



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:11 PM UTC

PDB ID : 1HXQ / pdb_00001hxq
Title : THE STRUCTURE OF NUCLEOTIDYLATED GALACTOSE-1-PHOSPHATE URIDYLYLTRANSFERASE FROM ESCHERICHIA COLI AT 1.86 ANGSTROMS RESOLUTION
Authors : Wedekind, J.E.; Frey, P.A.; Rayment, I.
Deposited on : 1996-06-16
Resolution : 1.86 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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

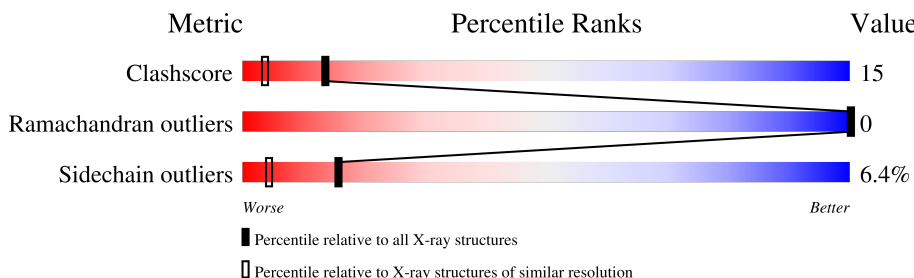
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)

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 ≥ 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	 67% 24% 5% ..
1	B	348	 61% 29% . . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6179 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 URIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2731	1732	484	502	13			
1	B	333	Total	C	N	O	S	0	0	1
			2674	1695	472	494	13			

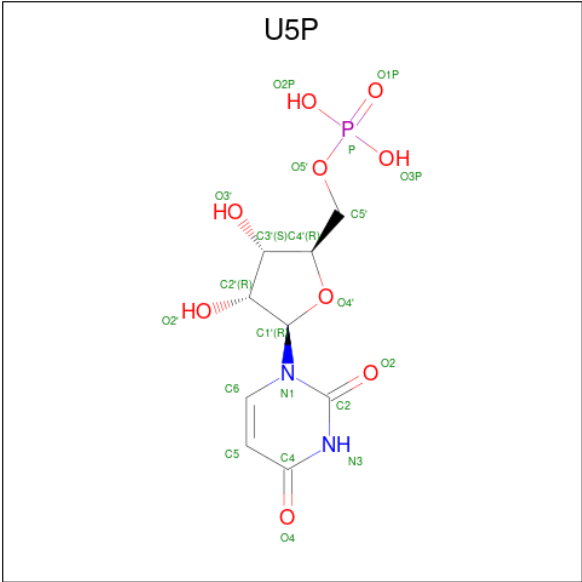
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 4 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: C₉H₁₃N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
4	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	400	Total	O	0	0
			400	400		
5	B	330	Total	O	0	0
			330	330		

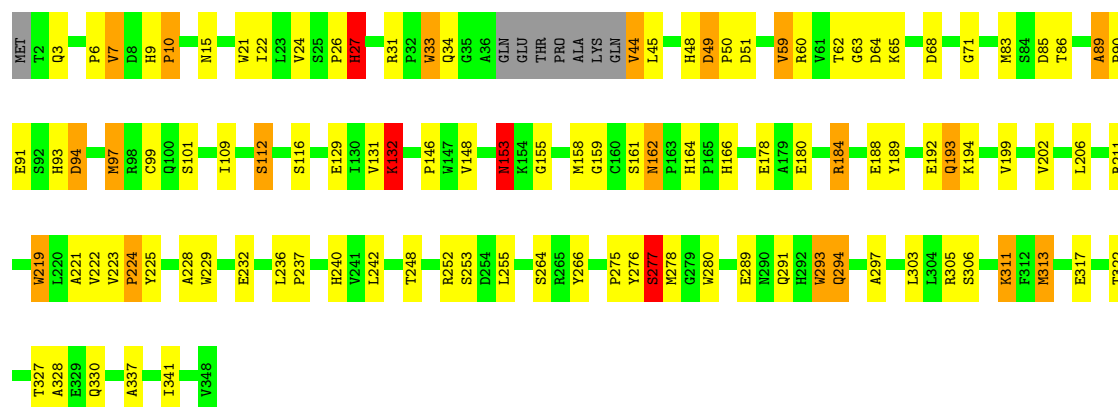
3 Residue-property plots

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. 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.

