



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:47 PM UTC

PDB ID : 1XTT / pdb_00001xtt
Title : Sulfolobus solfataricus uracil phosphoribosyltransferase in complex with
uridine 5'-monophosphate (UMP)
Authors : Arent, S.; Harris, P.; Jensen, K.F.; Larsen, S.
Deposited on : 2004-10-24
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

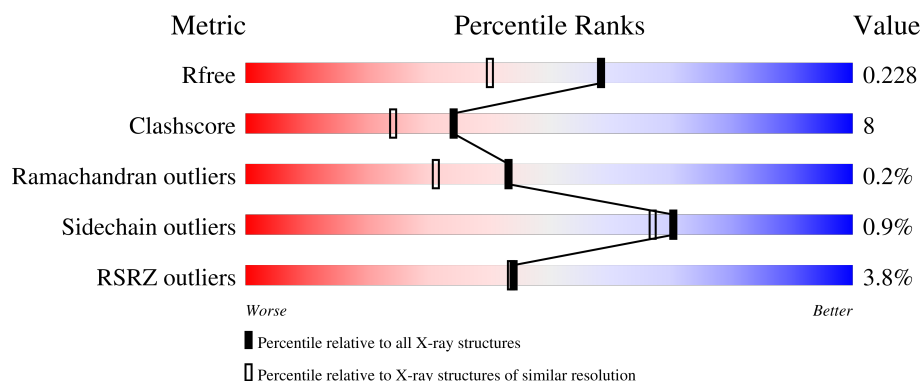
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	216	5% 76% 23%
1	B	216	4% 74% 21%
1	C	216	3% 79% 20%
1	D	216	4% 76% 19%

2 Entry composition [i](#)

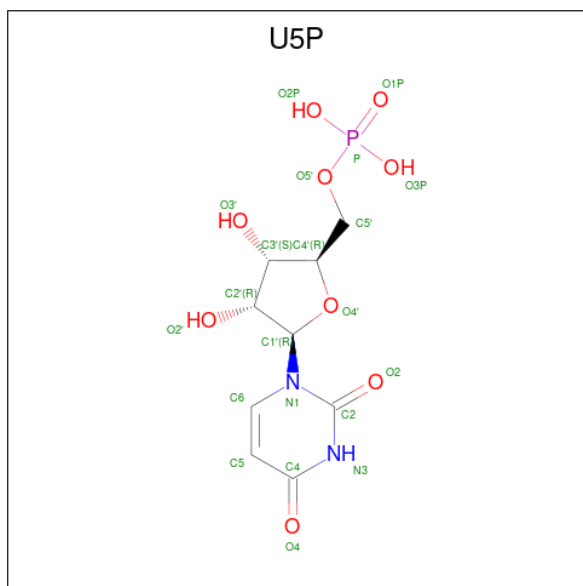
There are 4 unique types of molecules in this entry. The entry contains 7458 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable uracil phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1695	1102	279	311	3			
1	B	208	Total	C	N	O	S	0	0	0
			1642	1070	271	298	3			
1	C	215	Total	C	N	O	S	0	0	0
			1695	1102	279	311	3			
1	D	208	Total	C	N	O	S	0	0	0
			1642	1070	271	298	3			

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



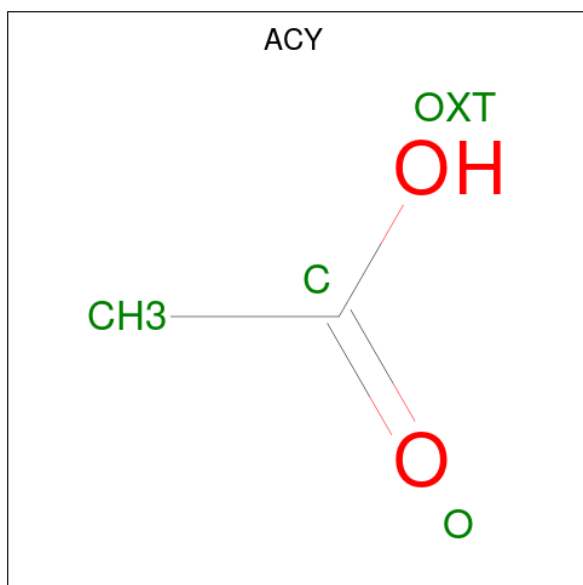
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

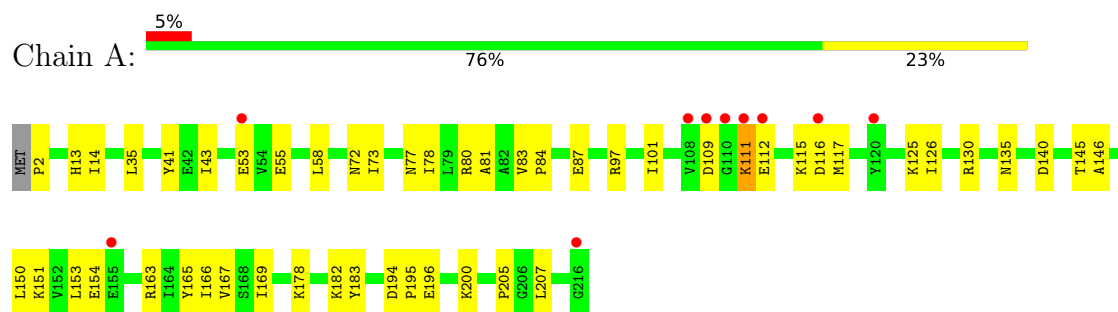
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	165	Total	O	0	0
			165	165		
4	B	180	Total	O	0	0
			180	180		
4	C	177	Total	O	0	0
			177	177		
4	D	170	Total	O	0	0
			170	170		

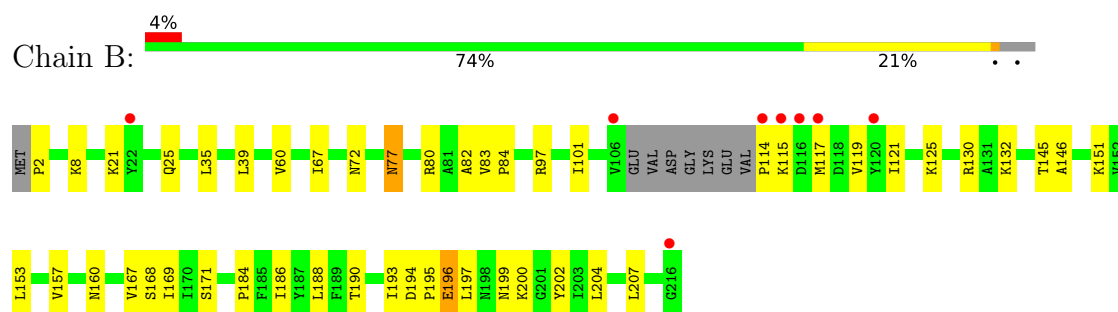
3 Residue-property plots [i](#)

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.

