Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 11:17 AM EDT

PDB ID	:	4KXU
Title	:	Human transketolase in covalent complex with donor ketose D-fructose-6-phosphate
Authors	:	Neumann, P.; Luedtke, S.; Ficner, R.; Tittmann, K.
Deposited on	:	2013-05-28
Resolution	:	0.98 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 (i) 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 (i)) were used in the production of this report:

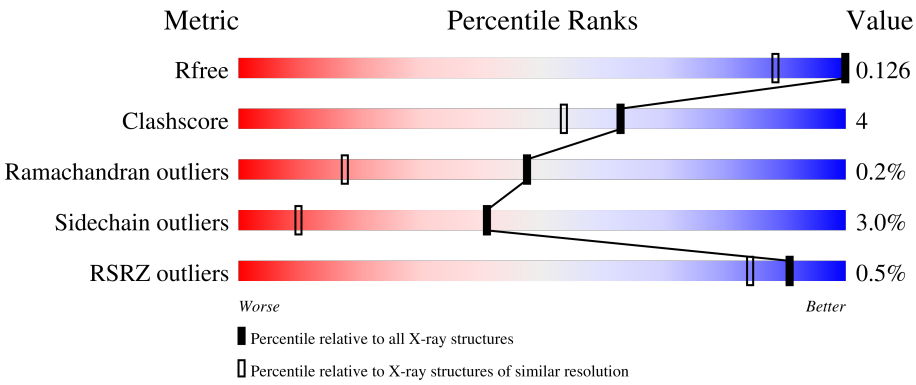
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 0.98 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	1166 (1.06-0.90)
Clashscore	141614	1241 (1.06-0.90)
Ramachandran outliers	138981	1159 (1.06-0.90)
Sidechain outliers	138945	1161 (1.06-0.90)
RSRZ outliers	127900	1132 (1.06-0.90)

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 <=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	637	85% 10% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1004[A]	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1005	-	X	-	-
2	EDO	A	1008	-	X	-	-
2	EDO	A	1011	-	X	-	-
2	EDO	A	1012	-	X	-	-
2	EDO	A	1013[A]	-	X	X	-
2	EDO	A	1013[B]	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6327 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.

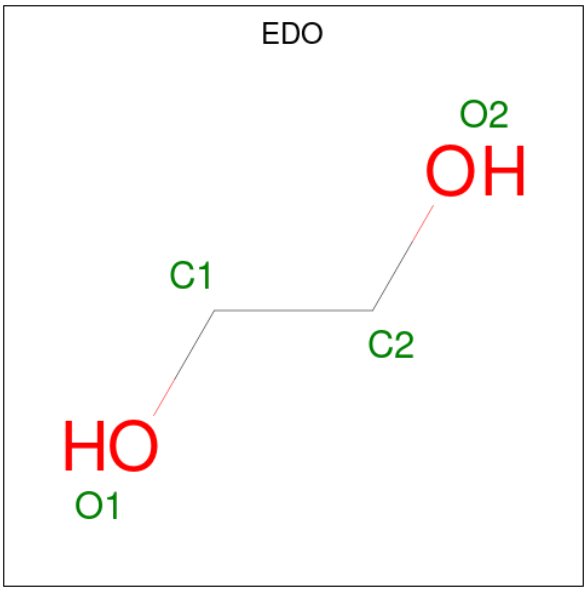
- Molecule 1 is a protein called Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	620	5360	3363	938	1030	29	0	76	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	LEU	-	expression tag	UNP P29401
A	625	VAL	-	expression tag	UNP P29401
A	626	PRO	-	expression tag	UNP P29401
A	627	ARG	-	expression tag	UNP P29401
A	628	GLY	-	expression tag	UNP P29401
A	629	SER	-	expression tag	UNP P29401
A	630	LEU	-	expression tag	UNP P29401
A	631	GLU	-	expression tag	UNP P29401
A	632	HIS	-	expression tag	UNP P29401
A	633	HIS	-	expression tag	UNP P29401
A	634	HIS	-	expression tag	UNP P29401
A	635	HIS	-	expression tag	UNP P29401
A	636	HIS	-	expression tag	UNP P29401
A	637	HIS	-	expression tag	UNP P29401

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 8	C 4	O 4	0	1
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 8	C 4	O 4	0	1

