



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:15 AM UTC

PDB ID : 2J4J / pdb_00002j4j
Title : Crystal structure of uridylylate kinase from *Sulfolobus solfataricus* in complex with UMP and AMPPCP to 2.1 Angstrom resolution
Authors : Jensen, K.S.; Johansson, E.; Jensen, K.F.
Deposited on : 2006-09-01
Resolution : 2.10 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:

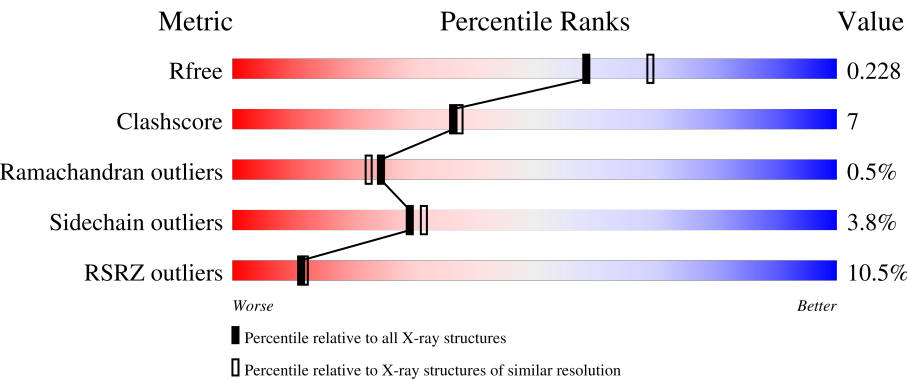
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	226	11% 78%14% . .
1	B	226	13% 84%10% . .
1	C	226	10% 81%12% . 5%
1	D	226	10% 81%13% . .
1	E	226	7% 79%16% . .

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Mol	Chain	Length	Quality of chain
1	F	226	11% 83% 17%

2 Entry composition [i](#)

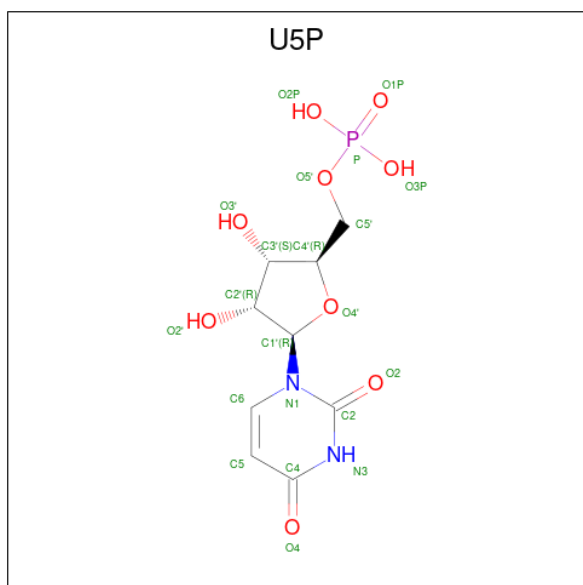
There are 7 unique types of molecules in this entry. The entry contains 10868 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 URIDYLATE KINASE.

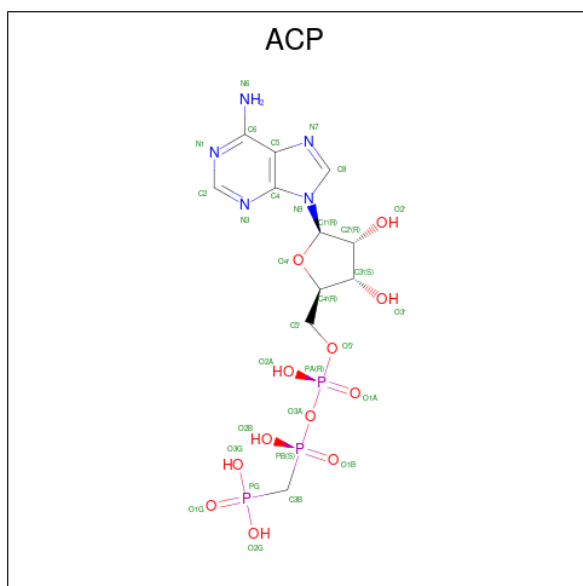
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1692	1085	288	315	4			
1	B	216	Total	C	N	O	S	0	0	0
			1692	1085	288	315	4			
1	C	215	Total	C	N	O	S	0	0	0
			1683	1080	287	312	4			
1	D	216	Total	C	N	O	S	0	0	0
			1692	1085	288	315	4			
1	E	216	Total	C	N	O	S	0	0	0
			1692	1085	288	315	4			
1	F	226	Total	C	N	O	S	0	0	0
			1761	1126	300	331	4			

- Molecule 2 is URIDINE-5'-MONOPHOSPHATE (CCD ID: U5P) (formula: C₉H₁₃N₂O₉P).



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

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

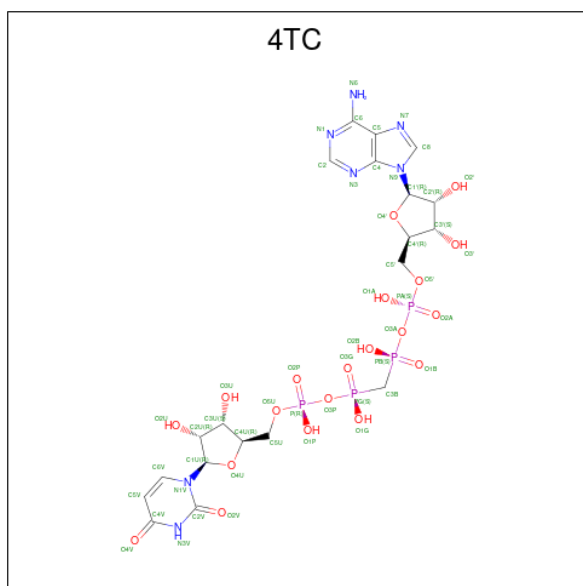
- Molecule 4 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Co 2 2	0	0
4	B	2	Total Co 2 2	0	0
4	C	1	Total Co 1 1	0	0
4	E	1	Total Co 1 1	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

- Molecule 6 is P1-(5'-ADENOSINE)P4-(5'-URIDINE)-BETA,GAMMA-METHYLENE TETRAPHOSPHATE (CCD ID: 4TC) (formula: C₂₀H₂₉N₇O₂₀P₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total C N O P 51 20 7 20 4	0	0

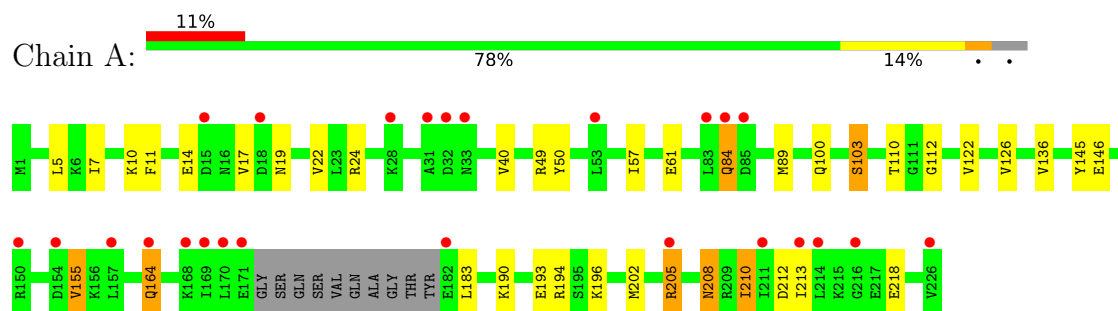
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	70	Total 70	O 70	0	0
7	B	68	Total 68	O 68	0	0
7	C	42	Total 42	O 42	0	0
7	D	40	Total 40	O 40	0	0
7	E	47	Total 47	O 47	0	0
7	F	70	Total 70	O 70	0	0

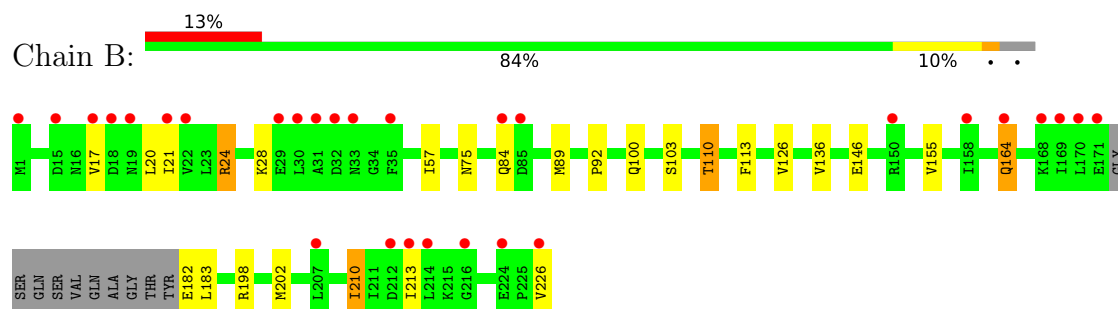
3 Residue-property plots [i](#)

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.

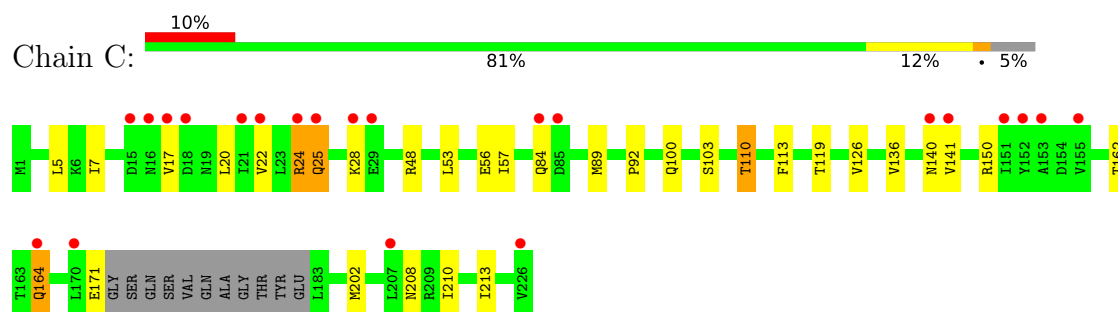
• Molecule 1: URIDYLATE KINASE



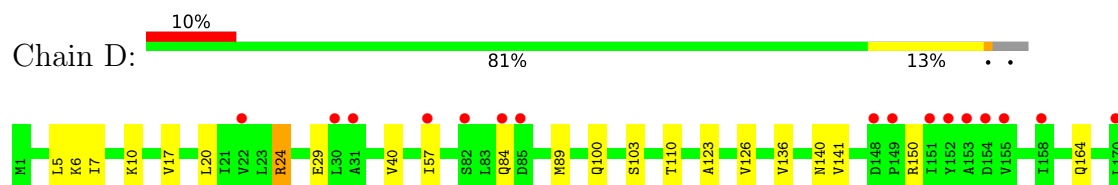
• Molecule 1: URIDYLATE KINASE



• Molecule 1: URIDYLATE KINASE

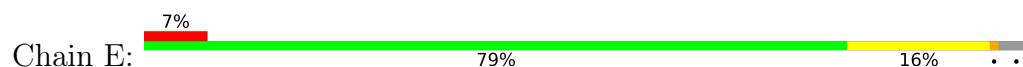


• Molecule 1: URIDYLATE KINASE

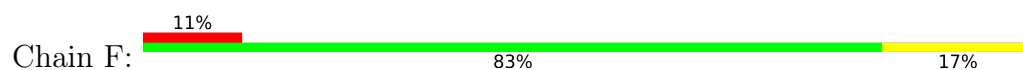




● Molecule 1: URIDYLATE KINASE



● Molecule 1: URIDYLATE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.17Å 126.44Å 134.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.10) 99.9 (25.00-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.242 0.222 , 0.228	Depositor DCC
R_{free} test set	4338 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10868	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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: MG, U5P, 4TC, CO, ACP

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	0.84	0/1716	0.92	3/2319 (0.1%)
1	B	0.83	0/1716	0.90	3/2319 (0.1%)
1	C	0.79	0/1707	0.90	2/2307 (0.1%)
1	D	0.77	0/1716	0.87	2/2319 (0.1%)
1	E	0.80	0/1716	0.90	2/2319 (0.1%)
1	F	0.85	1/1787 (0.1%)	0.94	4/2417 (0.2%)
All	All	0.82	1/10358 (0.0%)	0.91	16/14000 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	182	GLU	CA-C	8.40	1.64	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	182	GLU	N-CA-C	9.83	127.14	114.75
1	A	164	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	B	164	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	C	164	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	E	164	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	D	164	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	F	164	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	B	210	ILE	N-CA-C	6.92	117.68	110.62
1	E	164	GLN	CG-CD-NE2	6.67	126.41	116.40
1	C	164	GLN	CG-CD-NE2	6.67	126.41	116.40
1	A	164	GLN	CG-CD-NE2	6.66	126.39	116.40
1	B	164	GLN	CG-CD-NE2	6.66	126.39	116.40
1	D	164	GLN	CG-CD-NE2	6.66	126.39	116.40
1	F	164	GLN	CG-CD-NE2	6.65	126.37	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	151	ILE	CB-CA-C	-5.36	106.16	111.30
1	A	210	ILE	N-CA-C	5.09	115.81	110.62

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	1692	0	1759	34	0
1	B	1692	0	1759	25	0
1	C	1683	0	1753	23	0
1	D	1692	0	1759	29	0
1	E	1692	0	1759	24	0
1	F	1761	0	1822	28	0
2	A	21	0	11	1	0
2	B	21	0	11	1	0
2	C	21	0	11	1	0
2	D	21	0	11	1	0
2	E	21	0	11	0	0
3	A	31	0	14	4	0
3	B	31	0	14	3	0
3	C	31	0	14	4	0
3	D	31	0	14	6	0
3	E	31	0	14	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	F	51	0	25	4	0
7	A	70	0	0	2	0
7	B	68	0	0	0	0
7	C	42	0	0	0	0
7	D	40	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	47	0	0	2	0
7	F	70	0	0	3	0
All	All	10868	0	10761	153	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 7.

