Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:31 am BST

PDB ID	:	2J4K
Title	:	Crystal structure of uridylate kinase from Sulfolobus solfataricus in complex with UMP to 2.2 Angstrom resolution
Authors	:	Jensen, K.S.; Johansson, E.; Jensen, K.F.
Deposited on	:	2006-09-01
Resolution	:	2.20 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 following versions of software and data (see references ⓘ) were used in the production of this report:

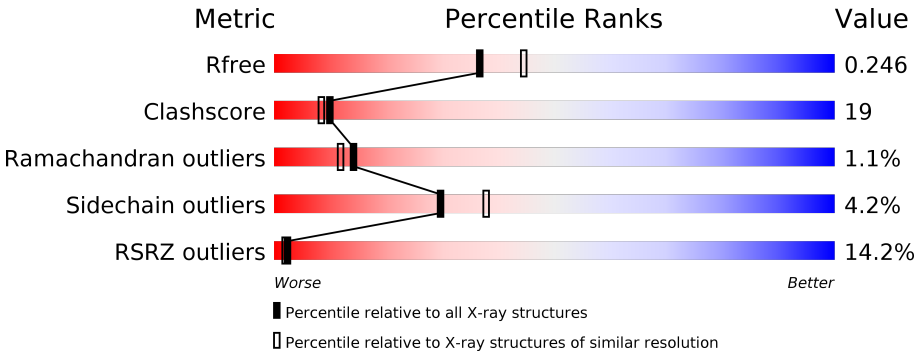
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	15% 59% 28% • 8%
1	B	226	9% 65% 27% • 5%
1	C	226	16% 57% 32% • 9%
1	D	226	15% 63% 34% •
1	E	226	13% 65% 30% • •
1	F	226	12% 55% 33% • 8%

2 Entry composition (i)

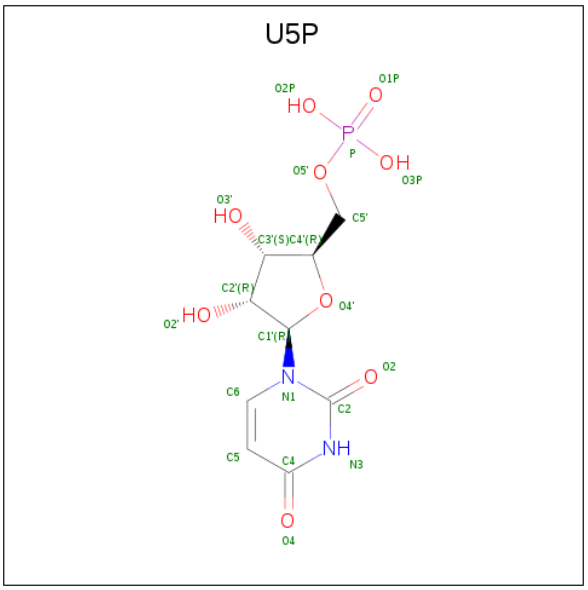
There are 5 unique types of molecules in this entry. The entry contains 10413 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	207	Total	C	N	O	S	0	0	0
			1620	1040	278	298	4			
1	B	214	Total	C	N	O	S	0	0	0
			1675	1074	286	311	4			
1	C	206	Total	C	N	O	S	0	0	0
			1612	1033	276	299	4			
1	D	226	Total	C	N	O	S	0	0	0
			1761	1126	300	331	4			
1	E	221	Total	C	N	O	S	0	0	0
			1722	1101	294	323	4			
1	F	208	Total	C	N	O	S	0	0	0
			1619	1039	276	300	4			

- Molecule 2 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U5P) (formula: $C_9H_{13}N_2O_9P$).



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		
2	F	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cd	0	0
			1	1		
3	E	2	Total	Cd	0	0
			2	2		
3	B	7	Total	Cd	0	0
			7	7		
3	C	3	Total	Cd	0	0
			3	3		
3	A	3	Total	Cd	0	0
			3	3		
3	F	2	Total	Cd	0	0
			2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	40	Total	O	0	0
			40	40		
5	B	49	Total	O	0	0
			49	49		

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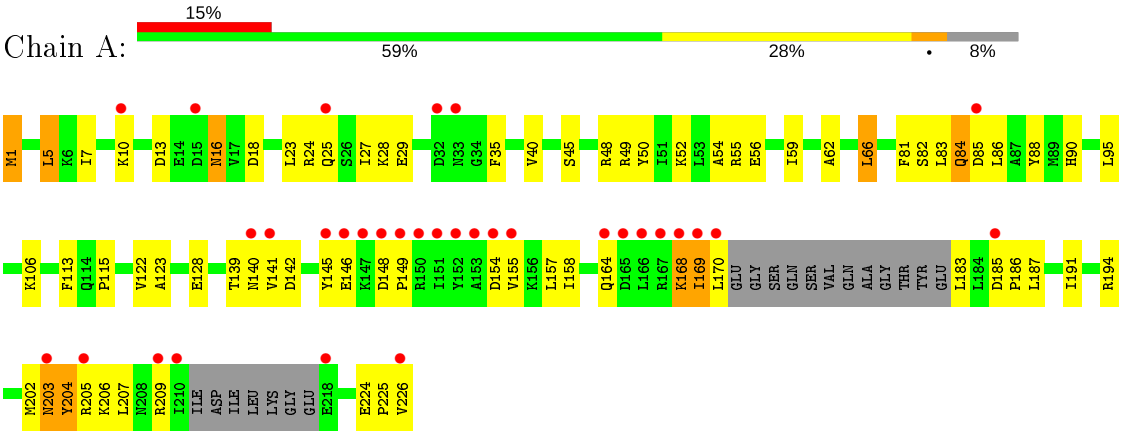
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	25	Total O 25 25	0	0
5	D	51	Total O 51 51	0	0
5	E	50	Total O 50 50	0	0
5	F	44	Total O 44 44	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

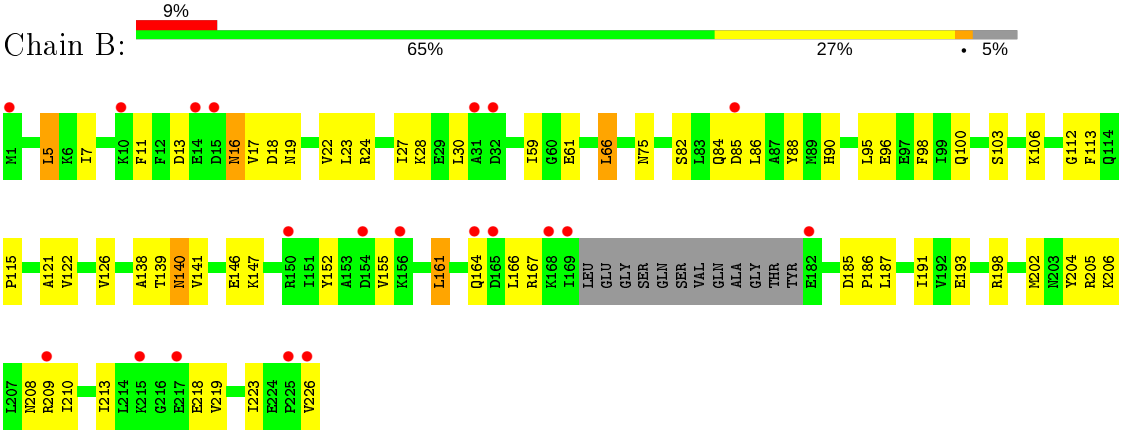
- Molecule 1: URIDYLATE KINASE

Chain A:



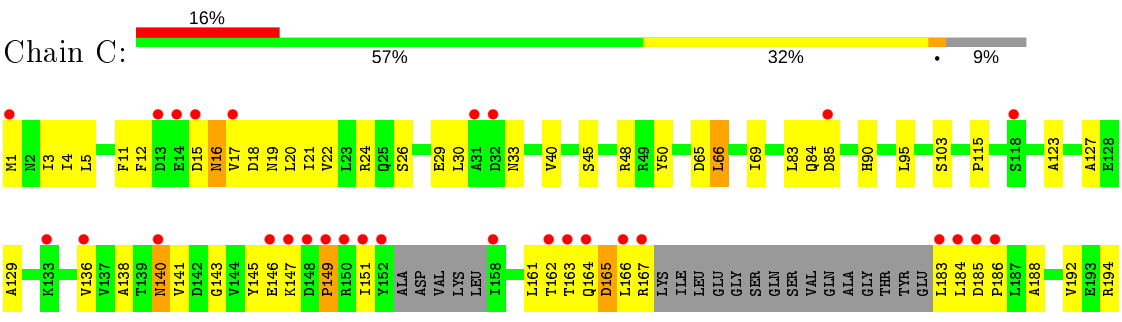
- Molecule 1: URIDYLATE KINASE

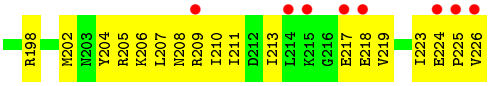
Chain B:



- Molecule 1: URIDYLATE KINASE

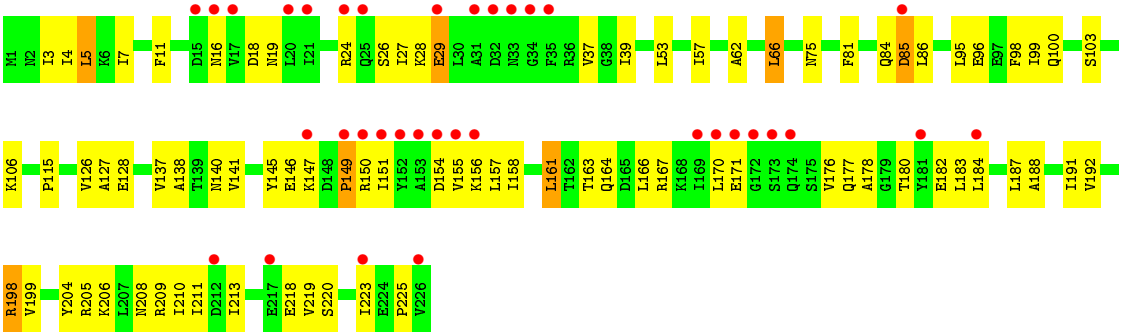
Chain C:





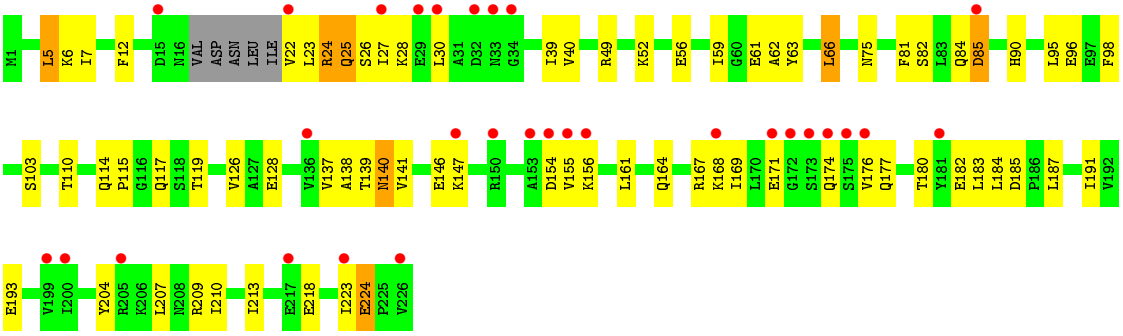
• Molecule 1: URIDYLATE KINASE

Chain D:



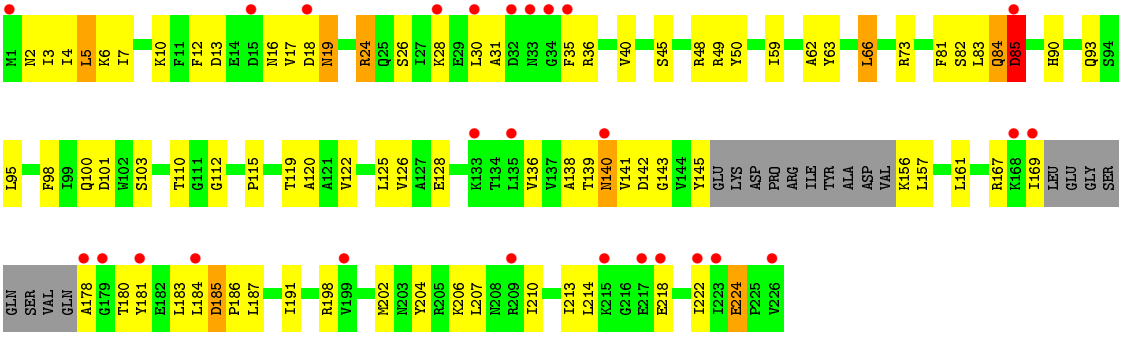
• Molecule 1: URIDYLATE KINASE

Chain E:



• Molecule 1: URIDYLATE KINASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.80Å 136.04Å 77.94Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	21.67 – 2.20 21.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (21.67-2.20) 99.1 (21.67-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 2.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.219 , 0.251 0.211 , 0.246	Depositor DCC
R_{free} test set	3363 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10413	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CD

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	0.33	0/1643	0.61	0/2220
1	B	0.33	0/1699	0.62	0/2296
1	C	0.33	0/1635	0.62	0/2209
1	D	0.34	0/1787	0.61	0/2417
1	E	0.33	0/1747	0.62	0/2360
1	F	0.35	0/1641	0.63	0/2216
All	All	0.33	0/10152	0.62	0/13718

There are no bond length outliers.

