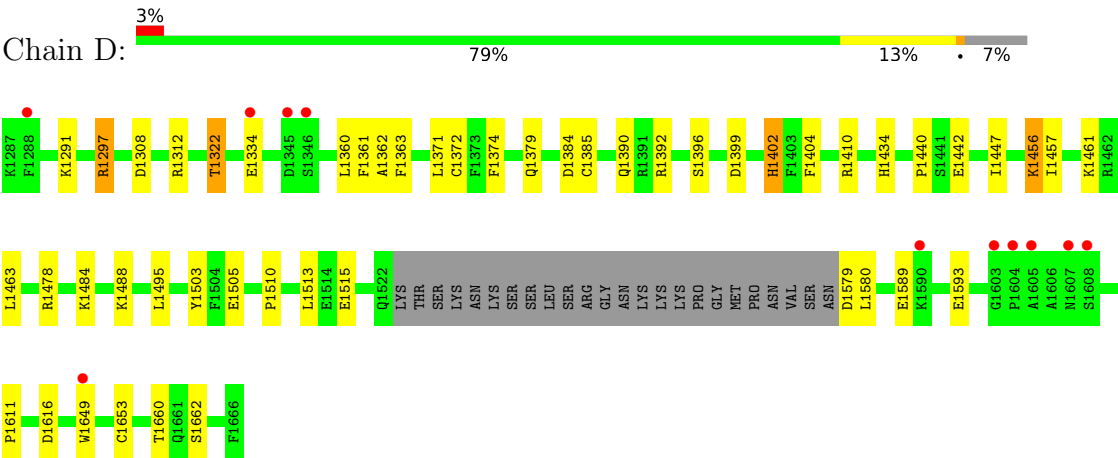


#### • Molecule 1: Histone acetyltransferase p300





● Molecule 1: Histone acetyltransferase p300



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.29Å 81.49Å 124.09Å 90.00° 117.31° 90.00°	Depositor
Resolution (Å)	74.58 – 2.61 74.58 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.1 (74.58-2.61) 99.1 (74.58-2.61)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 2.62Å)	Xtrriage
Refinement program	BUSTER 2.11.8 (11-DEC-2020)	Depositor
R, $R_{free}$	0.211 , 0.265 0.204 , 0.257	Depositor DCC
$R_{free}$ test set	1977 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.5	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.27 % 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 4.3153e-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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Y2P

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	0.43	0/2686	0.62	0/3635
1	B	0.42	0/2726	0.62	0/3687
1	C	0.44	0/2686	0.63	0/3635
1	D	0.39	0/2732	0.61	0/3696
All	All	0.42	0/10830	0.62	0/14653