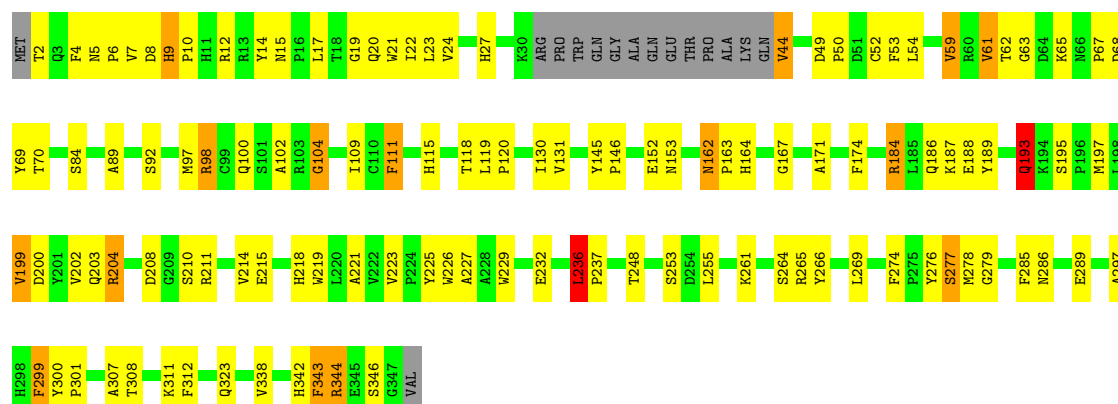
• Molecule 1: HEXOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

Chain A: 



• Molecule 1: HEXOSE-1-PHOSPHATE URIDYLYLTRANSFERASE

Chain B: 



4 Data and refinement statistics

Xtriage (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, α , β , γ	57.20Å 215.40Å 68.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.00 – 1.86	Depositor
% Data completeness (in resolution range)	97.0 (65.00-1.86)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6179	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, U5P, FE

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	0.97	2/2815 (0.1%)	1.70	63/3838 (1.6%)
1	B	0.98	1/2755 (0.0%)	1.66	50/3757 (1.3%)
All	All	0.98	3/5570 (0.1%)	1.68	113/7595 (1.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	MET	SD-CE	-9.17	1.56	1.79
1	B	346	SER	C-N	-5.49	1.25	1.33
1	A	153	ASN	CA-C	-5.11	1.46	1.52

