



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:48 PM UTC

PDB ID : 9DT6 / pdb_00009dt6
Title : Crystal structure of ADP-ribose diphosphatase from *Klebsiella pneumoniae* (CMP bound, P21 form)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-09-30
Resolution : 1.59 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

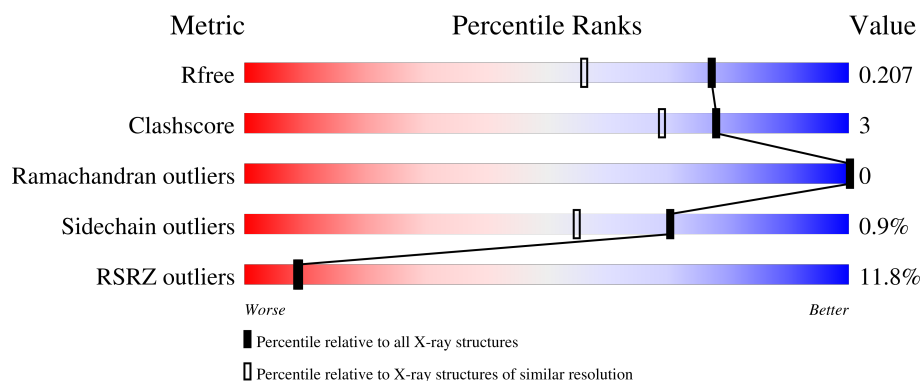
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 ≥ 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	218	9% 81% 8% 11%
1	B	218	17% 83% 8% 10%
1	C	218	7% 87% • 9%
1	D	218	12% 82% 8% 11%

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Mol	Chain	Length	Quality of chain
1	E	218	13% 86% 7% 6%
1	F	218	10% 83% 6% 11%
1	G	218	7% 87% 9%
1	H	218	11% 83% 6% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13926 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 ADP-ribose pyrophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	5	0
			1561	993	270	295	3			
1	B	197	Total	C	N	O	S	0	1	0
			1566	990	275	298	3			
1	C	199	Total	C	N	O	S	0	1	0
			1579	1000	277	299	3			
1	D	195	Total	C	N	O	S	0	2	0
			1564	988	278	295	3			
1	E	204	Total	C	N	O	S	0	2	0
			1635	1034	292	305	4			
1	F	195	Total	C	N	O	S	0	3	0
			1555	986	271	295	3			
1	G	198	Total	C	N	O	S	0	3	0
			1590	1009	278	300	3			
1	H	196	Total	C	N	O	S	0	4	0
			1571	996	273	299	3			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP A0A0H3GVQ7
A	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
A	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
A	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
A	0	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-7	MET	-	expression tag	UNP A0A0H3GVQ7
B	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
B	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-3	HIS	-	expression tag	UNP A0A0H3GVQ7

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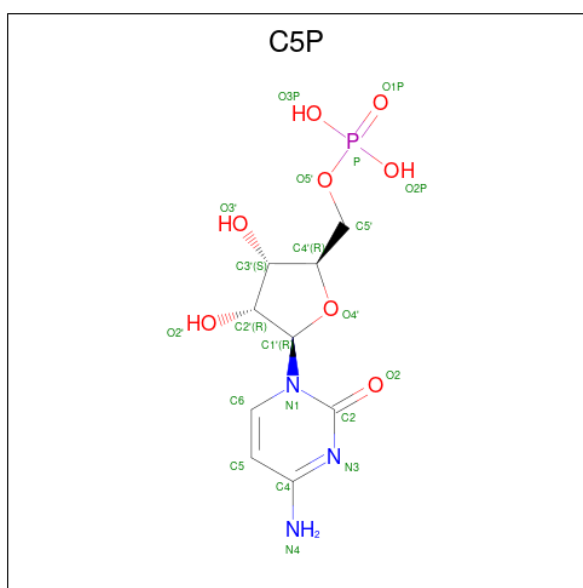
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
B	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
B	0	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-7	MET	-	expression tag	UNP A0A0H3GVQ7
C	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
C	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
C	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
C	0	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-7	MET	-	expression tag	UNP A0A0H3GVQ7
D	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
D	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
D	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
D	0	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-7	MET	-	expression tag	UNP A0A0H3GVQ7
E	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
E	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
E	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
E	0	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-7	MET	-	expression tag	UNP A0A0H3GVQ7
F	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
F	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
F	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
F	0	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-7	MET	-	expression tag	UNP A0A0H3GVQ7
G	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
G	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
G	-1	HIS	-	expression tag	UNP A0A0H3GVQ7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-7	MET	-	expression tag	UNP A0A0H3GVQ7
H	-6	ALA	-	expression tag	UNP A0A0H3GVQ7
H	-5	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-4	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-3	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-2	HIS	-	expression tag	UNP A0A0H3GVQ7
H	-1	HIS	-	expression tag	UNP A0A0H3GVQ7
H	0	HIS	-	expression tag	UNP A0A0H3GVQ7

- Molecule 2 is CYTIDINE-5'-MONOPHOSPHATE (CCD ID: C5P) (formula: $C_9H_{14}N_3O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
2	E	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
2	F	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
2	H	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

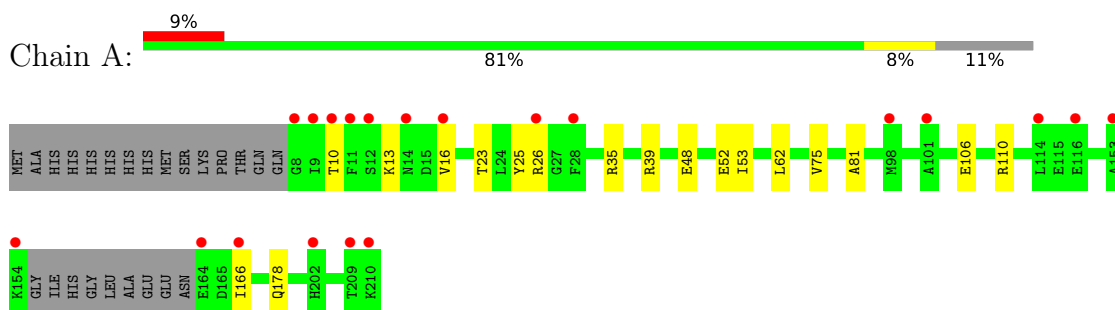
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	132	Total 132	O 132	0	0
3	B	143	Total 143	O 143	0	0
3	C	157	Total 157	O 157	0	0
3	D	136	Total 136	O 136	0	0
3	E	151	Total 151	O 151	0	0
3	F	164	Total 164	O 164	0	0
3	G	172	Total 172	O 172	0	0
3	H	166	Total 166	O 166	0	0