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 [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	A	2611	0	2565	15	0
1	B	2653	0	2599	30	0
1	C	2611	0	2565	24	0
1	D	2656	0	2604	27	0
2	A	44	0	0	0	0
2	B	44	0	0	2	0
2	C	44	0	0	0	0
2	D	44	0	0	0	0
3	A	122	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	137	0	0	0	0
3	C	135	0	0	3	0
3	D	99	0	0	0	0
All	All	11200	0	10333	93	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 (93) 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:C:1291:LYS:HE3	1:C:1322:THR:HB	1.35	1.06
1:D:1291:LYS:HE3	1:D:1322:THR:HB	1.47	0.97
1:C:1392:ARG:HH11	1:C:1434:HIS:HE1	1.23	0.87
1:D:1392:ARG:HH11	1:D:1434:HIS:HE1	1.22	0.87
1:A:1392:ARG:HH11	1:A:1434:HIS:HE1	1.23	0.86
1:B:1392:ARG:HH11	1:B:1434:HIS:HE1	1.23	0.85
1:D:1392:ARG:HH11	1:D:1434:HIS:CE1	1.99	0.81
1:B:1392:ARG:HH11	1:B:1434:HIS:CE1	2.01	0.79
1:C:1392:ARG:HH11	1:C:1434:HIS:CE1	2.00	0.79
1:A:1392:ARG:HH11	1:A:1434:HIS:CE1	2.00	0.79
1:B:1291:LYS:HG3	1:B:1322:THR:HG21	1.68	0.76
1:C:1291:LYS:CE	1:C:1322:THR:HB	2.16	0.74
1:B:1461:LYS:H	1:B:1461:LYS:HD3	1.54	0.73
1:C:1322:THR:HG22	3:C:1841:HOH:O	1.93	0.68
1:B:1464:GLN:HG2	1:B:1593:GLU:O	1.94	0.67
1:C:1300:THR:HA	1:C:1303:GLU:HG2	1.80	0.64
1:C:1440:PRO:HG2	1:C:1457:ILE:HG23	1.80	0.62
1:C:1371:LEU:HD21	1:C:1403:PHE:HB2	1.83	0.60
1:D:1322:THR:HG23	1:D:1363:PHE:HB2	1.83	0.60
1:D:1440:PRO:HG2	1:D:1457:ILE:HG23	1.82	0.60
1:A:1300:THR:HA	1:A:1303:GLU:HG2	1.84	0.59
1:C:1366:ILE:HD12	1:C:1371:LEU:HD23	1.83	0.58
1:B:1291:LYS:CG	1:B:1322:THR:HG21	2.33	0.57
1:B:1461:LYS:H	1:B:1461:LYS:CD	2.16	0.56
1:B:1300:THR:HA	1:B:1303:GLU:HG2	1.87	0.56
1:D:1361:PHE:HD1	1:D:1372:CYS:SG	2.29	0.55
1:C:1361:PHE:HD1	1:C:1372:CYS:SG	2.30	0.55
1:A:1361:PHE:HD1	1:A:1372:CYS:SG	2.31	0.54
1:B:1460:PRO:HD2	1:B:1461:LYS:NZ	2.24	0.52
1:B:1446:TYR:O	1:B:1627:ARG:HD2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1639:LEU:HB3	1:B:1650:SER:HB3	1.93	0.51
1:C:1444:ASP:HB3	3:C:1829:HOH:O	2.10	0.51
1:D:1362:ALA:HB3	1:D:1374:PHE:HB3	1.92	0.51
1:B:1484:LYS:HD3	1:B:1488:LYS:HG2	1.92	0.51
1:B:1457:ILE:HD11	2:B:1701:Y2P:O2	2.11	0.51
1:B:1361:PHE:HD1	1:B:1372:CYS:SG	2.34	0.50
1:D:1399:ASP:HB3	1:D:1447:ILE:HB	1.94	0.50
1:A:1484:LYS:HD3	1:A:1488:LYS:HG2	1.92	0.50
1:A:1299:GLY:HA3	3:A:1802:HOH:O	2.11	0.50
1:D:1484:LYS:HD3	1:D:1488:LYS:HG2	1.93	0.50
1:A:1291:LYS:HE3	1:A:1322:THR:OG1	2.11	0.49
1:C:1484:LYS:HD3	1:C:1488:LYS:HG2	1.93	0.49
1:D:1385:CYS:O	1:D:1390:GLN:HB3	2.11	0.49
1:C:1407:LYS:HG2	3:C:1836:HOH:O	2.13	0.49
1:A:1385:CYS:O	1:A:1390:GLN:HB3	2.13	0.48
1:B:1385:CYS:O	1:B:1390:GLN:HB3	2.12	0.48
1:B:1436:TRP:CD1	1:B:1594:VAL:HG12	2.49	0.48
1:B:1436:TRP:HD1	1:B:1594:VAL:HG12	1.79	0.48
1:C:1385:CYS:O	1:C:1390:GLN:HB3	2.13	0.48
1:D:1291:LYS:HE3	1:D:1322:THR:CB	2.33	0.48
1:D:1660:THR:HG22	1:D:1660:THR:O	2.14	0.47
1:A:1620:PRO:HD2	3:A:1893:HOH:O	2.14	0.47
1:D:1297:ARG:HG2	1:D:1616:ASP:OD1	2.14	0.47
1:C:1640:GLU:HB2	1:C:1646:ARG:HD3	1.96	0.46
1:A:1440:PRO:HG2	1:A:1457:ILE:HG23	1.98	0.46
1:A:1288:PHE:CD2	1:A:1288:PHE:N	2.84	0.46
1:A:1515:GLU:HB3	1:D:1611:PRO:HB2	1.98	0.46
1:B:1336:LYS:HD3	1:D:1478:ARG:NH2	2.30	0.46
1:B:1297:ARG:HG2	1:B:1616:ASP:OD1	2.15	0.46
1:B:1460:PRO:HD2	1:B:1461:LYS:HZ3	1.81	0.46
1:B:1611:PRO:HB2	1:C:1515:GLU:HB3	1.99	0.45
1:A:1392:ARG:NH1	1:A:1434:HIS:CE1	2.79	0.45
1:C:1392:ARG:NH1	1:C:1434:HIS:CE1	2.79	0.45
1:D:1291:LYS:CE	1:D:1322:THR:HB	2.31	0.45
1:C:1291:LYS:HE3	1:C:1322:THR:CB	2.26	0.45
1:D:1593:GLU:CD	1:D:1593:GLU:H	2.21	0.45
1:D:1649:TRP:CE2	1:D:1653:CYS:SG	3.10	0.45
1:C:1404:PHE:HB3	1:C:1410:ARG:HG2	1.99	0.44
1:B:1593:GLU:H	1:B:1593:GLU:CD	2.21	0.44
1:B:1620:PRO:HD2	1:B:1663:GLN:NE2	2.33	0.43
1:D:1649:TRP:CZ2	1:D:1653:CYS:SG	3.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1593:GLU:H	1:C:1593:GLU:CD	2.21	0.43
1:B:1287:LYS:HG3	1:B:1292:ARG:HG3	2.00	0.42
1:D:1297:ARG:HG2	1:D:1297:ARG:H	1.74	0.42
1:D:1379:GLN:HE22	1:D:1505:GLU:H	1.68	0.42
1:D:1456:LYS:HD3	1:D:1456:LYS:H	1.85	0.42
1:D:1361:PHE:CD1	1:D:1372:CYS:SG	3.12	0.42
1:C:1379:GLN:HE22	1:C:1505:GLU:H	1.68	0.42
1:A:1379:GLN:HE22	1:A:1505:GLU:H	1.68	0.41
1:B:1380:GLU:HG2	1:B:1393:VAL:HG12	2.02	0.41
1:B:1620:PRO:HD2	1:B:1663:GLN:HE22	1.85	0.41
1:C:1317:GLU:HB3	1:C:1405:ARG:HG2	2.02	0.41
1:B:1379:GLN:HE22	1:B:1505:GLU:H	1.69	0.41
1:D:1308:ASP:O	1:D:1312:ARG:HG3	2.21	0.41
1:D:1404:PHE:HB3	1:D:1410:ARG:HG3	2.02	0.41
1:B:1399:ASP:HB3	1:B:1447:ILE:HB	2.03	0.41
1:C:1380:GLU:HG2	1:C:1393:VAL:HG12	2.02	0.41
1:D:1503:TYR:CZ	1:D:1510:PRO:HB3	2.55	0.41
1:D:1392:ARG:NH1	1:D:1434:HIS:CE1	2.78	0.40
1:A:1308:ASP:O	1:A:1312:ARG:HG3	2.21	0.40
1:B:1457:ILE:HD11	2:B:1701:Y2P:C26	2.51	0.40
1:C:1297:ARG:HG2	1:C:1616:ASP:OD1	2.22	0.40
1:B:1308:ASP:O	1:B:1312:ARG:HG3	2.22	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	316/348 (91%)	308 (98%)	6 (2%)	2 (1%)	25 47
1	B	320/348 (92%)	312 (98%)	6 (2%)	2 (1%)	25 47
1	C	316/348 (91%)	308 (98%)	6 (2%)	2 (1%)	25 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	321/348 (92%)	312 (97%)	6 (2%)	3 (1%)	17	35
All	All	1273/1392 (92%)	1240 (97%)	24 (2%)	9 (1%)	22	43