There are no bond angle outliers.

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	1620	0	1687	78	0
1	B	1675	0	1742	68	0
1	C	1612	0	1669	68	0
1	D	1761	0	1822	76	0
1	E	1722	0	1780	72	0
1	F	1619	0	1684	70	0
2	A	21	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	21	0	11	1	0
2	C	21	0	11	0	0
2	D	21	0	11	0	0
2	E	21	0	11	0	0
2	F	21	0	11	0	0
3	A	3	0	0	0	0
3	B	7	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
5	A	40	0	0	6	0
5	B	49	0	0	2	0
5	C	25	0	0	1	0
5	D	51	0	0	2	0
5	E	50	0	0	3	0
5	F	44	0	0	2	0
All	All	10413	0	10450	394	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 19.

All (394) 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:D:145:TYR:H	1:D:177:GLN:HE22	1.00	0.98
1:D:137:VAL:HG21	1:D:183:LEU:HD21	1.44	0.97
1:C:146:GLU:HG3	1:C:147:LYS:HG2	1.43	0.97
1:B:30:LEU:HD21	1:B:210:ILE:HD13	1.48	0.95
1:B:185:ASP:HB2	1:B:186:PRO:HD2	1.50	0.93
1:A:139:THR:HG22	1:A:140:ASN:H	1.33	0.92
1:A:185:ASP:HB2	1:A:186:PRO:HD2	1.56	0.88
1:D:164:GLN:HA	1:D:167:ARG:HE	1.41	0.85
1:D:198:ARG:HB3	1:D:198:ARG:HH11	1.44	0.83
1:A:203:ASN:HB2	5:A:2036:HOH:O	1.80	0.80
1:A:207:LEU:HA	5:A:2037:HOH:O	1.81	0.79
1:F:181:TYR:HA	1:F:184:LEU:HD12	1.64	0.78
1:E:176:VAL:HG12	1:E:177:GLN:H	1.48	0.78
1:A:115:PRO:HG2	1:E:95:LEU:HD23	1.65	0.78
1:F:198:ARG:HH21	1:F:222:ILE:HG21	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:ILE:HD13	1:E:218:GLU:HB3	1.66	0.76
1:F:24:ARG:HH11	1:F:28:LYS:HE3	1.50	0.76
1:A:139:THR:HG22	1:A:140:ASN:N	2.01	0.76
1:B:164:GLN:HG3	1:B:226:VAL:CG2	2.16	0.76
1:C:162:THR:OG1	1:C:165:ASP:HB2	1.85	0.76
1:F:84:GLN:O	1:F:85:ASP:HB2	1.87	0.75
1:B:206:LYS:HG2	1:B:209:ARG:HH21	1.52	0.74
1:C:164:GLN:HG3	1:C:226:VAL:HG23	1.69	0.74
1:D:176:VAL:HG22	1:D:177:GLN:H	1.52	0.74
1:B:164:GLN:HG3	1:B:226:VAL:HG23	1.70	0.73
1:E:146:GLU:OE1	1:E:156:LYS:HE3	1.89	0.72
1:C:207:LEU:HD22	1:C:210:ILE:HD11	1.72	0.71
1:E:59:ILE:HD11	1:F:82:SER:HA	1.73	0.71
1:D:26:SER:O	1:D:29:GLU:HB2	1.91	0.70
1:B:28:LYS:HG2	1:B:86:LEU:HD11	1.74	0.70
1:C:185:ASP:HB2	1:C:186:PRO:HD2	1.74	0.70
1:B:213:ILE:HD13	1:B:218:GLU:HB3	1.73	0.70
1:D:145:TYR:N	1:D:177:GLN:HE22	1.84	0.70
1:E:52:LYS:O	1:E:56:GLU:HG3	1.92	0.70
1:F:10:LYS:HD3	1:F:140:ASN:OD1	1.93	0.69
1:C:207:LEU:O	1:C:210:ILE:HG13	1.93	0.68
1:D:84:GLN:O	1:D:85:ASP:HB2	1.91	0.68
1:B:84:GLN:O	1:B:85:ASP:HB2	1.93	0.68
1:E:147:LYS:HB2	1:E:155:VAL:HG11	1.77	0.67
1:C:11:PHE:CE1	1:C:19:ASN:HB3	2.31	0.66
1:B:66:LEU:HD13	1:B:115:PRO:HG3	1.76	0.66
1:C:138:ALA:HB1	1:C:204:TYR:HB3	1.78	0.66
1:B:209:ARG:O	1:B:213:ILE:HG12	1.96	0.66
1:B:166:LEU:HD22	1:B:223:ILE:HD13	1.76	0.66
1:D:167:ARG:O	1:D:171:GLU:HG3	1.96	0.65
1:E:164:GLN:O	1:E:168:LYS:HG2	1.97	0.65
1:B:61:GLU:HG2	1:C:194:ARG:HD2	1.79	0.65
1:B:96:GLU:HG3	5:C:2017:HOH:O	1.96	0.65
1:D:62:ALA:HB2	1:F:128:GLU:HG2	1.77	0.65
1:A:187:LEU:O	1:A:191:ILE:HG12	1.97	0.65
1:E:176:VAL:O	1:E:177:GLN:HG3	1.98	0.64
1:B:95:LEU:HD23	1:C:115:PRO:HG2	1.80	0.64
1:D:96:GLU:HG3	5:F:2026:HOH:O	1.97	0.64
1:A:95:LEU:HD23	1:E:115:PRO:HG2	1.80	0.63
1:C:20:LEU:HD13	1:D:57:ILE:HD13	1.79	0.63
1:A:139:THR:CG2	1:A:140:ASN:H	2.09	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:O	1:A:85:ASP:HB2	1.98	0.63
1:D:145:TYR:H	1:D:177:GLN:NE2	1.84	0.62
1:C:188:ALA:O	1:C:192:VAL:HG13	1.99	0.62
1:F:24:ARG:NH1	1:F:28:LYS:HE3	2.12	0.62
1:D:141:VAL:HG21	1:D:178:ALA:O	2.00	0.62
1:F:138:ALA:HB1	1:F:204:TYR:HB3	1.82	0.62
1:B:138:ALA:HB1	1:B:204:TYR:HB3	1.81	0.61
1:E:224:GLU:HG3	5:E:2048:HOH:O	2.01	0.61
1:A:168:LYS:HA	1:A:168:LYS:HE3	1.81	0.61
1:E:169:ILE:CD1	1:E:180:THR:HG21	2.31	0.61
1:B:98:PHE:CZ	1:B:126:VAL:HG13	2.35	0.61
1:D:164:GLN:HA	1:D:167:ARG:NE	2.13	0.61
1:D:81:PHE:O	1:D:84:GLN:HG3	2.01	0.61
1:A:141:VAL:HG12	1:A:142:ASP:N	2.16	0.60
1:D:161:LEU:N	1:D:161:LEU:HD23	2.16	0.60
1:D:176:VAL:HG22	1:D:177:GLN:N	2.14	0.60
1:A:203:ASN:HD21	1:A:206:LYS:CG	2.15	0.60
1:A:16:ASN:HD22	1:A:18:ASP:H	1.50	0.60
1:D:198:ARG:CB	1:D:198:ARG:HH11	2.13	0.60
1:D:100:GLN:O	1:D:103:SER:HB3	2.02	0.59
1:E:176:VAL:HG12	1:E:177:GLN:N	2.16	0.59
1:D:206:LYS:HG2	1:D:209:ARG:HH21	1.67	0.59
1:F:3:ILE:HD11	1:F:136:VAL:CG2	2.32	0.59
1:E:5:LEU:HD13	1:E:7:ILE:HD11	1.85	0.59
1:C:163:THR:HG23	1:C:225:PRO:HA	1.83	0.58
1:E:169:ILE:HG12	1:E:174:GLN:HB3	1.86	0.58
1:F:210:ILE:O	1:F:214:LEU:HG	2.03	0.58
1:C:164:GLN:NE2	1:C:226:VAL:OXT	2.36	0.58
1:F:45:SER:HA	1:F:48:ARG:NH1	2.18	0.58
1:B:140:ASN:HD22	1:B:141:VAL:N	2.02	0.58
1:C:213:ILE:HD13	1:C:218:GLU:HB3	1.85	0.57
1:F:198:ARG:NH2	1:F:222:ILE:HG21	2.20	0.57
1:A:115:PRO:HG2	1:E:95:LEU:CD2	2.35	0.57
1:B:185:ASP:CB	1:B:186:PRO:HD2	2.29	0.57
1:E:84:GLN:O	1:E:85:ASP:HB2	2.04	0.57
1:C:26:SER:HB2	1:C:210:ILE:HD12	1.86	0.57
1:E:138:ALA:HB1	1:E:204:TYR:HB3	1.87	0.56
1:E:169:ILE:HD13	1:E:180:THR:HG21	1.88	0.56
1:B:18:ASP:O	1:B:22:VAL:HG12	2.05	0.56
1:E:169:ILE:CG1	1:E:174:GLN:HB3	2.36	0.56
1:E:49:ARG:HH22	1:F:13:ASP:HA	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:VAL:O	1:C:21:ILE:HG12	2.04	0.56
1:A:169:ILE:O	1:A:169:ILE:HG22	2.06	0.56
1:A:203:ASN:HD21	1:A:206:LYS:HG3	1.71	0.56
1:C:163:THR:CG2	1:C:225:PRO:HA	2.36	0.56
1:D:28:LYS:HE3	1:D:86:LEU:HD21	1.87	0.56
1:C:26:SER:O	1:C:30:LEU:HD23	2.05	0.56
1:F:180:THR:O	1:F:184:LEU:HG	2.06	0.56
1:B:206:LYS:CG	1:B:209:ARG:HH21	2.17	0.55
1:F:66:LEU:HD13	1:F:115:PRO:HG3	1.86	0.55
1:E:82:SER:HA	1:F:59:ILE:HD11	1.88	0.55
1:B:206:LYS:HG2	1:B:209:ARG:NH2	2.21	0.55
1:D:177:GLN:H	1:D:180:THR:HG22	1.71	0.55
1:E:12:PHE:O	1:F:49:ARG:NH2	2.35	0.55
1:E:139:THR:HG23	1:E:141:VAL:H	1.71	0.55
1:E:75:ASN:ND2	1:F:50:TYR:OH	2.40	0.55
1:E:22:VAL:O	1:E:25:GLN:NE2	2.39	0.55
1:E:207:LEU:O	1:E:210:ILE:HG13	2.07	0.55
1:D:28:LYS:HG2	1:D:86:LEU:HD11	1.89	0.55
1:A:164:GLN:HG3	1:A:226:VAL:CG2	2.37	0.55
1:C:224:GLU:OE2	1:C:225:PRO:HD2	2.07	0.55
1:D:187:LEU:O	1:D:191:ILE:HG12	2.07	0.55
1:B:16:ASN:HD22	1:B:16:ASN:N	2.04	0.54
1:F:2:ASN:OD1	1:F:36:ARG:HB2	2.08	0.54
1:A:29:GLU:HB3	1:A:209:ARG:NH2	2.23	0.54
1:F:48:ARG:NH1	5:F:2010:HOH:O	2.40	0.54
1:A:28:LYS:HG2	1:A:86:LEU:HD11	1.89	0.54
1:A:115:PRO:CG	1:E:95:LEU:HD23	2.36	0.54
1:D:128:GLU:HG2	1:F:62:ALA:HB2	1.89	0.54
1:A:164:GLN:HG3	1:A:226:VAL:HG23	1.88	0.54
1:B:146:GLU:HG2	1:B:155:VAL:HG13	1.89	0.54
1:A:45:SER:HA	1:A:48:ARG:NH1	2.23	0.54
1:D:16:ASN:HD22	1:D:18:ASP:H	1.56	0.54
1:B:100:GLN:O	1:B:103:SER:HB2	2.07	0.54
1:B:140:ASN:ND2	1:B:141:VAL:HG13	2.23	0.54
1:C:208:ASN:OD1	1:C:209:ARG:HG3	2.08	0.53
1:D:66:LEU:HD13	1:D:115:PRO:HG3	1.90	0.53
1:F:141:VAL:HG12	1:F:143:GLY:H	1.73	0.53
1:F:26:SER:O	1:F:30:LEU:HB2	2.08	0.53
1:B:208:ASN:OD1	1:B:209:ARG:HG3	2.09	0.53
1:C:66:LEU:HD13	1:C:115:PRO:HG3	1.89	0.53
1:B:24:ARG:HD3	1:B:82:SER:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ILE:HD11	1:C:136:VAL:CG2	2.38	0.53
1:C:3:ILE:HD11	1:C:136:VAL:HG23	1.89	0.53
1:E:209:ARG:O	1:E:213:ILE:HG12	2.08	0.53
1:D:98:PHE:CZ	1:D:126:VAL:HG13	2.44	0.53
1:C:151:ILE:HG22	1:C:151:ILE:O	2.08	0.53
1:C:166:LEU:HD22	1:C:223:ILE:HD13	1.91	0.53
1:E:27:ILE:HD11	1:E:39:ILE:HD11	1.91	0.52
1:F:95:LEU:HD13	1:F:125:LEU:HB3	1.90	0.52
1:F:120:ALA:HB1	1:F:183:LEU:HD12	1.90	0.52
1:B:23:LEU:O	1:B:27:ILE:HG12	2.08	0.52
1:F:3:ILE:HD11	1:F:136:VAL:HG23	1.90	0.52
1:C:33:ASN:OD1	1:C:211:ILE:HD13	2.09	0.52
1:A:81:PHE:O	1:A:84:GLN:HG3	2.10	0.52
1:D:177:GLN:O	1:D:180:THR:HG22	2.09	0.52
1:E:30:LEU:HD21	1:E:210:ILE:CG2	2.40	0.52
1:C:206:LYS:HG2	1:C:209:ARG:HH21	1.74	0.52
1:C:140:ASN:HD22	1:C:140:ASN:H	1.58	0.52
1:D:27:ILE:HD11	1:D:39:ILE:HD11	1.91	0.52
1:E:174:GLN:NE2	5:E:2038:HOH:O	2.39	0.52
1:E:167:ARG:CZ	1:E:193:GLU:OE1	2.58	0.52
1:B:121:ALA:HB1	1:B:187:LEU:HD23	1.92	0.51
1:F:183:LEU:HG	1:F:183:LEU:O	2.10	0.51
1:B:11:PHE:CE1	1:B:19:ASN:HB3	2.45	0.51
1:A:66:LEU:HD13	1:A:115:PRO:HG3	1.91	0.51
1:C:95:LEU:HD11	1:C:129:ALA:HB2	1.91	0.51
1:C:140:ASN:N	1:C:140:ASN:HD22	2.07	0.51
1:C:141:VAL:HG12	1:C:143:GLY:H	1.75	0.51
1:B:206:LYS:HZ3	1:B:219:VAL:HB	1.75	0.51
1:C:84:GLN:O	1:C:85:ASP:HB2	2.11	0.51
1:D:4:ILE:HG13	1:D:127:ALA:HA	1.93	0.51
1:A:194:ARG:HD2	1:E:61:GLU:HG2	1.93	0.51
1:F:187:LEU:O	1:F:191:ILE:HG12	2.10	0.51
1:A:203:ASN:HD22	1:A:203:ASN:N	2.07	0.51
1:B:61:GLU:HG2	1:C:194:ARG:CD	2.41	0.51
1:A:24:ARG:O	1:A:28:LYS:HG3	2.10	0.50
1:B:115:PRO:HG2	1:C:95:LEU:HD23	1.92	0.50
1:B:66:LEU:HD13	1:B:115:PRO:CG	2.41	0.50
1:C:15:ASP:OD1	1:C:18:ASP:HB2	2.11	0.50
1:D:188:ALA:O	1:D:192:VAL:HG13	2.12	0.50
1:E:147:LYS:HB2	1:E:155:VAL:CG1	2.41	0.50
1:D:163:THR:HG23	1:D:225:PRO:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ASN:HD22	1:C:33:ASN:N	2.08	0.50
1:D:147:LYS:H	1:D:155:VAL:HG11	1.76	0.50
1:A:149:PRO:HG3	1:A:154:ASP:O	2.12	0.49
1:A:168:LYS:C	1:A:170:LEU:H	2.15	0.49
1:A:224:GLU:HG3	1:A:225:PRO:HD2	1.94	0.49
1:E:176:VAL:HG13	1:E:184:LEU:CD1	2.42	0.49
1:B:16:ASN:ND2	1:B:16:ASN:H	2.10	0.49
1:F:30:LEU:O	1:F:35:PHE:HB2	2.12	0.49
1:B:218:GLU:HG3	1:B:219:VAL:N	2.28	0.49
1:E:6:LYS:HE3	1:E:119:THR:OG1	2.13	0.49
1:A:155:VAL:HG23	1:A:155:VAL:O	2.13	0.49
1:A:209:ARG:HG3	5:A:2039:HOH:O	2.13	0.49
1:D:206:LYS:HG2	1:D:209:ARG:NH2	2.27	0.49
1:F:95:LEU:HG	1:F:95:LEU:O	2.13	0.49