All (153) 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:E:202:MET:HE2	1:E:213:ILE:HG21	1.40	1.02
1:C:202:MET:HE2	1:C:213:ILE:HG21	1.41	1.02
1:D:202:MET:HE2	1:D:213:ILE:HG21	1.42	1.00
1:A:202:MET:HE2	1:A:213:ILE:HG21	1.44	0.98
1:F:202:MET:HE2	1:F:213:ILE:HG21	1.42	0.96
1:B:202:MET:HE2	1:B:213:ILE:HG21	1.44	0.96
1:F:162:THR:OG1	1:F:164:GLN:HG2	1.66	0.95
1:E:190:LYS:HE3	7:E:2040:HOH:O	1.77	0.85
1:C:48:ARG:NH2	3:C:228:ACP:O1G	2.10	0.83
6:F:227:4TC:O1B	7:F:2068:HOH:O	1.98	0.81
1:A:205:ARG:NE	7:A:2061:HOH:O	2.21	0.73
1:F:10:LYS:NZ	6:F:227:4TC:O1A	2.22	0.73
1:F:202:MET:CE	1:F:213:ILE:HG21	2.18	0.73
1:A:202:MET:CE	1:A:213:ILE:HG21	2.19	0.72
1:C:202:MET:CE	1:C:213:ILE:HG21	2.19	0.72
1:D:202:MET:CE	1:D:213:ILE:HG21	2.20	0.72
1:E:202:MET:CE	1:E:213:ILE:HG21	2.19	0.72
1:B:202:MET:CE	1:B:213:ILE:HG21	2.20	0.68
1:A:212:ASP:OD2	7:A:2062:HOH:O	2.12	0.67
1:A:194:ARG:HB3	1:F:176:VAL:HG11	1.75	0.66
2:B:227:U5P:O3P	3:B:228:ACP:O3G	2.16	0.64
1:A:5:LEU:HG	1:A:7:ILE:HD11	1.82	0.62
1:C:56:GLU:HB2	1:D:17:VAL:HG11	1.83	0.60
2:A:227:U5P:O3P	3:A:228:ACP:O3G	2.20	0.60
1:E:84:GLN:O	1:E:89:MET:HE3	2.02	0.60
1:E:170:LEU:O	1:E:171:GLU:HB2	2.01	0.59
1:B:164:GLN:HG3	1:B:226:VAL:HG23	1.85	0.58
1:D:84:GLN:O	1:D:89:MET:HE3	2.03	0.58
1:E:24:ARG:HD3	7:E:2016:HOH:O	2.03	0.58
6:F:227:4TC:O1A	6:F:227:4TC:H3B2	2.03	0.58
1:C:92:PRO:HG2	1:C:110:THR:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PHE:CE1	1:A:19:ASN:HB3	2.38	0.57
1:C:84:GLN:O	1:C:89:MET:HE3	2.05	0.57
1:F:100:GLN:O	1:F:103:SER:HB2	2.04	0.57
3:B:228:ACP:H3B2	3:B:228:ACP:O2A	2.05	0.57
1:C:57:ILE:CG2	1:D:17:VAL:HB	2.35	0.57
1:B:100:GLN:O	1:B:103:SER:HB2	2.05	0.56
1:B:92:PRO:HG2	1:B:110:THR:HG23	1.88	0.56
1:E:49:ARG:NH2	1:F:15:ASP:HB2	2.20	0.56
1:E:213:ILE:HG13	1:E:218:GLU:HB3	1.88	0.56
1:A:194:ARG:HB3	1:F:176:VAL:CG1	2.35	0.56
3:A:228:ACP:O2A	3:A:228:ACP:H3B2	2.06	0.56
1:E:20:LEU:HD13	1:F:57:ILE:HD13	1.87	0.55
1:A:17:VAL:HG23	1:B:57:ILE:CG2	2.37	0.55
1:A:84:GLN:O	1:A:89:MET:HE3	2.06	0.55
1:B:84:GLN:O	1:B:89:MET:HE3	2.07	0.54
1:A:208:ASN:HD22	1:A:208:ASN:H	1.56	0.54
1:C:53:LEU:HD12	1:D:17:VAL:HG13	1.90	0.54
1:F:5:LEU:HG	1:F:7:ILE:HD11	1.90	0.54
1:E:40:VAL:HG22	1:E:110:THR:CG2	2.38	0.54
1:B:110:THR:HG21	1:B:113:PHE:CE1	2.44	0.53
3:A:228:ACP:O2A	3:A:228:ACP:C3B	2.56	0.53
1:B:17:VAL:HG22	1:B:21:ILE:HD12	1.90	0.53
1:D:100:GLN:O	1:D:103:SER:HB2	2.09	0.53
6:F:227:4TC:H3B2	7:F:2069:HOH:O	2.09	0.53
1:C:5:LEU:HG	1:C:7:ILE:HD11	1.89	0.53
1:C:17:VAL:HG23	1:D:57:ILE:CG2	2.39	0.53
1:F:202:MET:HE1	1:F:210:ILE:HD12	1.91	0.52
3:D:228:ACP:H3B2	3:D:228:ACP:O2A	2.09	0.52
1:E:202:MET:HE1	1:E:210:ILE:HD12	1.92	0.52
1:B:202:MET:HE1	1:B:210:ILE:HD12	1.91	0.52
1:E:146:GLU:OE2	1:E:156:LYS:HB2	2.10	0.51
1:E:5:LEU:HG	1:E:7:ILE:HD11	1.92	0.51
1:E:167:ARG:O	1:E:171:GLU:N	2.44	0.51
1:D:205:ARG:HH11	1:D:205:ARG:HG2	1.76	0.51
1:A:193:GLU:O	1:A:196:LYS:HE2	2.11	0.51
1:D:202:MET:HE1	1:D:210:ILE:HD12	1.93	0.50
1:E:100:GLN:O	1:E:103:SER:HB2	2.10	0.50
1:A:17:VAL:CG2	1:B:57:ILE:HG22	2.42	0.50
1:B:136:VAL:HG13	1:B:202:MET:HE3	1.94	0.50
1:A:100:GLN:O	1:A:103:SER:HB2	2.12	0.50
1:C:119:THR:OG1	2:C:227:U5P:O2P	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:MET:HE1	1:A:210:ILE:HD12	1.94	0.49
1:C:20:LEU:HD23	1:D:57:ILE:HD13	1.93	0.49
1:F:5:LEU:HG	1:F:7:ILE:CD1	2.43	0.49
1:C:100:GLN:O	1:C:103:SER:HB2	2.13	0.49
1:D:5:LEU:HG	1:D:7:ILE:HD11	1.96	0.48
1:C:17:VAL:CG2	1:D:57:ILE:HG22	2.43	0.48
1:A:145:TYR:HB3	1:A:155:VAL:HG13	1.94	0.48
1:D:205:ARG:HD2	7:D:2004:HOH:O	2.13	0.48
3:E:228:ACP:O2A	3:E:228:ACP:H3B2	2.14	0.48
1:D:40:VAL:HG22	1:D:110:THR:CG2	2.44	0.47
1:B:24:ARG:HD3	1:B:28:LYS:NZ	2.29	0.47
1:F:160:HIS:NE2	1:F:224:GLU:OE2	2.47	0.47
1:A:136:VAL:HG13	1:A:202:MET:HE3	1.96	0.47
1:A:202:MET:HE1	1:A:210:ILE:CD1	2.44	0.47
1:A:190:LYS:CG	1:F:176:VAL:HG13	2.44	0.47
1:A:14:GLU:OE1	1:A:205:ARG:NH2	2.48	0.47
1:F:5:LEU:CD2	1:F:7:ILE:HD11	2.45	0.47
1:F:167:ARG:O	1:F:171:GLU:HB3	2.15	0.47
1:C:17:VAL:HG23	1:D:57:ILE:HG22	1.97	0.47
1:C:136:VAL:HG13	1:C:202:MET:HE3	1.95	0.47
1:E:142:ASP:OD2	1:E:206:LYS:NZ	2.48	0.47
1:F:10:LYS:NZ	1:F:181:TYR:CD1	2.82	0.47
1:A:11:PHE:CZ	1:A:19:ASN:HB3	2.50	0.47
1:C:162:THR:OG1	1:C:164:GLN:HG2	2.16	0.46
1:D:213:ILE:HG13	1:D:218:GLU:HB3	1.96	0.46
1:A:50:TYR:OH	1:B:75:ASN:ND2	2.49	0.46
1:D:136:VAL:HG13	1:D:202:MET:HE3	1.98	0.46
1:E:57:ILE:HD13	1:F:20:LEU:HD13	1.97	0.46
1:F:84:GLN:O	1:F:89:MET:HE3	2.15	0.46
1:B:136:VAL:CG1	1:B:202:MET:HE3	2.45	0.46
1:E:57:ILE:CG2	1:F:17:VAL:HG23	2.46	0.46
1:E:136:VAL:HG13	1:E:202:MET:HE3	1.97	0.45
1:B:17:VAL:HG22	1:B:21:ILE:CD1	2.45	0.45
1:C:22:VAL:HA	1:C:25:GLN:CG	2.45	0.45
1:A:17:VAL:HG23	1:B:57:ILE:HG23	1.98	0.45
1:B:164:GLN:HG3	1:B:226:VAL:CG2	2.46	0.45
1:F:160:HIS:HE2	1:F:224:GLU:CG	2.29	0.45
1:E:50:TYR:OH	1:F:75:ASN:ND2	2.49	0.45
1:F:136:VAL:HG13	1:F:202:MET:HE3	1.99	0.45
1:B:202:MET:HE1	1:B:210:ILE:CD1	2.47	0.44
1:A:57:ILE:CG2	1:B:17:VAL:HG23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:MET:HE1	1:D:210:ILE:CD1	2.47	0.44
1:C:140:ASN:OD1	3:C:228:ACP:O3'	2.28	0.44
1:F:209:ARG:HD3	1:F:218:GLU:OE2	2.17	0.44
1:E:209:ARG:HB3	1:E:212:ASP:HB2	1.99	0.44
1:A:40:VAL:HG22	1:A:110:THR:CG2	2.48	0.44
1:C:110:THR:HG21	1:C:113:PHE:CE1	2.53	0.44
3:B:228:ACP:O2A	3:B:228:ACP:C3B	2.67	0.43
1:D:10:LYS:HD3	1:D:140:ASN:ND2	2.33	0.43
2:D:227:U5P:O3P	3:D:228:ACP:O3G	2.36	0.43
1:D:182:GLU:HA	1:D:182:GLU:OE1	2.18	0.43
1:A:10:LYS:NZ	3:A:228:ACP:H3B1	2.34	0.43
1:B:146:GLU:HG3	1:B:155:VAL:HG22	2.00	0.43
1:C:5:LEU:HG	1:C:7:ILE:CD1	2.49	0.42
1:D:20:LEU:O	1:D:24:ARG:HB2	2.19	0.42
1:A:136:VAL:CG1	1:A:202:MET:HE3	2.49	0.42
1:C:24:ARG:O	1:C:28:LYS:HG3	2.18	0.42
1:D:10:LYS:NZ	3:D:228:ACP:H3B1	2.35	0.42
1:F:5:LEU:CG	1:F:7:ILE:HD11	2.49	0.42
1:B:110:THR:HG21	1:B:113:PHE:HE1	1.83	0.42
3:C:228:ACP:H3B2	3:C:228:ACP:O2A	2.20	0.42
1:A:57:ILE:HD13	1:B:20:LEU:HD13	2.02	0.42
1:A:146:GLU:HB2	1:A:155:VAL:HG22	2.01	0.42
3:D:228:ACP:O2A	3:D:228:ACP:C3B	2.67	0.42
1:A:17:VAL:CG2	1:B:57:ILE:CG2	2.96	0.42
1:D:40:VAL:HG21	1:D:123:ALA:HA	2.02	0.41
1:A:61:GLU:HG2	1:F:194:ARG:HD2	2.02	0.41
1:A:112:GLY:HA2	1:A:122:VAL:HG21	2.02	0.41
1:D:203:ASN:OD1	1:D:205:ARG:HG2	2.20	0.41
1:F:198:ARG:HD2	7:F:2064:HOH:O	2.21	0.41
1:A:57:ILE:HG22	1:B:17:VAL:CG2	2.50	0.41
1:E:147:LYS:HG3	1:E:152:TYR:CD2	2.56	0.41
1:C:150:ARG:HG2	3:C:228:ACP:O2'	2.21	0.41
1:D:150:ARG:HG2	3:D:228:ACP:O2'	2.21	0.41
1:F:40:VAL:HG21	1:F:123:ALA:HA	2.03	0.41
1:D:182:GLU:O	1:D:184:LEU:N	2.54	0.40
1:A:213:ILE:HG13	1:A:218:GLU:HB3	2.03	0.40
1:D:6:LYS:NZ	7:D:2002:HOH:O	2.54	0.40
1:E:40:VAL:HG22	1:E:110:THR:HG22	2.01	0.40
1:E:136:VAL:CG1	1:E:202:MET:HE3	2.50	0.40
1:D:10:LYS:NZ	3:D:228:ACP:C3B	2.84	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	212/226 (94%)	209 (99%)	1 (0%)	2 (1%)	14	10
1	B	212/226 (94%)	209 (99%)	2 (1%)	1 (0%)	24	22
1	C	211/226 (93%)	205 (97%)	6 (3%)	0	100	100
1	D	212/226 (94%)	208 (98%)	3 (1%)	1 (0%)	24	22
1	E	212/226 (94%)	208 (98%)	3 (1%)	1 (0%)	24	22
1	F	224/226 (99%)	220 (98%)	3 (1%)	1 (0%)	30	28
All	All	1283/1356 (95%)	1259 (98%)	18 (1%)	6 (0%)	24	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	D	183	LEU
1	E	183	LEU
1	F	183	LEU
1	A	183	LEU
1	B	183	LEU