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1396	SER
1	C	1396	SER
1	A	1402	HIS
1	B	1402	HIS
1	C	1402	HIS
1	D	1396	SER
1	D	1402	HIS
1	B	1661	GLN
1	D	1662	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	287/313 (92%)	266 (93%)	21 (7%)	14	28
1	B	291/313 (93%)	273 (94%)	18 (6%)	18	37
1	C	287/313 (92%)	265 (92%)	22 (8%)	13	25
1	D	292/313 (93%)	275 (94%)	17 (6%)	20	40
All	All	1157/1252 (92%)	1079 (93%)	78 (7%)	16	33

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1287	LYS
1	A	1297	ARG
1	A	1311	ARG
1	A	1360	LEU
1	A	1371	LEU

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Mol	Chain	Res	Type
1	A	1384	ASP
1	A	1396	SER
1	A	1402	HIS
1	A	1438[A]	CYS
1	A	1438[B]	CYS
1	A	1456	LYS
1	A	1461	LYS
1	A	1463	LEU
1	A	1495	LEU
1	A	1513	LEU
1	A	1515	GLU
1	A	1579	ASP
1	A	1580	LEU
1	A	1589	GLU
1	A	1645	ARG
1	A	1656	VAL
1	B	1297	ARG
1	B	1360	LEU
1	B	1369	VAL
1	B	1384	ASP
1	B	1396	SER
1	B	1402	HIS
1	B	1432	THR
1	B	1456	LYS
1	B	1461	LYS
1	B	1492	GLU
1	B	1495	LEU
1	B	1513	LEU
1	B	1515	GLU
1	B	1579	ASP
1	B	1580	LEU
1	B	1589	GLU
1	B	1656	VAL
1	B	1665	ARG
1	C	1291	LYS
1	C	1297	ARG
1	C	1322	THR
1	C	1334	GLU
1	C	1342	ARG
1	C	1360	LEU
1	C	1384	ASP
1	C	1396	SER