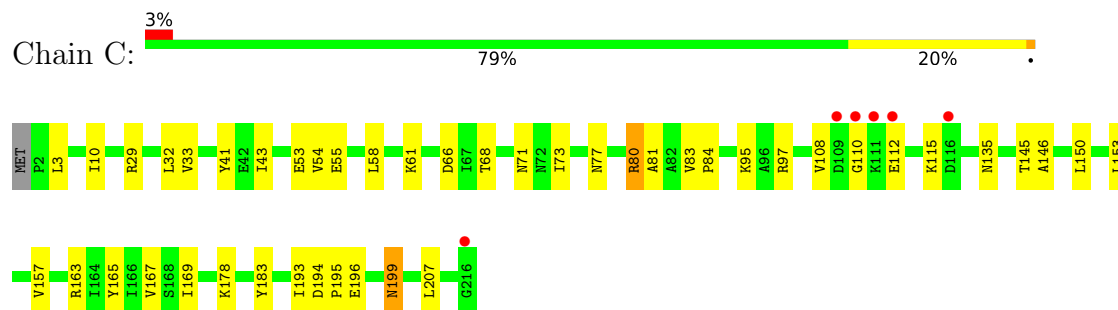
- Molecule 1: Probable uracil phosphoribosyltransferase



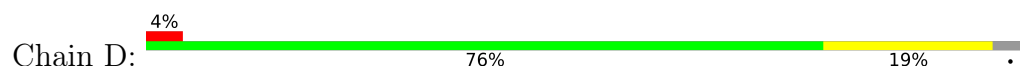
- Molecule 1: Probable uracil phosphoribosyltransferase

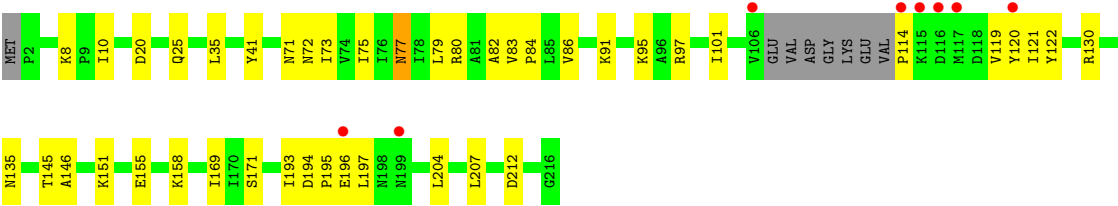


- Molecule 1: Probable uracil phosphoribosyltransferase



- Molecule 1: Probable uracil phosphoribosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.84Å 97.48Å 73.44Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	24.43 – 1.80 24.43 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.2 (24.43-1.80) 94.2 (24.43-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.60Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.228 0.193 , 0.228	Depositor DCC
R_{free} test set	3217 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7458	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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 51.59 % 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 5.4930e-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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/1724	0.92	8/2338 (0.3%)
1	B	0.36	0/1670	0.87	5/2263 (0.2%)
1	C	0.35	0/1724	0.92	10/2338 (0.4%)
1	D	0.35	0/1670	0.90	6/2263 (0.3%)
All	All	0.36	0/6788	0.90	29/9202 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	81	ALA	N-CA-C	7.35	120.23	111.33
1	D	97	ARG	N-CA-C	-7.18	99.28	110.42
1	C	196	GLU	N-CA-C	6.96	118.34	108.74
1	D	196	GLU	N-CA-C	6.93	119.46	109.14
1	A	196	GLU	N-CA-C	6.68	117.95	108.74
1	B	196	GLU	N-CA-C	6.19	118.36	109.14
1	B	97	ARG	N-CA-C	-6.07	101.01	110.42
1	B	195	PRO	N-CA-C	6.04	121.50	113.40
1	D	79	LEU	N-CA-C	5.90	118.26	109.59
1	A	169	ILE	N-CA-C	-5.86	106.77	111.81
1	C	81	ALA	N-CA-C	5.78	118.52	111.82
1	C	169	ILE	N-CA-C	-5.77	106.19	111.67
1	D	195	PRO	N-CA-C	5.73	121.49	113.53
1	A	194	ASP	CA-C-N	5.70	125.38	119.05
1	A	194	ASP	C-N-CA	5.70	125.38	119.05
1	D	194	ASP	CA-C-N	5.67	125.34	119.05
1	D	194	ASP	C-N-CA	5.67	125.34	119.05
1	A	115	LYS	N-CA-C	-5.64	106.53	113.41
1	A	97	ARG	N-CA-C	-5.61	102.22	110.52
1	C	195	PRO	N-CA-C	5.58	121.18	113.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	TYR	CA-C-N	5.56	125.23	119.56
1	C	183	TYR	C-N-CA	5.56	125.23	119.56
1	A	195	PRO	N-CA-C	5.42	121.07	113.53
1	C	194	ASP	CA-C-N	5.28	125.09	119.28
1	C	194	ASP	C-N-CA	5.28	125.09	119.28
1	C	115	LYS	N-CA-C	-5.27	107.02	113.50
1	C	97	ARG	N-CA-C	-5.20	102.05	110.32
1	B	194	ASP	CA-C-N	5.05	124.36	118.85
1	B	194	ASP	C-N-CA	5.05	124.36	118.85

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	1695	0	1789	31	0
1	B	1642	0	1739	31	0
1	C	1695	0	1789	30	0
1	D	1642	0	1739	27	0
2	A	21	0	11	0	0
2	B	21	0	11	0	0
2	C	21	0	11	0	0
2	D	21	0	11	0	0
3	B	4	0	3	0	0
3	D	4	0	3	0	0
4	A	165	0	0	2	0
4	B	180	0	0	1	0
4	C	177	0	0	1	0
4	D	170	0	0	2	0
All	All	7458	0	7106	106	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 8.