1:E:30:LEU:HD21	1:E:210:ILE:HG22	1.94	0.49
1:E:24:ARG:NH1	1:E:28:LYS:HE3	2.28	0.49
1:E:49:ARG:NH2	1:F:13:ASP:HA	2.28	0.49
1:D:11:PHE:CZ	1:D:19:ASN:HB2	2.48	0.49
1:D:5:LEU:HD13	1:D:7:ILE:HD11	1.95	0.48
1:E:140:ASN:HD22	1:E:140:ASN:N	2.11	0.48
1:C:17:VAL:HG23	1:C:18:ASP:N	2.28	0.48
1:D:16:ASN:HB2	1:D:18:ASP:OD1	2.12	0.48
1:F:112:GLY:HA2	1:F:122:VAL:HG21	1.94	0.48
1:A:24:ARG:NH2	1:A:28:LYS:NZ	2.61	0.48
1:A:28:LYS:HE2	1:A:86:LEU:HD11	1.94	0.48
1:C:164:GLN:CG	1:C:226:VAL:HG23	2.42	0.48
1:D:146:GLU:HB3	1:D:158:ILE:HD11	1.95	0.48
1:C:163:THR:O	1:C:167:ARG:HG3	2.13	0.48
1:D:209:ARG:O	1:D:213:ILE:HG12	2.13	0.48
1:C:16:ASN:HB3	1:D:53:LEU:CD1	2.43	0.48
1:B:164:GLN:HB2	5:B:2038:HOH:O	2.14	0.48
1:B:16:ASN:ND2	1:B:16:ASN:N	2.62	0.48
1:B:11:PHE:CZ	1:B:19:ASN:HB3	2.49	0.48
1:D:166:LEU:HD12	1:D:166:LEU:N	2.29	0.48
1:E:81:PHE:O	1:E:84:GLN:HG3	2.14	0.48
1:E:114:GLN:O	1:E:117:GLN:HG2	2.13	0.48
1:A:141:VAL:HG12	1:A:142:ASP:H	1.79	0.47
1:A:203:ASN:O	1:A:203:ASN:ND2	2.47	0.47
1:F:81:PHE:O	1:F:84:GLN:HG3	2.13	0.47
1:C:12:PHE:C	1:C:16:ASN:HD21	2.18	0.47
1:C:24:ARG:HA	1:C:83:LEU:HD21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:PHE:CD2	1:E:126:VAL:HG22	2.49	0.47
1:C:11:PHE:CZ	1:C:19:ASN:HB3	2.49	0.47
1:D:149:PRO:O	1:D:151:ILE:N	2.47	0.47
1:D:170:LEU:HD21	1:D:184:LEU:HB3	1.95	0.47
1:E:183:LEU:HD13	1:E:223:ILE:HD12	1.96	0.47
1:C:205:ARG:HG3	1:C:205:ARG:HH11	1.80	0.47
1:A:203:ASN:HD21	1:A:206:LYS:HD2	1.79	0.47
1:A:23:LEU:O	1:A:27:ILE:HG13	2.14	0.47
1:A:62:ALA:HB2	1:E:128:GLU:HG2	1.95	0.47
1:A:204:TYR:O	1:A:204:TYR:HD1	1.98	0.47
1:A:203:ASN:HD21	1:A:206:LYS:CD	2.27	0.47
1:B:185:ASP:HB2	1:B:186:PRO:CD	2.36	0.47
1:E:25:GLN:CD	1:E:25:GLN:H	2.17	0.47
1:F:141:VAL:CG1	1:F:145:TYR:HE2	2.27	0.47
1:A:141:VAL:CG1	1:A:145:TYR:HE2	2.27	0.47
1:D:84:GLN:O	1:D:85:ASP:CB	2.62	0.47
1:A:88:TYR:CE2	1:A:90:HIS:HB3	2.50	0.47
1:D:177:GLN:N	1:D:180:THR:HG22	2.30	0.47
1:E:23:LEU:HD12	1:E:26:SER:OG	2.14	0.47
1:F:3:ILE:HD11	1:F:136:VAL:HG21	1.95	0.47
1:A:5:LEU:HD13	1:A:7:ILE:HD11	1.97	0.46
1:D:11:PHE:CE1	1:D:19:ASN:HB2	2.50	0.46
1:F:98:PHE:CD2	1:F:126:VAL:HG22	2.50	0.46
1:D:199:VAL:HB	1:D:223:ILE:HB	1.97	0.46
1:D:19:ASN:ND2	5:D:2005:HOH:O	2.47	0.46
1:A:54:ALA:HB1	1:A:59:ILE:HG13	1.95	0.46
1:A:203:ASN:H	1:A:203:ASN:ND2	2.14	0.46
1:F:98:PHE:CZ	1:F:126:VAL:HG13	2.50	0.46
1:C:183:LEU:O	1:C:184:LEU:HD23	2.15	0.46
1:D:138:ALA:HB1	1:D:204:TYR:HB3	1.97	0.46
1:A:203:ASN:C	1:A:205:ARG:H	2.19	0.46
1:A:203:ASN:HD22	1:A:203:ASN:H	1.63	0.46
1:B:17:VAL:CG2	1:B:18:ASP:N	2.79	0.46
1:E:49:ARG:NH2	1:F:12:PHE:O	2.50	0.45
1:A:146:GLU:OE1	1:A:149:PRO:HA	2.16	0.45
1:D:213:ILE:HD13	1:D:218:GLU:HB3	1.99	0.45
1:A:95:LEU:CD2	1:E:115:PRO:HG2	2.44	0.45
1:B:205:ARG:HG3	1:B:205:ARG:HH11	1.80	0.45
1:F:17:VAL:C	1:F:19:ASN:N	2.69	0.45
1:C:145:TYR:CD2	1:C:149:PRO:HD3	2.52	0.45
1:C:185:ASP:CB	1:C:186:PRO:HD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ILE:HD13	1:F:63:TYR:CE1	2.51	0.45
1:A:10:LYS:HD2	1:A:140:ASN:HB2	1.98	0.45
1:A:157:LEU:HD23	1:A:158:ILE:N	2.32	0.45
1:D:100:GLN:HG3	1:E:90:HIS:HB2	1.99	0.45
1:E:66:LEU:HD13	1:E:115:PRO:HG3	1.98	0.45
1:A:55:ARG:HD2	5:A:2013:HOH:O	2.15	0.45
1:A:82:SER:HA	1:B:59:ILE:HD11	1.99	0.45
1:F:213:ILE:HD13	1:F:218:GLU:HB3	1.99	0.45
1:A:28:LYS:CG	1:A:86:LEU:HD11	2.47	0.45
1:F:5:LEU:HD13	1:F:7:ILE:HD11	1.99	0.45
1:B:17:VAL:HG22	5:B:2006:HOH:O	2.17	0.44
1:B:17:VAL:HG23	1:B:18:ASP:N	2.31	0.44
1:C:206:LYS:NZ	1:C:219:VAL:HB	2.32	0.44
1:F:73:ARG:NH2	1:F:93:GLN:HB3	2.31	0.44
1:B:164:GLN:HG3	1:B:226:VAL:HG21	1.95	0.44
1:D:29:GLU:HB3	1:D:211:ILE:HD11	1.99	0.44
1:A:1:MET:O	1:A:35:PHE:HA	2.17	0.44
1:F:141:VAL:HG12	1:F:142:ASP:N	2.32	0.44
1:C:18:ASP:O	1:C:22:VAL:HG12	2.18	0.44
1:D:19:ASN:ND2	5:D:2004:HOH:O	2.51	0.44
1:E:63:TYR:CD2	1:F:84:GLN:NE2	2.85	0.44
1:E:23:LEU:HD12	1:E:23:LEU:O	2.17	0.44
1:F:16:ASN:HD21	1:F:18:ASP:CG	2.20	0.44
1:A:183:LEU:O	1:A:183:LEU:HD23	2.18	0.44
1:D:3:ILE:CG2	1:D:37:VAL:HG22	2.47	0.44
1:D:208:ASN:OD1	1:D:209:ARG:HG3	2.18	0.44
1:D:210:ILE:O	1:D:213:ILE:HB	2.17	0.44
5:A:2030:HOH:O	1:E:96:GLU:HG3	2.18	0.44
1:B:30:LEU:CD2	1:B:210:ILE:HG21	2.48	0.44
1:F:185:ASP:HA	1:F:186:PRO:HD2	1.88	0.44
1:E:24:ARG:HH11	1:E:24:ARG:CG	2.30	0.44
1:F:4:ILE:HG13	1:F:126:VAL:HG12	1.99	0.43
1:A:139:THR:O	1:A:203:ASN:HA	2.17	0.43
1:D:155:VAL:HG12	1:D:156:LYS:N	2.33	0.43
1:A:49:ARG:NE	5:A:2011:HOH:O	2.51	0.43
1:C:209:ARG:O	1:C:213:ILE:HG12	2.18	0.43
1:E:25:GLN:OE1	1:E:25:GLN:N	2.51	0.43
1:F:178:ALA:C	1:F:180:THR:H	2.22	0.43
1:C:161:LEU:N	1:C:161:LEU:HD23	2.33	0.43
1:C:16:ASN:HB3	1:D:53:LEU:HD11	2.00	0.43
1:F:198:ARG:NE	1:F:224:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:ASP:CG	1:F:206:LYS:HZ1	2.22	0.43
1:A:204:TYR:O	1:A:204:TYR:CD1	2.70	0.43
1:D:145:TYR:CE1	1:D:157:LEU:HG	2.53	0.43
1:A:25:GLN:HG2	1:A:29:GLU:OE1	2.19	0.43
1:A:83:LEU:O	1:A:84:GLN:C	2.56	0.43
1:B:146:GLU:CG	1:B:155:VAL:HG13	2.48	0.43
1:C:40:VAL:HG21	1:C:123:ALA:HA	2.00	0.43
1:D:182:GLU:O	1:D:183:LEU:HD23	2.18	0.43
1:B:13:ASP:C	1:B:16:ASN:HD21	2.21	0.43
1:B:112:GLY:HA3	2:B:227:U5P:C5	2.47	0.43
1:B:167:ARG:NH2	1:B:193:GLU:OE1	2.52	0.43
1:D:95:LEU:HD23	1:F:115:PRO:HG2	2.01	0.43
1:B:161:LEU:HD23	1:B:161:LEU:N	2.33	0.43
1:A:106:LYS:HE3	1:C:103:SER:O	2.18	0.42
1:A:66:LEU:HA	1:A:66:LEU:HD12	1.87	0.42
1:C:146:GLU:O	1:C:147:LYS:HD2	2.18	0.42
1:F:139:THR:HG23	1:F:141:VAL:H	1.84	0.42
1:F:140:ASN:HD22	1:F:140:ASN:C	2.23	0.42
1:D:5:LEU:CD1	1:D:7:ILE:HD11	2.48	0.42
1:B:106:LYS:HE3	1:E:103:SER:O	2.19	0.42
1:E:169:ILE:HG21	1:E:184:LEU:HD11	2.01	0.42
1:B:5:LEU:HD22	1:B:7:ILE:CD1	2.49	0.42
1:E:156:LYS:H	1:E:156:LYS:HG2	1.63	0.42
1:F:31:ALA:HA	1:F:35:PHE:O	2.19	0.42
1:C:45:SER:HA	1:C:48:ARG:NH1	2.33	0.42
1:D:3:ILE:HG23	1:D:37:VAL:HG22	2.00	0.42
1:A:40:VAL:HG21	1:A:123:ALA:HA	2.02	0.42
1:C:217:GLU:O	1:C:218:GLU:HB2	2.19	0.42
1:B:103:SER:O	1:D:106:LYS:HE3	2.20	0.42
1:F:204:TYR:O	1:F:207:LEU:HG	2.20	0.42
1:B:139:THR:OG1	1:B:140:ASN:N	2.52	0.42
1:E:22:VAL:C	1:E:25:GLN:NE2	2.72	0.42
1:F:167:ARG:O	1:F:169:ILE:HG22	2.20	0.42
1:A:203:ASN:ND2	1:A:203:ASN:N	2.68	0.42
1:B:113:PHE:CE2	1:B:122:VAL:HG13	2.54	0.42
1:C:65:ASP:O	1:C:69:ILE:HG13	2.20	0.42
1:C:90:HIS:HB2	1:F:100:GLN:HG3	2.02	0.42
1:E:137:VAL:HG11	1:E:182:GLU:HB3	2.01	0.42
1:D:176:VAL:HG23	1:D:184:LEU:HD11	2.00	0.42
1:E:95:LEU:HD21	5:E:2028:HOH:O	2.19	0.42
1:F:5:LEU:HD22	1:F:7:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:HD12	1:C:69:ILE:HD12	2.02	0.42
1:D:205:ARG:HG3	1:D:205:ARG:NH1	2.35	0.42
1:D:24:ARG:O	1:D:28:LYS:HG3	2.20	0.42
1:A:203:ASN:ND2	1:A:206:LYS:HG3	2.35	0.41
1:D:205:ARG:HG3	1:D:205:ARG:HH11	1.83	0.41
1:D:115:PRO:HG2	1:F:95:LEU:CD2	2.50	0.41
1:A:113:PHE:CE2	1:A:122:VAL:HG13	2.55	0.41
1:A:10:LYS:HA	1:A:13:ASP:OD2	2.20	0.41
1:A:157:LEU:C	1:A:157:LEU:HD23	2.40	0.41
1:C:29:GLU:HG2	1:C:211:ILE:HD11	2.02	0.41
1:F:19:ASN:OD1	1:F:19:ASN:N	2.51	0.41
1:F:140:ASN:HB3	1:F:204:TYR:OH	2.20	0.41
1:F:40:VAL:HG22	1:F:110:THR:CG2	2.50	0.41
1:F:90:HIS:ND1	1:F:101:ASP:OD2	2.45	0.41
1:A:52:LYS:O	1:A:56:GLU:HG3	2.19	0.41
1:C:4:ILE:HG13	1:C:127:ALA:HA	2.03	0.41
1:C:95:LEU:HD11	1:C:129:ALA:CB	2.50	0.41
1:D:219:VAL:O	1:D:220:SER:HB3	2.20	0.41
1:D:4:ILE:HG13	1:D:127:ALA:CA	2.51	0.41
1:B:147:LYS:O	1:B:155:VAL:HG11	2.21	0.41
1:C:205:ARG:HG3	1:C:205:ARG:NH1	2.35	0.41
1:B:24:ARG:HG2	1:B:28:LYS:HE3	2.02	0.41
1:C:50:TYR:OH	1:D:75:ASN:ND2	2.53	0.41
1:E:176:VAL:CG1	1:E:177:GLN:H	2.27	0.41
1:A:128:GLU:HG2	1:E:62:ALA:HB2	2.03	0.41
1:A:5:LEU:CD1	1:A:7:ILE:HD11	2.51	0.41
1:E:164:GLN:HA	1:E:167:ARG:HE	1.86	0.41
1:F:6:LYS:HE3	1:F:119:THR:OG1	2.20	0.41
1:B:206:LYS:CD	1:B:209:ARG:HH21	2.34	0.41
1:E:187:LEU:O	1:E:191:ILE:HG12	2.20	0.41
1:A:50:TYR:OH	1:B:75:ASN:ND2	2.53	0.41
1:B:185:ASP:CB	1:B:186:PRO:CD	2.98	0.41
1:B:187:LEU:O	1:B:191:ILE:HG12	2.21	0.41
1:A:141:VAL:CG1	1:A:142:ASP:N	2.82	0.41
1:B:147:LYS:HB3	1:B:152:TYR:CD2	2.55	0.40
1:B:30:LEU:HD21	1:B:210:ILE:HG21	2.02	0.40
1:E:140:ASN:H	1:E:140:ASN:HD22	1.67	0.40
1:B:75:ASN:HD22	1:B:75:ASN:HA	1.73	0.40
1:C:164:GLN:H	1:C:226:VAL:CG2	2.34	0.40
1:A:194:ARG:CD	1:E:61:GLU:HG2	2.51	0.40
1:F:16:ASN:ND2	1:F:18:ASP:OD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLU:HG2	1:C:194:ARG:NE	2.37	0.40
1:D:100:GLN:O	1:D:103:SER:CB	2.69	0.40
1:E:167:ARG:O	1:E:171:GLU:HG3	2.21	0.40
1:A:168:LYS:HE3	1:A:168:LYS:CA	2.49	0.40
1:E:114:GLN:HA	1:E:115:PRO:HD3	1.93	0.40
1:F:83:LEU:O	1:F:84:GLN:C	2.59	0.40
1:B:88:TYR:CE2	1:B:90:HIS:HB3	2.56	0.40
1:E:40:VAL:HG22	1:E:110:THR:CG2	2.52	0.40
1:F:156:LYS:HG2	1:F:157:LEU:N	2.36	0.40
1:F:98:PHE:CG	1:F:126:VAL:HG22	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	201/226 (89%)	189 (94%)	9 (4%)	3 (2%)	10 8
1	B	210/226 (93%)	199 (95%)	10 (5%)	1 (0%)	29 31
1	C	200/226 (88%)	186 (93%)	12 (6%)	2 (1%)	15 14
1	D	224/226 (99%)	210 (94%)	9 (4%)	5 (2%)	6 4
1	E	217/226 (96%)	209 (96%)	7 (3%)	1 (0%)	29 31
1	F	202/226 (89%)	193 (96%)	7 (4%)	2 (1%)	15 14
All	All	1254/1356 (92%)	1186 (95%)	54 (4%)	14 (1%)	14 12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	149	PRO
1	D	154	ASP