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	185/192 (96%)	176 (95%)	9 (5%)	22	22
1	B	185/192 (96%)	180 (97%)	5 (3%)	39	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	184/192 (96%)	176 (96%)	8 (4%)	26	27
1	D	185/192 (96%)	179 (97%)	6 (3%)	34	38
1	E	185/192 (96%)	177 (96%)	8 (4%)	26	27
1	F	192/192 (100%)	186 (97%)	6 (3%)	35	39
All	All	1116/1152 (97%)	1074 (96%)	42 (4%)	29	32

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	24	ARG
1	A	49	ARG
1	A	103	SER
1	A	126	VAL
1	A	155	VAL
1	A	164	GLN
1	A	205	ARG
1	A	208	ASN
1	B	24	ARG
1	B	110	THR
1	B	126	VAL
1	B	182	GLU
1	B	198	ARG
1	C	24	ARG
1	C	25	GLN
1	C	110	THR
1	C	126	VAL
1	C	141	VAL
1	C	171	GLU
1	C	208	ASN
1	C	210	ILE
1	D	24	ARG
1	D	29	GLU
1	D	126	VAL
1	D	141	VAL
1	D	182	GLU
1	D	208	ASN
1	E	17	VAL
1	E	24	ARG
1	E	28	LYS
1	E	103	SER

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Mol	Chain	Res	Type
1	E	126	VAL
1	E	141	VAL
1	E	182	GLU
1	E	215	LYS
1	F	1	MET
1	F	24	ARG
1	F	26	SER
1	F	48	ARG
1	F	126	VAL
1	F	155	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	208	ASN
1	B	16	ASN
1	B	75	ASN
1	B	84	GLN
1	C	33	ASN
1	C	75	ASN
1	C	100	GLN
1	D	33	ASN
1	D	75	ASN
1	D	100	GLN
1	E	75	ASN
1	F	16	ASN
1	F	25	GLN
1	F	33	ASN
1	F	75	ASN
1	F	208	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 ⓘ

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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
3	ACP	B	228	4	31,33,33	1.89	6 (19%)	47,52,52	2.11	15 (31%)
6	4TC	F	227	5	53,55,55	1.95	11 (20%)	77,86,86	1.89	17 (22%)
2	U5P	E	227	4	22,22,22	1.33	3 (13%)	32,33,33	1.54	4 (12%)
2	U5P	C	227	4	22,22,22	1.29	2 (9%)	32,33,33	1.45	5 (15%)
2	U5P	B	227	4	22,22,22	1.30	2 (9%)	32,33,33	1.51	4 (12%)
3	ACP	A	228	4	31,33,33	1.70	6 (19%)	47,52,52	2.31	14 (29%)
3	ACP	E	228	4	31,33,33	1.74	6 (19%)	47,52,52	2.15	14 (29%)
2	U5P	D	227	5	22,22,22	1.15	3 (13%)	32,33,33	1.48	4 (12%)
3	ACP	C	228	4	31,33,33	2.02	8 (25%)	47,52,52	2.06	12 (25%)
3	ACP	D	228	5	31,33,33	1.64	6 (19%)	47,52,52	2.18	13 (27%)
2	U5P	A	227	4	22,22,22	1.16	2 (9%)	32,33,33	1.55	7 (21%)

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
3	ACP	B	228	4	-	4/19/38/38	0/3/3/3
6	4TC	F	227	5	-	12/32/70/70	0/5/5/5
2	U5P	E	227	4	-	3/10/26/26	0/2/2/2
2	U5P	C	227	4	-	1/10/26/26	0/2/2/2
2	U5P	B	227	4	-	2/10/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACP	A	228	4	-	2/19/38/38	0/3/3/3
3	ACP	E	228	4	-	3/19/38/38	0/3/3/3
2	U5P	D	227	5	-	1/10/26/26	0/2/2/2
3	ACP	C	228	4	-	3/19/38/38	0/3/3/3
3	ACP	D	228	5	-	4/19/38/38	0/3/3/3
2	U5P	A	227	4	-	2/10/26/26	0/2/2/2

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	228	ACP	PB-O3A	6.67	1.65	1.58
6	F	227	4TC	PB-O3A	6.33	1.65	1.58
6	F	227	4TC	O4V-C4V	6.22	1.36	1.24
3	A	228	ACP	PB-O3A	5.90	1.65	1.58
3	C	228	ACP	PB-O3A	5.82	1.64	1.58
6	F	227	4TC	PG-O3P	5.69	1.64	1.58
3	C	228	ACP	PA-O3A	5.61	1.65	1.59
3	E	228	ACP	PB-O3A	5.52	1.64	1.58
3	B	228	ACP	C5-C4	4.99	1.48	1.39
3	E	228	ACP	C5-C4	4.73	1.47	1.39
3	D	228	ACP	C5-C4	4.59	1.47	1.39
6	F	227	4TC	PA-O3A	4.45	1.64	1.59
3	C	228	ACP	C5-C4	4.34	1.46	1.39
3	D	228	ACP	PB-O3A	4.21	1.63	1.58
3	A	228	ACP	C5-C4	3.80	1.45	1.39
2	E	227	U5P	C4-N3	-3.49	1.32	1.38
2	C	227	U5P	C4-N3	-3.31	1.32	1.38
6	F	227	4TC	C2V-N1V	3.01	1.43	1.38
2	B	227	U5P	C5-C4	-2.98	1.37	1.43
3	C	228	ACP	PB-O2B	-2.93	1.49	1.56
6	F	227	4TC	C6V-C5V	2.81	1.41	1.35
2	C	227	U5P	C6-C5	2.67	1.41	1.35
6	F	227	4TC	C8-N9	-2.62	1.33	1.37
3	A	228	ACP	C5-C6	2.61	1.48	1.41
2	E	227	U5P	C2-N1	2.60	1.42	1.38
3	B	228	ACP	C5-N7	-2.59	1.34	1.39
2	D	227	U5P	C4-N3	-2.56	1.34	1.38
3	D	228	ACP	C5-N7	-2.55	1.34	1.39
2	B	227	U5P	C2-N3	-2.54	1.33	1.38
3	B	228	ACP	C5-C6	2.50	1.48	1.41
3	D	228	ACP	PA-O3A	2.49	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	228	ACP	PB-O2B	-2.49	1.50	1.56
3	E	228	ACP	PA-O3A	2.45	1.62	1.59
3	D	228	ACP	C5-C6	2.44	1.47	1.41
3	E	228	ACP	C5-C6	2.41	1.47	1.41
3	D	228	ACP	C8-N7	2.36	1.36	1.31
3	C	228	ACP	C5-N7	-2.31	1.34	1.39
2	D	227	U5P	C6-C5	2.29	1.40	1.35
3	C	228	ACP	C5-C6	2.27	1.47	1.41
2	E	227	U5P	C6-C5	2.27	1.40	1.35
3	A	228	ACP	C5-N7	-2.26	1.35	1.39
3	E	228	ACP	C8-N7	2.25	1.36	1.31
2	A	227	U5P	C2-N3	-2.23	1.34	1.38
6	F	227	4TC	O2V-C2V	2.23	1.27	1.23
2	D	227	U5P	C2-N3	-2.19	1.34	1.38
3	B	228	ACP	C4-N9	-2.15	1.33	1.37
3	A	228	ACP	C8-N7	2.12	1.35	1.31
6	F	227	4TC	C4V-N3V	-2.11	1.35	1.38
6	F	227	4TC	P-O3P	2.07	1.61	1.59
3	B	228	ACP	PB-O2B	-2.07	1.51	1.56
3	E	228	ACP	C5-N7	-2.06	1.35	1.39
3	C	228	ACP	C8-N7	2.03	1.35	1.31
6	F	227	4TC	C5-N7	-2.03	1.35	1.39
2	A	227	U5P	C4-N3	-2.02	1.35	1.38
3	C	228	ACP	C4-N9	-2.01	1.33	1.37