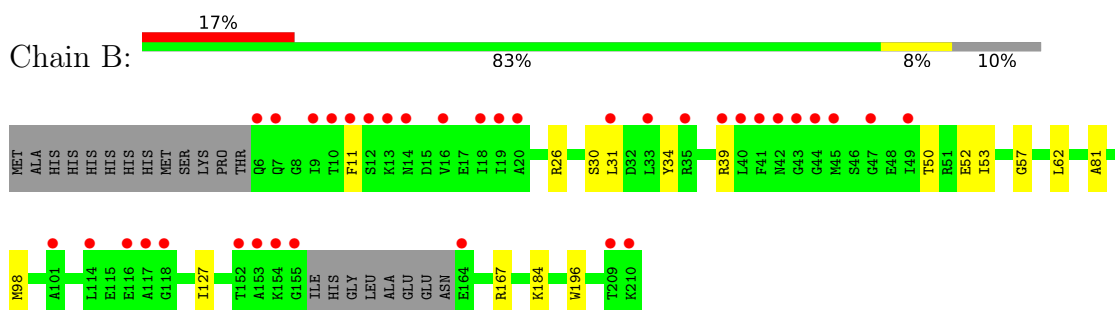
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

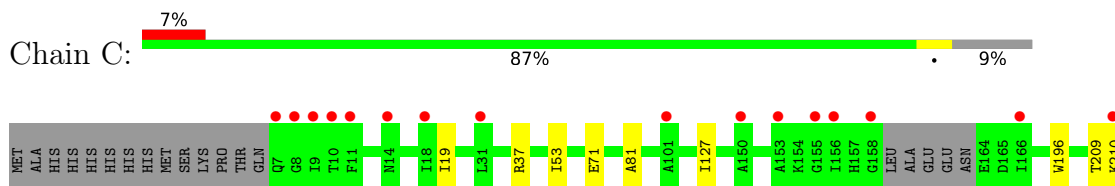
- Molecule 1: ADP-ribose pyrophosphatase



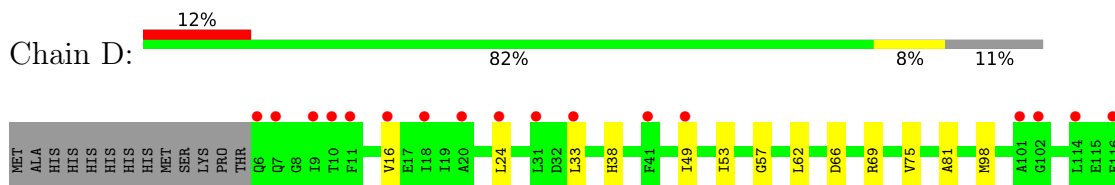
- Molecule 1: ADP-ribose pyrophosphatase

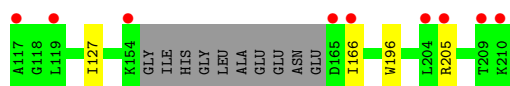


- Molecule 1: ADP-ribose pyrophosphatase

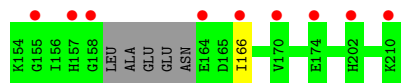
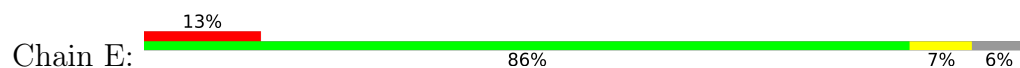


- Molecule 1: ADP-ribose pyrophosphatase

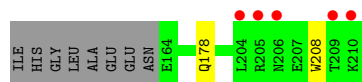
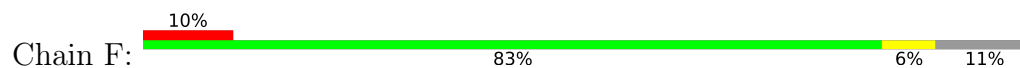




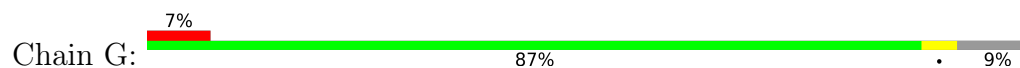
- Molecule 1: ADP-ribose pyrophosphatase



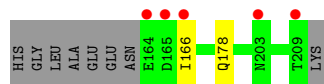
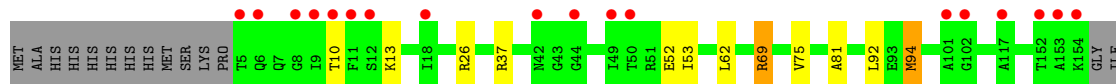
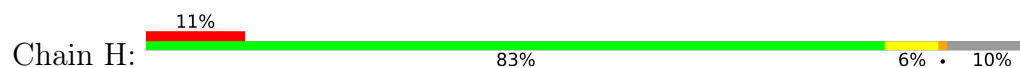
- Molecule 1: ADP-ribose pyrophosphatase



- Molecule 1: ADP-ribose pyrophosphatase



- Molecule 1: ADP-ribose pyrophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.94Å 80.06Å 115.79Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	72.59 – 1.59 72.59 – 1.59	Depositor EDS
% Data completeness (in resolution range)	97.2 (72.59-1.59) 97.3 (72.59-1.59)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.59Å)	Xtriage
Refinement program	PHENIX (dev_5295: ???)	Depositor
R, R_{free}	0.170 , 0.202 0.179 , 0.207	Depositor DCC
R_{free} test set	11200 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13926	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.23 % 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 3.2574e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: C5P

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	0.36	0/1602	0.56	0/2172
1	B	0.38	0/1598	0.57	0/2162
1	C	0.42	0/1612	0.61	0/2182
1	D	0.38	0/1599	0.57	0/2163
1	E	0.41	0/1675	0.59	0/2266
1	F	0.42	0/1593	0.59	0/2156
1	G	0.47	0/1630	0.64	0/2207
1	H	0.51	2/1612 (0.1%)	0.69	4/2185 (0.2%)
All	All	0.42	2/12921 (0.0%)	0.60	4/17493 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	69[A]	ARG	C-O	5.86	1.31	1.24
1	H	69[B]	ARG	C-O	5.86	1.31	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	69[A]	ARG	CA-C-O	6.86	127.34	119.18
1	H	69[B]	ARG	CA-C-O	6.86	127.34	119.18
1	H	69[A]	ARG	N-CA-C	5.31	119.75	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	69[B]	ARG	N-CA-C	5.31	119.75	113.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	69[A]	ARG	Sidechain
1	H	69[B]	ARG	Sidechain

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	1561	0	1537	14	0
1	B	1566	0	1529	14	0
1	C	1579	0	1546	6	0
1	D	1564	0	1528	10	0
1	E	1635	0	1592	11	0
1	F	1555	0	1525	8	0
1	G	1590	0	1563	6	0
1	H	1571	0	1535	14	0
2	C	21	0	12	0	0
2	E	21	0	12	0	0
2	F	21	0	12	1	0
2	H	21	0	12	0	0
3	A	132	0	0	2	0
3	B	143	0	0	1	0
3	C	157	0	0	0	0
3	D	136	0	0	1	0
3	E	151	0	0	0	0
3	F	164	0	0	1	0
3	G	172	0	0	1	0
3	H	166	0	0	4	0
All	All	13926	0	12403	69	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 3.