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Mol	Chain	Res	Type
1	A	169	ILE
1	B	16	ASN
1	C	16	ASN
1	D	85	ASP
1	D	150	ARG
1	A	84	GLN
1	A	204	TYR
1	D	29	GLU
1	E	85	ASP
1	F	85	ASP
1	F	84	GLN
1	C	149	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	177/192 (92%)	169 (96%)	8 (4%)	27	34
1	B	183/192 (95%)	177 (97%)	6 (3%)	38	49
1	C	176/192 (92%)	169 (96%)	7 (4%)	31	40
1	D	192/192 (100%)	187 (97%)	5 (3%)	46	58
1	E	187/192 (97%)	178 (95%)	9 (5%)	25	32
1	F	176/192 (92%)	165 (94%)	11 (6%)	18	20
All	All	1091/1152 (95%)	1045 (96%)	46 (4%)	30	38

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	LEU
1	A	16	ASN
1	A	66	LEU
1	A	148	ASP
1	A	168	LYS

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Mol	Chain	Res	Type
1	A	202	MET
1	A	203	ASN
1	B	5	LEU
1	B	66	LEU
1	B	140	ASN
1	B	161	LEU
1	B	198	ARG
1	B	202	MET
1	C	1	MET
1	C	5	LEU
1	C	66	LEU
1	C	140	ASN
1	C	165	ASP
1	C	198	ARG
1	C	202	MET
1	D	5	LEU
1	D	66	LEU
1	D	140	ASN
1	D	161	LEU
1	D	198	ARG
1	E	5	LEU
1	E	24	ARG
1	E	25	GLN
1	E	66	LEU
1	E	140	ASN
1	E	154	ASP
1	E	161	LEU
1	E	185	ASP
1	E	224	GLU
1	F	5	LEU
1	F	19	ASN
1	F	24	ARG
1	F	66	LEU
1	F	85	ASP
1	F	103	SER
1	F	140	ASN
1	F	161	LEU
1	F	185	ASP
1	F	202	MET
1	F	224	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	33	ASN
1	A	75	ASN
1	A	93	GLN
1	A	114	GLN
1	A	117	GLN
1	A	203	ASN
1	B	16	ASN
1	B	75	ASN
1	B	114	GLN
1	B	117	GLN
1	B	140	ASN
1	C	16	ASN
1	C	33	ASN
1	C	75	ASN
1	C	93	GLN
1	C	114	GLN
1	C	117	GLN
1	C	140	ASN
1	D	16	ASN
1	D	19	ASN
1	D	33	ASN
1	D	75	ASN
1	D	114	GLN
1	D	117	GLN
1	D	140	ASN
1	D	177	GLN
1	E	75	ASN
1	E	114	GLN
1	E	117	GLN
1	E	140	ASN
1	F	33	ASN
1	F	75	ASN
1	F	114	GLN
1	F	117	GLN
1	F	140	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 19 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	U5P	D	227	-	18,22,22	4.65	7 (38%)	21,33,33	1.93	5 (23%)
2	U5P	E	227	-	18,22,22	4.70	7 (38%)	21,33,33	1.89	4 (19%)
2	U5P	F	227	-	18,22,22	4.60	7 (38%)	21,33,33	1.88	3 (14%)
2	U5P	C	227	-	18,22,22	4.91	7 (38%)	21,33,33	1.80	4 (19%)
2	U5P	A	227	4	18,22,22	4.68	6 (33%)	21,33,33	1.83	3 (14%)
2	U5P	B	227	-	18,22,22	4.84	7 (38%)	21,33,33	1.86	3 (14%)