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	228	ACP	O1G-PG-C3B	-6.30	97.63	111.37
3	D	228	ACP	O1G-PG-C3B	-6.29	97.65	111.37
3	D	228	ACP	C5-C4-N3	-6.21	118.17	126.72
6	F	227	4TC	C5-C4-N3	-6.15	118.25	126.72
3	C	228	ACP	O1G-PG-C3B	-5.96	98.39	111.37
3	A	228	ACP	C5-C4-N3	-5.88	118.63	126.72
3	B	228	ACP	O1G-PG-C3B	-5.79	98.75	111.37
3	E	228	ACP	C5-C4-N3	-5.71	118.85	126.72
3	C	228	ACP	C5-C4-N3	-5.64	118.95	126.72
3	A	228	ACP	O1G-PG-C3B	-5.59	99.19	111.37
3	A	228	ACP	N3-C4-N9	5.51	136.54	127.17
3	D	228	ACP	N3-C4-N9	5.44	136.43	127.17
3	B	228	ACP	C5-C4-N3	-5.43	119.25	126.72
3	E	228	ACP	N3-C4-N9	5.20	136.02	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	228	ACP	N3-C4-N9	4.79	135.31	127.17
3	B	228	ACP	N3-C4-N9	4.71	135.17	127.17
6	F	227	4TC	N3-C2-N1	-4.51	121.76	128.58
6	F	227	4TC	N3-C4-N9	4.50	134.82	127.17
6	F	227	4TC	C4V-N3V-C2V	-4.45	121.08	126.61
3	A	228	ACP	C4-N9-C8	4.29	110.24	105.74
2	B	227	U5P	C4-N3-C2	-4.15	121.45	126.61
3	C	228	ACP	N3-C2-N1	-4.09	122.39	128.58
2	D	227	U5P	N3-C2-N1	4.01	120.11	114.89
3	A	228	ACP	N3-C2-N1	-3.96	122.58	128.58
2	E	227	U5P	N3-C2-N1	3.95	120.03	114.89
3	A	228	ACP	C2-N3-C4	3.89	121.33	111.83
3	D	228	ACP	C2-N3-C4	3.82	121.17	111.83
2	A	227	U5P	C5-C4-N3	3.82	120.15	114.80
3	B	228	ACP	O3G-PG-O2G	3.80	118.80	107.96
3	C	228	ACP	C2-N3-C4	3.80	121.11	111.83
3	E	228	ACP	C2-N3-C4	3.77	121.05	111.83
6	F	227	4TC	N3V-C2V-N1V	3.76	119.79	114.89
3	E	228	ACP	N3-C2-N1	-3.74	122.92	128.58
6	F	227	4TC	C5V-C4V-N3V	3.72	120.01	114.80
2	A	227	U5P	C4-N3-C2	-3.68	122.04	126.61
6	F	227	4TC	O4'-C1'-N9	3.67	115.14	108.09
3	A	228	ACP	O3G-PG-O1G	3.64	121.81	112.39
3	E	228	ACP	C4-N9-C8	3.64	109.56	105.74
6	F	227	4TC	C2-N3-C4	3.62	120.68	111.83
3	D	228	ACP	N3-C2-N1	-3.60	123.14	128.58
2	B	227	U5P	C5-C4-N3	3.60	119.84	114.80
2	B	227	U5P	N3-C2-N1	3.59	119.56	114.89
2	C	227	U5P	N3-C2-N1	3.58	119.55	114.89
2	D	227	U5P	C4-N3-C2	-3.54	122.22	126.61
2	E	227	U5P	C4-N3-C2	-3.42	122.37	126.61
3	B	228	ACP	C2-N3-C4	3.34	120.00	111.83
3	A	228	ACP	N9-C8-N7	-3.33	109.21	113.94
3	D	228	ACP	C4-N9-C8	3.27	109.17	105.74
3	A	228	ACP	C5-N7-C8	3.25	108.55	103.45
3	B	228	ACP	N3-C2-N1	-3.19	123.76	128.58
2	E	227	U5P	C5-C4-N3	3.16	119.23	114.80
6	F	227	4TC	N9-C8-N7	-3.15	109.47	113.94
2	D	227	U5P	C5-C4-N3	3.08	119.11	114.80
3	D	228	ACP	C4-C5-N7	-3.08	107.06	110.58
6	F	227	4TC	O1G-PG-O3G	3.03	119.81	109.95
3	A	228	ACP	PB-O3A-PA	-3.02	122.50	132.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	227	U5P	C5-C4-N3	3.00	119.00	114.80
2	A	227	U5P	N3-C2-N1	3.00	118.80	114.89
3	A	228	ACP	C4-C5-N7	-2.99	107.16	110.58
3	D	228	ACP	O2B-PB-O1B	2.97	119.61	109.95
3	B	228	ACP	C4-C5-N7	-2.90	107.27	110.58
2	C	227	U5P	C4-N3-C2	-2.86	123.07	126.61
6	F	227	4TC	C5-N7-C8	2.84	107.92	103.45
3	E	228	ACP	C4-C5-N7	-2.83	107.34	110.58
3	C	228	ACP	C4-N9-C8	2.80	108.68	105.74
3	D	228	ACP	C5-N7-C8	2.75	107.78	103.45
3	E	228	ACP	C5-N7-C8	2.74	107.75	103.45
6	F	227	4TC	O3G-PG-C3B	-2.73	101.87	109.05
3	E	228	ACP	O2B-PB-O1B	2.72	118.81	109.95
6	F	227	4TC	O2B-PB-O1B	2.69	118.71	109.95
2	A	227	U5P	O2-C2-N1	-2.67	119.32	122.80
2	E	227	U5P	O5'-P-O1P	-2.63	99.33	106.44
2	A	227	U5P	O3P-P-O2P	2.63	117.65	107.80
3	A	228	ACP	C4'-O4'-C1'	-2.62	103.67	109.47
3	E	228	ACP	N9-C8-N7	-2.62	110.22	113.94
3	C	228	ACP	C4-C5-N7	-2.61	107.60	110.58
6	F	227	4TC	C4-C5-N7	-2.61	107.60	110.58
3	E	228	ACP	O3G-PG-O2G	2.60	115.36	107.96
3	B	228	ACP	C4-N9-C8	2.57	108.44	105.74
2	A	227	U5P	O4-C4-C5	-2.56	120.75	125.16
3	D	228	ACP	PB-O3A-PA	-2.53	124.10	132.37
2	C	227	U5P	O2-C2-N1	-2.53	119.50	122.80
3	B	228	ACP	PB-O3A-PA	-2.45	124.38	132.37
3	C	228	ACP	C3'-C2'-C1'	2.43	106.05	101.46
6	F	227	4TC	O1G-PG-C3B	-2.41	96.74	106.73
2	B	227	U5P	O4-C4-C5	-2.40	121.03	125.16
3	D	228	ACP	N9-C8-N7	-2.37	110.58	113.94
6	F	227	4TC	PA-O3A-PB	-2.31	124.84	132.37
2	A	227	U5P	C2'-C1'-N1	2.30	119.65	113.25
3	C	228	ACP	O3G-PG-O2G	2.28	114.47	107.96
2	D	227	U5P	O5'-P-O1P	-2.28	100.28	106.44
3	E	228	ACP	PB-O3A-PA	-2.27	124.95	132.37
2	C	227	U5P	O5'-P-O1P	-2.27	100.30	106.44
3	E	228	ACP	O3G-PG-O1G	2.26	118.22	112.39
6	F	227	4TC	C4-N9-C8	2.22	108.07	105.74
3	B	228	ACP	O2B-PB-O1B	2.21	117.16	109.95
3	D	228	ACP	C1'-N9-C8	-2.18	122.25	127.09
3	C	228	ACP	C5-N7-C8	2.18	106.87	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	228	ACP	C2-N1-C6	2.17	122.30	118.73
3	C	228	ACP	O2B-PB-O1B	2.16	116.99	109.95
3	B	228	ACP	O2B-PB-C3B	2.16	115.67	106.73
3	E	228	ACP	C6-C5-N7	2.13	136.19	132.09
3	B	228	ACP	C1'-N9-C8	-2.12	122.38	127.09
3	B	228	ACP	C2-N1-C6	2.11	122.20	118.73
3	D	228	ACP	O3G-PG-O1G	2.10	117.83	112.39
3	B	228	ACP	C3'-C2'-C1'	2.10	105.44	101.46
3	B	228	ACP	C5-N7-C8	2.04	106.66	103.45
3	A	228	ACP	C6-C5-N7	2.04	136.03	132.09
3	A	228	ACP	C1'-N9-C8	-2.01	122.62	127.09

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	227	U5P	C5'-O5'-P-O2P
2	B	227	U5P	C5'-O5'-P-O2P
6	F	227	4TC	C5U-O5U-P-O3P
6	F	227	4TC	C5U-O5U-P-O2P
6	F	227	4TC	PG-C3B-PB-O1B
6	F	227	4TC	PG-C3B-PB-O2B
6	F	227	4TC	C5'-O5'-PA-O3A
6	F	227	4TC	C5'-O5'-PA-O1A
6	F	227	4TC	PB-O3A-PA-O2A
3	C	228	ACP	C2'-C1'-N9-C4
6	F	227	4TC	C4U-C5U-O5U-P
6	F	227	4TC	C3'-C4'-C5'-O5'
3	B	228	ACP	PB-C3B-PG-O2G
3	B	228	ACP	C5'-O5'-PA-O1A
6	F	227	4TC	C5U-O5U-P-O1P
2	B	227	U5P	C4'-C5'-O5'-P
2	E	227	U5P	C3'-C4'-C5'-O5'
2	C	227	U5P	C4'-C5'-O5'-P
3	D	228	ACP	C2'-C1'-N9-C4
2	E	227	U5P	C4'-C5'-O5'-P
2	A	227	U5P	C4'-C5'-O5'-P
2	D	227	U5P	C4'-C5'-O5'-P
3	E	228	ACP	C3'-C4'-C5'-O5'
3	E	228	ACP	C2'-C1'-N9-C4
6	F	227	4TC	C2'-C1'-N9-C4
3	C	228	ACP	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
3	B	228	ACP	PB-C3B-PG-O1G
3	D	228	ACP	C2'-C1'-N9-C8
3	C	228	ACP	PB-O3A-PA-O1A
3	D	228	ACP	PB-O3A-PA-O1A
3	B	228	ACP	O4'-C1'-N9-C8
3	D	228	ACP	O4'-C1'-N9-C8
6	F	227	4TC	O4'-C1'-N9-C8
3	A	228	ACP	C2'-C1'-N9-C4
2	E	227	U5P	O4'-C4'-C5'-O5'
3	A	228	ACP	O4'-C1'-N9-C8
3	E	228	ACP	O4'-C1'-N9-C8

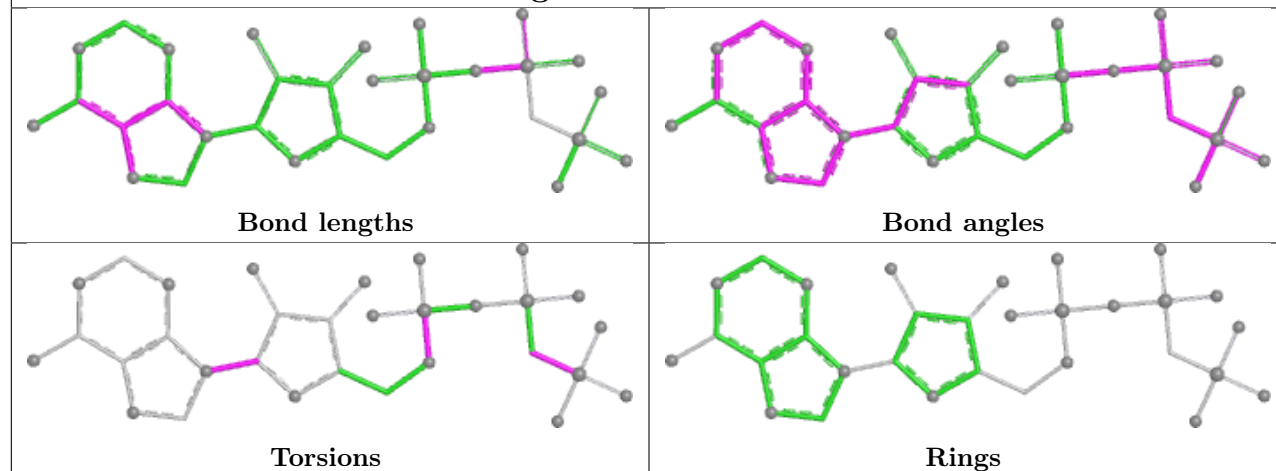
There are no ring outliers.

10 monomers are involved in 23 short contacts:

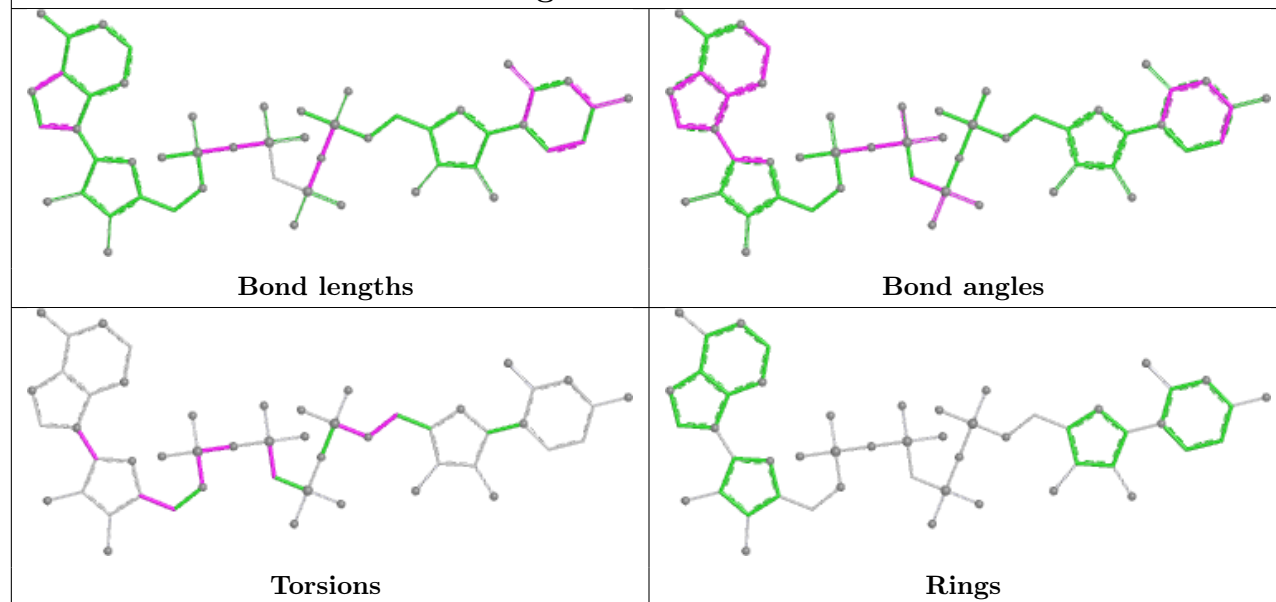
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	228	ACP	3	0
6	F	227	4TC	4	0
2	C	227	U5P	1	0
2	B	227	U5P	1	0
3	A	228	ACP	4	0
3	E	228	ACP	1	0
2	D	227	U5P	1	0
3	C	228	ACP	4	0
3	D	228	ACP	6	0
2	A	227	U5P	1	0

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.