All (106) 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:58:LEU:HD13	1:B:204:LEU:HD23	1.55	0.87
1:B:114:PRO:HD2	1:B:197:LEU:HD12	1.57	0.86
1:D:35:LEU:HD13	1:D:169:ILE:HD12	1.66	0.76
1:A:83:VAL:O	1:A:87:GLU:HG3	1.89	0.73
1:D:155:GLU:HA	1:D:158:LYS:HD3	1.71	0.72
1:B:101:ILE:HD11	1:B:121:ILE:HD13	1.72	0.72
1:A:151:LYS:O	1:A:154:GLU:HG2	1.91	0.71
1:D:77:ASN:C	1:D:77:ASN:HD22	1.99	0.70
1:B:115:LYS:HD2	1:B:117:MET:HB2	1.72	0.70
1:A:13:HIS:HD2	1:B:67:ILE:H	1.43	0.67
1:B:35:LEU:HD13	1:B:169:ILE:HD12	1.74	0.67
1:D:73:ILE:HD13	1:D:135:ASN:HB2	1.74	0.67
1:A:73:ILE:HD13	1:A:135:ASN:HB2	1.78	0.65
1:D:101:ILE:HD11	1:D:121:ILE:HD13	1.78	0.64
1:C:73:ILE:HD13	1:C:135:ASN:HB2	1.81	0.62
1:A:13:HIS:CD2	1:B:67:ILE:H	2.20	0.60
1:B:132:LYS:HE2	1:B:160:ASN:OD1	2.04	0.58
1:C:108:VAL:HG11	4:C:3360:HOH:O	2.04	0.57
1:D:119:VAL:O	1:D:151:LYS:HE3	2.05	0.57
1:A:58:LEU:HD13	1:B:204:LEU:CD2	2.33	0.56
1:D:114:PRO:HD2	1:D:197:LEU:HD12	1.87	0.56
1:C:110:GLY:HA2	1:C:199:ASN:CG	2.32	0.54
1:A:78:ILE:HD12	1:A:140:ASP:HB2	1.88	0.54
1:C:112:GLU:N	1:C:199:ASN:HD21	2.06	0.54
1:A:55:GLU:HG2	1:B:21:LYS:HD2	1.90	0.54
1:C:83:VAL:HB	1:C:84:PRO:HD3	1.90	0.53
1:B:83:VAL:HB	1:B:84:PRO:HD3	1.91	0.53
1:A:2:PRO:HG3	4:A:1409:HOH:O	2.09	0.52
1:B:199:ASN:ND2	1:B:200:LYS:HE2	2.25	0.52
1:C:43:ILE:HD11	1:C:167:VAL:HG22	1.92	0.52
1:A:109:ASP:OD2	1:A:200:LYS:HD3	2.10	0.52
1:D:35:LEU:CD1	1:D:169:ILE:HD12	2.38	0.51
1:D:71:ASN:HD21	1:D:95:LYS:NZ	2.08	0.51
1:D:77:ASN:C	1:D:77:ASN:ND2	2.67	0.51
1:C:71:ASN:ND2	1:C:95:LYS:HD3	2.26	0.50
1:B:171:SER:O	1:B:193:ILE:HA	2.11	0.50
1:B:119:VAL:O	1:B:151:LYS:HE3	2.12	0.49
1:C:53:GLU:CD	1:C:61:LYS:HD3	2.37	0.49
1:A:111:LYS:NZ	1:A:111:LYS:HB2	2.27	0.49
1:C:77:ASN:C	1:C:77:ASN:HD22	2.20	0.49
1:C:150:LEU:HD11	1:C:178:LYS:HG2	1.94	0.49
1:A:83:VAL:HB	1:A:84:PRO:HD3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:O	1:B:157:VAL:HG22	2.11	0.49
1:C:43:ILE:HD11	1:C:167:VAL:CG2	2.43	0.49
1:A:101:ILE:HD11	1:A:126:ILE:HD11	1.95	0.48
1:B:196:GLU:HG3	1:B:204:LEU:HB2	1.94	0.48
1:C:112:GLU:C	1:C:199:ASN:HD21	2.21	0.48
1:A:53:GLU:HG2	4:A:1382:HOH:O	2.14	0.47
1:A:145:THR:O	1:A:146:ALA:HB3	2.14	0.47
1:A:43:ILE:HD11	1:A:167:VAL:HG22	1.95	0.47
1:A:80:ARG:HD2	4:D:4323:HOH:O	2.14	0.47
1:D:71:ASN:ND2	1:D:95:LYS:NZ	2.63	0.47
1:D:77:ASN:ND2	1:D:82:ALA:HB3	2.30	0.47
1:B:77:ASN:C	1:B:77:ASN:HD22	2.22	0.47
1:D:83:VAL:HB	1:D:84:PRO:HD3	1.96	0.46
1:A:41:TYR:OH	1:B:8:LYS:HD2	2.15	0.46
1:A:150:LEU:HD11	1:A:178:LYS:HG2	1.98	0.46
1:C:55:GLU:HG2	1:C:61:LYS:HG2	1.97	0.46
1:C:145:THR:O	1:C:146:ALA:HB3	2.16	0.46
1:A:125:LYS:HE2	1:D:212:ASP:HA	1.97	0.46
1:C:112:GLU:C	1:C:199:ASN:ND2	2.74	0.46
1:A:163:ARG:HD2	1:A:165:TYR:CE1	2.52	0.45
1:C:41:TYR:OH	1:D:8:LYS:HD2	2.16	0.45
1:A:182:LYS:HE3	1:A:183:TYR:CZ	2.52	0.45
1:B:39:LEU:HD13	1:B:167:VAL:HG13	1.97	0.45
1:B:188:LEU:C	1:B:188:LEU:HD23	2.42	0.45
1:C:71:ASN:HD21	1:C:95:LYS:NZ	2.15	0.45
1:D:91:LYS:HE3	4:D:4257:HOH:O	2.16	0.45
1:C:3:LEU:HD21	1:C:193:ILE:HD11	1.98	0.44
1:C:207:LEU:C	1:C:207:LEU:HD12	2.42	0.44
1:A:111:LYS:HG3	1:A:112:GLU:HG3	1.99	0.44
1:D:207:LEU:HD12	1:D:207:LEU:C	2.43	0.44
1:D:145:THR:O	1:D:146:ALA:HB3	2.17	0.44
1:D:171:SER:O	1:D:193:ILE:HA	2.18	0.44
1:C:53:GLU:OE1	1:C:61:LYS:HD3	2.18	0.44
1:A:77:ASN:HD22	1:A:77:ASN:C	2.27	0.43
1:C:163:ARG:HD2	1:C:165:TYR:CE1	2.54	0.43
1:C:41:TYR:CD1	1:D:10:ILE:HG21	2.54	0.43
1:B:207:LEU:C	1:B:207:LEU:HD12	2.44	0.43
1:D:71:ASN:HD21	1:D:95:LYS:HZ3	1.67	0.43
1:A:14:ILE:HG21	1:A:35:LEU:HG	2.01	0.43
1:B:72:ASN:OD1	1:B:130:ARG:NH2	2.51	0.43
1:C:58:LEU:HG	1:D:204:LEU:HD23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:C	1:A:207:LEU:HD12	2.44	0.42
1:B:125:LYS:NZ	4:B:2431:HOH:O	2.52	0.42
1:B:199:ASN:HD21	1:B:200:LYS:HE2	1.84	0.42
1:B:197:LEU:HA	1:B:202:TYR:O	2.19	0.42
1:C:10:ILE:HG21	1:D:41:TYR:CD1	2.55	0.42
1:A:153:LEU:HD11	1:A:166:ILE:HD11	2.00	0.42
1:B:168:SER:O	1:B:190:THR:HA	2.19	0.42
1:B:145:THR:O	1:B:146:ALA:HB3	2.19	0.41
1:A:116:ASP:O	1:A:117:MET:HG3	2.20	0.41
1:A:205:PRO:HA	1:B:60:VAL:HG21	2.03	0.41
1:C:32:LEU:HD23	1:C:84:PRO:HB2	2.01	0.41
1:C:29:ARG:O	1:C:33:VAL:HG23	2.21	0.41
1:B:2:PRO:HD3	1:B:184:PRO:O	2.21	0.41
1:C:80:ARG:H	1:C:80:ARG:HG3	1.60	0.41
1:C:153:LEU:O	1:C:157:VAL:HG23	2.21	0.41
1:B:77:ASN:ND2	1:B:82:ALA:HB3	2.36	0.41
1:D:72:ASN:OD1	1:D:130:ARG:NH2	2.54	0.41
1:D:120:TYR:CE1	1:D:122:TYR:HB3	2.56	0.41
1:D:75:ILE:HG21	1:D:86:VAL:HG13	2.02	0.40
1:C:66:ASP:OD2	1:C:68:THR:HG22	2.20	0.40
1:B:2:PRO:HD2	1:B:186:ILE:O	2.22	0.40
1:A:72:ASN:OD1	1:A:130:ARG:NH2	2.55	0.40
1:C:54:VAL:CG2	1:D:20:ASP:HA	2.52	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	213/216 (99%)	205 (96%)	8 (4%)	0	100	100
1	B	204/216 (94%)	194 (95%)	9 (4%)	1 (0%)	24	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	213/216 (99%)	203 (95%)	10 (5%)	0	100	100
1	D	204/216 (94%)	192 (94%)	11 (5%)	1 (0%)	24	14
All	All	834/864 (96%)	794 (95%)	38 (5%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	ARG
1	D	80	ARG

