



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:02 pm BST

PDB ID : 1HXP  
Title : NUCLEOTIDE TRANSFERASE  
Authors : Wedekind, J.E.; Frey, P.A.; Rayment, I.  
Deposited on : 1995-06-09  
Resolution : 1.80 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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

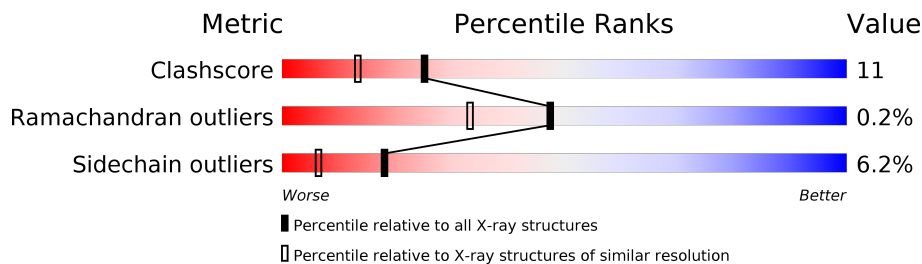
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	
1	B	348	

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	BME	A	354	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5889 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 HEXOSE-1-PHOSPHATE URIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2713	1720	478	502	13	0	0	0
1	B	329	2641	1675	464	489	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLU	GLN	CONFLICT	UNP P09148
B	34	GLU	GLN	CONFLICT	UNP P09148

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

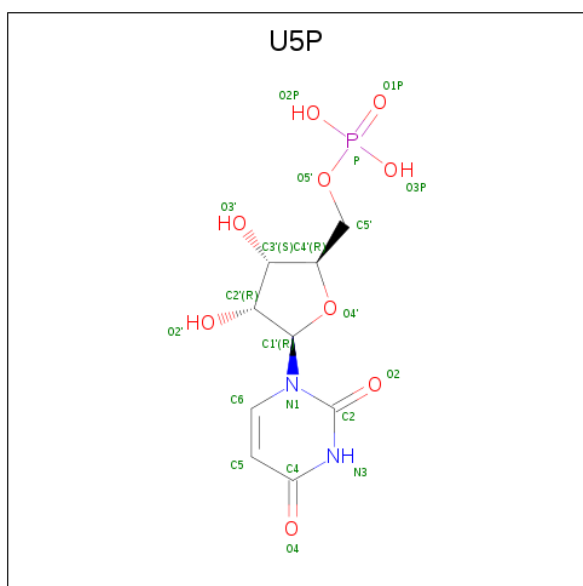
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



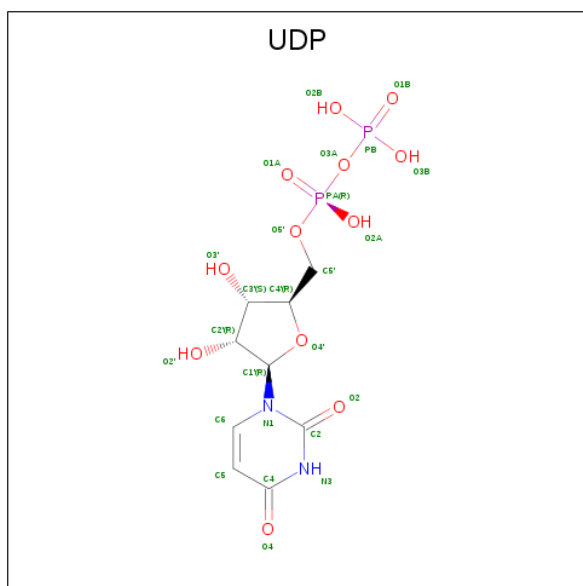
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			S
4	A	1	4	2	1	1	0	0
4	A	1	4	2	1	1	0	0
4	A	1	4	2	1	1	0	0
4	B	1	4	2	1	1	0	0