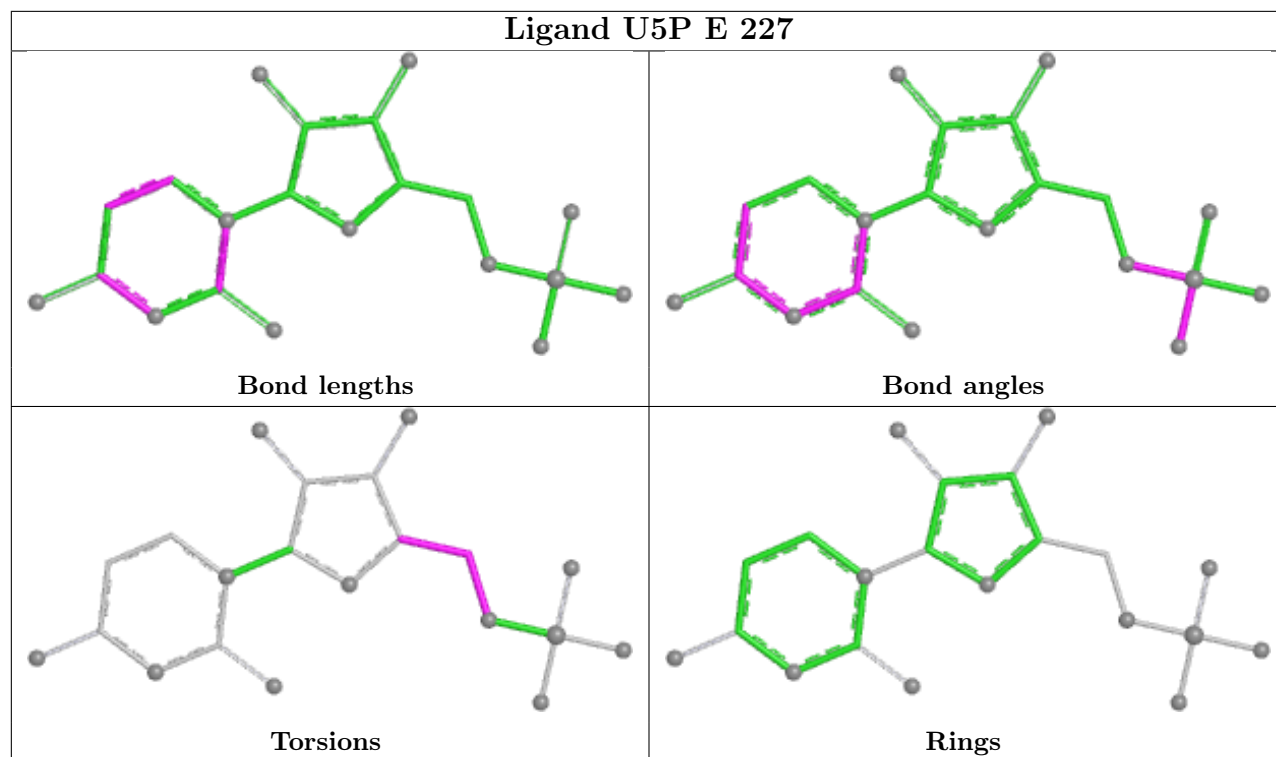
Ligand ACP B 228



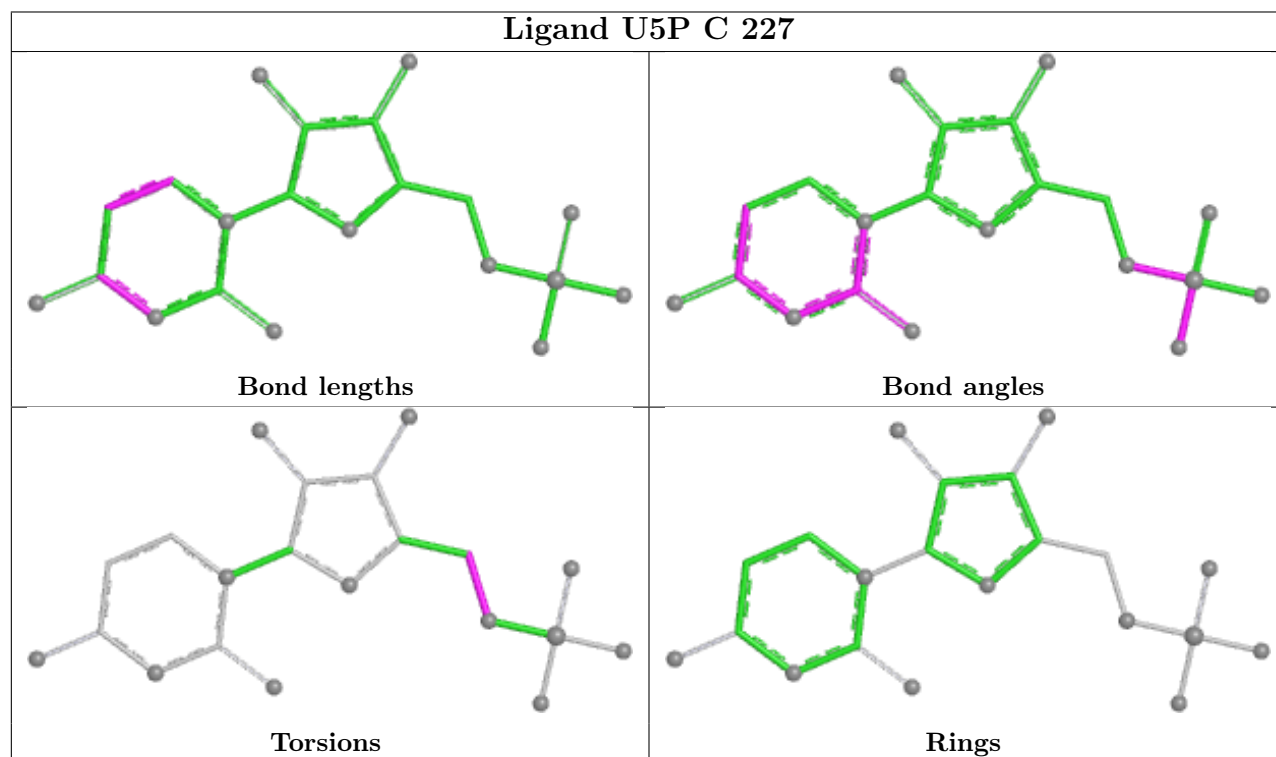
Ligand 4TC F 227



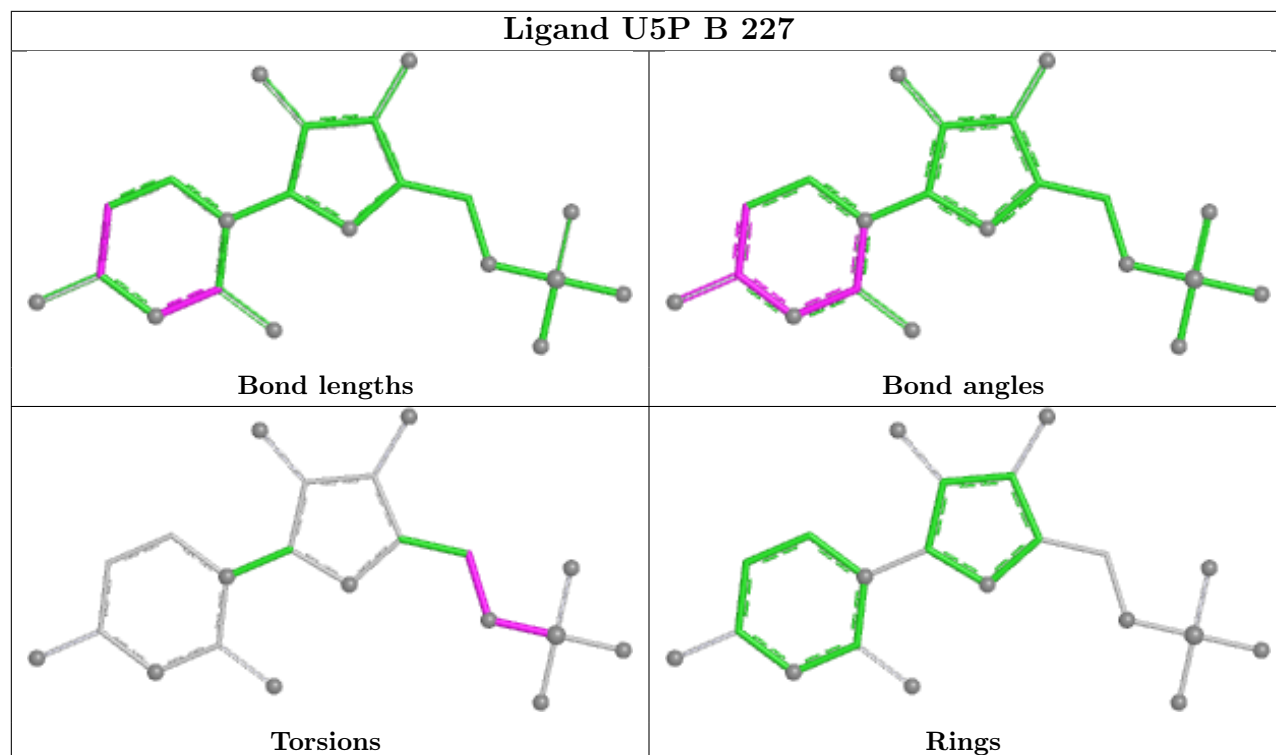
Ligand U5P E 227



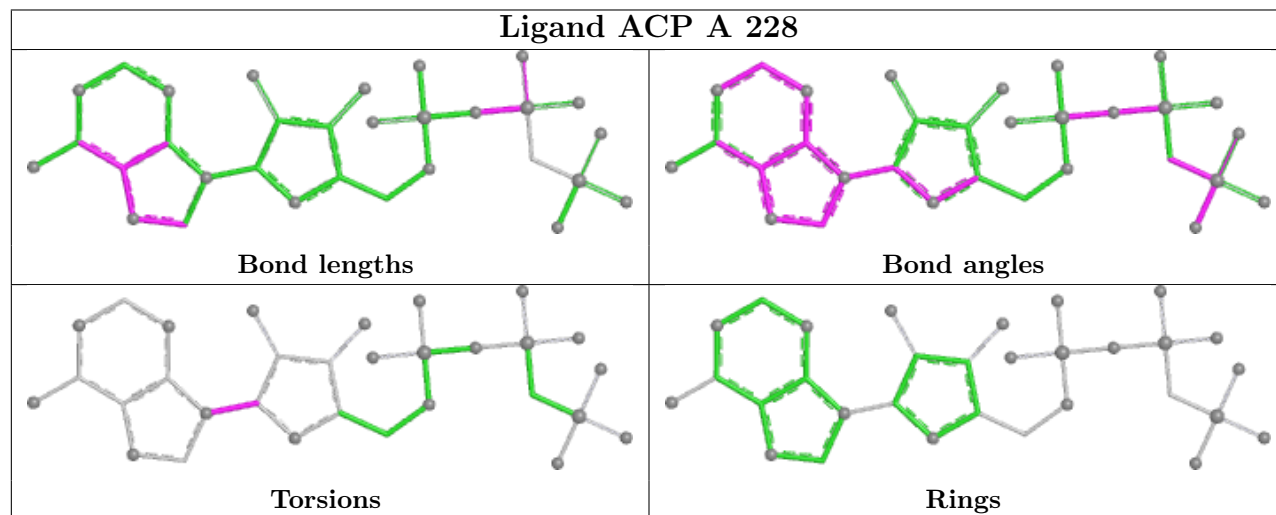
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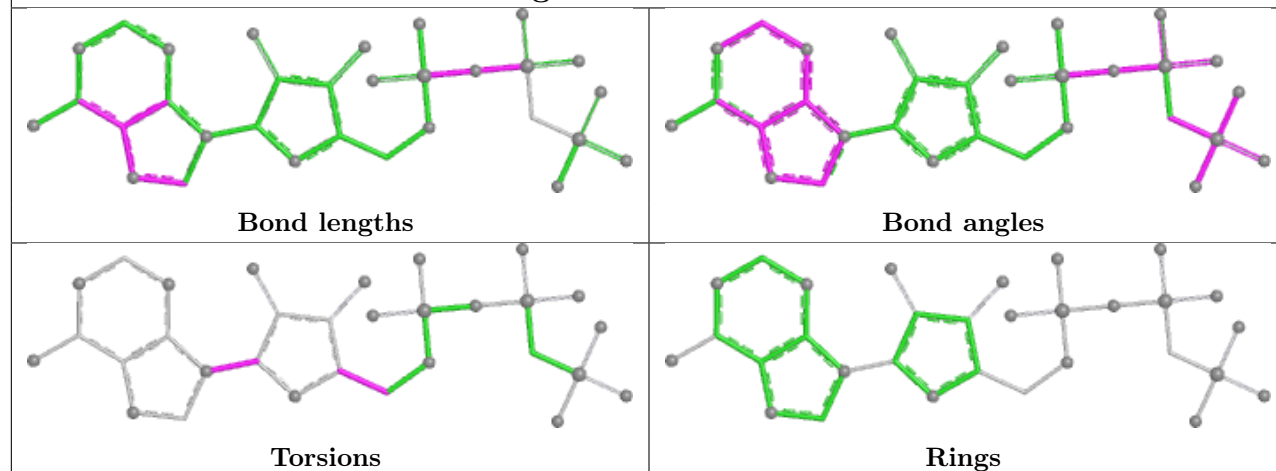
Ligand U5P B 227