All (69) 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:178:GLN:NE2	3:A:401:HOH:O	2.22	0.72
1:H:75:VAL:HG13	1:H:166:ILE:HG23	1.71	0.72
1:D:75:VAL:HG13	1:D:166:ILE:HG23	1.73	0.69
1:C:81:ALA:HB2	1:D:53:ILE:HD12	1.74	0.69
1:A:75[A]:VAL:HG13	1:A:166:ILE:HG23	1.75	0.69
1:H:75:VAL:HG13	1:H:166:ILE:CG2	2.22	0.69
1:A:13:LYS:NZ	3:A:402:HOH:O	2.25	0.68
1:D:75:VAL:HG13	1:D:166:ILE:CG2	2.23	0.68
1:A:81:ALA:HB2	1:B:53:ILE:HD12	1.75	0.68
1:E:81:ALA:HB2	1:F:53:ILE:HD12	1.75	0.66
1:H:13:LYS:NZ	3:H:405:HOH:O	2.30	0.64
1:F:52:GLU:O	1:F:53:ILE:HD13	1.97	0.64
1:E:35:ARG:NH1	1:E:48:GLU:OE2	2.25	0.64
1:E:75[A]:VAL:HG13	1:E:166:ILE:HG23	1.79	0.63
1:G:53:ILE:HD12	1:H:81:ALA:HB2	1.81	0.63
1:H:52:GLU:O	1:H:53:ILE:HD13	2.02	0.59
1:C:53:ILE:HD12	1:D:81:ALA:HB2	1.87	0.56
1:A:39:ARG:NH1	1:C:71:GLU:OE2	2.29	0.56
1:A:35:ARG:NH1	1:A:48[A]:GLU:OE2	2.34	0.56
1:A:23:THR:HG23	1:A:26:ARG:NH1	2.20	0.56
1:A:53:ILE:HD12	1:B:81:ALA:HB2	1.87	0.55
1:E:75[B]:VAL:CG2	1:E:166:ILE:HG23	2.36	0.54
1:A:25:TYR:CD2	1:B:31:LEU:HD22	2.42	0.54
1:A:75[A]:VAL:HG13	1:A:166:ILE:CG2	2.36	0.54
1:B:11:PHE:CE1	1:B:39:ARG:HD2	2.43	0.53
1:G:81:ALA:HB2	1:H:53:ILE:HD12	1.91	0.53
1:E:57:GLY:HA3	1:E:98:MET:HE3	1.91	0.53
1:A:10:THR:OG1	1:B:167:ARG:NH1	2.43	0.52
1:G:35:ARG:NH1	1:G:48:GLU:OE2	2.35	0.52
1:H:178[A]:GLN:NE2	3:H:407:HOH:O	2.42	0.52
1:B:184:LYS:HG3	3:B:350:HOH:O	2.10	0.52
1:E:75[B]:VAL:HG23	1:E:166:ILE:HG23	1.91	0.51
1:B:52:GLU:O	1:B:53:ILE:HD13	2.11	0.50
1:H:26:ARG:NH1	3:H:401:HOH:O	2.24	0.50
1:D:24:LEU:HD11	1:D:33:LEU:HB2	1.94	0.49
1:H:75:VAL:CG1	1:H:166:ILE:HG23	2.42	0.49
1:E:53:ILE:HD12	1:F:81:ALA:HB2	1.95	0.49
1:D:57:GLY:HA3	1:D:98:MET:HE3	1.95	0.49
1:B:26[A]:ARG:CZ	1:B:30:SER:OG	2.62	0.48
1:D:38:HIS:CD2	1:D:49:ILE:HD12	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:ARG:HD3	1:F:48:GLU:OE2	2.14	0.47
1:B:26[A]:ARG:NE	1:B:30:SER:OG	2.47	0.47
1:C:19:ILE:HD11	1:C:37:ARG:HG3	1.97	0.47
1:D:205:ARG:NH1	3:D:303:HOH:O	2.30	0.46
1:B:34:TYR:O	1:B:50:THR:HA	2.16	0.45
1:F:178:GLN:HG3	3:F:514:HOH:O	2.14	0.45
1:A:25:TYR:CE2	1:B:31:LEU:CD2	2.99	0.45
1:C:209:THR:O	1:C:210:LYS:CB	2.65	0.44
1:B:127:ILE:HG23	1:B:196:TRP:CG	2.52	0.44
1:C:127:ILE:HG23	1:C:196:TRP:CG	2.52	0.44
1:G:9:ILE:CD1	1:H:92:LEU:HG	2.47	0.44
1:H:94:MET:HA	1:H:94:MET:HE2	2.00	0.44
1:G:167:ARG:NH1	1:H:10:THR:OG1	2.42	0.44
1:D:66:ASP:OD2	1:D:69[B]:ARG:HD2	2.18	0.43
1:E:119:LEU:HD21	1:E:153:ALA:HB2	2.00	0.43
1:F:34:TYR:O	1:F:50:THR:HA	2.18	0.43
1:G:119:LEU:HD21	1:G:153:ALA:HB2	1.99	0.43
1:A:52:GLU:O	1:A:53:ILE:HD13	2.19	0.42
1:B:11:PHE:CD1	1:B:39:ARG:HD2	2.55	0.42
1:E:26:ARG:HD3	1:E:30:SER:OG	2.20	0.42
1:E:37:ARG:NH1	1:E:46:SER:O	2.53	0.42
1:B:57:GLY:HA3	1:B:98:MET:HE3	2.01	0.42
1:A:106:GLU:OE2	1:A:110:ARG:NE	2.46	0.42
3:G:322:HOH:O	1:H:13:LYS:HE3	2.19	0.42
1:F:123:ARG:NH2	1:F:208:TRP:O	2.53	0.41
1:D:127:ILE:HG23	1:D:196:TRP:CG	2.55	0.41
1:F:24:LEU:HD11	1:F:33:LEU:HB2	2.01	0.41
1:E:51:ARG:NH1	2:F:301:C5P:H3'	2.35	0.41
1:H:37:ARG:HD3	3:H:494:HOH:O	2.22	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	195/218 (89%)	187 (96%)	8 (4%)	0	100	100
1	B	194/218 (89%)	185 (95%)	9 (5%)	0	100	100
1	C	196/218 (90%)	189 (96%)	7 (4%)	0	100	100
1	D	193/218 (88%)	186 (96%)	7 (4%)	0	100	100
1	E	200/218 (92%)	196 (98%)	4 (2%)	0	100	100
1	F	194/218 (89%)	187 (96%)	7 (4%)	0	100	100
1	G	197/218 (90%)	191 (97%)	6 (3%)	0	100	100
1	H	196/218 (90%)	188 (96%)	8 (4%)	0	100	100
All	All	1565/1744 (90%)	1509 (96%)	56 (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	164/183 (90%)	161 (98%)	3 (2%)	51	28
1	B	162/183 (88%)	161 (99%)	1 (1%)	78	66
1	C	164/183 (90%)	164 (100%)	0	100	100
1	D	162/183 (88%)	160 (99%)	2 (1%)	63	43
1	E	171/183 (93%)	170 (99%)	1 (1%)	78	66
1	F	162/183 (88%)	160 (99%)	2 (1%)	63	43
1	G	167/183 (91%)	165 (99%)	2 (1%)	63	43
1	H	164/183 (90%)	162 (99%)	2 (1%)	63	43
All	All	1316/1464 (90%)	1303 (99%)	13 (1%)	70	50