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	188/189 (100%)	187 (100%)	1 (0%)	81	80
1	B	182/189 (96%)	180 (99%)	2 (1%)	65	60
1	C	188/189 (100%)	186 (99%)	2 (1%)	65	60
1	D	182/189 (96%)	180 (99%)	2 (1%)	65	60
All	All	740/756 (98%)	733 (99%)	7 (1%)	70	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	B	25	GLN
1	B	77	ASN
1	C	80	ARG
1	C	199	ASN
1	D	25	GLN
1	D	77	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	71	ASN
1	A	77	ASN
1	A	98	GLN
1	A	160	ASN
1	B	27	ASN
1	C	71	ASN
1	C	77	ASN
1	C	98	GLN
1	C	160	ASN
1	C	199	ASN
1	D	71	ASN
1	D	77	ASN
1	D	160	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	U5P	C	3250	-	22,22,22	2.39	5 (22%)	32,33,33	1.69	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	U5P	A	1250	-	22,22,22	2.38	5 (22%)	32,33,33	1.71	8 (25%)
3	ACY	B	2252	-	3,3,3	1.26	0	3,3,3	1.60	1 (33%)
2	U5P	B	2250	-	22,22,22	1.93	5 (22%)	32,33,33	1.39	4 (12%)
2	U5P	D	4250	-	22,22,22	1.94	7 (31%)	32,33,33	1.41	4 (12%)
3	ACY	D	4252	-	3,3,3	1.21	0	3,3,3	1.64	1 (33%)

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	U5P	C	3250	-	-	2/10/26/26	0/2/2/2
2	U5P	B	2250	-	-	2/10/26/26	0/2/2/2
2	U5P	D	4250	-	-	2/10/26/26	0/2/2/2
2	U5P	A	1250	-	-	2/10/26/26	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3250	U5P	O2-C2	6.15	1.34	1.23
2	B	2250	U5P	O2-C2	6.13	1.33	1.23
2	A	1250	U5P	C6-C5	6.01	1.49	1.35
2	A	1250	U5P	O2-C2	5.99	1.33	1.23
2	D	4250	U5P	O2-C2	5.90	1.33	1.23
2	C	3250	U5P	C6-C5	5.71	1.48	1.35
2	A	1250	U5P	C2-N1	3.36	1.43	1.38
2	C	3250	U5P	C2-N3	3.18	1.43	1.38
2	C	3250	U5P	C2-N1	3.17	1.43	1.38
2	C	3250	U5P	C1'-N1	3.05	1.56	1.47
2	A	1250	U5P	C1'-N1	2.95	1.55	1.47
2	D	4250	U5P	C6-N1	-2.89	1.31	1.38
2	A	1250	U5P	C2-N3	2.75	1.42	1.38
2	B	2250	U5P	C6-N1	-2.74	1.31	1.38
2	D	4250	U5P	C2-N1	2.39	1.42	1.38
2	B	2250	U5P	C2-N1	2.34	1.42	1.38
2	B	2250	U5P	O2'-C2'	-2.26	1.37	1.43
2	D	4250	U5P	O2'-C2'	-2.20	1.37	1.43
2	B	2250	U5P	O4'-C4'	2.12	1.49	1.45
2	D	4250	U5P	O4'-C4'	2.11	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4250	U5P	C1'-N1	2.06	1.53	1.47
2	D	4250	U5P	C3'-C2'	2.01	1.58	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4250	U5P	C4-N3-C2	-4.22	121.38	126.61
2	B	2250	U5P	C4-N3-C2	-4.14	121.47	126.61
2	C	3250	U5P	C5-C4-N3	3.76	120.07	114.80
2	A	1250	U5P	C5-C4-N3	3.76	120.06	114.80
2	A	1250	U5P	O5'-C5'-C4'	3.69	121.56	108.99
2	C	3250	U5P	O5'-C5'-C4'	3.65	121.42	108.99
2	C	3250	U5P	C4-N3-C2	-3.42	122.37	126.61
2	A	1250	U5P	C4-N3-C2	-3.38	122.42	126.61
2	D	4250	U5P	C5-C4-N3	3.35	119.49	114.80
2	B	2250	U5P	C5-C4-N3	3.31	119.44	114.80
2	A	1250	U5P	C6-N1-C2	3.16	124.84	121.00
2	C	3250	U5P	C6-N1-C2	3.09	124.75	121.00
2	C	3250	U5P	O4'-C4'-C3'	2.83	110.76	105.15
2	A	1250	U5P	O4'-C4'-C3'	2.77	110.65	105.15
2	C	3250	U5P	O4-C4-C5	-2.54	120.79	125.16
2	D	4250	U5P	C6-C5-C4	-2.53	116.30	119.53
2	A	1250	U5P	O4-C4-C5	-2.46	120.92	125.16
2	A	1250	U5P	C5-C6-N1	-2.45	117.86	121.84
2	B	2250	U5P	C6-C5-C4	-2.44	116.41	119.53
2	D	4250	U5P	O4-C4-C5	-2.25	121.29	125.16
3	D	4252	ACY	O-C-CH3	-2.24	113.35	122.53
2	B	2250	U5P	O4-C4-C5	-2.21	121.36	125.16
2	C	3250	U5P	C5-C6-N1	-2.18	118.30	121.84
3	B	2252	ACY	O-C-CH3	-2.18	113.59	122.53
2	A	1250	U5P	O4'-C4'-C5'	-2.09	102.64	109.33
2	C	3250	U5P	O4'-C4'-C5'	-2.06	102.73	109.33

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1250	U5P	C3'-C4'-C5'-O5'
2	A	1250	U5P	O4'-C4'-C5'-O5'
2	C	3250	U5P	O4'-C4'-C5'-O5'
2	C	3250	U5P	C3'-C4'-C5'-O5'
2	B	2250	U5P	O4'-C4'-C5'-O5'

Continued on next page...