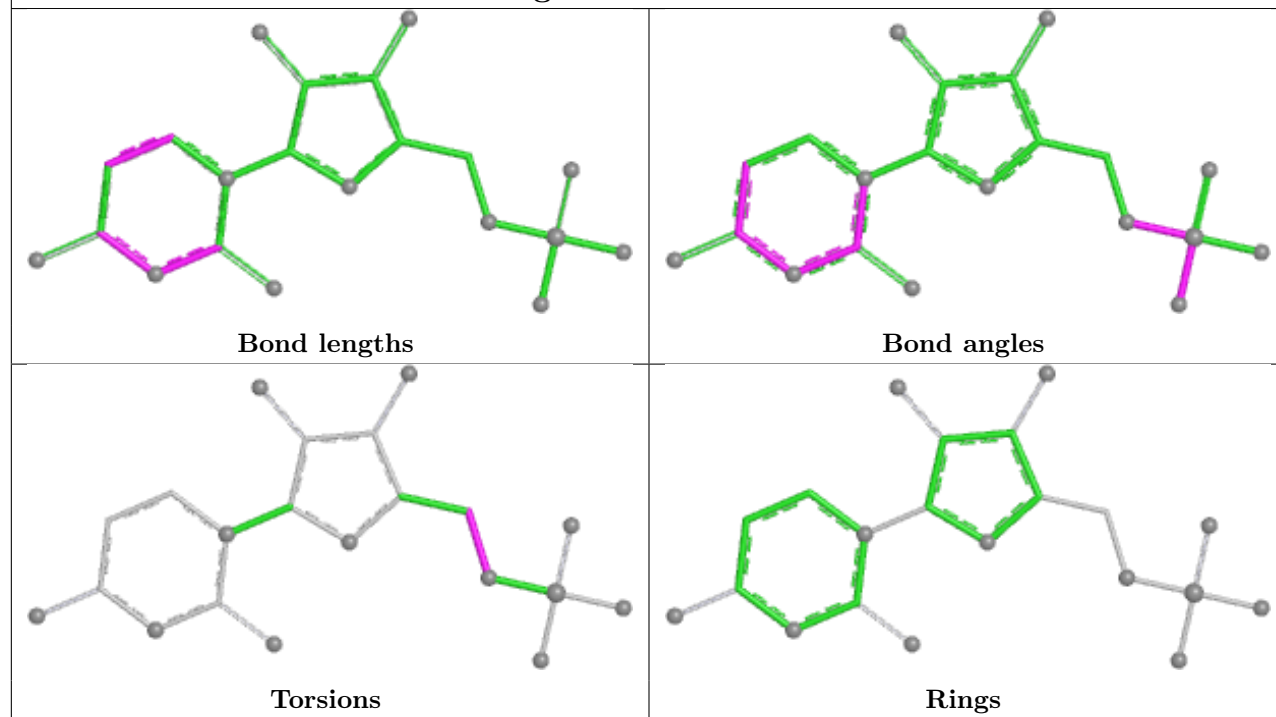
Ligand ACP A 228



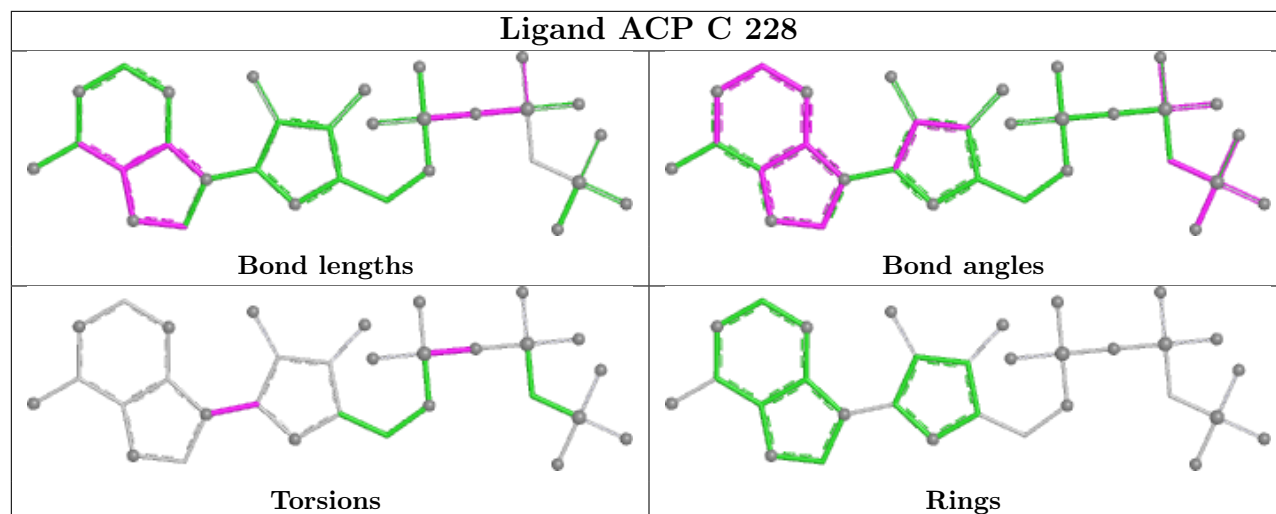
Ligand ACP E 228



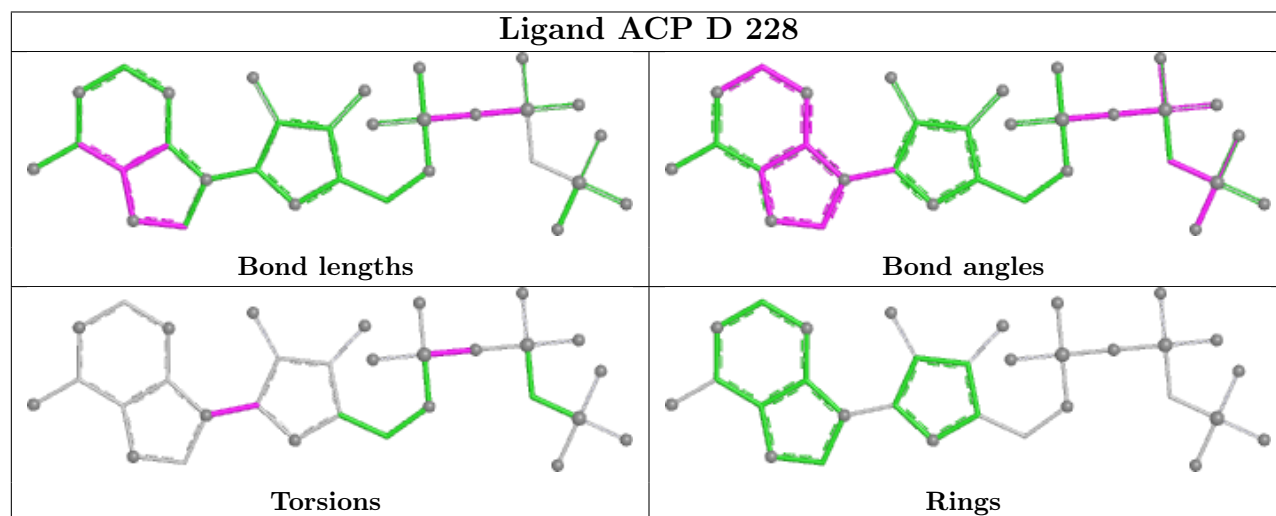
Ligand U5P D 227

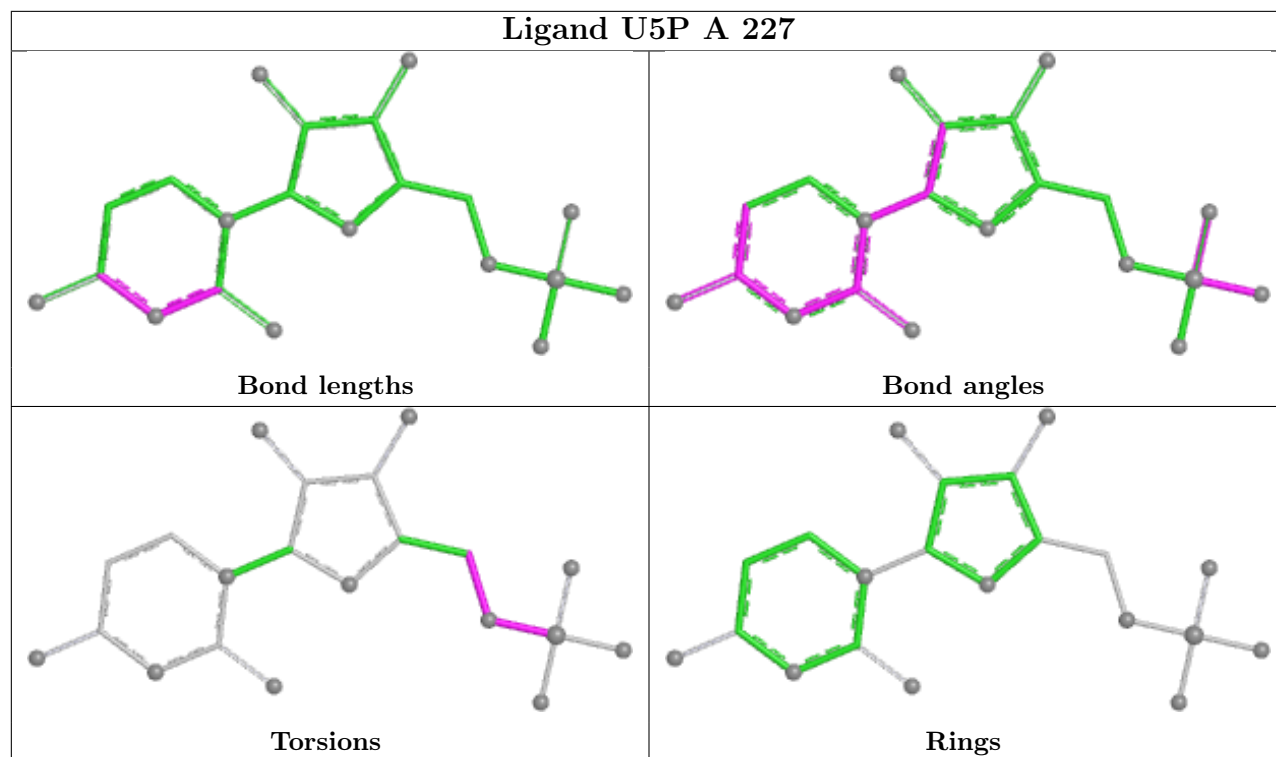


Ligand ACP C 228



Ligand ACP D 228





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	216/226 (95%)	0.54	25 (11%)	9 10	15, 27, 45, 56	0
1	B	216/226 (95%)	0.68	29 (13%)	7 7	15, 27, 46, 55	0
1	C	215/226 (95%)	0.60	22 (10%)	12 12	15, 27, 51, 58	0
1	D	216/226 (95%)	0.62	22 (10%)	12 12	16, 28, 51, 62	0
1	E	216/226 (95%)	0.60	15 (6%)	23 24	16, 28, 48, 57	0
1	F	226/226 (100%)	0.60	24 (10%)	11 12	15, 27, 47, 55	0
All	All	1305/1356 (96%)	0.61	137 (10%)	11 12	15, 27, 49, 62	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	GLY	4.4
1	B	226	VAL	4.2
1	D	170	LEU	4.1
1	B	164	GLN	4.0
1	F	176	VAL	3.9
1	D	153	ALA	3.7
1	B	15	ASP	3.7
1	F	154	ASP	3.7
1	D	151	ILE	3.6
1	D	152	TYR	3.5
1	C	226	VAL	3.5
1	B	33	ASN	3.5
1	C	151	ILE	3.4
1	A	226	VAL	3.4
1	A	85	ASP	3.4
1	A	84	GLN	3.4
1	F	173	SER	3.3
1	F	31	ALA	3.3
1	F	169	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	181	TYR	3.3
1	B	85	ASP	3.2
1	C	141	VAL	3.2
1	A	171	GLU	3.1
1	B	171	GLU	3.1
1	A	33	ASN	3.1
1	E	170	LEU	3.1
1	B	170	LEU	3.1
1	D	211	ILE	3.1
1	B	29	GLU	3.0
1	C	17	VAL	3.0
1	B	169	ILE	3.0
1	D	85	ASP	3.0
1	B	84	GLN	2.9
1	B	21	ILE	2.9
1	F	226	VAL	2.9
1	B	1	MET	2.9
1	A	168	LYS	2.8
1	A	214	LEU	2.8
1	E	226	VAL	2.8
1	E	169	ILE	2.8
1	B	17	VAL	2.8
1	D	84	GLN	2.7
1	A	170	LEU	2.7
1	F	164	GLN	2.7
1	A	154	ASP	2.7
1	C	153	ALA	2.7
1	D	149	PRO	2.7
1	E	216	GLY	2.7
1	E	154	ASP	2.7
1	E	212	ASP	2.7
1	E	213	ILE	2.7
1	F	15	ASP	2.7
1	B	150	ARG	2.7
1	F	26	SER	2.6
1	A	169	ILE	2.6
1	A	205	ARG	2.6
1	C	21	ILE	2.6
1	D	226	VAL	2.6
1	F	216	GLY	2.6
1	C	28	LYS	2.5
1	A	18	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	85	ASP	2.5
1	F	175	SER	2.5
1	C	170	LEU	2.5
1	B	22	VAL	2.5
1	D	155	VAL	2.5
1	D	158	ILE	2.5
1	D	205	ARG	2.5
1	F	177	GLN	2.5
1	B	30	LEU	2.5
1	F	183	LEU	2.5
1	B	212	ASP	2.5
1	C	15	ASP	2.5
1	A	31	ALA	2.5
1	E	168	LYS	2.5
1	E	211	ILE	2.5
1	C	84	GLN	2.4
1	C	155	VAL	2.4
1	D	154	ASP	2.4
1	D	214	LEU	2.4
1	B	19	ASN	2.4
1	A	32	ASP	2.4
1	A	213	ILE	2.4
1	B	158	ILE	2.4
1	D	57	ILE	2.4
1	A	182	GLU	2.4
1	B	35	PHE	2.4
1	B	31	ALA	2.3
1	F	172	GLY	2.3
1	F	1	MET	2.3
1	F	180	THR	2.3
1	A	216	GLY	2.3
1	F	18	ASP	2.3
1	C	24	ARG	2.3
1	D	213	ILE	2.3
1	D	31	ALA	2.3
1	A	15	ASP	2.3
1	A	83	LEU	2.3
1	E	84	GLN	2.3
1	E	158	ILE	2.3
1	F	17	VAL	2.3
1	C	16	ASN	2.3