- Molecule 5 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula:  $C_9H_{13}N_2O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	21	9	2	9	1	0	0

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	B	1	25	9	2	12	2	0	0

- Molecule 7 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	254	Total O 254 254	0	0
7	B	215	Total O 215 215	0	0

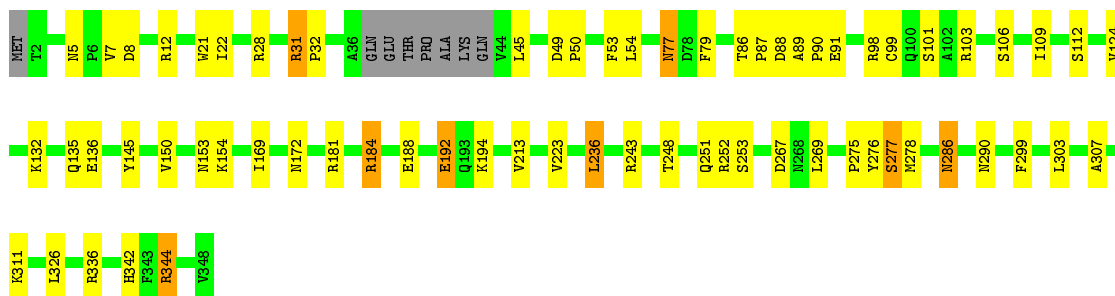
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

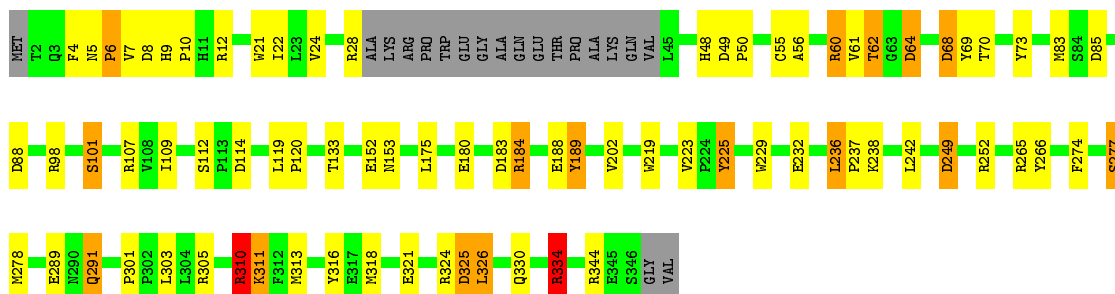
- Molecule 1: HEXOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

Chain A: 



- Molecule 1: HEXOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

Chain B: 



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.60Å 217.20Å 69.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.80)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5889	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 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: UDP, FE, ZN, U5P, BME