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	D	227	-	-	1/8/26/26	0/2/2/2
2	U5P	E	227	-	-	1/8/26/26	0/2/2/2
2	U5P	F	227	-	-	1/8/26/26	0/2/2/2
2	U5P	C	227	-	-	1/8/26/26	0/2/2/2
2	U5P	A	227	4	-	0/8/26/26	0/2/2/2
2	U5P	B	227	-	-	1/8/26/26	0/2/2/2

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	227	U5P	C6-N1	12.63	1.51	1.35
2	D	227	U5P	C6-N1	12.50	1.51	1.35
2	B	227	U5P	C6-N1	12.38	1.51	1.35
2	A	227	U5P	C6-N1	12.35	1.51	1.35
2	E	227	U5P	C6-N1	12.07	1.50	1.35
2	C	227	U5P	O4-C4	11.52	1.53	1.24
2	F	227	U5P	C6-N1	11.51	1.50	1.35
2	B	227	U5P	O4-C4	11.50	1.53	1.24
2	A	227	U5P	O4-C4	11.22	1.52	1.24
2	E	227	U5P	O4-C4	11.15	1.52	1.24
2	F	227	U5P	O4-C4	10.96	1.52	1.24
2	D	227	U5P	O4-C4	10.49	1.50	1.24
2	B	227	U5P	O4'-C1'	6.84	1.50	1.41
2	C	227	U5P	O4'-C1'	6.70	1.50	1.41
2	C	227	U5P	C4-N3	6.56	1.44	1.33
2	F	227	U5P	C4-N3	6.35	1.44	1.33
2	B	227	U5P	C4-N3	6.20	1.43	1.33
2	E	227	U5P	C4-N3	6.17	1.43	1.33
2	D	227	U5P	C4-N3	6.01	1.43	1.33
2	E	227	U5P	O4'-C1'	5.93	1.49	1.41
2	A	227	U5P	O4'-C1'	5.89	1.49	1.41
2	F	227	U5P	O4'-C1'	5.84	1.49	1.41
2	A	227	U5P	C4-N3	5.71	1.43	1.33
2	D	227	U5P	O4'-C1'	5.54	1.48	1.41
2	F	227	U5P	C2'-C1'	5.09	1.61	1.53
2	D	227	U5P	C2'-C1'	5.07	1.61	1.53
2	E	227	U5P	C2'-C1'	4.87	1.61	1.53
2	A	227	U5P	C2'-C1'	4.83	1.61	1.53
2	C	227	U5P	C2'-C1'	4.83	1.61	1.53
2	B	227	U5P	C2'-C1'	4.61	1.60	1.53
2	D	227	U5P	O4'-C4'	-3.49	1.37	1.45
2	E	227	U5P	O4'-C4'	-3.39	1.37	1.45
2	B	227	U5P	O4'-C4'	-3.24	1.37	1.45
2	A	227	U5P	O4'-C4'	-3.23	1.37	1.45
2	C	227	U5P	O4'-C4'	-3.12	1.38	1.45
2	F	227	U5P	O4'-C4'	-3.10	1.38	1.45
2	C	227	U5P	C2-N3	2.45	1.43	1.38
2	B	227	U5P	C2-N3	2.32	1.42	1.38
2	E	227	U5P	C2-N3	2.24	1.42	1.38
2	D	227	U5P	P-O5'	-2.11	1.53	1.60
2	F	227	U5P	P-O5'	-2.08	1.53	1.60

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	227	U5P	O2'-C2'-C3'	5.50	129.63	111.82
2	C	227	U5P	O2'-C2'-C3'	5.47	129.51	111.82
2	A	227	U5P	O2'-C2'-C3'	5.45	129.44	111.82
2	D	227	U5P	O2'-C2'-C3'	5.38	129.22	111.82
2	F	227	U5P	O2'-C2'-C3'	5.32	129.02	111.82
2	E	227	U5P	O2'-C2'-C3'	5.28	128.89	111.82
2	E	227	U5P	O4'-C1'-C2'	-3.03	102.50	106.93
2	F	227	U5P	O4'-C1'-C2'	-2.95	102.61	106.93
2	D	227	U5P	O4'-C1'-C2'	-2.93	102.64	106.93
2	D	227	U5P	C3'-C2'-C1'	-2.68	96.94	100.98
2	A	227	U5P	O4'-C1'-C2'	-2.58	103.15	106.93
2	B	227	U5P	O4'-C1'-C2'	-2.50	103.28	106.93
2	B	227	U5P	C3'-C2'-C1'	-2.41	97.35	100.98
2	F	227	U5P	C3'-C2'-C1'	-2.33	97.46	100.98
2	C	227	U5P	O4'-C1'-C2'	-2.25	103.64	106.93
2	E	227	U5P	C3'-C2'-C1'	-2.23	97.63	100.98
2	D	227	U5P	O4'-C4'-C5'	-2.18	102.20	109.37
2	A	227	U5P	C3'-C2'-C1'	-2.13	97.77	100.98
2	D	227	U5P	C5'-C4'-C3'	2.11	123.09	115.18
2	E	227	U5P	O4'-C4'-C5'	-2.06	102.61	109.37
2	C	227	U5P	C3'-C2'-C1'	-2.05	97.89	100.98
2	C	227	U5P	P-O5'-C5'	2.02	123.85	118.30

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	227	U5P	O4'-C1'-N1-C6
2	B	227	U5P	O4'-C1'-N1-C6
2	D	227	U5P	C3'-C4'-C5'-O5'
2	E	227	U5P	C3'-C4'-C5'-O5'
2	F	227	U5P	C3'-C4'-C5'-O5'

There are no ring outliers.

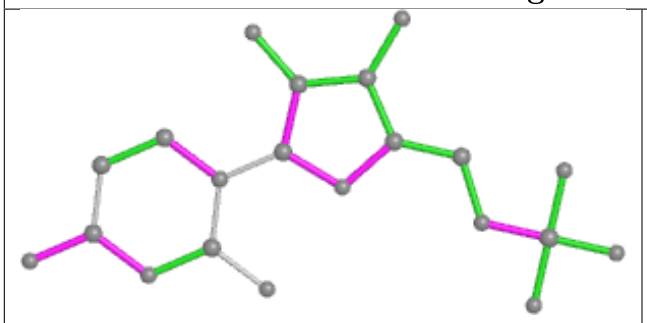
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	227	U5P	1	0

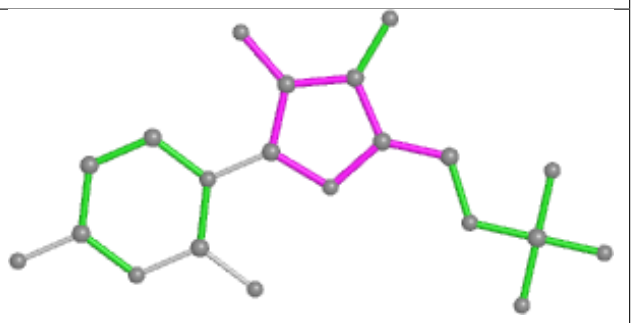
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