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Mol	Chain	Res	Type
1	C	1402	HIS
1	C	1432	THR
1	C	1438[A]	CYS
1	C	1438[B]	CYS
1	C	1456	LYS
1	C	1463	LEU
1	C	1495	LEU
1	C	1513	LEU
1	C	1515	GLU
1	C	1579	ASP
1	C	1580	LEU
1	C	1589	GLU
1	C	1645	ARG
1	C	1661	GLN
1	D	1297	ARG
1	D	1322	THR
1	D	1334	GLU
1	D	1360	LEU
1	D	1371	LEU
1	D	1384	ASP
1	D	1402	HIS
1	D	1442	GLU
1	D	1456	LYS
1	D	1461	LYS
1	D	1463	LEU
1	D	1495	LEU
1	D	1513	LEU
1	D	1515	GLU
1	D	1579	ASP
1	D	1580	LEU
1	D	1589	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1379	GLN
1	A	1434	HIS
1	B	1379	GLN
1	B	1434	HIS
1	B	1663	GLN
1	C	1379	GLN
1	C	1402	HIS

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Mol	Chain	Res	Type
1	C	1434	HIS
1	C	1659	HIS
1	C	1661	GLN
1	D	1379	GLN
1	D	1402	HIS
1	D	1434	HIS

### 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 ⓘ

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	$\# Z  > 2$
2	Y2P	A	1701	-	42,48,48	0.38	0	49,73,73	0.79	3 (6%)
2	Y2P	B	1701	-	42,48,48	0.38	0	49,73,73	0.78	2 (4%)
2	Y2P	C	1701	-	42,48,48	0.48	0	49,73,73	0.91	3 (6%)
2	Y2P	D	1701	-	42,48,48	0.32	0	49,73,73	0.79	3 (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	Y2P	A	1701	-	-	1/31/66/66	0/5/5/5
2	Y2P	B	1701	-	-	0/31/66/66	0/5/5/5
2	Y2P	C	1701	-	-	0/31/66/66	0/5/5/5
2	Y2P	D	1701	-	-	2/31/66/66	0/5/5/5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1701	Y2P	C17-C16-C15	3.03	114.23	107.36
2	C	1701	Y2P	C21-C16-C15	-2.80	125.11	130.81
2	A	1701	Y2P	C17-C16-C15	2.74	113.58	107.36
2	D	1701	Y2P	C17-C16-C15	2.62	113.29	107.36
2	C	1701	Y2P	C20-C21-C16	-2.51	119.50	122.09
2	B	1701	Y2P	C20-C21-C16	-2.44	119.57	122.09
2	D	1701	Y2P	C20-C21-C16	-2.37	119.65	122.09
2	B	1701	Y2P	C17-C16-C15	2.35	112.70	107.36
2	A	1701	Y2P	C21-C16-C15	-2.33	126.08	130.81
2	D	1701	Y2P	C21-C16-C15	-2.18	126.38	130.81
2	A	1701	Y2P	C20-C21-C16	-2.12	119.90	122.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1701	Y2P	N3-C25-C26-O2
2	A	1701	Y2P	C2-C1-N-C3
2	D	1701	Y2P	N3-C25-C26-N4