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	0.86	0/2795	1.39	21/3812 (0.6%)
1	B	0.86	1/2721 (0.0%)	1.42	30/3711 (0.8%)
All	All	0.86	1/5516 (0.0%)	1.40	51/7523 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	TYR	CD1-CE1	5.22	1.47	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	A	344	ARG	NE-CZ-NH1	-11.03	114.79	120.30
1	A	243	ARG	NE-CZ-NH2	9.82	125.21	120.30
1	A	344	ARG	NE-CZ-NH2	8.78	124.69	120.30
1	B	249	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	A	103	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	A	223	VAL	N-CA-C	-7.95	89.53	111.00
1	A	336	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	B	223	VAL	N-CA-C	-7.70	90.22	111.00
1	B	28	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	B	318	MET	CG-SD-CE	-7.18	88.71	100.20
1	B	321	GLU	OE1-CD-OE2	-7.18	114.69	123.30
1	B	265	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	265	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	243	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	A	181	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	B	183	ASP	CB-CG-OD1	6.79	124.41	118.30
1	B	107	ARG	NE-CZ-NH1	6.56	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	252	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	85	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	64	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	B	180	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	B	324	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	184	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	A	326	LEU	CB-CG-CD2	-5.83	101.09	111.00
1	A	236	LEU	CB-CA-C	-5.76	99.26	110.20
1	B	334	ARG	CB-CG-CD	5.72	126.48	111.60
1	B	344	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	B	249	ASP	OD1-CG-OD2	5.70	134.13	123.30
1	A	336	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	277	SER	N-CA-C	-5.63	95.79	111.00
1	A	269	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	A	124	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	B	242	LEU	CB-CG-CD2	5.57	120.47	111.00
1	B	236	LEU	CB-CA-C	-5.56	99.63	110.20
1	B	60	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	114	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	12	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	225	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	A	136	GLU	OE1-CD-OE2	5.49	129.88	123.30
1	A	213	VAL	CG1-CB-CG2	-5.46	102.17	110.90
1	B	326	LEU	CB-CG-CD2	-5.34	101.91	111.00
1	B	325	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	98	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	8	ASP	CB-CG-OD1	-5.32	113.52	118.30
1	B	98	ARG	NH1-CZ-NH2	5.30	125.23	119.40
1	A	299	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	B	68	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	A	154	LYS	N-CA-CB	-5.17	101.29	110.60
1	A	277	SER	N-CA-C	-5.12	97.18	111.00
1	B	310	ARG	N-CA-CB	-5.08	101.46	110.60

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	2713	0	2568	61	0
1	B	2641	0	2508	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	12	0	15	11	0
4	B	4	0	5	1	0
5	A	21	0	11	5	0
6	B	25	0	11	3	0
7	A	254	0	0	1	0
7	B	215	0	0	5	0
All	All	5889	0	5118	113	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 11.