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16[A]	VAL
1	A	16[B]	VAL

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Mol	Chain	Res	Type
1	A	62	LEU
1	B	62	LEU
1	D	16	VAL
1	D	62	LEU
1	E	114	LEU
1	F	16	VAL
1	F	62	LEU
1	G	9	ILE
1	G	16	VAL
1	H	62	LEU
1	H	94	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	77	GLN
1	C	175	GLN
1	D	7	GLN
1	D	175	GLN
1	E	157	HIS
1	F	175	GLN
1	F	187	ASN

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 oligosaccharides 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	C5P	H	301	-	22,22,22	0.52	0	32,33,33	0.79	1 (3%)
2	C5P	F	301	-	22,22,22	0.50	0	32,33,33	0.79	1 (3%)
2	C5P	E	301	-	22,22,22	0.44	0	32,33,33	0.73	1 (3%)
2	C5P	C	301	-	22,22,22	0.53	0	32,33,33	0.94	2 (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	C5P	H	301	-	-	0/10/26/26	0/2/2/2
2	C5P	F	301	-	-	0/10/26/26	0/2/2/2
2	C5P	E	301	-	-	2/10/26/26	0/2/2/2
2	C5P	C	301	-	-	0/10/26/26	0/2/2/2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	C5P	O3P-P-O5'	-2.81	99.34	106.67
2	C	301	C5P	O3P-P-O5'	-2.77	99.45	106.67
2	F	301	C5P	O3P-P-O5'	-2.44	100.31	106.67
2	C	301	C5P	C4-N3-C2	2.21	123.75	120.26
2	H	301	C5P	O3P-P-O5'	-2.20	100.94	106.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

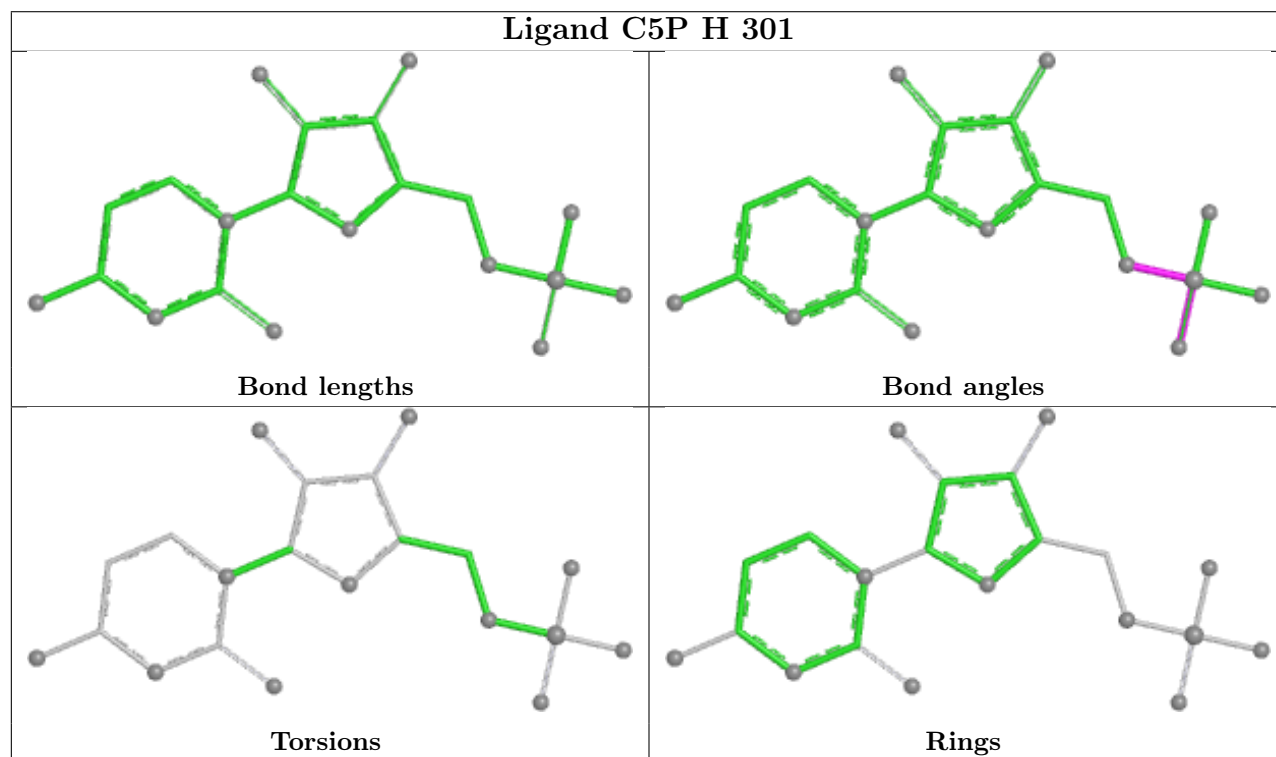
Mol	Chain	Res	Type	Atoms
2	E	301	C5P	O4'-C4'-C5'-O5'
2	E	301	C5P	C3'-C4'-C5'-O5'

There are no ring outliers.