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	VAL	N-CA-C	-19.43	88.32	107.55
1	A	49	ASP	CA-C-N	9.67	129.78	119.05
1	A	49	ASP	C-N-CA	9.67	129.78	119.05
1	A	94	ASP	CA-C-N	-9.33	111.32	120.83
1	A	94	ASP	C-N-CA	-9.33	111.32	120.83
1	B	223	VAL	N-CA-C	-9.19	89.04	108.88
1	B	69	TYR	N-CA-C	8.73	122.06	110.53
1	A	289	GLU	N-CA-C	-8.55	96.17	109.25
1	B	193	GLN	N-CA-C	8.13	123.38	113.38
1	B	277	SER	N-CA-C	-8.08	95.11	108.76
1	B	289	GLU	N-CA-C	-7.99	97.05	109.76
1	A	9	HIS	N-CA-C	7.92	121.24	110.31
1	B	248	THR	N-CA-C	-7.91	100.33	110.53
1	B	344	ARG	N-CA-C	-7.90	102.55	112.90
1	A	112	SER	N-CA-C	-7.90	101.02	108.13
1	A	291	GLN	CB-CA-C	-7.76	97.48	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	THR	CA-C-N	-7.72	112.60	123.11
1	B	308	THR	C-N-CA	-7.72	112.60	123.11
1	B	285	PHE	CA-C-N	-7.65	110.59	122.37
1	B	285	PHE	C-N-CA	-7.65	110.59	122.37
1	B	62	THR	CA-C-N	-7.43	110.83	122.86
1	B	62	THR	C-N-CA	-7.43	110.83	122.86
1	B	153	ASN	CB-CA-C	-7.42	98.79	110.74
1	B	84	SER	N-CA-C	7.36	121.51	112.54
1	A	153	ASN	CB-CA-C	-7.31	99.58	110.62
1	A	62	THR	CB-CA-C	-7.28	96.90	110.01
1	A	328	ALA	N-CA-C	-7.14	103.50	111.71
1	A	294	GLN	N-CA-C	-6.78	96.47	108.13
1	A	306	SER	N-CA-C	-6.60	98.88	107.73
1	B	274	PHE	CA-C-N	-6.35	114.08	120.31
1	B	274	PHE	C-N-CA	-6.35	114.08	120.31
1	B	146	PRO	CA-C-N	-6.35	112.45	122.73
1	B	146	PRO	C-N-CA	-6.35	112.45	122.73
1	A	166	HIS	CA-CB-CG	6.29	120.09	113.80
1	A	158	MET	N-CA-C	-6.28	105.20	112.92
1	A	93	HIS	CB-CA-C	6.26	121.41	110.64
1	B	65	LYS	N-CA-C	6.20	119.06	109.07
1	A	293	TRP	N-CA-C	6.17	118.87	110.55
1	A	248	THR	N-CA-C	-6.14	102.61	110.53
1	B	111	PHE	N-CA-C	6.13	117.96	111.28
1	B	68	ASP	N-CA-C	-6.13	100.43	109.62
1	A	178	GLU	CB-CA-C	-6.04	100.76	110.79
1	B	6	PRO	CA-C-N	-6.03	111.91	121.02
1	B	6	PRO	C-N-CA	-6.03	111.91	121.02
1	A	148	VAL	N-CA-C	-6.00	99.48	108.12
1	B	153	ASN	N-CA-C	-5.99	97.53	108.02
1	A	242	LEU	N-CA-C	5.95	119.01	111.69
1	A	45	LEU	N-CA-C	5.93	118.09	110.39
1	A	193	GLN	N-CA-C	5.91	120.56	113.23
1	B	104	GLY	N-CA-C	-5.90	102.78	110.45
1	A	255	LEU	N-CA-C	-5.86	104.97	111.36
1	B	186	GLN	N-CA-C	-5.85	104.99	111.36
1	A	162	ASN	CA-C-N	5.83	126.59	120.12
1	A	162	ASN	C-N-CA	5.83	126.59	120.12
1	B	62	THR	CB-CA-C	-5.83	100.00	110.37
1	B	195	SER	N-CA-C	-5.83	100.59	108.11
1	B	102	ALA	N-CA-C	5.81	117.71	107.61
1	B	200	ASP	N-CA-C	-5.75	105.09	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	PHE	N-CA-C	5.75	119.81	112.34
1	A	45	LEU	CA-C-N	5.73	125.92	120.31
1	A	45	LEU	C-N-CA	5.73	125.92	120.31
1	A	159	GLY	N-CA-C	5.69	122.60	115.21
1	B	17	LEU	N-CA-C	-5.67	105.86	112.89
1	A	164	HIS	N-CA-C	-5.66	102.64	109.83
1	A	221	ALA	N-CA-C	-5.65	99.69	108.90
1	B	59	VAL	CB-CA-C	-5.64	103.48	111.21
1	A	15	ASN	CB-CA-C	-5.62	103.93	110.17
1	A	62	THR	CA-C-N	-5.60	113.72	122.51
1	A	62	THR	C-N-CA	-5.60	113.72	122.51
1	A	86	THR	CA-C-N	-5.57	114.52	120.03
1	A	86	THR	C-N-CA	-5.57	114.52	120.03
1	A	222	VAL	CB-CA-C	-5.49	101.90	110.52
1	B	199	VAL	N-CA-C	-5.46	105.05	111.00
1	A	337	ALA	N-CA-C	5.45	117.98	111.71
1	A	68	ASP	N-CA-C	-5.45	103.11	110.68
1	A	155	GLY	N-CA-C	5.45	119.48	112.18
1	A	166	HIS	N-CA-CB	-5.45	102.42	111.57
1	A	224	PRO	N-CA-C	5.40	119.80	111.21
1	B	162	ASN	CA-C-O	5.40	123.32	119.32
1	A	264	SER	N-CA-C	-5.39	105.07	111.69
1	B	307	ALA	CA-C-N	-5.34	114.14	122.37
1	B	307	ALA	C-N-CA	-5.34	114.14	122.37
1	A	132	LYS	CB-CA-C	-5.34	101.92	110.79
1	A	89	ALA	N-CA-C	-5.34	102.44	110.24
1	A	146	PRO	CA-C-N	-5.32	114.55	122.74
1	A	146	PRO	C-N-CA	-5.32	114.55	122.74
1	A	7	VAL	N-CA-C	-5.30	105.13	112.50
1	A	26	PRO	N-CA-C	5.28	120.77	113.65
1	B	312	PHE	N-CA-C	-5.27	100.31	108.90
1	B	299	PHE	N-CA-C	-5.25	99.73	108.34
1	B	264	SER	N-CA-C	-5.24	105.65	111.36
1	B	9	HIS	N-CA-C	5.24	117.54	110.31
1	A	192	GLU	N-CA-C	5.23	117.78	111.40
1	B	236	LEU	N-CA-C	5.22	112.92	108.22
1	B	184	ARG	N-CA-C	5.21	116.96	111.28
1	A	6	PRO	CA-C-N	-5.20	112.11	120.64
1	A	6	PRO	C-N-CA	-5.20	112.11	120.64
1	A	85	ASP	N-CA-C	5.19	118.92	112.59
1	A	59	VAL	CB-CA-C	-5.14	104.03	111.68
1	B	98	ARG	N-CA-CB	-5.13	101.97	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	TYR	CB-CA-C	-5.13	103.68	110.34
1	A	63	GLY	CA-C-N	-5.10	113.35	122.07
1	A	63	GLY	C-N-CA	-5.10	113.35	122.07
1	A	27	HIS	CA-C-N	-5.10	113.15	122.38
1	A	27	HIS	C-N-CA	-5.10	113.15	122.38
1	B	89	ALA	N-CA-C	-5.09	103.26	110.29
1	A	219	TRP	N-CA-C	5.09	117.40	109.52
1	B	218	HIS	N-CA-C	5.08	120.33	113.72
1	A	277	SER	N-CA-C	-5.07	100.19	108.76
1	B	67	PRO	N-CA-C	-5.05	104.15	111.22
1	A	199	VAL	CA-C-O	5.05	126.11	120.71
1	A	116	SER	N-CA-C	5.03	120.05	113.30
1	B	195	SER	CA-C-O	5.02	124.63	119.76