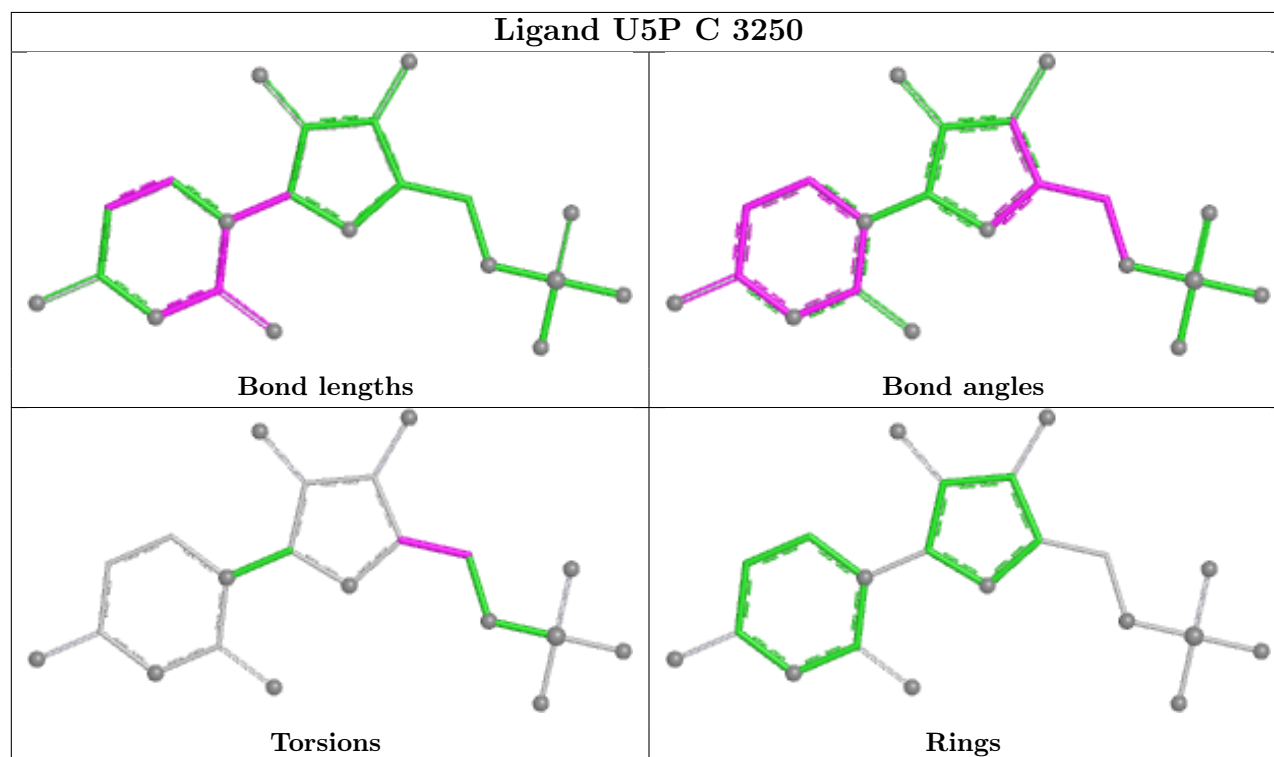
Continued from previous page...