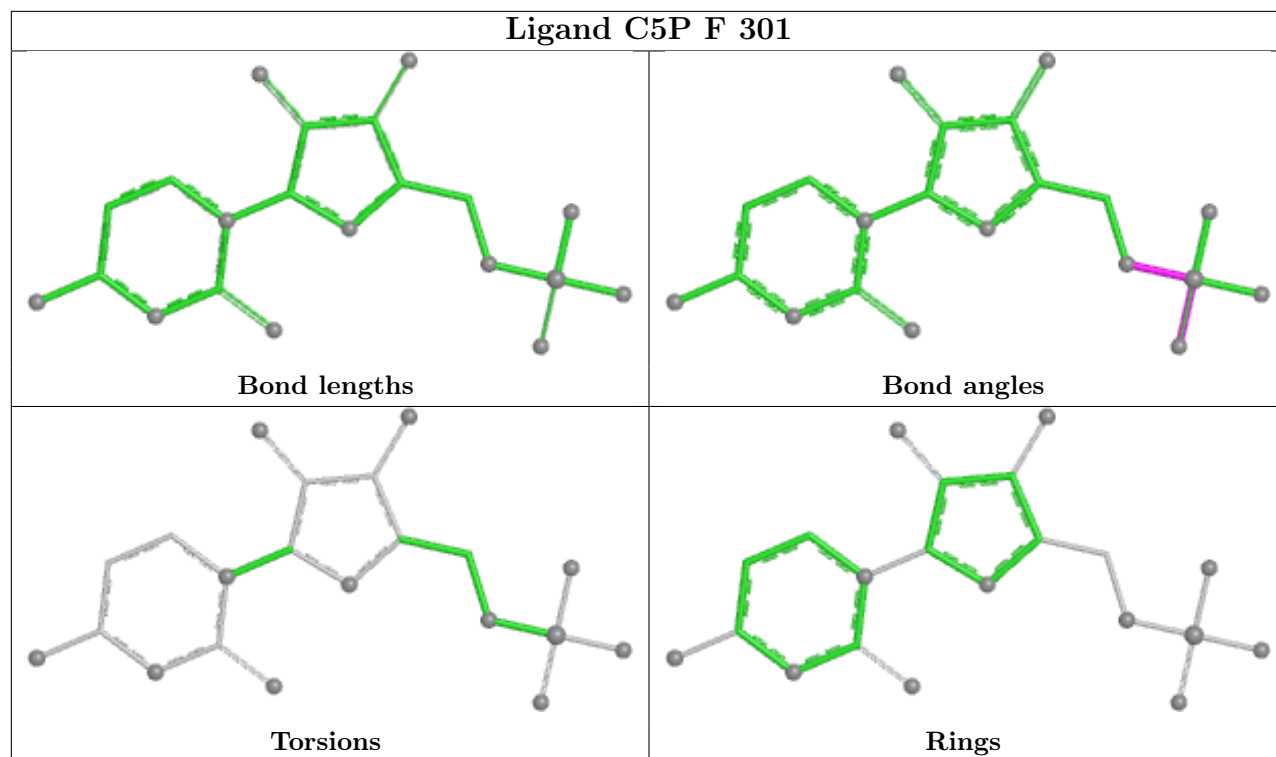
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	C5P	1	0

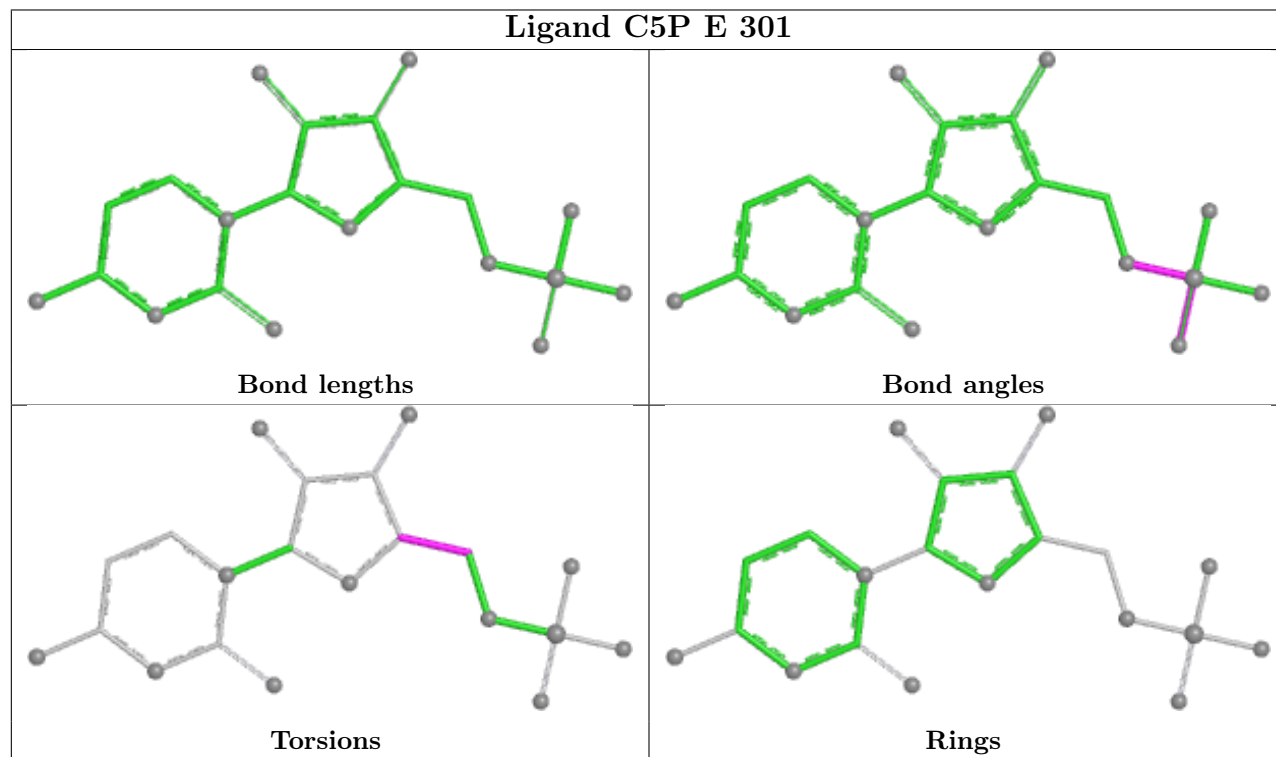
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