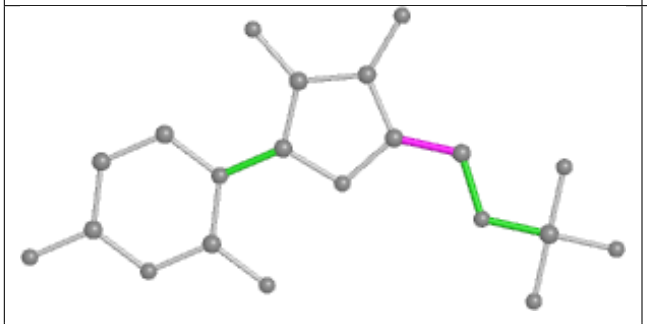
Ligand U5P D 227



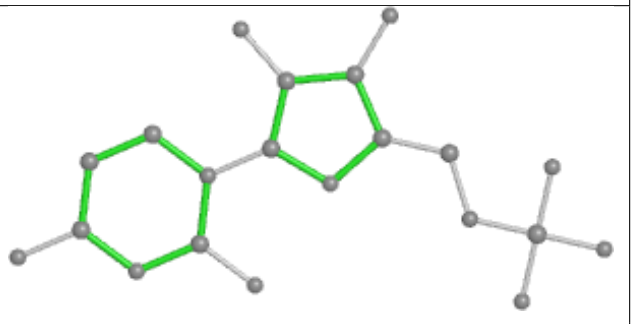
Bond lengths



Bond angles

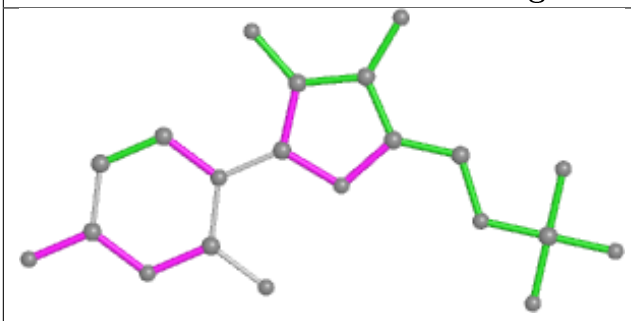


Torsions

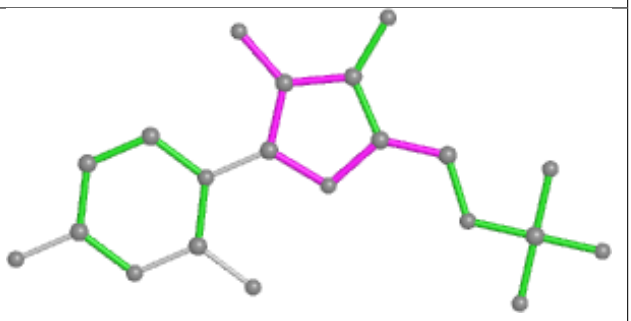


Rings

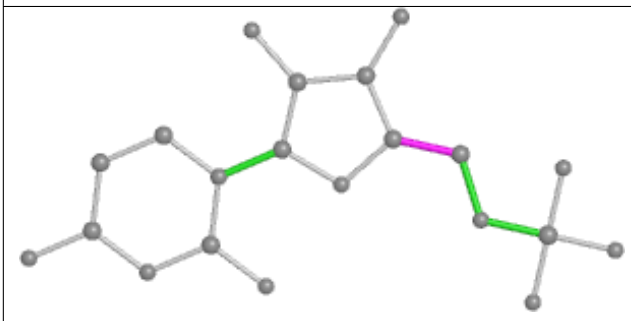
Ligand U5P E 227



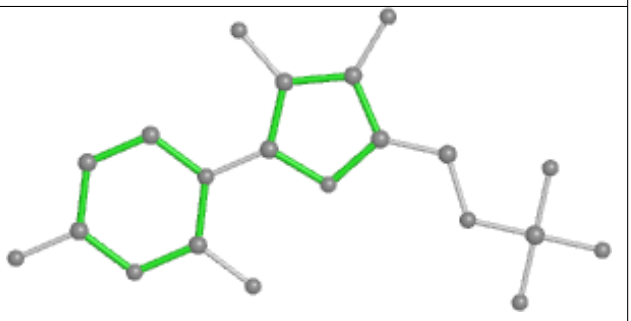
Bond lengths



Bond angles

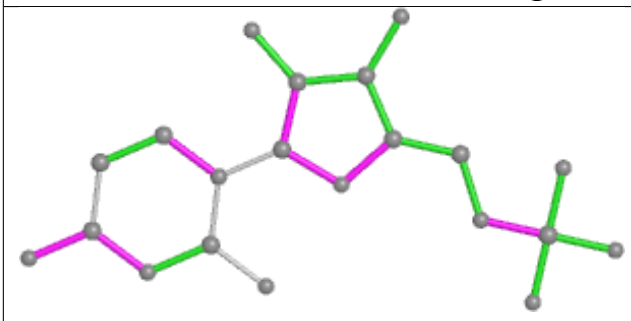


Torsions

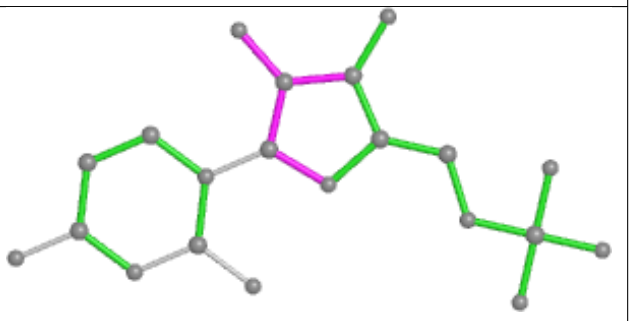


Rings

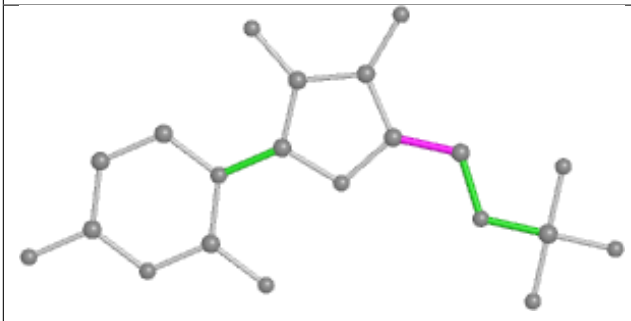
Ligand U5P F 227



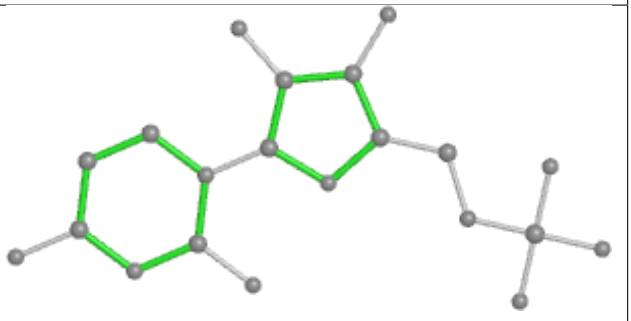
Bond lengths



Bond angles

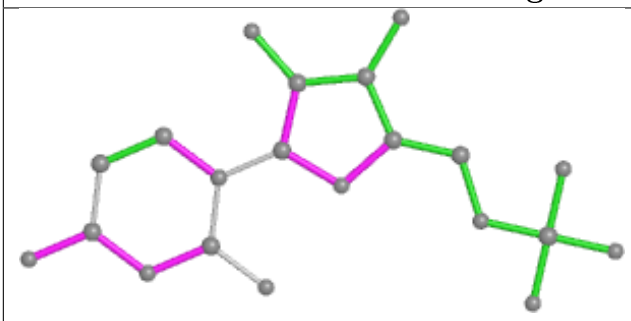


Torsions

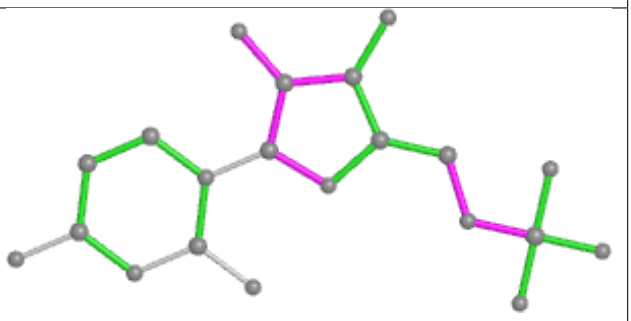


Rings

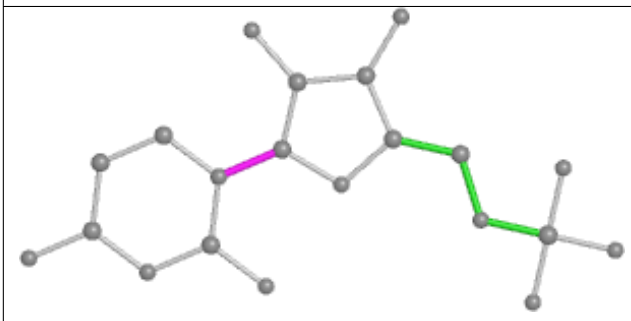
Ligand U5P C 227



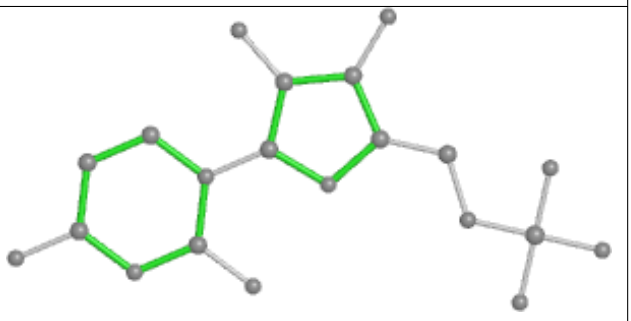
Bond lengths



Bond angles

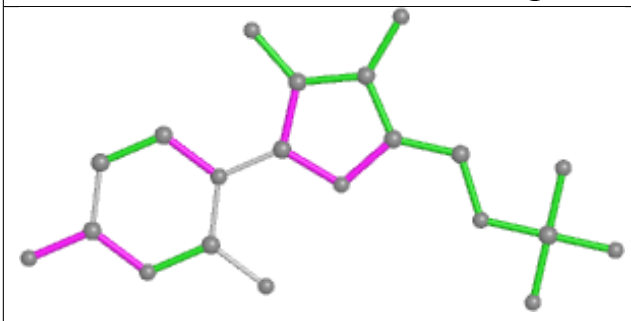


Torsions

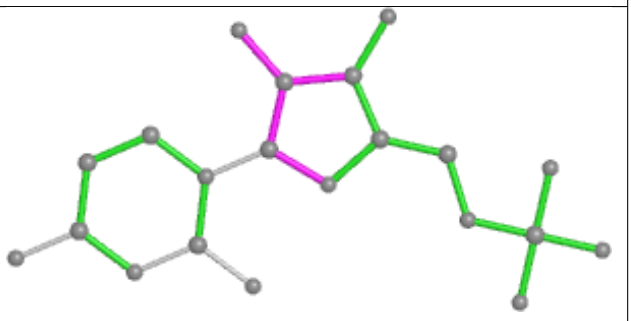


Rings

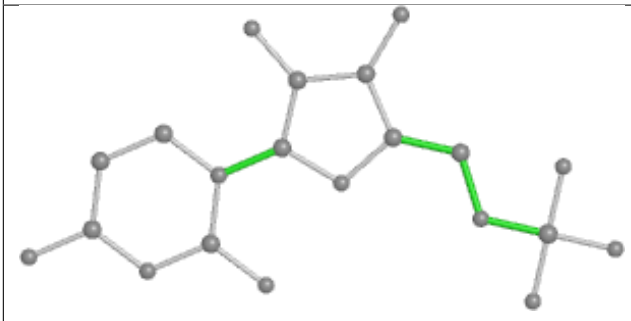
Ligand U5P A 227



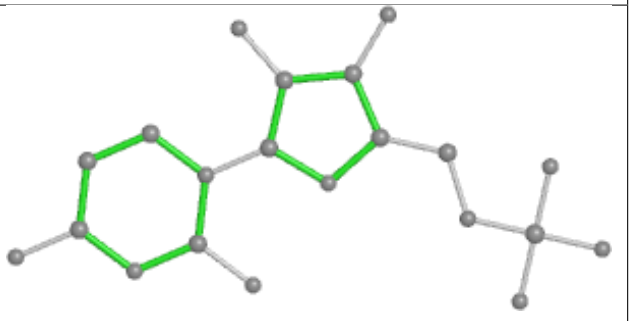
Bond lengths



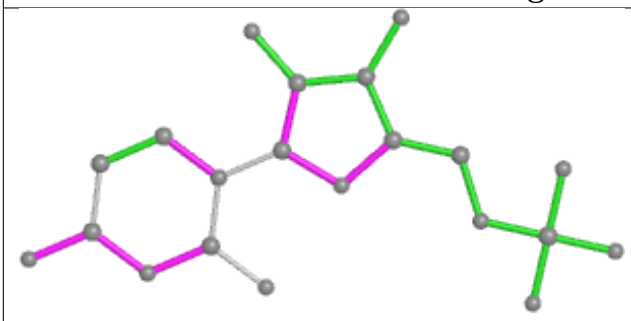
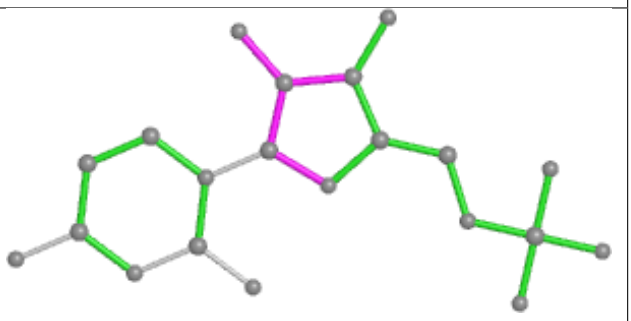
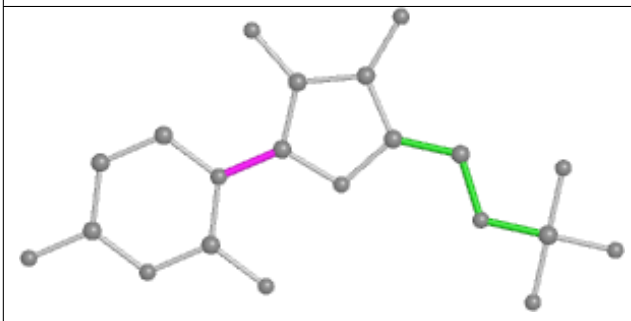
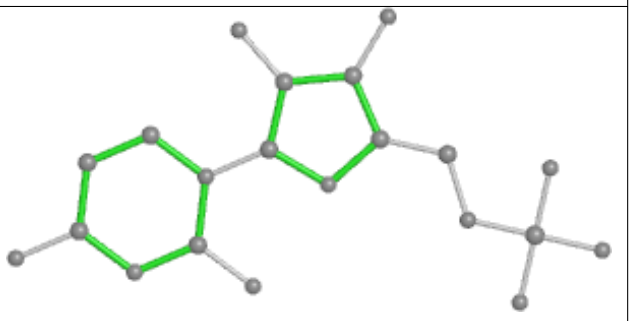
Bond angles