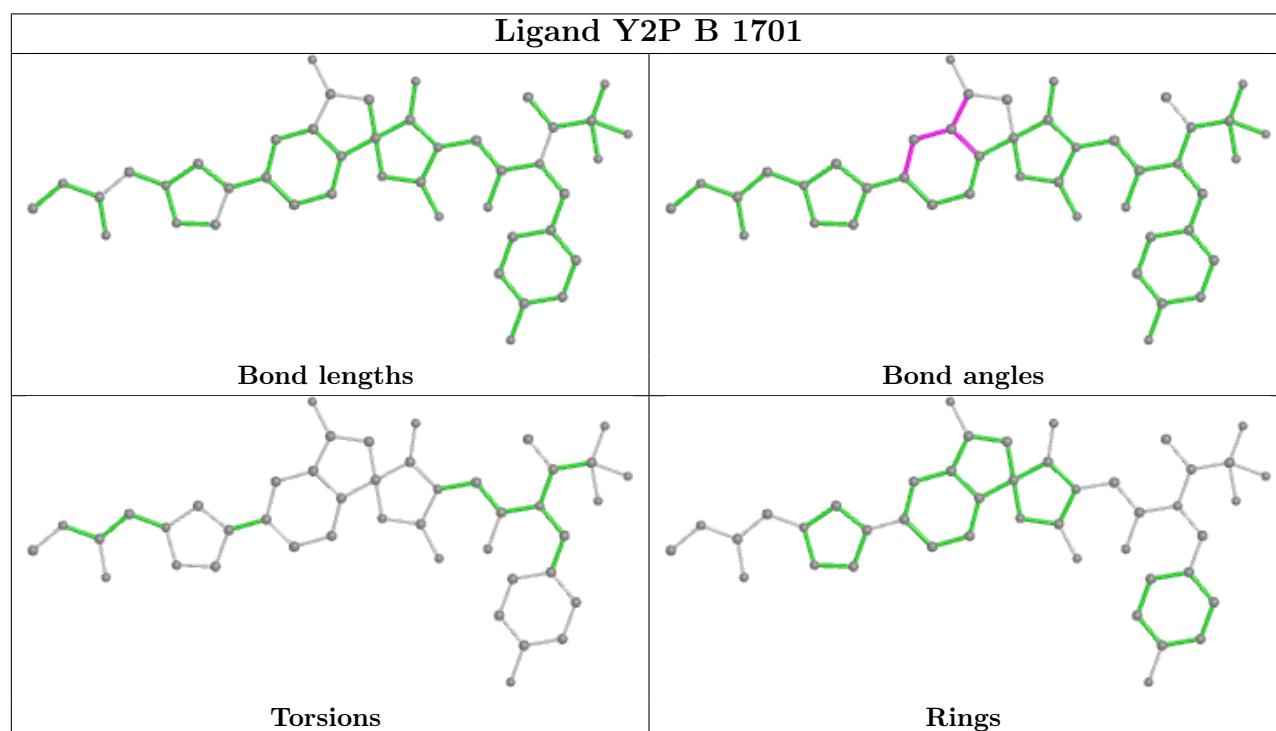
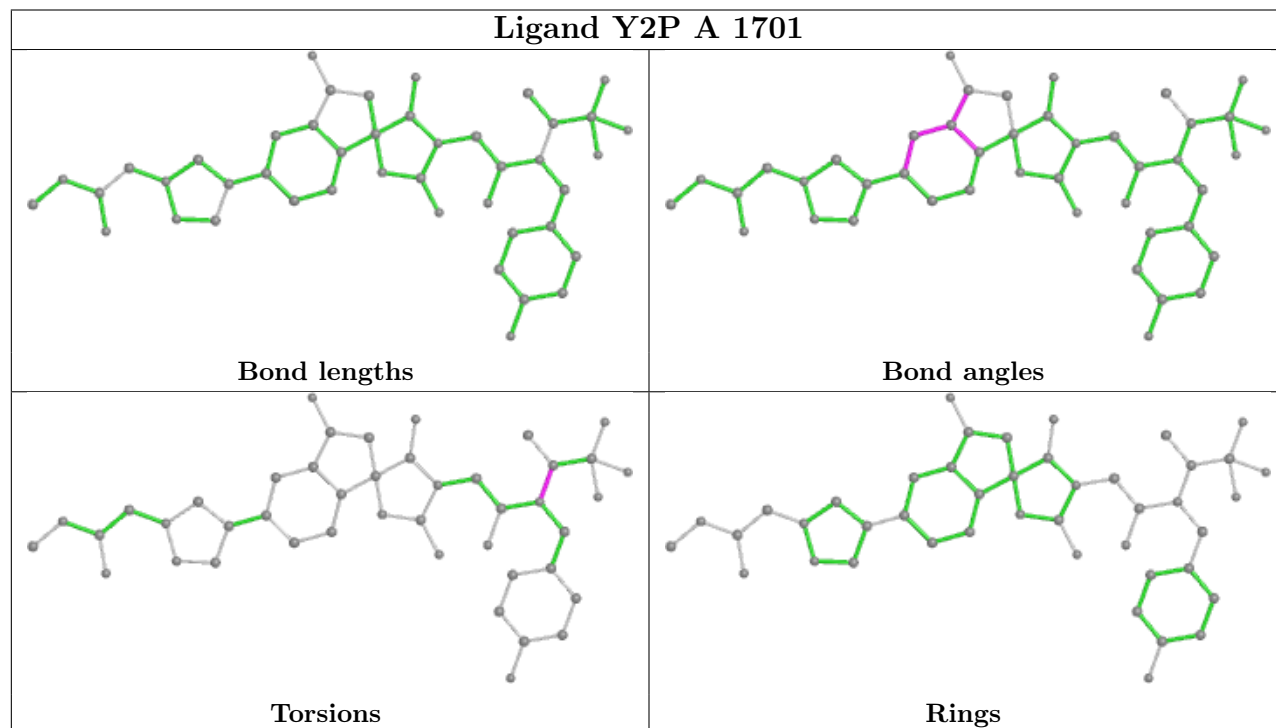
There are no ring outliers.