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	2731	0	2606	80	0
1	B	2674	0	2552	87	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	20	0	11	0	0
4	B	20	0	11	2	0
5	A	400	0	0	15	0
5	B	330	0	0	13	0
All	All	6179	0	5180	155	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 15.

All (155) 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:311:LYS:HE3	1:A:313:MET:CE	1.59	1.32
1:A:311:LYS:HE3	1:A:313:MET:HE2	1.41	1.01
1:A:33:TRP:CD1	1:A:33:TRP:N	2.26	1.00
1:B:61:VAL:HG13	4:B:352:U5P:O4	1.63	0.97
1:A:33:TRP:CD1	1:A:33:TRP:H	1.78	0.97
1:A:311:LYS:HE3	1:A:313:MET:HE1	1.46	0.95
1:B:14:TYR:OH	5:B:538:HOH:O	1.83	0.94
1:B:344:ARG:NH2	5:B:551:HOH:O	2.00	0.94
1:A:94:ASP:OD2	1:B:204:ARG:NH2	2.00	0.94
1:A:90:PRO:HD2	5:A:660:HOH:O	1.73	0.88
1:B:184:ARG:HD2	5:B:631:HOH:O	1.72	0.88
1:B:342:HIS:CE1	1:B:344:ARG:HG3	2.10	0.86
1:A:162:ASN:ND2	5:A:744:HOH:O	2.08	0.85
1:A:188:GLU:OE1	5:A:547:HOH:O	1.94	0.83
1:A:240:HIS:HE1	1:A:293:TRP:O	1.62	0.82
1:A:311:LYS:CE	1:A:313:MET:CE	2.54	0.78
1:A:7:VAL:HG12	1:A:7:VAL:O	1.84	0.77
1:A:89:ALA:HA	1:B:4:PHE:CD2	2.20	0.76
1:A:97:MET:HE3	1:B:225:TYR:HB2	1.69	0.74
1:B:342:HIS:HE1	1:B:344:ARG:HG3	1.52	0.73
1:B:44:VAL:O	5:B:550:HOH:O	2.06	0.73
1:A:27:HIS:CD2	1:A:27:HIS:H	2.03	0.73
1:B:215:GLU:CD	5:B:644:HOH:O	2.33	0.71
1:A:184:ARG:O	1:A:188:GLU:HG3	1.95	0.67
1:A:276:TYR:CD1	1:A:276:TYR:C	2.73	0.67
1:A:132:LYS:HE3	5:A:715:HOH:O	1.95	0.66
1:B:184:ARG:O	1:B:188:GLU:HG3	1.95	0.66
1:A:33:TRP:N	1:A:33:TRP:HD1	1.89	0.65
1:B:118:THR:OG1	1:B:120:PRO:HD2	1.96	0.64
1:A:97:MET:HA	5:A:448:HOH:O	1.97	0.63
1:A:49:ASP:OD1	1:A:51:ASP:N	2.30	0.63
1:B:202:VAL:HG23	1:B:236:LEU:HD11	1.81	0.62
1:A:49:ASP:OD1	1:A:50:PRO:HD2	1.99	0.62
1:A:311:LYS:CE	1:A:313:MET:HE2	2.23	0.62
1:A:240:HIS:CE1	1:A:293:TRP:O	2.50	0.61
1:B:49:ASP:OD1	1:B:50:PRO:HD2	2.00	0.60
1:B:92:SER:HB2	5:B:592:HOH:O	1.99	0.60
1:B:5:ASN:N	1:B:9:HIS:ND1	2.47	0.60
1:B:109:ILE:O	1:B:109:ILE:HG23	2.00	0.60
1:B:162:ASN:OD1	1:B:164:HIS:HB2	2.02	0.60
1:B:21:TRP:C	1:B:22:ILE:HD12	2.28	0.58
1:B:162:ASN:OD1	1:B:164:HIS:N	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:VAL:O	1:B:202:VAL:HG12	2.04	0.58
1:A:49:ASP:OD1	1:A:49:ASP:C	2.47	0.57
1:A:275:PRO:O	1:A:276:TYR:HB3	2.04	0.57
1:B:52:CYS:SG	1:B:115:HIS:HE1	2.27	0.57
1:B:219:TRP:CE2	1:B:255:LEU:HB2	2.39	0.57
1:A:311:LYS:HE2	5:A:593:HOH:O	2.04	0.56