All (113) 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:B:311:LYS:HE3	1:B:313:MET:HG3	1.33	1.06
1:A:89:ALA:HA	1:B:4:PHE:CD2	2.00	0.94
1:B:334:ARG:HD2	7:B:470:HOH:O	1.69	0.92
1:A:90:PRO:HD3	1:B:4:PHE:CD2	2.04	0.92
1:A:90:PRO:HD3	1:B:4:PHE:HD2	1.32	0.91
1:A:77:ASN:HD22	1:A:79:PHE:H	1.06	0.90
1:A:135:GLN:HE22	1:A:252:ARG:HH11	1.15	0.88
1:B:330:GLN:O	1:B:334:ARG:HG2	1.74	0.88
1:A:303:LEU:HD11	4:A:354:BME:C1	2.04	0.87
1:B:62:THR:HB	1:B:64:ASP:OD2	1.80	0.82
1:A:303:LEU:HD11	4:A:354:BME:C2	2.11	0.81
1:A:184:ARG:HD2	7:A:420:HOH:O	1.81	0.79
1:A:21:TRP:C	1:A:22:ILE:HD12	2.03	0.79
1:A:342:HIS:HD2	1:A:344:ARG:H	1.28	0.79
1:B:311:LYS:CE	1:B:313:MET:HG3	2.12	0.78
1:A:303:LEU:HD11	4:A:354:BME:H22	1.64	0.78
4:A:352:BME:H22	1:B:225:TYR:OH	1.84	0.77
1:A:77:ASN:ND2	1:A:79:PHE:H	1.80	0.77
1:A:342:HIS:CD2	1:A:344:ARG:H	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LEU:CD1	4:A:354:BME:H22	2.15	0.76
1:B:5:ASN:ND2	1:B:8:ASP:OD2	2.21	0.72
1:B:311:LYS:HE2	1:B:313:MET:CE	2.20	0.71
1:A:248:THR:H	1:A:251:GLN:HE21	1.39	0.71
1:A:77:ASN:HD22	1:A:79:PHE:N	1.85	0.69
1:A:87:PRO:HG2	1:B:9:HIS:CE1	2.27	0.69
1:B:310:ARG:HG2	1:B:311:LYS:N	2.06	0.69
1:A:22:ILE:N	1:A:22:ILE:HD12	2.09	0.68
1:B:289:GLU:HG2	1:B:291:GLN:HG2	1.77	0.65
1:B:153:ASN:HD22	4:B:351:BME:H11	1.63	0.64
1:A:303:LEU:HD11	4:A:354:BME:H12	1.80	0.63
1:A:89:ALA:HA	1:B:4:PHE:CE2	2.34	0.62
1:A:135:GLN:NE2	1:A:252:ARG:HH11	1.94	0.61
1:A:53:PHE:CE1	1:A:54:LEU:HD21	2.35	0.61
1:B:109:ILE:HD12	1:B:133:THR:HG21	1.82	0.61
1:A:88:ASP:O	1:B:4:PHE:HB2	2.01	0.60
1:B:311:LYS:HE2	1:B:313:MET:HE2	1.83	0.60
1:B:101:SER:HA	7:B:366:HOH:O	2.01	0.60
1:B:60:ARG:HB3	6:B:352:UDP:O4	2.02	0.60
1:A:307:ALA:HA	4:A:354:BME:H22	1.84	0.59
1:A:53:PHE:CE1	5:A:355:U5P:C6	2.87	0.57
1:A:150:VAL:HG22	1:A:169:ILE:HD12	1.87	0.57
1:A:307:ALA:O	4:A:354:BME:C2	2.53	0.56
1:A:5:ASN:ND2	1:A:7:VAL:HB	2.21	0.56
1:B:152:GLU:HB3	1:B:278:MET:HG3	1.87	0.56
1:B:21:TRP:C	1:B:22:ILE:HD12	2.26	0.56
1:B:311:LYS:HE2	1:B:313:MET:HE3	1.88	0.56
1:A:53:PHE:CZ	5:A:355:U5P:C6	2.90	0.55
1:B:109:ILE:HD12	1:B:133:THR:CG2	2.35	0.55
1:A:90:PRO:CD	1:B:4:PHE:CD2	2.84	0.55
1:B:5:ASN:O	1:B:7:VAL:N	2.40	0.55
1:B:61:VAL:HG12	1:B:62:THR:N	2.20	0.55
1:B:69:TYR:CG	1:B:73:TYR:HB2	2.43	0.54
1:B:48:HIS:CE1	1:B:55:CYS:HB3	2.43	0.54
1:B:184:ARG:O	1:B:188:GLU:HG3	2.07	0.54
1:A:7:VAL:O	1:A:7:VAL:HG12	2.08	0.53
1:A:53:PHE:CE1	1:A:54:LEU:CD2	2.92	0.52
1:B:229:TRP:CZ3	1:B:311:LYS:HD3	2.45	0.52
1:B:310:ARG:HG2	1:B:311:LYS:H	1.72	0.52
1:A:31:ARG:NH2	6:B:352:UDP:O2A	2.36	0.51
1:A:248:THR:H	1:A:251:GLN:NE2	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:HIS:CD2	1:A:344:ARG:HB2	2.46	0.50