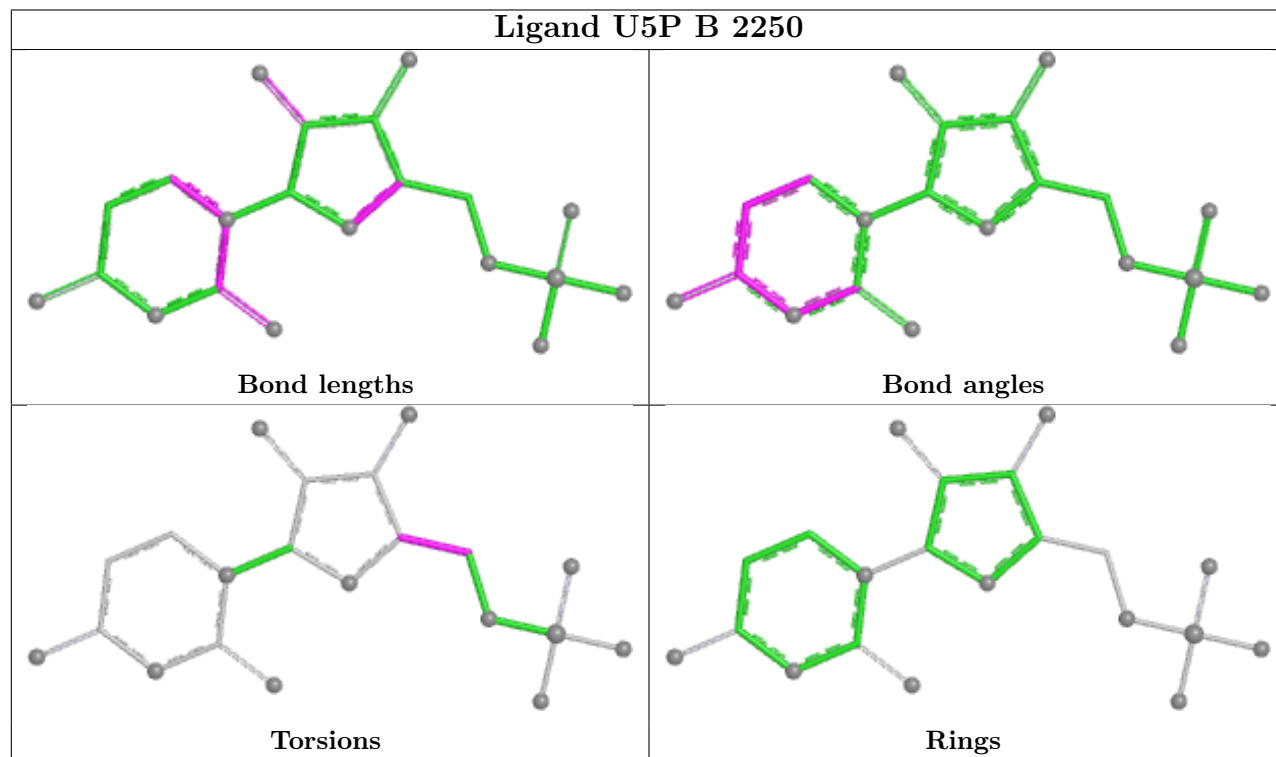
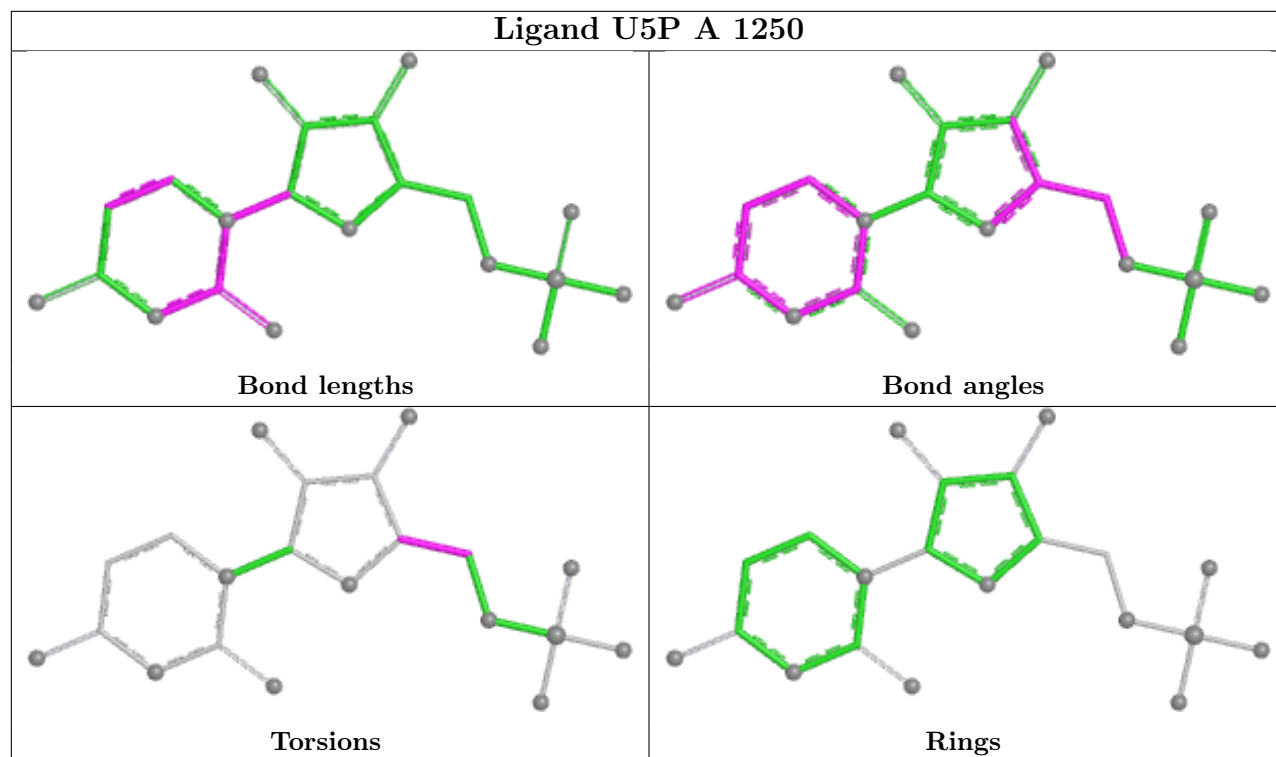
Mol	Chain	Res	Type	Atoms
2	D	4250	U5P	O4'-C4'-C5'-O5'
2	B	2250	U5P	C3'-C4'-C5'-O5'
2	D	4250	U5P	C3'-C4'-C5'-O5'

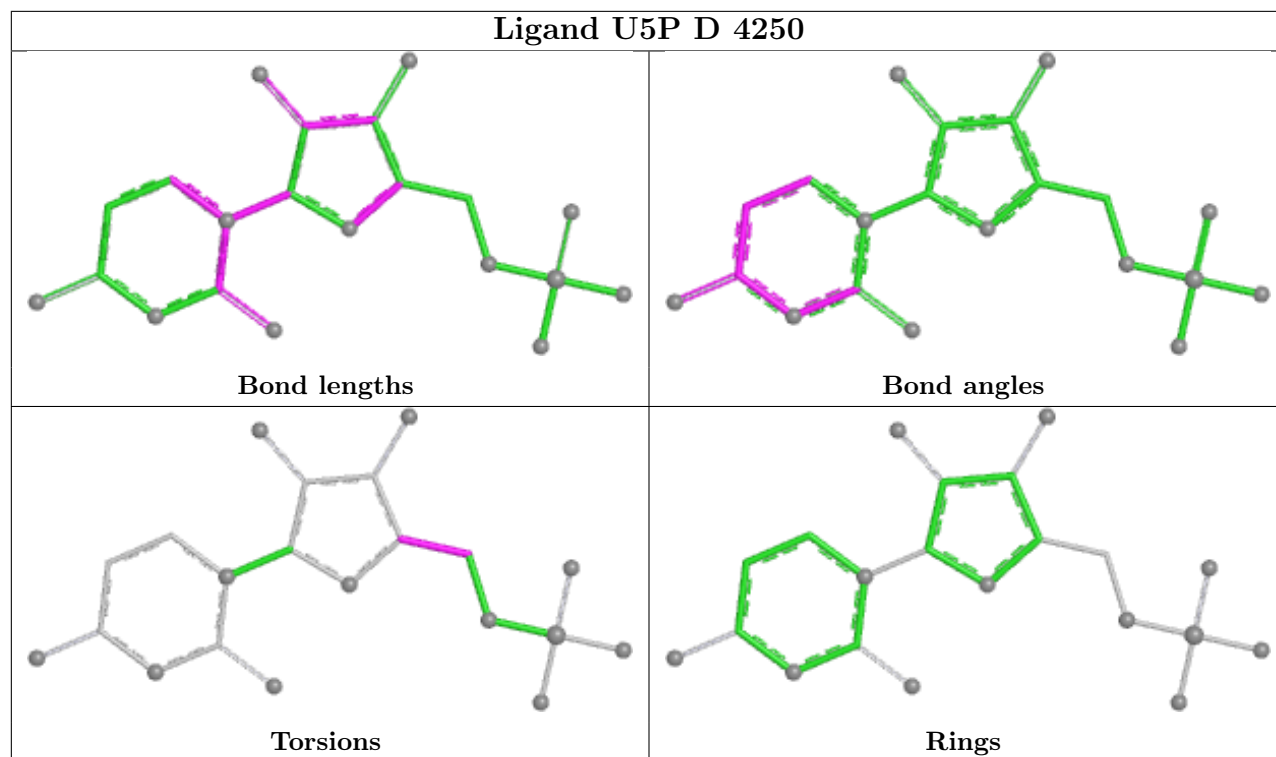
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	215/216 (99%)	0.01	10 (4%) 36 35	8, 16, 33, 55	0
1	B	208/216 (96%)	-0.01	8 (3%) 44 44	8, 16, 32, 69	0
1	C	215/216 (99%)	-0.07	6 (2%) 55 55	7, 15, 35, 62	0
1	D	208/216 (96%)	-0.03	8 (3%) 44 44	10, 16, 32, 68	0
All	All	846/864 (97%)	-0.03	32 (3%) 44 44	7, 16, 33, 69	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	GLY	5.8
1	D	106	VAL	5.5
1	D	114	PRO	5.1
1	B	114	PRO	4.9
1	C	109	ASP	4.7
1	D	115	LYS	4.0
1	A	120	TYR	3.8
1	B	120	TYR	3.7
1	B	117	MET	3.6
1	A	116	ASP	3.5
1	B	106	VAL	3.5
1	D	116	ASP	3.5
1	C	116	ASP	3.2
1	D	199	ASN	3.1
1	B	216	GLY	3.1
1	B	116	ASP	2.9
1	A	216	GLY	2.9
1	A	112	GLU	2.8
1	D	117	MET	2.8
1	C	112	GLU	2.8
1	B	115	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	108	VAL	2.7
1	A	111	LYS	2.6
1	A	109	ASP	2.6
1	B	22	TYR	2.5
1	A	110	GLY	2.3
1	A	53	GLU	2.3
1	C	216	GLY	2.2
1	D	196	GLU	2.2
1	C	111	LYS	2.2
1	D	120	TYR	2.1
1	A	155	GLU	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](#)