1:A:31:ARG:HB3	5:A:358:HOH:O	2.04	0.56
1:B:261:LYS:NZ	5:B:470:HOH:O	2.37	0.56
1:B:188:GLU:OE1	5:B:543:HOH:O	2.18	0.56
1:B:193:GLN:NE2	5:B:545:HOH:O	2.20	0.56
1:B:7:VAL:O	1:B:7:VAL:HG12	2.05	0.55
1:B:276:TYR:C	1:B:276:TYR:CD1	2.83	0.55
1:A:7:VAL:O	1:A:7:VAL:CG1	2.50	0.55
1:A:27:HIS:CD2	1:A:27:HIS:N	2.74	0.55
1:A:94:ASP:CG	1:B:204:ARG:NH2	2.65	0.55
1:B:53:PHE:CE2	1:B:61:VAL:HG12	2.42	0.55
1:B:61:VAL:HG13	4:B:352:U5P:C4	2.35	0.54
1:A:7:VAL:HG13	5:A:400:HOH:O	2.06	0.54
1:B:208:ASP:OD1	1:B:210:SER:CB	2.56	0.54
1:B:229:TRP:HB2	1:B:232:GLU:HB2	1.90	0.53
1:A:89:ALA:HA	1:B:4:PHE:CG	2.43	0.53
1:A:65:LYS:HE2	5:A:749:HOH:O	2.08	0.53
1:A:60:ARG:N	1:A:64:ASP:O	2.31	0.53
1:A:71:GLY:O	1:A:112:SER:HA	2.09	0.53
1:A:97:MET:HE1	1:B:211:ARG:NH2	2.23	0.53
1:B:219:TRP:CZ3	1:B:237:PRO:HD3	2.43	0.52
1:B:236:LEU:HD12	1:B:236:LEU:O	2.10	0.52
1:B:8:ASP:HA	5:B:535:HOH:O	2.10	0.52
1:A:49:ASP:CG	1:A:50:PRO:HD2	2.35	0.51
1:A:237:PRO:HG2	1:A:294:GLN:NE2	2.26	0.51
1:B:49:ASP:HB3	1:B:52:CYS:HB2	1.93	0.51
1:B:215:GLU:CG	5:B:644:HOH:O	2.57	0.51
1:A:276:TYR:C	1:A:276:TYR:HD1	2.15	0.51
1:B:10:PRO:HG3	1:B:27:HIS:CE1	2.46	0.50
1:B:12:ARG:HA	1:B:22:ILE:O	2.11	0.50
1:B:236:LEU:C	1:B:236:LEU:CD1	2.85	0.49
1:B:8:ASP:CA	5:B:535:HOH:O	2.59	0.49
1:B:49:ASP:OD1	1:B:50:PRO:CD	2.60	0.49
1:A:211:ARG:NH2	1:B:97:MET:HE1	2.27	0.49
1:B:214:VAL:HB	1:B:221:ALA:HB3	1.94	0.49
1:B:236:LEU:HD12	1:B:236:LEU:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:SER:CB	5:B:592:HOH:O	2.57	0.49
1:A:131:VAL:HG11	1:A:252:ARG:HG3	1.95	0.49
1:A:65:LYS:CE	5:A:749:HOH:O	2.61	0.48
1:B:59:VAL:HG13	1:B:63:GLY:O	2.13	0.47
1:A:97:MET:CE	1:B:225:TYR:HB2	2.42	0.47
1:B:208:ASP:OD1	1:B:210:SER:HB2	2.14	0.47
1:B:343:PHE:CD1	1:B:344:ARG:HG2	2.49	0.47
1:A:313:MET:HE2	1:A:317:GLU:OE1	2.15	0.47
1:B:15:ASN:OD1	1:B:15:ASN:C	2.58	0.47
1:B:219:TRP:CZ2	1:B:255:LEU:HB2	2.49	0.47
1:A:44:VAL:O	1:A:44:VAL:CG1	2.62	0.46
1:B:286:ASN:OD1	1:B:286:ASN:N	2.48	0.46
1:B:162:ASN:OD1	1:B:164:HIS:CB	2.63	0.46
1:A:228:ALA:HB1	1:A:322:THR:HG21	1.98	0.45
1:A:278:MET:C	1:A:278:MET:SD	3.00	0.45
1:B:152:GLU:HB3	1:B:278:MET:HG3	1.98	0.45
1:B:7:VAL:O	1:B:7:VAL:CG1	2.61	0.45
1:B:10:PRO:HA	1:B:24:VAL:O	2.16	0.45
1:B:163:PRO:O	1:B:164:HIS:C	2.59	0.45
1:B:278:MET:C	1:B:278:MET:SD	3.00	0.45
1:B:104:GLY:HA2	1:B:145:TYR:CE1	2.51	0.45
1:A:129:GLU:OE2	1:A:132:LYS:HE2	2.17	0.45