Torsions



Rings

Ligand U5P B 227	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	207/226 (91%)	0.81	33 (15%) 1 1	14, 30, 70, 85	0
1	B	214/226 (94%)	0.53	20 (9%) 8 7	17, 30, 55, 67	0
1	C	206/226 (91%)	0.89	37 (17%) 1 1	17, 31, 67, 88	0
1	D	226/226 (100%)	0.82	35 (15%) 2 1	15, 32, 65, 73	0
1	E	221/226 (97%)	0.75	30 (13%) 3 2	14, 28, 66, 72	0
1	F	208/226 (92%)	0.71	27 (12%) 3 3	14, 27, 58, 76	0
All	All	1282/1356 (94%)	0.75	182 (14%) 2 2	14, 30, 64, 88	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	VAL	8.7
1	C	151	ILE	7.7
1	F	181	TYR	7.5
1	C	164	GLN	7.3
1	C	152	TYR	6.8
1	C	150	ARG	6.5
1	D	152	TYR	6.4
1	A	170	LEU	6.2
1	E	173	SER	6.1
1	C	147	LYS	5.7
1	A	226	VAL	5.7
1	E	176	VAL	5.6
1	E	32	ASP	5.6
1	B	15	ASP	5.5
1	F	217	GLU	5.4
1	D	170	LEU	5.4
1	D	15	ASP	5.4
1	C	148	ASP	5.4
1	B	164	GLN	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	150	ARG	5.1
1	D	32	ASP	5.1
1	D	226	VAL	5.0
1	C	149	PRO	5.0
1	B	14	GLU	4.9
1	E	154	ASP	4.9
1	F	15	ASP	4.9
1	A	169	ILE	4.9
1	C	15	ASP	4.9
1	F	1	MET	4.8
1	A	203	ASN	4.7
1	E	153	ALA	4.7
1	A	147	LYS	4.7
1	A	33	ASN	4.7
1	D	154	ASP	4.7
1	E	172	GLY	4.7
1	D	85	ASP	4.6
1	A	167	ARG	4.6
1	E	15	ASP	4.5
1	B	32	ASP	4.5
1	A	164	GLN	4.5
1	B	150	ARG	4.4
1	F	169	ILE	4.4
1	C	14	GLU	4.4
1	C	1	MET	4.4
1	A	15	ASP	4.3
1	D	151	ILE	4.3
1	C	225	PRO	4.2
1	C	146	GLU	4.2
1	D	153	ALA	4.2
1	C	13	ASP	4.1
1	D	150	ARG	4.1
1	F	33	ASN	4.0
1	C	158	ILE	4.0
1	A	148	ASP	3.9
1	A	85	ASP	3.9
1	C	166	LEU	3.8
1	B	31	ALA	3.7
1	A	25	GLN	3.7
1	E	156	LYS	3.7
1	A	32	ASP	3.7
1	E	174	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	179	GLY	3.6
1	F	226	VAL	3.6
1	D	181	TYR	3.6
1	D	31	ALA	3.6
1	A	152	TYR	3.6
1	E	168	LYS	3.5
1	C	85	ASP	3.5
1	D	172	GLY	3.5
1	A	218	GLU	3.5
1	E	29	GLU	3.4
1	A	209	ARG	3.4
1	C	136	VAL	3.4
1	E	175	SER	3.4
1	E	223	ILE	3.4
1	D	217	GLU	3.4
1	D	155	VAL	3.4
1	A	149	PRO	3.4
1	A	153	ALA	3.4
1	D	149	PRO	3.3
1	D	17	VAL	3.3
1	A	145	TYR	3.3
1	C	217	GLU	3.2
1	F	32	ASP	3.2
1	E	171	GLU	3.2
1	B	168	LYS	3.2
1	B	154	ASP	3.2
1	B	1	MET	3.1
1	D	171	GLU	3.1
1	F	199	VAL	3.1
1	A	141	VAL	3.1
1	E	147	LYS	3.1
1	A	140	ASN	3.1
1	B	85	ASP	3.0
1	A	151	ILE	3.0
1	B	217	GLU	3.0
1	E	33	ASN	2.9
1	F	184	LEU	2.9
1	E	155	VAL	2.9
1	E	34	GLY	2.9
1	C	140	ASN	2.9
1	E	150	ARG	2.9
1	F	34	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	21	ILE	2.8
1	B	226	VAL	2.8
1	D	212	ASP	2.8
1	A	155	VAL	2.8
1	E	22	VAL	2.8
1	A	146	GLU	2.8
1	A	168	LYS	2.8
1	C	167	ARG	2.8
1	E	85	ASP	2.7
1	D	20	LEU	2.7
1	E	217	GLU	2.7
1	F	209	ARG	2.7
1	D	174	GLN	2.7
1	F	178	ALA	2.7
1	C	186	PRO	2.6
1	D	33	ASN	2.6
1	B	182	GLU	2.6
1	C	185	ASP	2.6
1	B	156	LYS	2.6
1	C	118	SER	2.6
1	B	10	LYS	2.6
1	F	218	GLU	2.5
1	F	28	LYS	2.5
1	A	165	ASP	2.5
1	D	29	GLU	2.5
1	D	16	ASN	2.5
1	D	35	PHE	2.5
1	E	226	VAL	2.5
1	F	18	ASP	2.5
1	E	205	ARG	2.4
1	F	35	PHE	2.4
1	A	210	ILE	2.4
1	C	184	LEU	2.4
1	C	133	LYS	2.4
1	C	31	ALA	2.4
1	F	223	ILE	2.4
1	A	185	ASP	2.4
1	D	173	SER	2.4
1	C	32	ASP	2.3
1	A	166	LEU	2.3
1	D	34	GLY	2.3
1	B	225	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	168	LYS	2.3
1	C	183	LEU	2.3
1	A	154	ASP	2.3
1	B	165	ASP	2.3
1	E	200	ILE	2.3
1	E	181	TYR	2.2
1	F	133	LYS	2.2
1	B	169	ILE	2.2
1	C	17	VAL	2.2
1	C	224	GLU	2.2
1	D	24	ARG	2.2
1	F	215	LYS	2.2
1	C	214	LEU	2.2
1	D	169	ILE	2.2
1	F	135	LEU	2.2
1	A	10	LYS	2.1
1	F	140	ASN	2.1
1	F	30	LEU	2.1
1	B	215	LYS	2.1
1	D	156	LYS	2.1
1	E	136	VAL	2.1
1	C	209	ARG	2.1
1	D	223	ILE	2.1
1	E	30	LEU	2.1
1	F	85	ASP	2.1
1	E	199	VAL	2.1
1	D	25	GLN	2.1
1	D	184	LEU	2.1
1	C	218	GLU	2.0
1	E	27	ILE	2.0
1	C	163	THR	2.0
1	A	205	ARG	2.0
1	F	222	ILE	2.0
1	C	162	THR	2.0
1	B	209	ARG	2.0
1	C	215	LYS	2.0
1	D	147	LYS	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 carbohydrates in this entry.

6.4 Ligands (i)

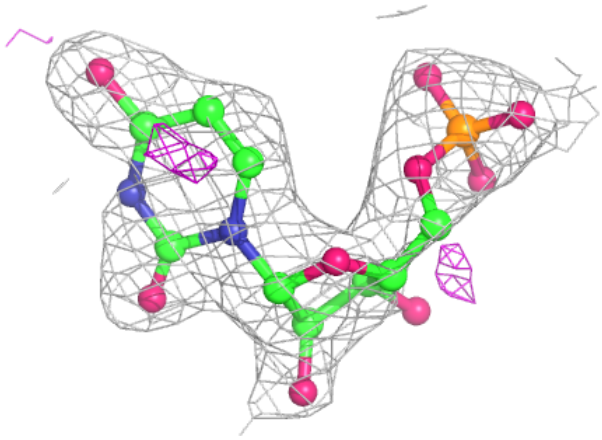
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

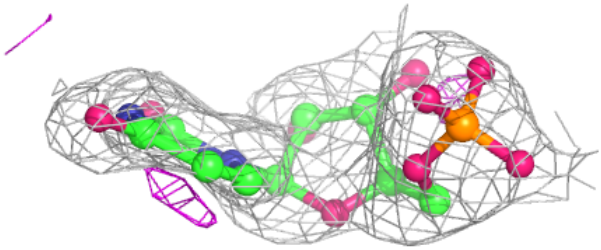
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	U5P	C	227	21/21	0.76	0.28	48,59,60,61	0
3	CD	B	232	1/1	0.80	0.08	131,131,131,131	0
2	U5P	B	227	21/21	0.87	0.19	30,43,47,49	0
2	U5P	A	227	21/21	0.91	0.16	26,32,37,39	0
4	MG	A	231	1/1	0.91	0.17	33,33,33,33	0
3	CD	A	230	1/1	0.92	0.03	102,102,102,102	0
2	U5P	E	227	21/21	0.93	0.13	22,26,29,30	0
3	CD	C	231	1/1	0.94	0.08	56,56,56,56	1
2	U5P	D	227	21/21	0.95	0.11	13,23,28,29	0
3	CD	B	234	1/1	0.96	0.07	61,61,61,61	1
2	U5P	F	227	21/21	0.96	0.12	18,23,28,32	0
3	CD	B	230	1/1	0.96	0.07	78,78,78,78	0
3	CD	B	231	1/1	0.97	0.04	80,80,80,80	0
3	CD	C	229	1/1	0.97	0.04	78,78,78,78	0
3	CD	F	229	1/1	0.98	0.06	52,52,52,52	0
3	CD	C	228	1/1	0.98	0.05	49,49,49,49	0
3	CD	E	229	1/1	0.98	0.07	47,47,47,47	0
3	CD	B	229	1/1	0.99	0.04	46,46,46,46	0
3	CD	B	233	1/1	0.99	0.04	45,45,45,45	0
3	CD	A	229	1/1	0.99	0.05	43,43,43,43	0
3	CD	D	228	1/1	0.99	0.03	41,41,41,41	0
3	CD	E	228	1/1	0.99	0.04	42,42,42,42	0
3	CD	F	228	1/1	0.99	0.04	38,38,38,38	0
3	CD	A	228	1/1	1.00	0.09	27,27,27,27	0
3	CD	B	228	1/1	1.00	0.09	23,23,23,23	0

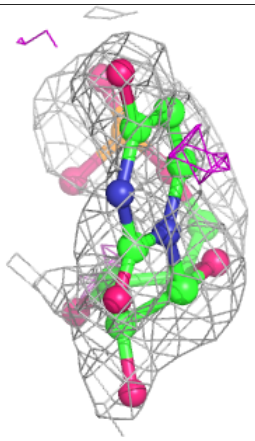
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U5P C 227:

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

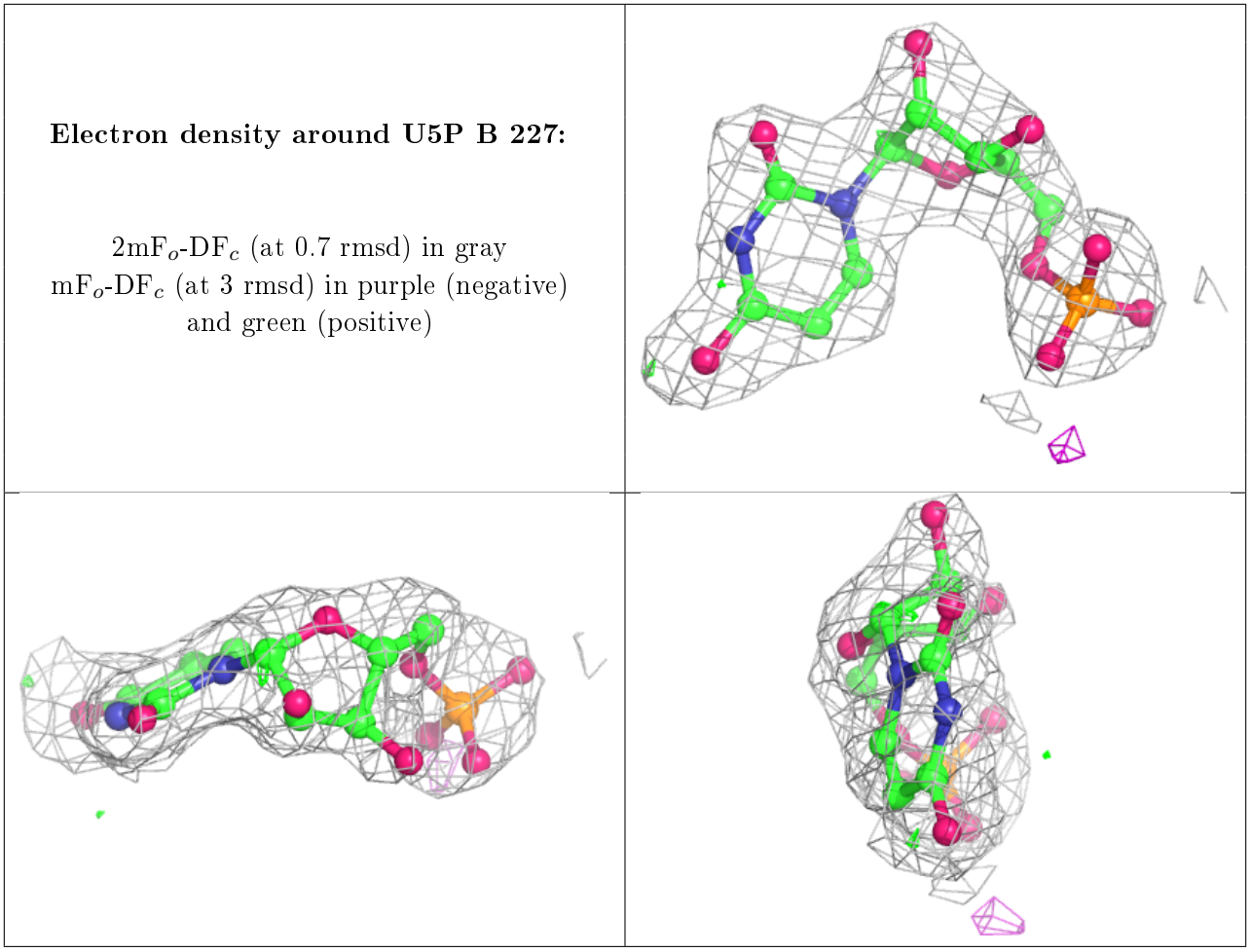






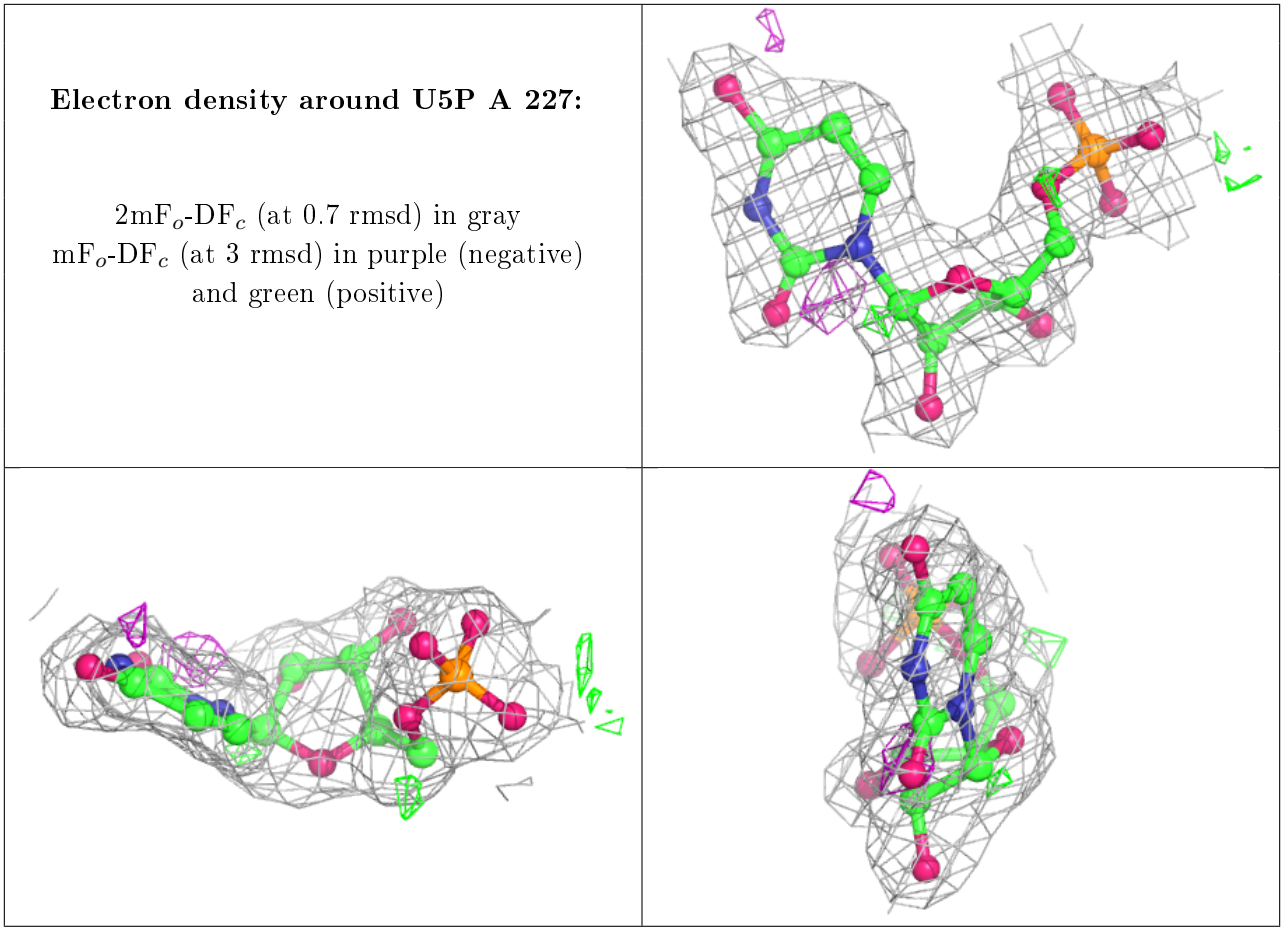
Electron density around U5P B 227:

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



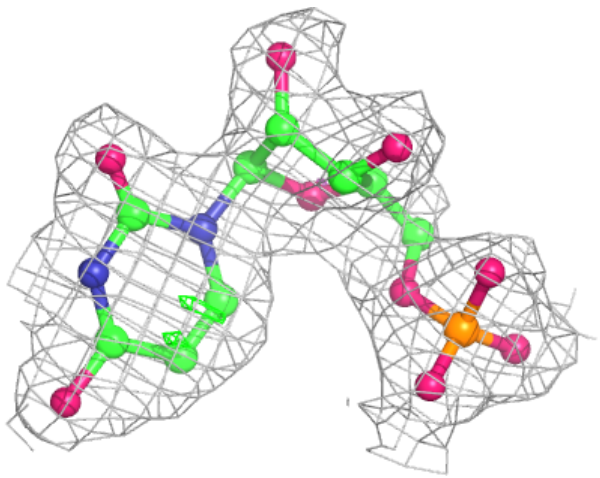
Electron density around U5P A 227:

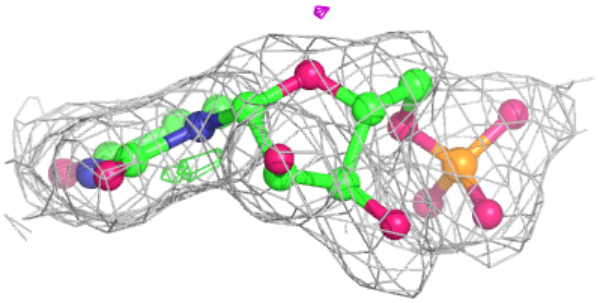
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around U5P E 227:

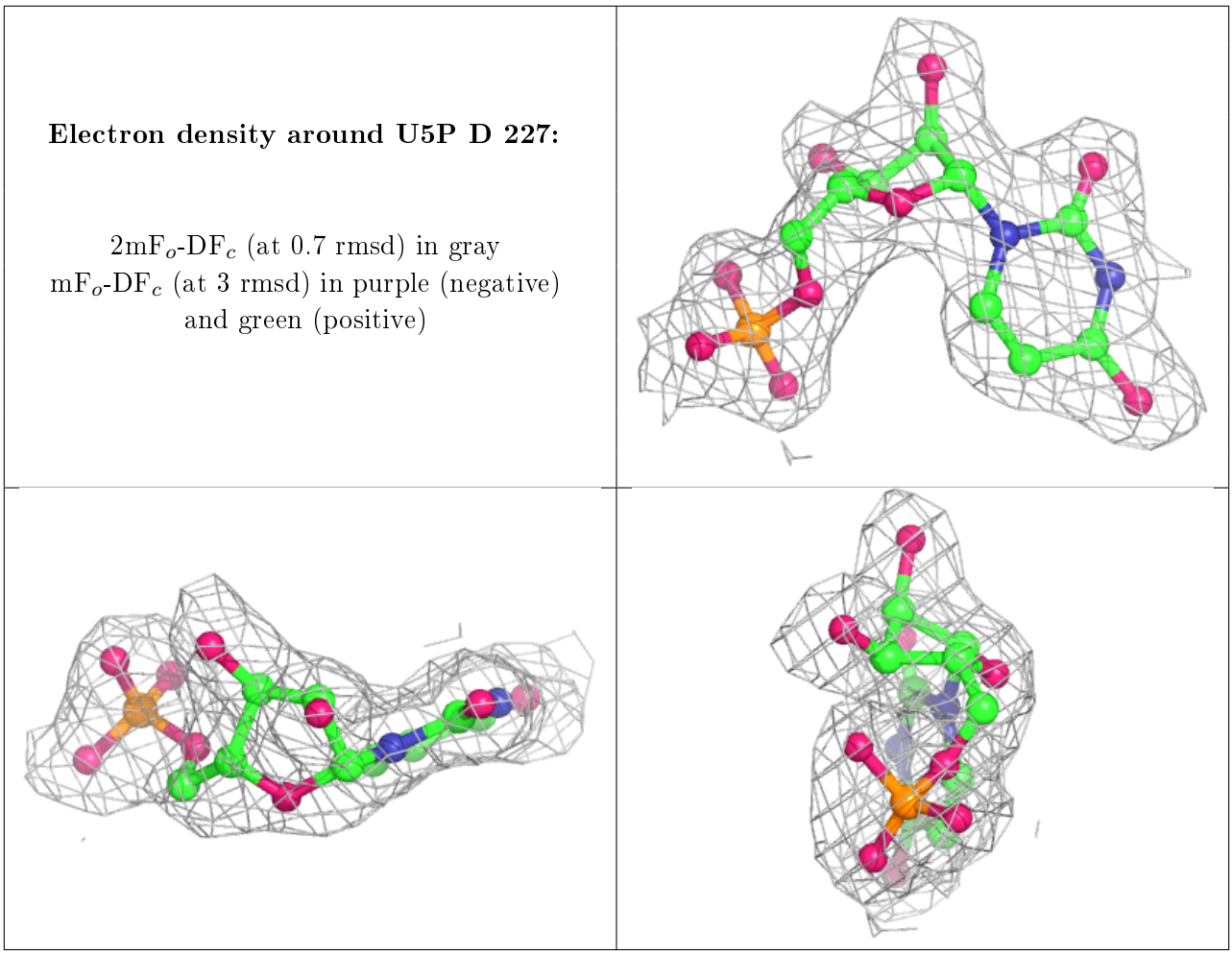
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





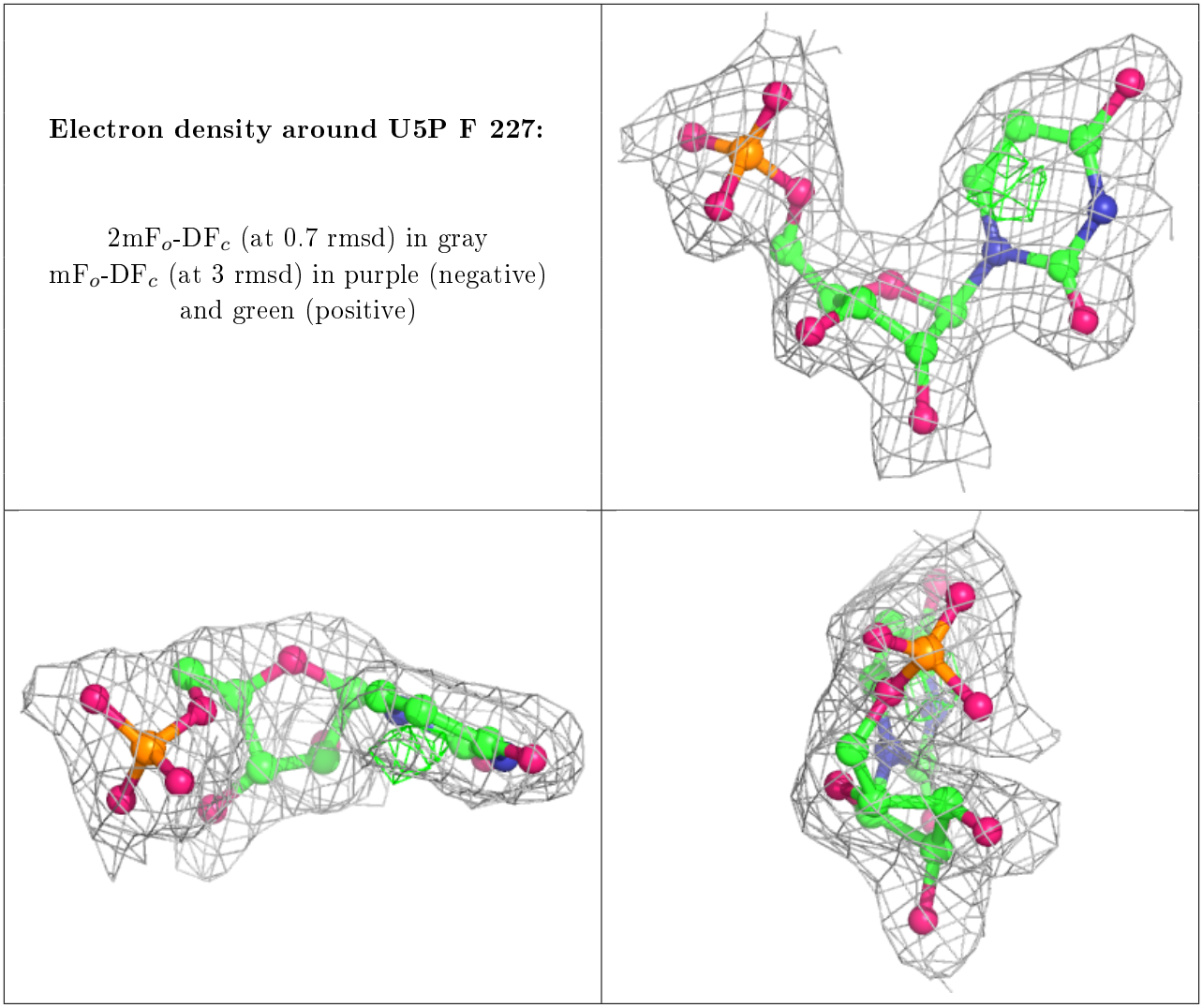
Electron density around U5P D 227:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.