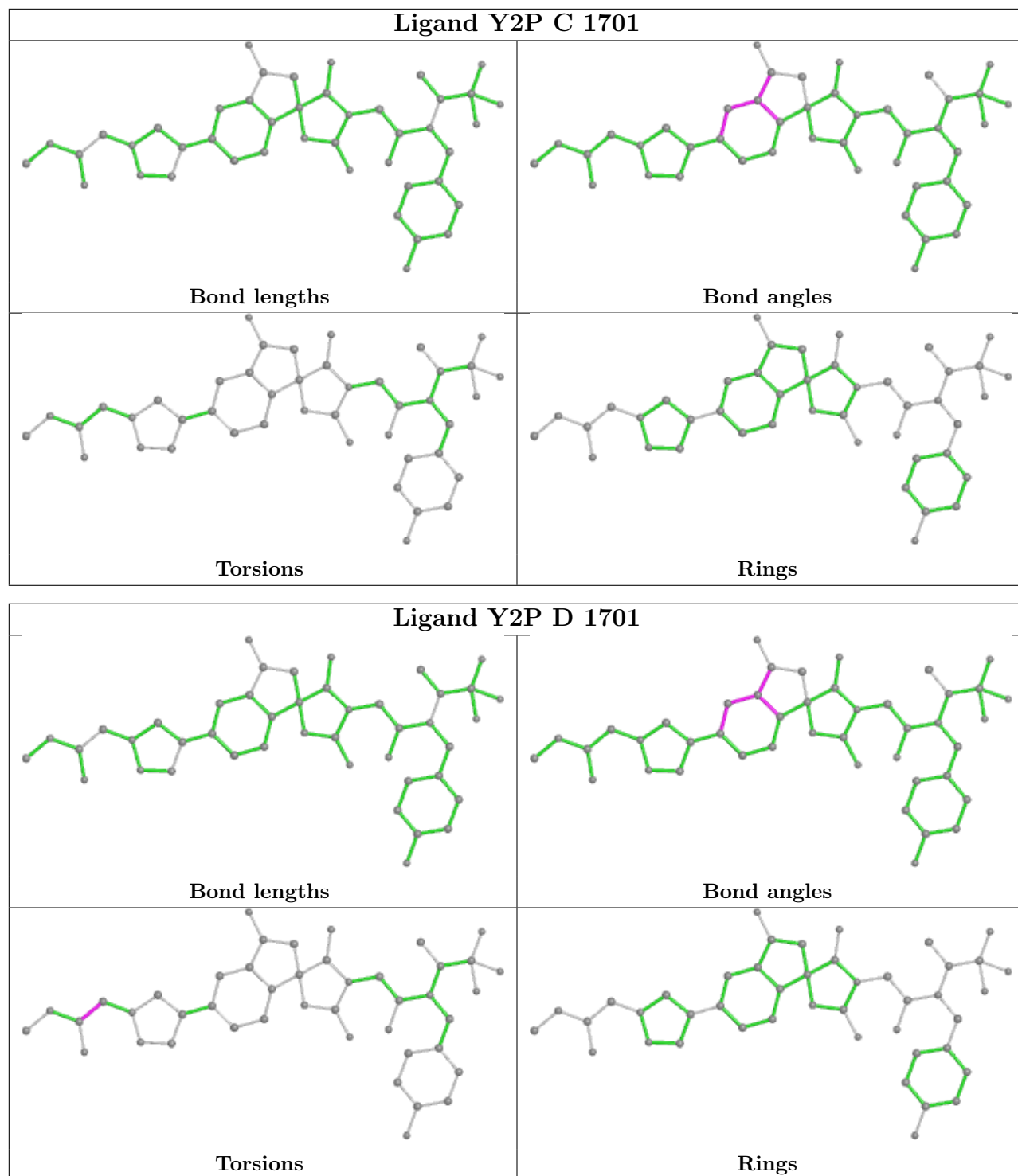
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1701	Y2P	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 ⓘ