1:A:189:TYR:CD1	1:A:189:TYR:C	2.96	0.44
1:A:21:TRP:C	1:A:22:ILE:HD12	2.43	0.44
1:B:189:TYR:CE1	1:B:197:MET:HA	2.52	0.44
1:B:199:VAL:O	1:B:203:GLN:HG2	2.18	0.44
1:A:129:GLU:O	1:A:132:LYS:HB2	2.16	0.44
1:A:65:LYS:HG2	5:A:749:HOH:O	2.18	0.44
1:A:34:GLN:HB3	5:A:581:HOH:O	2.17	0.44
1:B:5:ASN:C	1:B:7:VAL:N	2.73	0.44
1:A:180:GLU:HG2	5:A:538:HOH:O	2.17	0.44
1:B:265:ARG:NH1	1:B:338:VAL:O	2.50	0.44
1:B:111:PHE:CE2	1:B:119:LEU:HD21	2.52	0.44
1:B:15:ASN:O	1:B:19:GLY:N	2.50	0.43
1:B:23:LEU:O	1:B:323:GLN:HA	2.18	0.43
1:B:279:GLY:O	1:B:297:ALA:HA	2.19	0.43
1:A:49:ASP:OD1	1:A:50:PRO:CD	2.64	0.43
1:A:49:ASP:CG	1:A:50:PRO:CD	2.91	0.43
1:B:104:GLY:HA3	1:B:171:ALA:O	2.18	0.43
1:A:280:TRP:CE3	1:A:297:ALA:HB2	2.54	0.43
1:A:27:HIS:H	1:A:27:HIS:HD2	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:OE2	1:A:132:LYS:CE	2.65	0.43
1:A:224:PRO:O	1:A:225:TYR:C	2.61	0.43
1:A:44:VAL:O	1:A:44:VAL:HG13	2.18	0.43
1:A:89:ALA:CB	1:B:4:PHE:CE2	3.02	0.43
1:B:5:ASN:C	1:B:7:VAL:H	2.27	0.43
1:B:343:PHE:CE1	1:B:344:ARG:HG2	2.53	0.43
1:A:327:THR:OG1	1:A:330:GLN:HG3	2.18	0.42
1:B:14:TYR:CZ	1:B:19:GLY:HA2	2.54	0.42
1:B:109:ILE:HG22	1:B:167:GLY:C	2.44	0.42
1:B:14:TYR:OH	1:B:19:GLY:HA2	2.18	0.42
1:A:10:PRO:HA	1:A:24:VAL:O	2.19	0.42
1:A:83:MET:HE2	1:A:83:MET:HB2	1.82	0.42
1:A:193:GLN:O	1:A:194:LYS:HB2	2.20	0.42
1:B:226:TRP:O	1:B:227:ALA:C	2.62	0.42
1:A:59:VAL:HA	1:A:65:LYS:HA	2.00	0.42
1:B:22:ILE:HD12	1:B:22:ILE:N	2.34	0.41
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.84	0.41
1:B:130:ILE:O	1:B:131:VAL:C	2.62	0.41
1:B:174:PHE:CD1	1:B:174:PHE:N	2.87	0.41
1:A:21:TRP:CH2	1:B:100:GLN:HG3	2.55	0.41
1:A:59:VAL:O	1:A:59:VAL:HG23	2.20	0.41
1:A:97:MET:HE2	1:B:225:TYR:CD1	2.56	0.41
1:A:99:CYS:HA	1:B:12:ARG:O	2.21	0.41
1:A:219:TRP:CZ3	1:A:237:PRO:HD3	2.54	0.41
1:A:59:VAL:HG22	5:A:371:HOH:O	2.21	0.41
1:A:311:LYS:HE3	1:A:313:MET:HE3	1.81	0.41
1:A:303:LEU:HD23	1:A:303:LEU:HA	1.75	0.40
1:A:229:TRP:HB2	1:A:232:GLU:HB2	2.02	0.40
1:A:48:HIS:HD2	5:A:364:HOH:O	2.04	0.40
1:A:153:ASN:ND2	1:A:277:SER:OG	2.54	0.40
1:B:299:PHE:O	1:B:301:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	329/348 (94%)	314 (95%)	15 (5%)	0	100	100
All	All	665/696 (96%)	635 (96%)	30 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	291/299 (97%)	270 (93%)	21 (7%)	13	3
1	B	287/299 (96%)	271 (94%)	16 (6%)	19	6
All	All	578/598 (97%)	541 (94%)	37 (6%)	16	4