1	B	18	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	164	GLN	2.2
1	B	213	ILE	2.2
1	A	53	LEU	2.2
1	A	157	LEU	2.2
1	B	224	GLU	2.2
1	F	146	GLU	2.2
1	F	84	GLN	2.2
1	B	168	LYS	2.2
1	B	32	ASP	2.2
1	C	25	GLN	2.2
1	B	214	LEU	2.2
1	A	150	ARG	2.2
1	D	82	SER	2.2
1	C	29	GLU	2.1
1	C	207	LEU	2.1
1	C	18	ASP	2.1
1	E	171	GLU	2.1
1	F	205	ARG	2.1
1	A	28	LYS	2.1
1	F	28	LYS	2.1
1	C	140	ASN	2.1
1	C	85	ASP	2.1
1	C	22	VAL	2.1
1	B	207	LEU	2.1
1	F	24	ARG	2.1
1	D	208	ASN	2.0
1	C	164	GLN	2.0
1	D	148	ASP	2.0
1	C	152	TYR	2.0
1	A	211	ILE	2.0
1	D	22	VAL	2.0
1	E	182	GLU	2.0
1	D	30	LEU	2.0
1	E	164	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

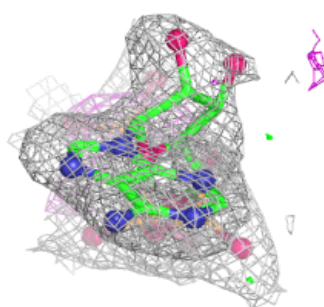
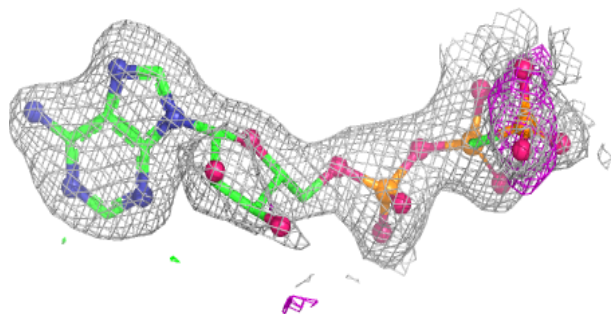
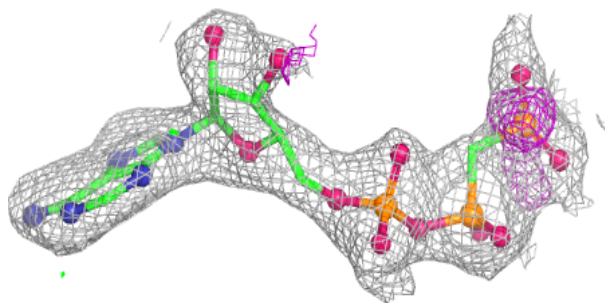
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	F	229	1/1	0.84	0.12	50,50,50,50	0
3	ACP	E	228	31/31	0.86	0.11	35,43,46,48	0
3	ACP	D	228	31/31	0.87	0.11	49,51,54,55	0
5	MG	D	229	1/1	0.89	0.17	44,44,44,44	0
3	ACP	A	228	31/31	0.89	0.09	19,24,35,37	0
6	4TC	F	227	51/51	0.89	0.10	13,25,42,45	0
3	ACP	B	228	31/31	0.90	0.10	20,25,38,38	0
4	CO	E	229	1/1	0.93	0.08	70,70,70,70	0
2	U5P	C	227	21/21	0.94	0.07	18,22,26,28	0
2	U5P	E	227	21/21	0.94	0.08	17,22,34,34	0
3	ACP	C	228	31/31	0.94	0.08	29,37,42,43	0
2	U5P	D	227	21/21	0.95	0.06	16,23,31,33	0
2	U5P	A	227	21/21	0.96	0.06	12,15,23,26	0
2	U5P	B	227	21/21	0.96	0.06	10,13,25,27	0
4	CO	B	230	1/1	0.97	0.07	26,26,26,26	0
4	CO	C	229	1/1	0.97	0.06	43,43,43,43	0
4	CO	A	229	1/1	0.98	0.13	50,50,50,50	0
4	CO	A	230	1/1	0.98	0.07	27,27,27,27	0
4	CO	B	229	1/1	0.98	0.04	53,53,53,53	0

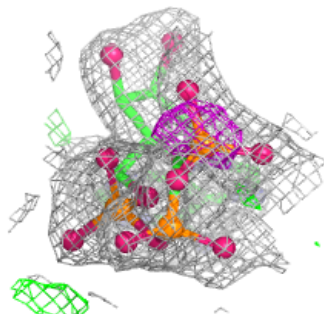
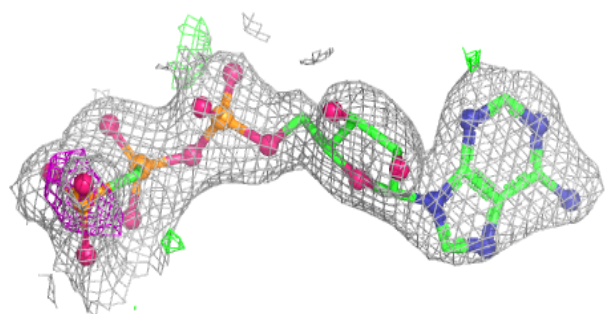
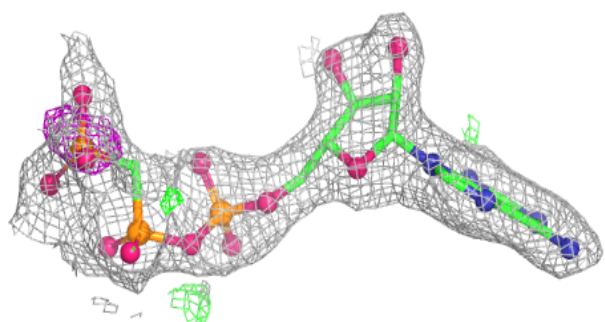
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ACP E 228:

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

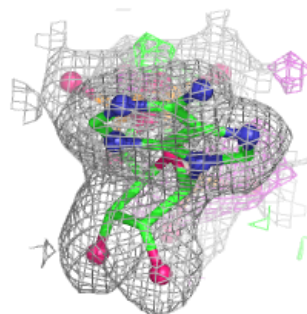
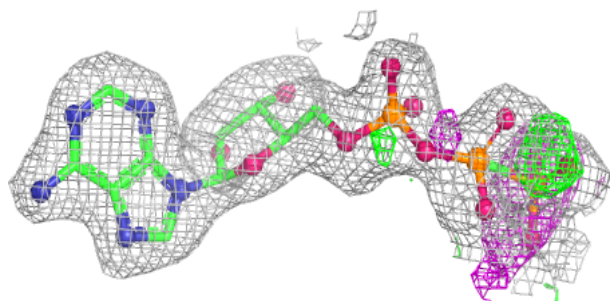
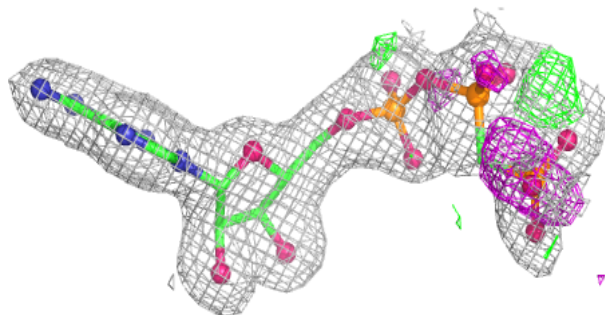
**Electron density around ACP D 228:**

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

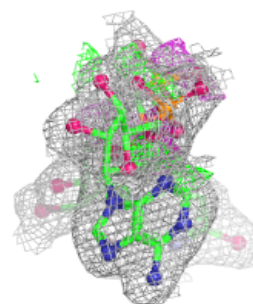
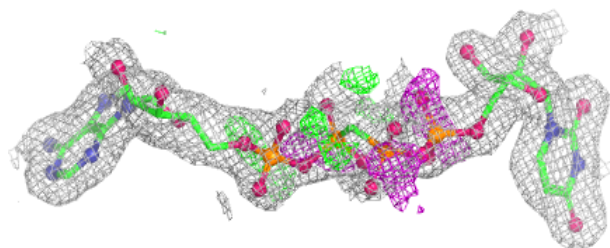
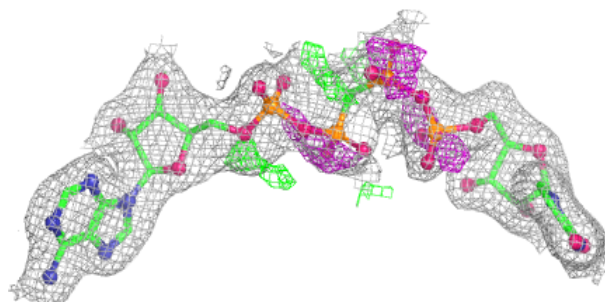


Electron density around ACP A 228:

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

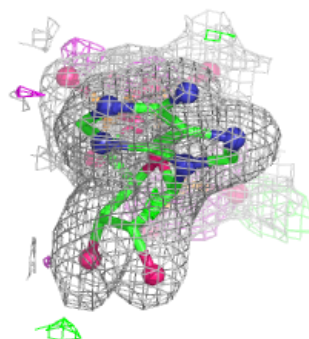
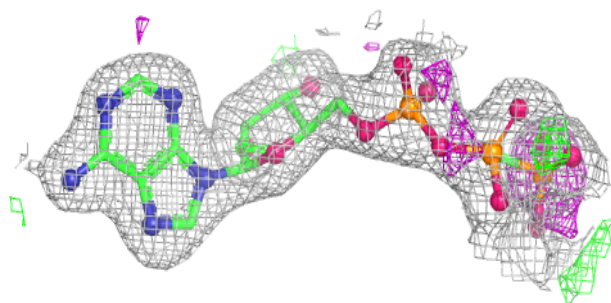
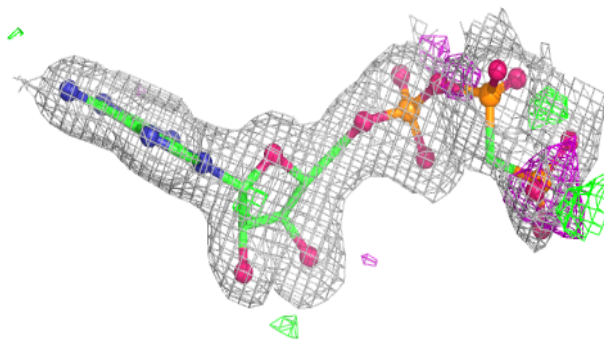
**Electron density around 4TC F 227:**