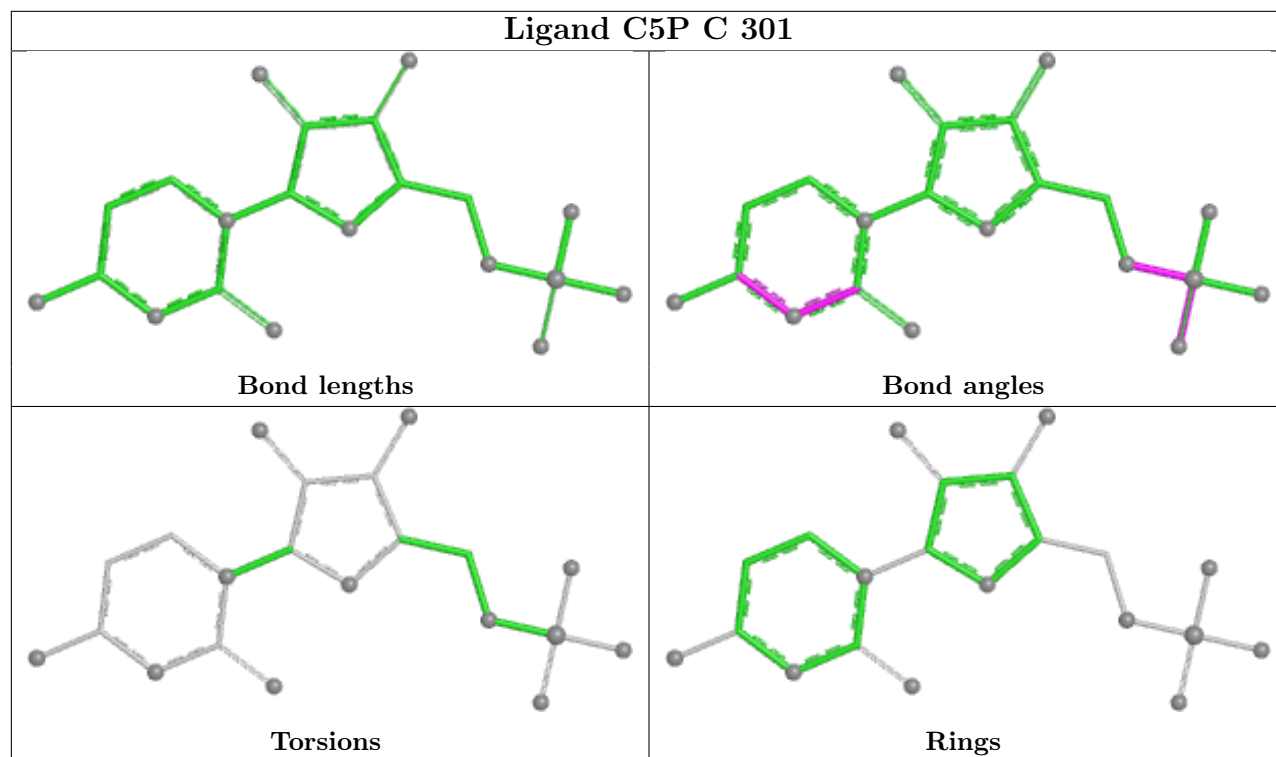


Ligand C5P F 301



Ligand C5P E 301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q < 0.9
1	A	194/218 (88%)	0.78	20 (10%)	12 12	16, 33, 58, 82	5 (2%)
1	B	197/218 (90%)	0.98	36 (18%)	3 3	20, 35, 72, 84	1 (0%)
1	C	199/218 (91%)	0.59	16 (8%)	18 18	14, 30, 47, 74	1 (0%)
1	D	195/218 (89%)	0.88	26 (13%)	7 7	18, 34, 66, 79	2 (1%)
1	E	204/218 (93%)	0.87	29 (14%)	6 6	14, 32, 56, 76	2 (0%)
1	F	195/218 (89%)	0.71	21 (10%)	11 10	17, 31, 61, 78	3 (1%)
1	G	198/218 (90%)	0.51	15 (7%)	20 20	12, 26, 49, 64	3 (1%)
1	H	196/218 (89%)	0.72	23 (11%)	9 9	15, 30, 54, 80	4 (2%)
All	All	1578/1744 (90%)	0.75	186 (11%)	9 9	12, 31, 61, 84	21 (1%)