1:A:22:ILE:N	1:A:22:ILE:CD1	2.75	0.49
6:B:352:UDP:O3B	6:B:352:UDP:H5'1	2.12	0.49
1:B:5:ASN:O	1:B:8:ASP:N	2.32	0.49
1:A:342:HIS:HD2	1:A:344:ARG:N	2.05	0.48
1:A:99:CYS:HA	1:B:12:ARG:O	2.14	0.48
1:B:109:ILE:CD1	1:B:133:THR:HG21	2.44	0.48
1:B:219:TRP:CZ3	1:B:237:PRO:HD3	2.49	0.48
1:A:88:ASP:O	1:B:4:PHE:CB	2.63	0.47
1:B:101:SER:HB3	7:B:366:HOH:O	2.14	0.47
1:A:53:PHE:CE1	5:A:355:U5P:C5	2.98	0.47
1:A:276:TYR:CD1	1:A:276:TYR:C	2.89	0.47
1:A:172:ASN:ND2	1:B:316:TYR:OH	2.47	0.47
1:A:49:ASP:OD1	1:A:49:ASP:C	2.54	0.46
1:A:307:ALA:O	4:A:354:BME:H21	2.14	0.46
1:A:89:ALA:HA	1:B:4:PHE:CG	2.47	0.45
1:B:49:ASP:OD1	1:B:50:PRO:HD2	2.16	0.45
1:B:229:TRP:CE2	1:B:313:MET:CE	3.00	0.45
1:B:303:LEU:HA	1:B:303:LEU:HD23	1.73	0.45
1:B:22:ILE:N	1:B:22:ILE:HD12	2.31	0.45
1:A:5:ASN:HD21	1:A:7:VAL:HB	1.80	0.45
1:B:229:TRP:CE3	1:B:311:LYS:HD2	2.52	0.45
1:B:229:TRP:CE2	1:B:313:MET:HE1	2.53	0.44
1:B:274:PHE:CE2	1:B:301:PRO:HB3	2.53	0.44
1:A:145:TYR:HB3	1:A:172:ASN:O	2.16	0.44
1:B:189:TYR:CD1	1:B:189:TYR:C	2.91	0.44
1:A:49:ASP:HA	1:A:50:PRO:HD2	1.66	0.44
1:A:267:ASP:OD2	1:A:342:HIS:HE1	2.01	0.43
1:A:86:THR:HA	1:A:87:PRO:HD3	1.93	0.43
1:A:31:ARG:HG2	1:A:32:PRO:HD2	2.00	0.43
1:B:5:ASN:C	1:B:7:VAL:N	2.72	0.43
1:B:119:LEU:N	1:B:120:PRO:HD2	2.34	0.43
1:A:53:PHE:CD1	5:A:355:U5P:C5	3.01	0.43
1:B:48:HIS:CE1	1:B:56:ALA:O	2.71	0.43
1:A:275:PRO:O	1:A:276:TYR:HB3	2.19	0.42
1:B:10:PRO:HA	1:B:24:VAL:O	2.20	0.42
1:B:49:ASP:OD1	1:B:49:ASP:C	2.58	0.42
1:A:278:MET:C	1:A:278:MET:SD	2.98	0.42
1:B:325:ASP:OD1	1:B:326:LEU:N	2.52	0.42
1:A:286:ASN:HD21	1:A:290:ASN:HD21	1.67	0.41
1:A:188:GLU:O	1:A:192:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:PHE:CE2	1:B:6:PRO:HG3	2.55	0.41
1:A:153:ASN:HD22	4:A:353:BME:H11	1.86	0.41
1:B:310:ARG:NE	1:B:311:LYS:O	2.37	0.41
1:B:49:ASP:HA	1:B:50:PRO:HD3	1.80	0.41
1:A:307:ALA:O	4:A:354:BME:C1	2.68	0.41
1:A:53:PHE:CZ	5:A:355:U5P:H6	2.56	0.41
1:A:5:ASN:C	1:A:7:VAL:H	2.25	0.41
1:B:229:TRP:HB2	1:B:232:GLU:HB2	2.03	0.41
1:B:238:LYS:NZ	7:B:531:HOH:O	2.54	0.41
1:B:83:MET:HE3	7:B:376:HOH:O	2.20	0.40
1:B:334:ARG:HG2	1:B:334:ARG:H	1.73	0.40
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.82	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	336/348 (97%)	321 (96%)	15 (4%)	0	100	100
1	B	325/348 (93%)	313 (96%)	11 (3%)	1 (0%)	41	27
All	All	661/696 (95%)	634 (96%)	26 (4%)	1 (0%)	47	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	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	286/299 (96%)	268 (94%)	18 (6%)	18	6
1	B	282/299 (94%)	265 (94%)	17 (6%)	19	7
All	All	568/598 (95%)	533 (94%)	35 (6%)	18	6