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	10	PRO
1	A	27	HIS
1	A	33	TRP
1	A	44	VAL
1	A	91	GLU
1	A	101	SER
1	A	109	ILE
1	A	132	LYS
1	A	153	ASN
1	A	161	SER
1	A	184	ARG
1	A	202	VAL
1	A	236	LEU
1	A	253	SER

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Mol	Chain	Res	Type
1	A	266	TYR
1	A	277	SER
1	A	305	ARG
1	A	311	LYS
1	A	313	MET
1	A	341	ILE
1	B	2	THR
1	B	20	GLN
1	B	44	VAL
1	B	54	LEU
1	B	61	VAL
1	B	70	THR
1	B	98	ARG
1	B	187	LYS
1	B	193	GLN
1	B	204	ARG
1	B	236	LEU
1	B	253	SER
1	B	266	TYR
1	B	269	LEU
1	B	277	SER
1	B	311	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	48	HIS
1	A	93	HIS
1	A	100	GLN
1	A	153	ASN
1	A	193	GLN
1	A	240	HIS
1	A	290	ASN
1	B	20	GLN
1	B	172	ASN

5.3.3 RNA ⓘ

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](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
4	U5P	A	352	1	18,21,22	0.94	0	25,30,33	1.17	2 (8%)
4	U5P	B	352	1	18,21,22	0.95	2 (11%)	25,30,33	1.58	6 (24%)

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
4	U5P	A	352	1	-	0/7/25/26	0/2/2/2
4	U5P	B	352	1	-	0/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	352	U5P	C2-N1	-2.25	1.34	1.38
4	B	352	U5P	O2-C2	2.02	1.26	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	352	U5P	O4'-C1'-N1	-4.00	99.29	108.36
4	A	352	U5P	O4'-C1'-C2'	-2.93	100.35	106.62
4	B	352	U5P	O4'-C1'-C2'	-2.87	100.48	106.62
4	B	352	U5P	O2-C2-N1	-2.74	119.23	122.80
4	B	352	U5P	C5-C4-N3	-2.28	111.60	114.80
4	B	352	U5P	C4'-O4'-C1'	-2.20	104.61	109.47
4	A	352	U5P	C4-N3-C2	-2.09	124.02	126.61
4	B	352	U5P	C6-C5-C4	2.02	122.11	119.53

There are no chirality outliers.