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	209	THR	7.2
1	E	9	ILE	7.1
1	H	5	THR	6.5
1	F	8	GLY	6.0
1	A	9	ILE	5.6
1	A	154	LYS	5.2
1	D	10	THR	5.1
1	A	10	THR	4.7
1	F	209	THR	4.7
1	G	163	ASN	4.6
1	F	10	THR	4.5
1	G	9	ILE	4.5
1	A	8	GLY	4.4
1	F	210	LYS	4.4
1	H	153	ALA	4.3
1	E	158	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	153	ALA	4.0
1	H	9	ILE	3.9
1	B	49	ILE	3.9
1	B	209	THR	3.8
1	E	-2	HIS	3.8
1	B	7	GLN	3.7
1	A	114	LEU	3.6
1	B	101	ALA	3.6
1	C	7	GLN	3.6
1	F	19	ILE	3.6
1	D	9	ILE	3.5
1	D	101	ALA	3.5
1	D	6	GLN	3.5
1	E	-4	HIS	3.5
1	E	0	HIS	3.5
1	B	19	ILE	3.5
1	D	209	THR	3.5
1	B	44	GLY	3.4
1	B	14	ASN	3.4
1	E	114	LEU	3.4
1	B	6	GLN	3.4
1	G	10	THR	3.4
1	B	155	GLY	3.3
1	H	10	THR	3.3
1	C	9	ILE	3.3
1	D	49	ILE	3.3
1	F	11	PHE	3.3
1	E	101	ALA	3.3
1	C	210	LYS	3.3
1	H	164	GLU	3.3
1	B	20	ALA	3.3
1	B	154	LYS	3.2
1	E	117	ALA	3.2
1	D	31	LEU	3.2
1	A	11	PHE	3.1
1	A	164	GLU	3.1
1	E	2	SER	3.1
1	B	18	ILE	3.1
1	B	47	GLY	3.1
1	D	18	ILE	3.1
1	H	165	ASP	3.0
1	C	158	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	8	GLY	3.0
1	D	114	LEU	3.0
1	F	102	GLY	3.0
1	D	117	ALA	2.9
1	A	166	ILE	2.9
1	B	42	ASN	2.9
1	B	31	LEU	2.9
1	D	24	LEU	2.9
1	E	155	GLY	2.9
1	C	18	ILE	2.9
1	H	166	ILE	2.9
1	F	28	PHE	2.9
1	A	153	ALA	2.8
1	B	11	PHE	2.8
1	C	8	GLY	2.8
1	B	210	LYS	2.8
1	F	154	LYS	2.8
1	B	35	ARG	2.8
1	E	28	PHE	2.8
1	D	166	ILE	2.8
1	D	7	GLN	2.8
1	D	210	LYS	2.8
1	G	153	ALA	2.7
1	H	8	GLY	2.7
1	D	11	PHE	2.7
1	A	14	ASN	2.7
1	F	9	ILE	2.7
1	E	174	GLU	2.7
1	H	44	GLY	2.7
1	A	209	THR	2.7
1	B	10	THR	2.7
1	B	152	THR	2.7
1	B	13	LYS	2.7
1	F	155	GLY	2.7
1	G	26	ARG	2.7
1	B	164	GLU	2.6
1	H	203	ASN	2.6
1	H	101	ALA	2.6
1	D	102	GLY	2.6
1	C	166	ILE	2.6
1	F	18	ILE	2.6
1	H	152	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	154	LYS	2.5
1	B	41	PHE	2.5
1	B	114	LEU	2.5
1	E	118	GLY	2.5
1	H	102	GLY	2.5
1	B	16	VAL	2.5
1	E	10	THR	2.5
1	A	26	ARG	2.5
1	G	101	ALA	2.5
1	G	114	LEU	2.5
1	F	206	ASN	2.5
1	H	50	THR	2.5
1	B	153	ALA	2.4
1	E	150	ALA	2.4
1	A	210	LYS	2.4
1	F	204	LEU	2.4
1	C	14	ASN	2.4
1	F	115	GLU	2.4
1	A	202	HIS	2.4
1	A	98	MET	2.4
1	E	1	MET	2.4
1	E	202	HIS	2.4
1	F	14	ASN	2.4
1	G	102	GLY	2.4
1	A	101	ALA	2.3
1	E	99	ILE	2.3
1	E	157	HIS	2.3
1	C	11	PHE	2.3
1	D	41	PHE	2.3
1	A	12	SER	2.3
1	E	75[A]	VAL	2.3
1	B	116	GLU	2.3
1	D	116	GLU	2.3
1	H	42	ASN	2.3
1	D	154	LYS	2.3
1	A	28	PHE	2.3
1	E	170	VAL	2.3
1	D	205	ARG	2.3
1	F	118	GLY	2.3
1	G	118	GLY	2.3
1	B	33	LEU	2.3
1	A	116	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	164	GLU	2.3
1	F	49	ILE	2.3
1	D	165	ASP	2.2
1	H	11	PHE	2.2
1	H	12	SER	2.2
1	C	101	ALA	2.2
1	F	205	ARG	2.2
1	G	164	GLU	2.2
1	B	43	GLY	2.2
1	H	6	GLN	2.2
1	C	31	LEU	2.2
1	E	-1	HIS	2.2
1	E	210	LYS	2.2
1	H	49	ILE	2.1
1	E	151	SER	2.1
1	G	14	ASN	2.1
1	A	16[A]	VAL	2.1
1	G	12	SER	2.1
1	B	117	ALA	2.1
1	C	150	ALA	2.1
1	D	20	ALA	2.1
1	D	204	LEU	2.1
1	C	10	THR	2.1
1	E	166	ILE	2.1
1	G	99	ILE	2.1
1	D	16	VAL	2.1
1	E	73	VAL	2.1
1	C	153	ALA	2.1
1	B	40	LEU	2.1
1	G	202[A]	HIS	2.1
1	B	118	GLY	2.1
1	H	117	ALA	2.0
1	B	39	ARG	2.0
1	B	9	ILE	2.0
1	C	156	ILE	2.0
1	H	18	ILE	2.0
1	B	12	SER	2.0
1	C	155	GLY	2.0
1	E	152	THR	2.0
1	F	113	ALA	2.0
1	B	45	MET	2.0
1	D	33	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	119	LEU	2.0
1	F	98	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

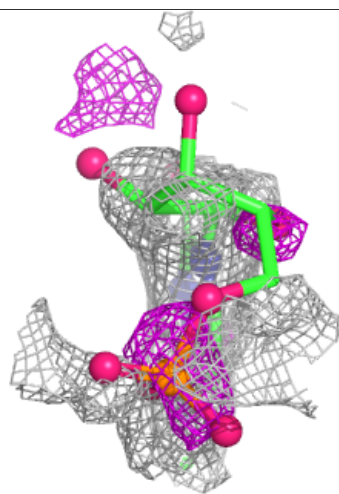
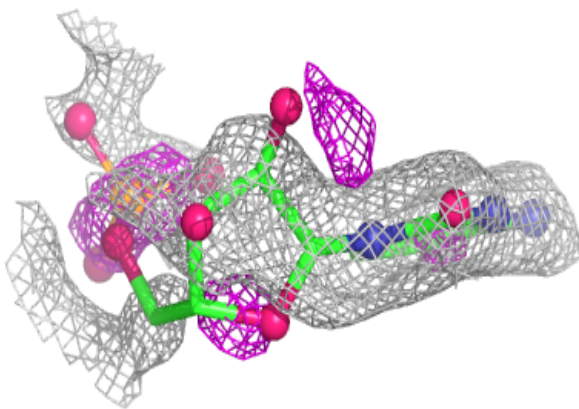
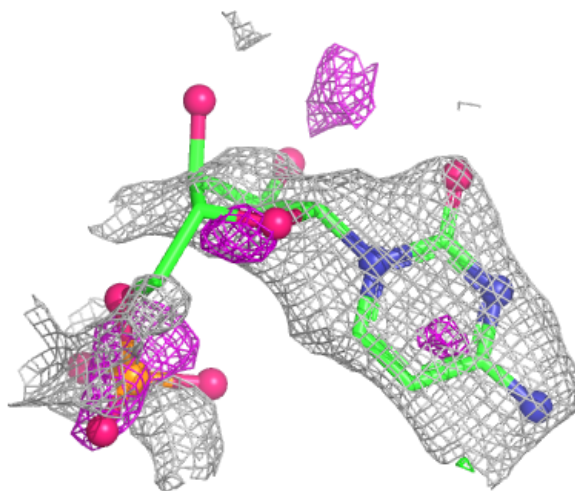
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C5P	E	301	21/21	0.49	0.16	55,75,99,113	0
2	C5P	F	301	21/21	0.61	0.16	30,65,77,97	0
2	C5P	C	301	21/21	0.65	0.14	28,61,89,107	0
2	C5P	H	301	21/21	0.74	0.14	28,55,75,93	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.