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	31	ARG
1	A	45	LEU
1	A	77	ASN
1	A	91	GLU
1	A	101	SER
1	A	106	SER
1	A	109	ILE
1	A	112	SER
1	A	132	LYS
1	A	184	ARG
1	A	192	GLU
1	A	194	LYS
1	A	236	LEU
1	A	253	SER
1	A	277	SER
1	A	286	ASN
1	A	311	LYS
1	B	62	THR
1	B	68	ASP
1	B	70	THR
1	B	88	ASP
1	B	101	SER
1	B	112	SER
1	B	175	LEU
1	B	202	VAL
1	B	236	LEU

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Mol	Chain	Res	Type
1	B	249	ASP
1	B	266	TYR
1	B	277	SER
1	B	291	GLN
1	B	305	ARG
1	B	310	ARG
1	B	311	LYS
1	B	334	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	77	ASN
1	A	135	GLN
1	A	172	ASN
1	A	251	GLN
1	A	286	ASN
1	A	342	HIS
1	B	172	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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
5	U5P	A	355	-	18,22,22	1.54	3 (16%)	21,33,33	1.89	4 (19%)
4	BME	A	354	1	3,3,3	0.70	0	1,2,2	0.49	0
4	BME	B	351	1	3,3,3	0.78	0	1,2,2	1.19	0
4	BME	A	353	1	3,3,3	0.84	0	1,2,2	1.95	0
6	UDP	B	352	-	20,26,26	1.65	4 (20%)	25,40,40	1.69	5 (20%)
4	BME	A	352	1	3,3,3	0.41	0	1,2,2	0.90	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	U5P	A	355	-	-	4/8/26/26	0/2/2/2
4	BME	A	354	1	-	1/1/1/1	-
4	BME	B	351	1	-	1/1/1/1	-
4	BME	A	353	1	-	1/1/1/1	-
6	UDP	B	352	-	-	2/14/32/32	0/2/2/2
4	BME	A	352	1	-	0/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	352	UDP	C4-N3	4.03	1.40	1.33
5	A	355	U5P	C4-N3	3.76	1.39	1.33
6	B	352	UDP	PB-O1B	3.23	1.61	1.50
5	A	355	U5P	P-O3P	3.12	1.66	1.54
6	B	352	UDP	C6-C5	-2.93	1.31	1.38
5	A	355	U5P	C6-C5	-2.92	1.31	1.38
6	B	352	UDP	C6-N1	2.45	1.38	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	355	U5P	C5-C4-N3	-4.49	113.42	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	355	U5P	O5'-P-O1P	4.32	118.59	106.47
6	B	352	UDP	C5-C4-N3	-4.17	114.15	123.31
6	B	352	UDP	O3B-PB-O1B	3.94	126.09	110.68
6	B	352	UDP	O5'-C5'-C4'	3.36	120.57	108.99
5	A	355	U5P	O3'-C3'-C4'	3.22	120.36	111.05
6	B	352	UDP	O4'-C4'-C5'	2.50	117.59	109.37
6	B	352	UDP	O3A-PB-O1B	-2.19	99.03	111.19
5	A	355	U5P	O2P-P-O1P	-2.00	102.84	110.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	355	U5P	C2'-C1'-N1-C6
5	A	355	U5P	O4'-C1'-N1-C6
4	A	354	BME	O1-C1-C2-S2
6	B	352	UDP	O4'-C1'-N1-C6
6	B	352	UDP	PB-O3A-PA-O5'
4	B	351	BME	O1-C1-C2-S2
4	A	353	BME	O1-C1-C2-S2
5	A	355	U5P	C4'-C5'-O5'-P
5	A	355	U5P	O4'-C4'-C5'-O5'