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



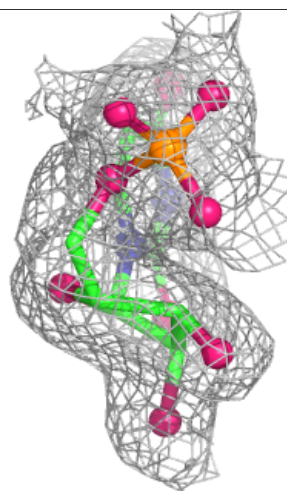
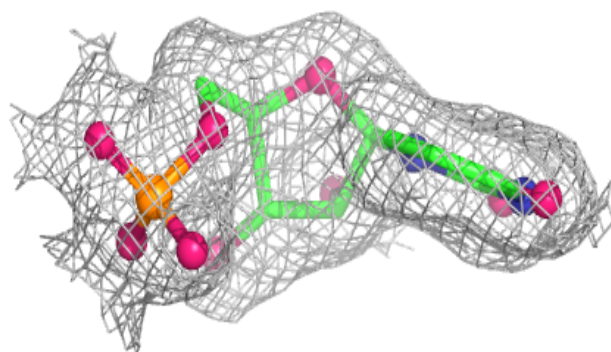
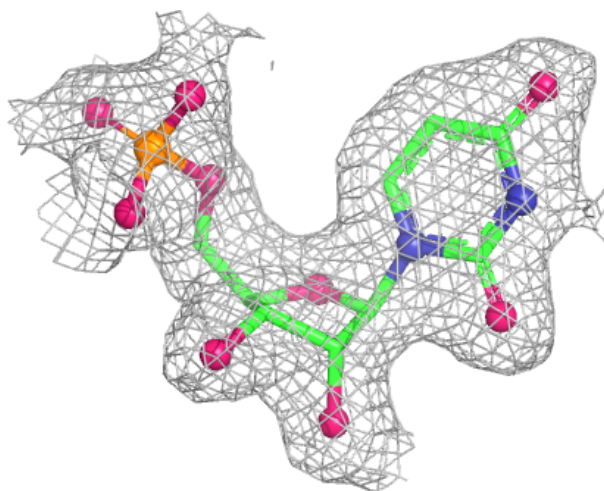
Electron density around ACP B 228:

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



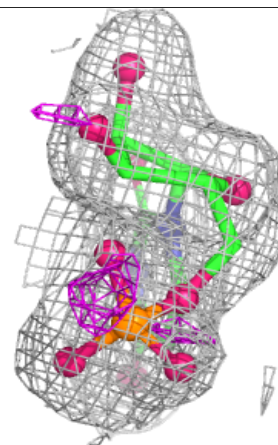
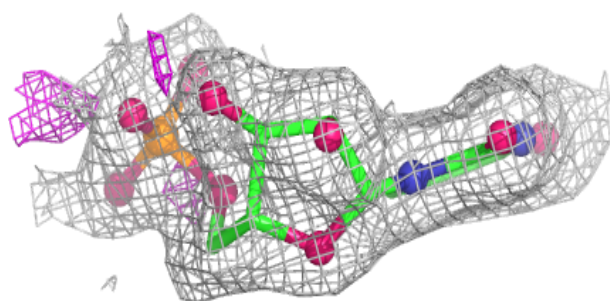
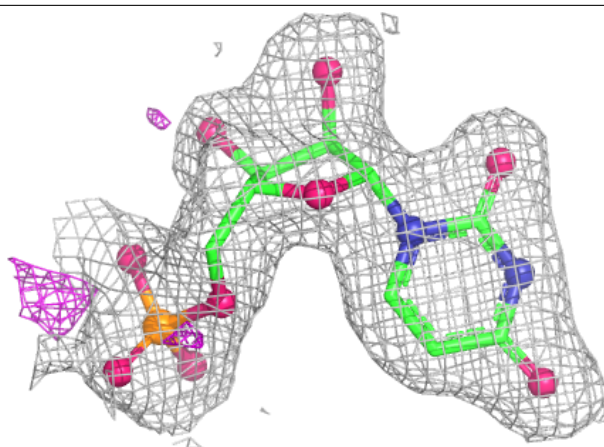
Electron density around U5P C 227:

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

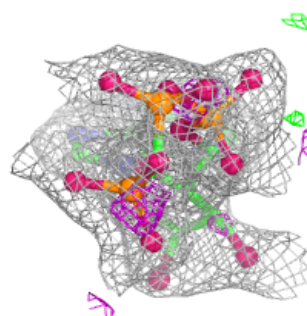
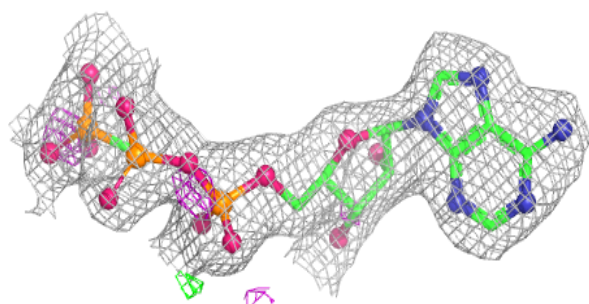
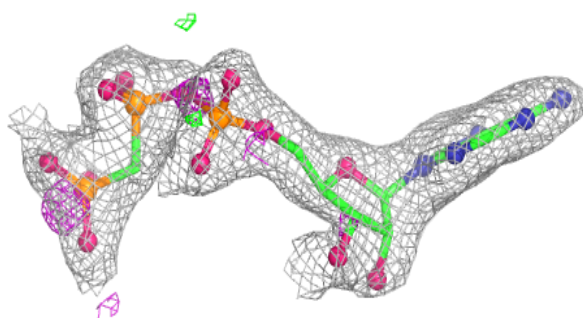


Electron density around U5P E 227:

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

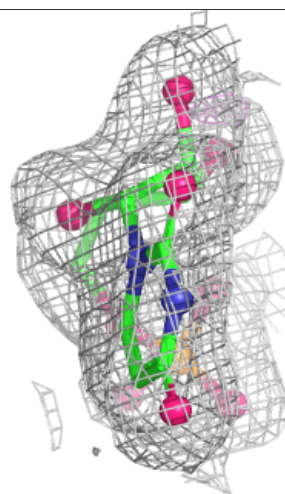
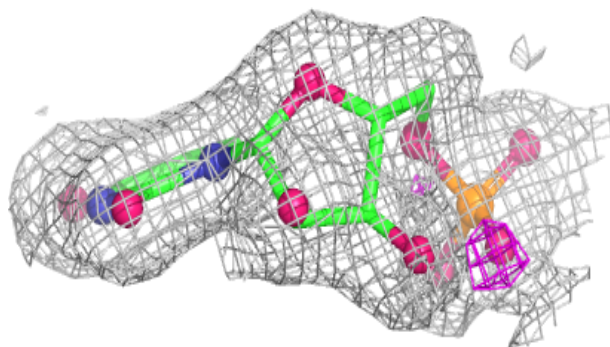
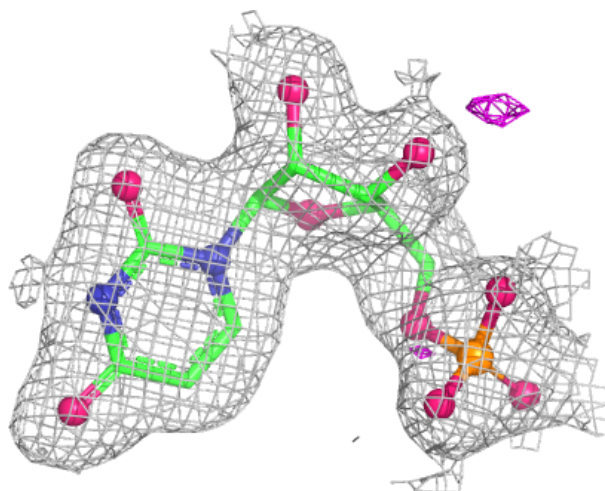
**Electron density around ACP C 228:**

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



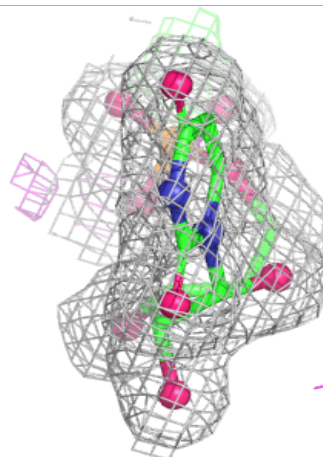
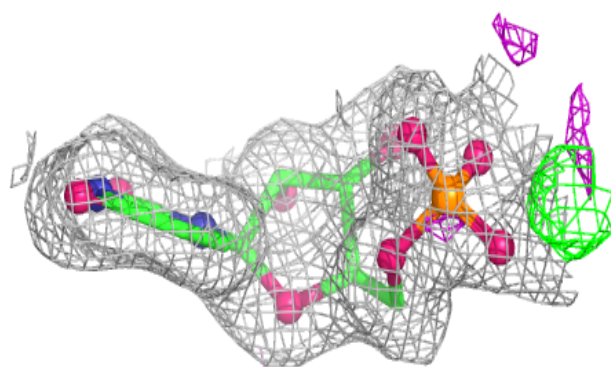
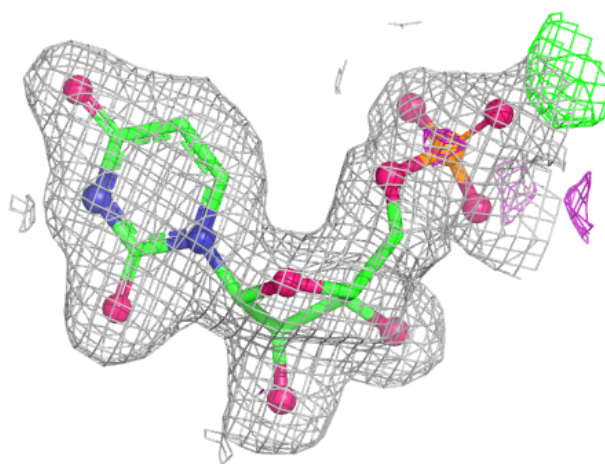
Electron density around U5P D 227:

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



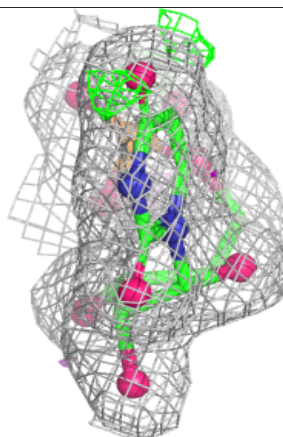
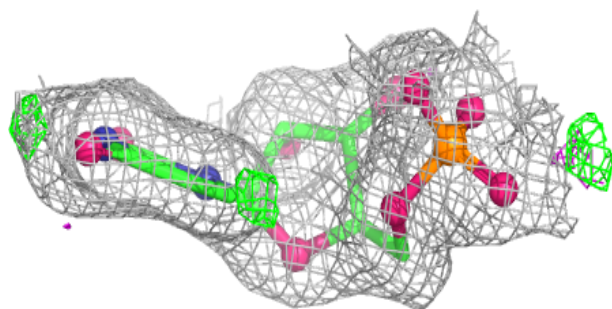
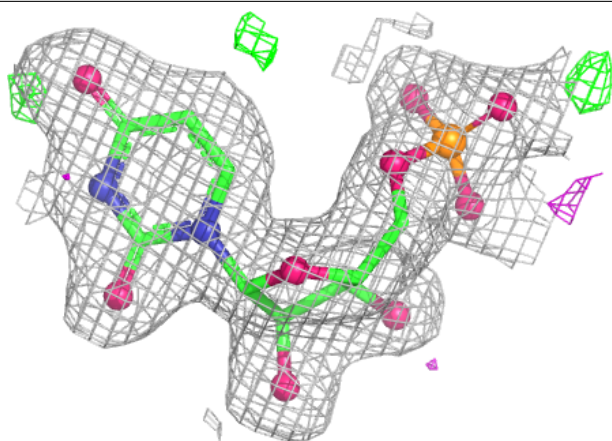
Electron density around U5P A 227:

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



Electron density around U5P B 227:

$2mF_o-DF_c$ (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.