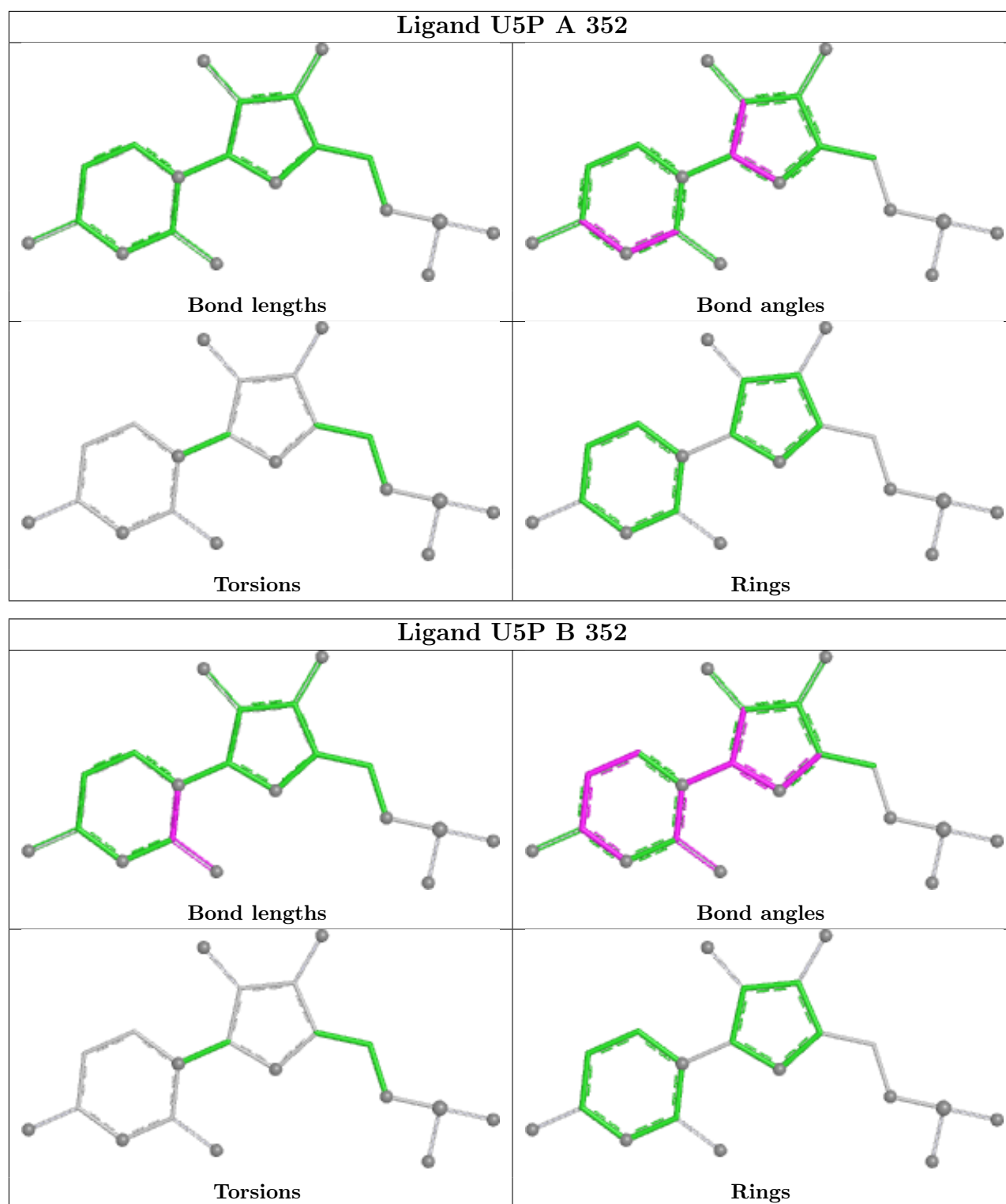
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	352	U5P	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

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.