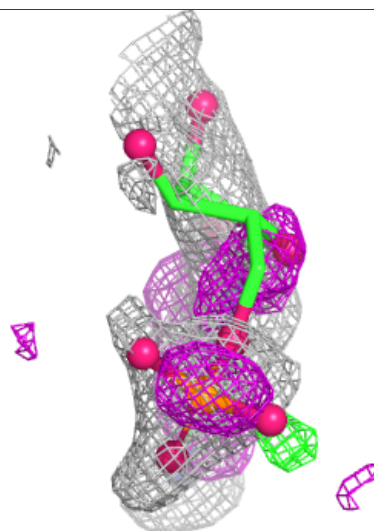
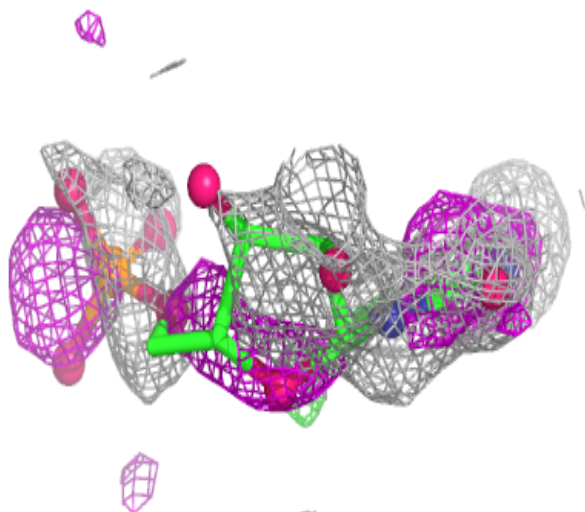
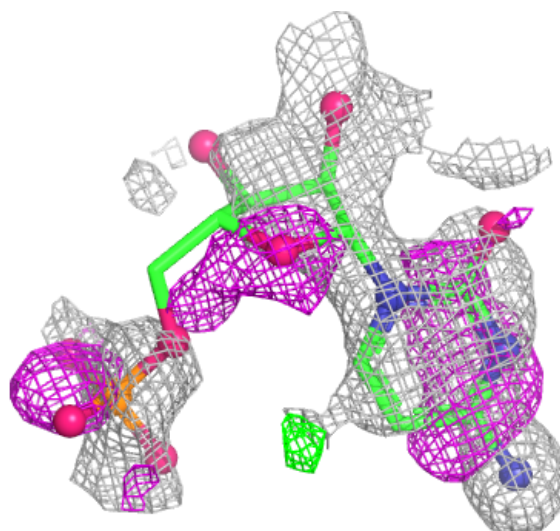
Electron density around C5P E 301:

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



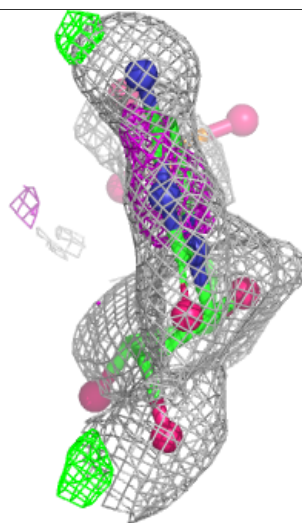
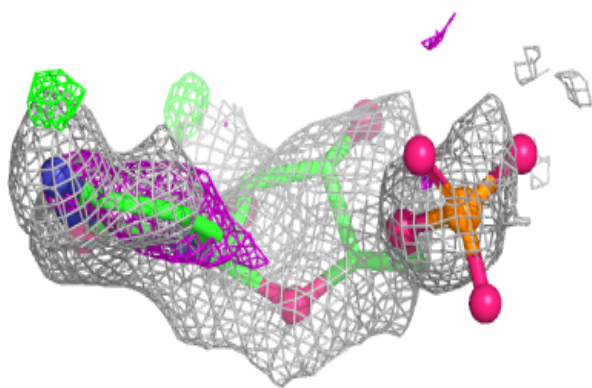
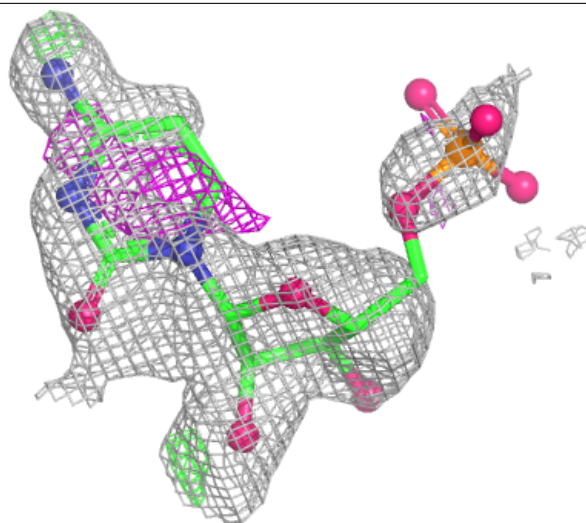
Electron density around C5P F 301:

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



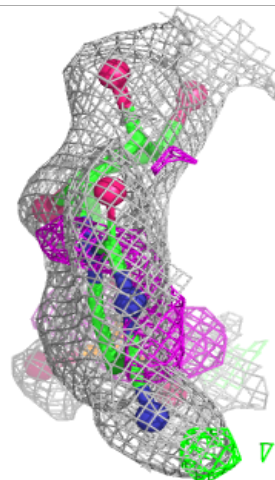
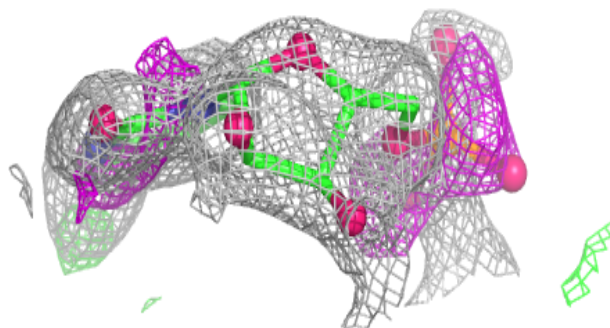
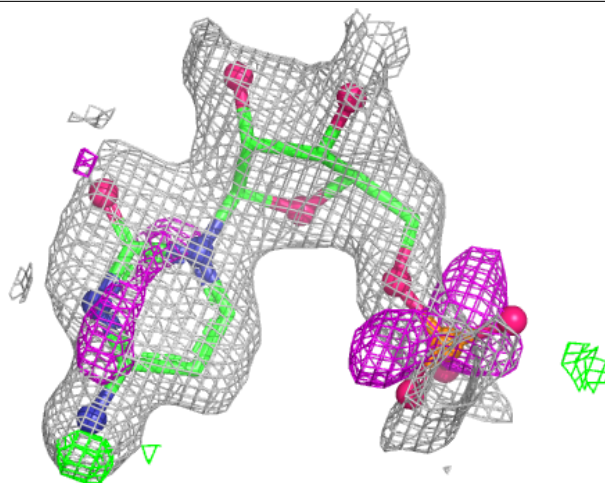
Electron density around C5P C 301:

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



Electron density around C5P H 301:

$2mF_o-DF_c$ (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.