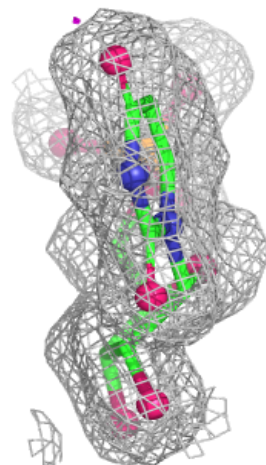
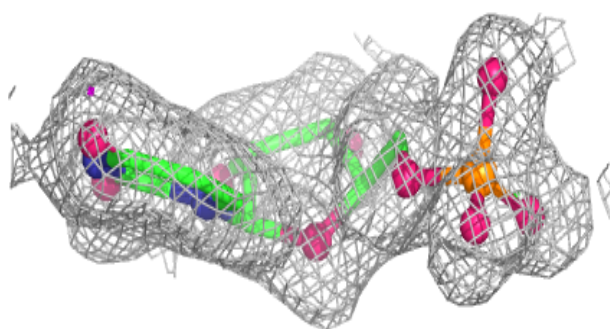
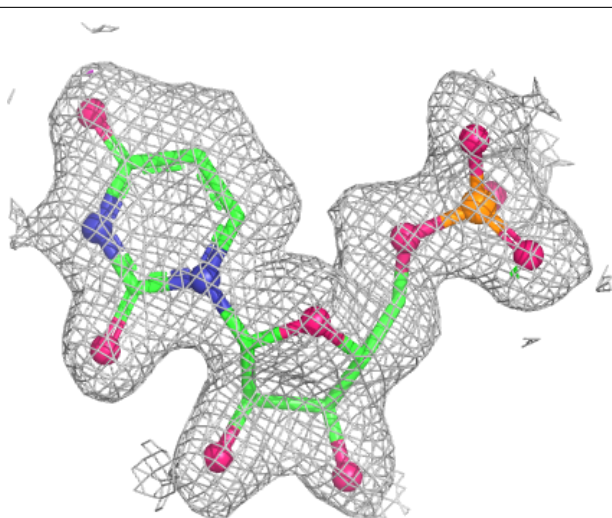
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
3	ACY	D	4252	4/4	0.93	0.10	16,17,18,18	0
3	ACY	B	2252	4/4	0.94	0.10	12,12,16,17	0
2	U5P	C	3250	21/21	0.95	0.07	8,13,16,21	0
2	U5P	D	4250	21/21	0.96	0.06	12,15,21,28	0
2	U5P	B	2250	21/21	0.96	0.06	11,14,18,24	0
2	U5P	A	1250	21/21	0.96	0.06	12,14,17,20	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.

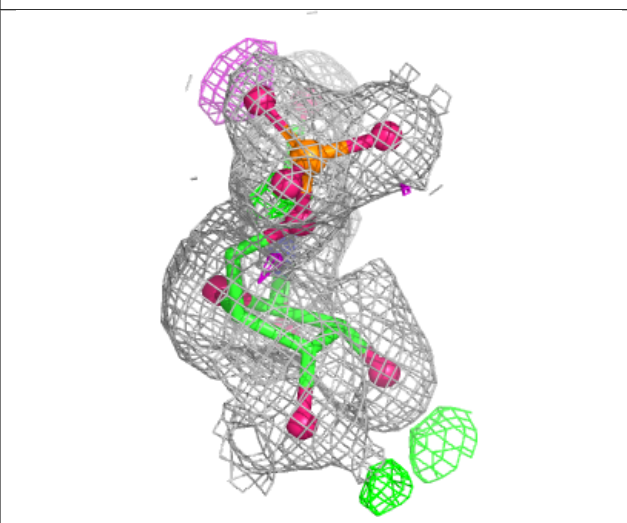
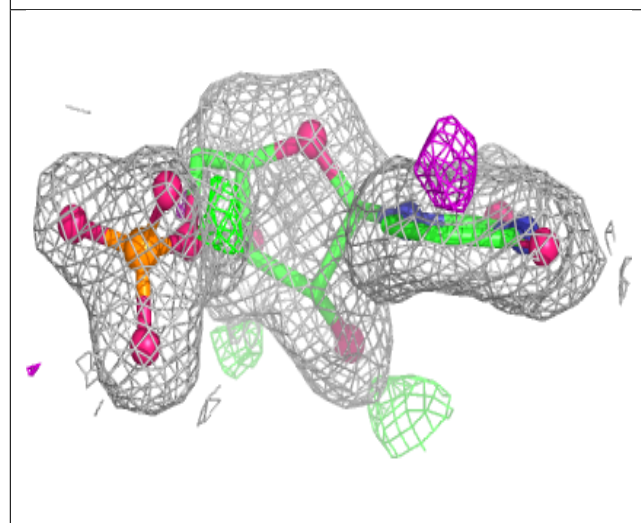
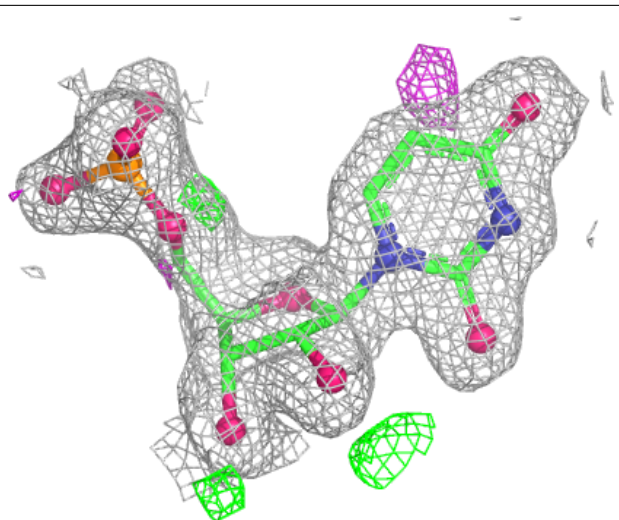
Electron density around U5P C 3250:

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



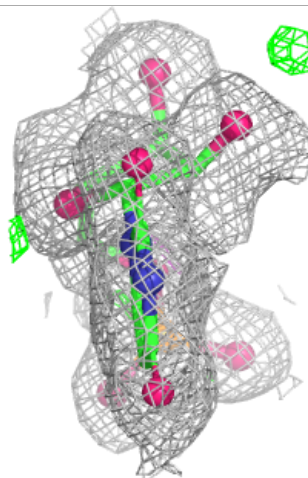
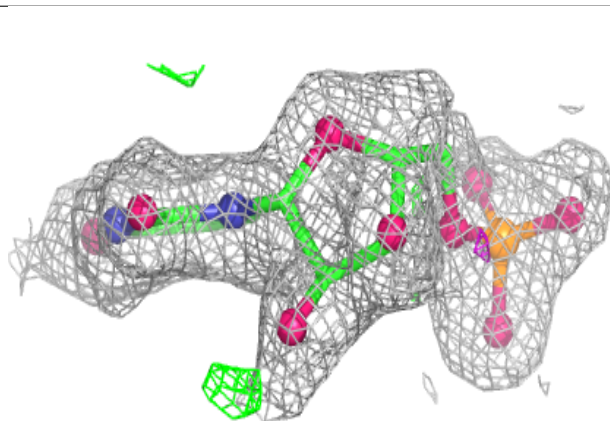
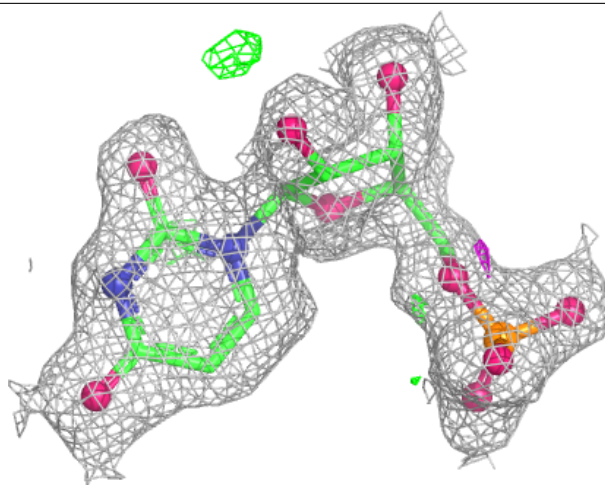
Electron density around U5P D 4250:

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



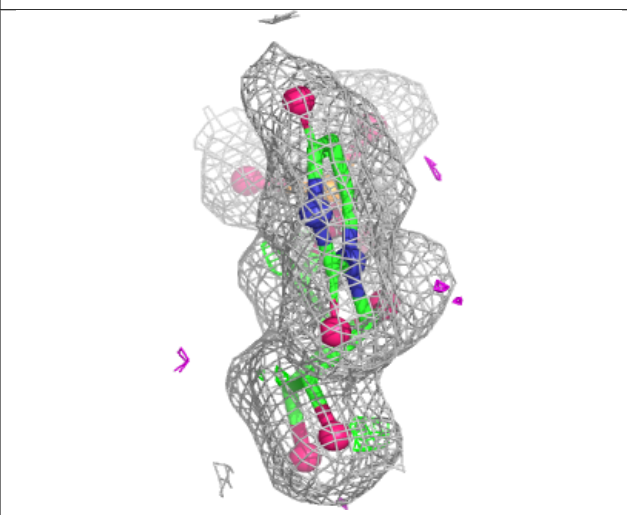
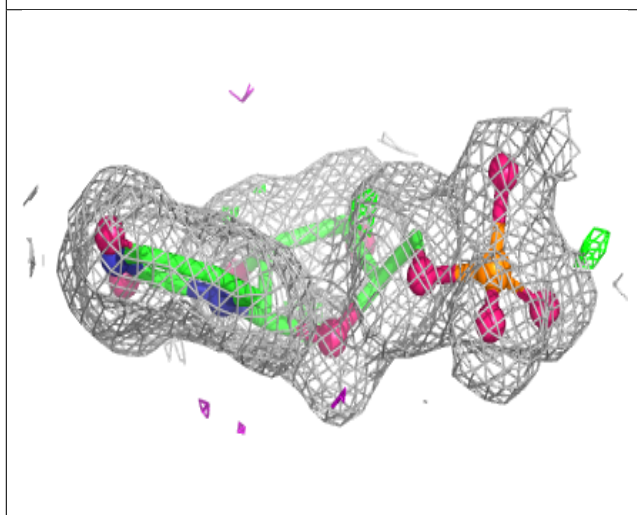
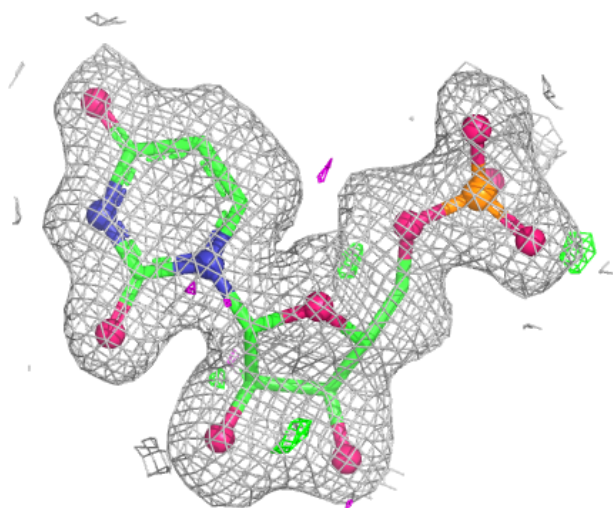
Electron density around U5P B 2250:

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



Electron density around U5P A 1250:

$2mF_o-DF_c$ (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.