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	319/348 (91%)	-0.21	4 (1%) 77 73	19, 41, 62, 82	8 (2%)
1	B	324/348 (93%)	-0.11	7 (2%) 62 56	25, 44, 67, 82	8 (2%)
1	C	319/348 (91%)	-0.30	3 (0%) 84 82	19, 40, 57, 78	8 (2%)
1	D	324/348 (93%)	0.06	11 (3%) 45 38	27, 50, 76, 93	8 (2%)
All	All	1286/1392 (92%)	-0.14	25 (1%) 66 62	19, 43, 68, 93	32 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1608	SER	6.9
1	D	1604	PRO	4.6
1	B	1608	SER	3.8
1	B	1604	PRO	3.7
1	B	1522	GLN	3.5
1	C	1603	GLY	3.5
1	C	1604	PRO	3.3
1	A	1607	ASN	3.1
1	D	1649	TRP	3.0
1	A	1604	PRO	2.6
1	D	1288	PHE	2.6
1	C	1608	SER	2.5
1	D	1345	ASP	2.4
1	A	1603	GLY	2.4
1	D	1607	ASN	2.4
1	A	1608	SER	2.4
1	D	1603	GLY	2.4
1	B	1438	CYS	2.3
1	D	1605	ALA	2.3
1	D	1334	GLU	2.3
1	B	1478	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1442	GLU	2.1
1	D	1346	SER	2.1
1	D	1590	LYS	2.0
1	B	1603	GLY	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 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.

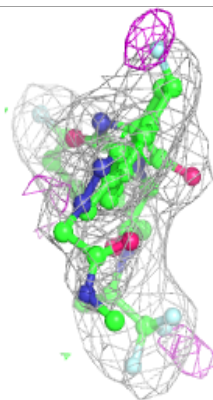
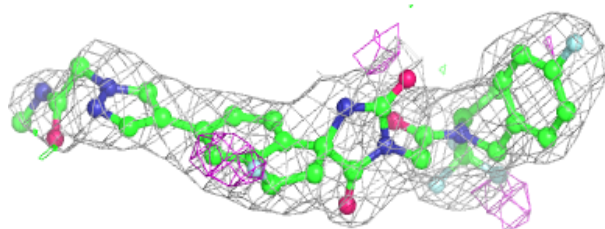
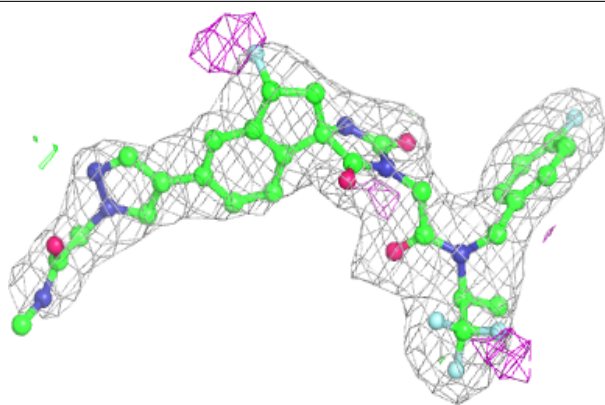
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	Y2P	B	1701	44/44	0.93	0.17	36,41,53,53	0
2	Y2P	D	1701	44/44	0.93	0.18	43,47,60,61	0
2	Y2P	C	1701	44/44	0.95	0.17	32,36,42,42	0
2	Y2P	A	1701	44/44	0.95	0.17	29,33,38,39	0

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.