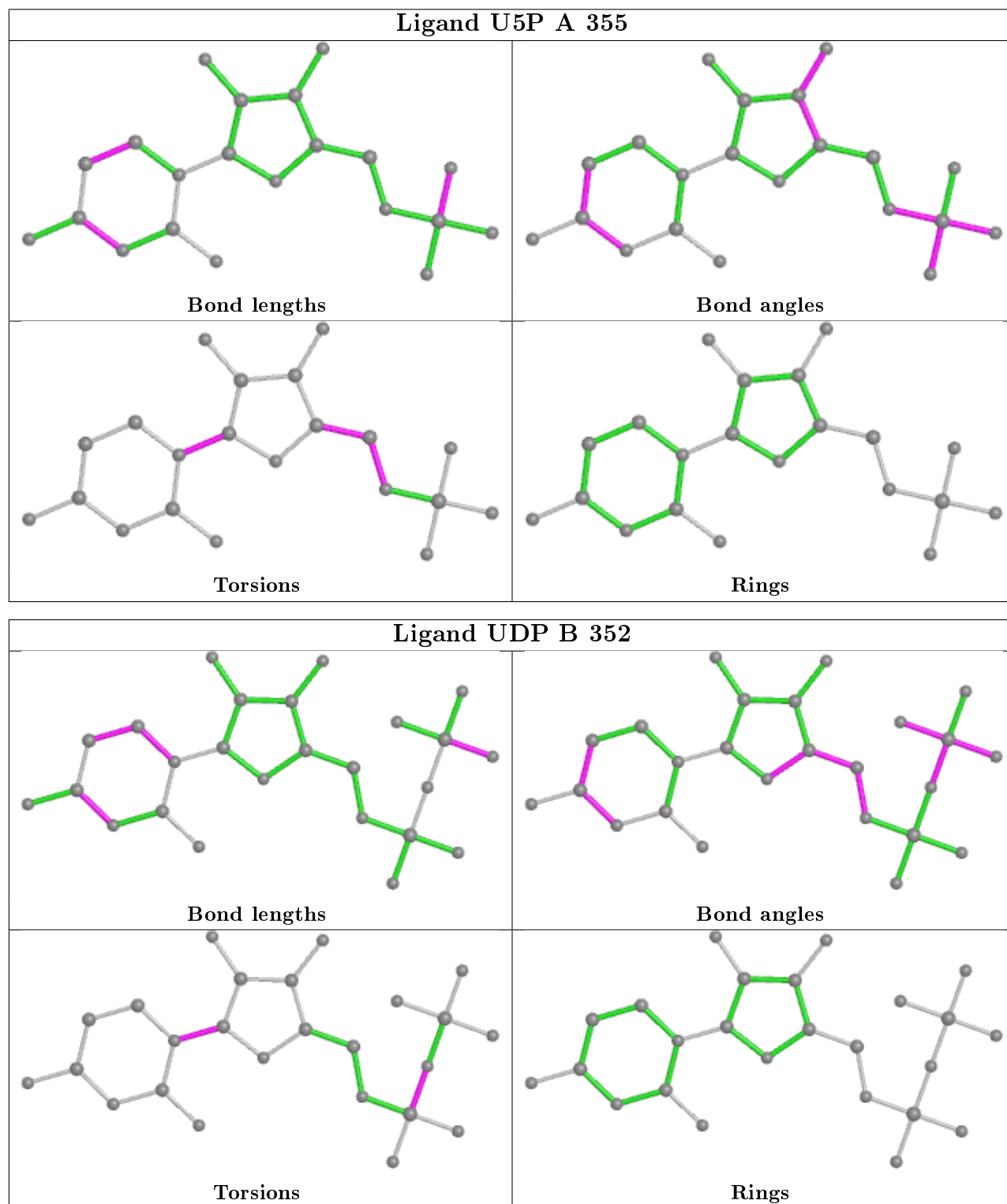
There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	355	U5P	5	0
4	A	354	BME	9	0
4	B	351	BME	1	0
4	A	353	BME	1	0
6	B	352	UDP	3	0
4	A	352	BME	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.



## 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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.