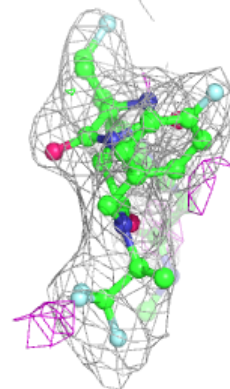
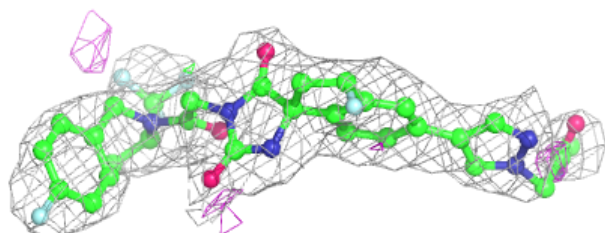
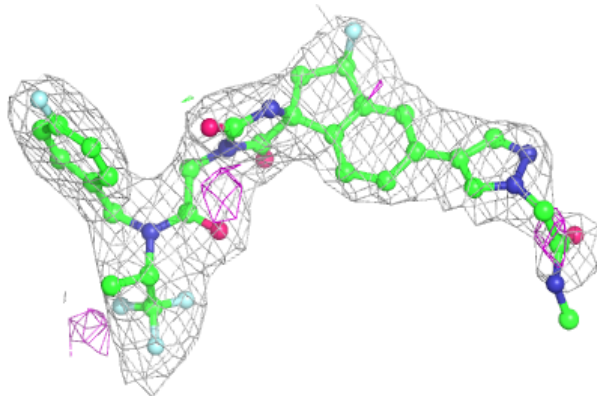


**Electron density around Y2P B 1701:**

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

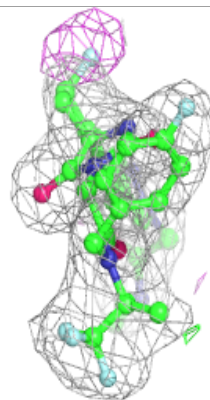
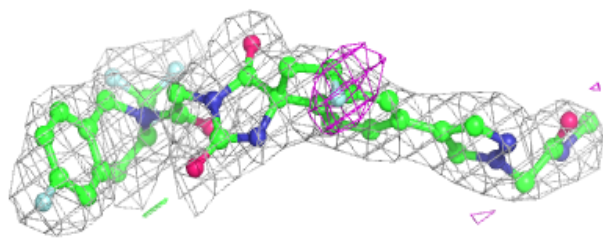
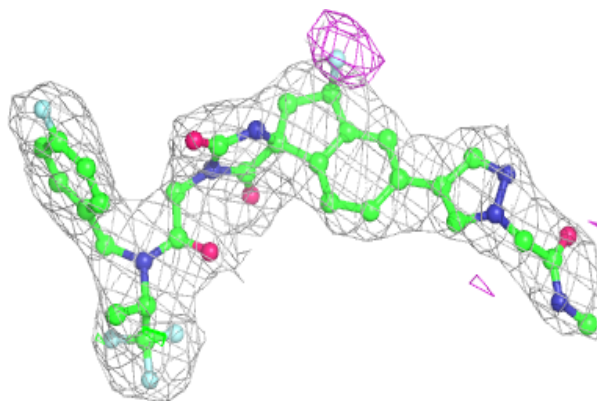
**Electron density around Y2P D 1701:**

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

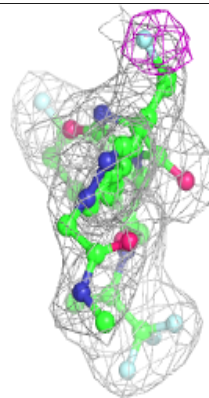
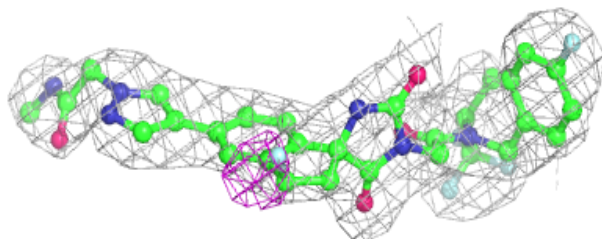
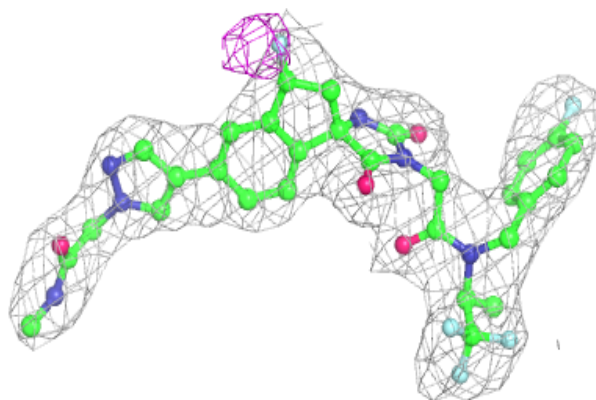


**Electron density around Y2P C 1701:**

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

**Electron density around Y2P A 1701:**

$2mF_o-DF_c$  (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.