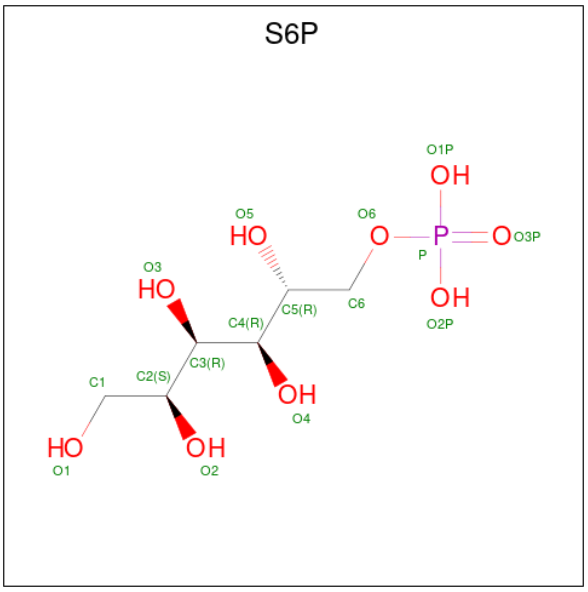
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

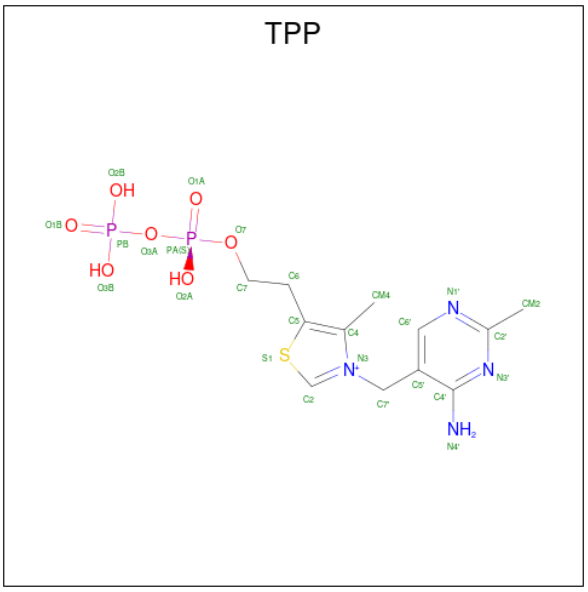
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	1	1	1	0	0

- Molecule 5 is D-SORBITOL-6-PHOSPHATE (three-letter code: S6P) (formula: $C_6H_{15}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	A	1	16	6	9	1	0	1

- Molecule 6 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
6	A	1	26	12	4	7	2	1	0	0

- Molecule 7 is water.

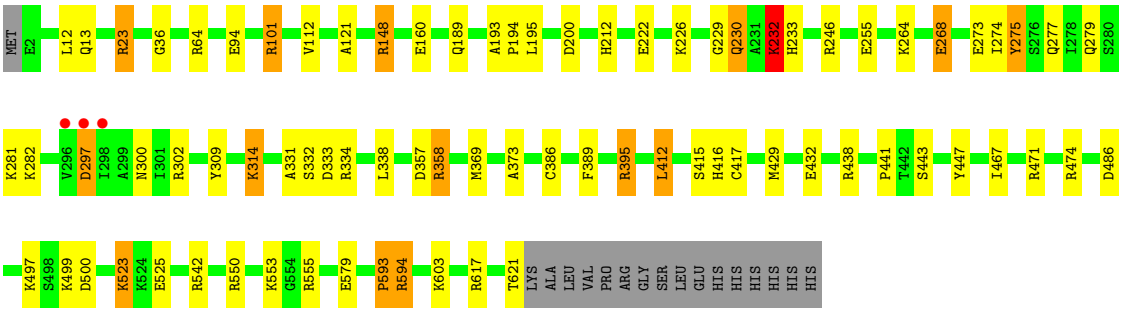
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	820	871	871	0	119

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: Transketolase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.76Å 85.88Å 72.99Å 90.00° 125.31° 90.00°	Depositor
Resolution (Å)	30.00 – 0.98 46.42 – 0.98	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-0.98) 88.2 (46.42-0.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 0.98Å)	Xtriage
Refinement program	SHELX, SHELXL	Depositor
R, R_{free}	0.102 , 0.122 0.109 , 0.126	Depositor DCC
R_{free} test set	3007 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	6.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 70.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6327	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, MG, EDO, NA, S6P

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	0.72	1/5463 (0.0%)	1.18	51/7388 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	GLU	CD-OE2	5.18	1.31	1.25

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	232[A]	LYS	CA-CB-CG	11.23	138.11	113.40
1	A	232[B]	LYS	CA-CB-CG	11.23	138.11	113.40
1	A	148	ARG	NE-CZ-NH2	10.67	125.64	120.30
1	A	412[A]	LEU	CA-CB-CG	10.65	139.80	115.30
1	A	412[B]	LEU	CA-CB-CG	10.65	139.80	115.30
1	A	621	THR	CA-C-O	10.18	141.49	120.10
1	A	121	ALA	O-C-N	-9.22	107.94	122.70
1	A	334	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	A	200[A]	ASP	CB-CG-OD1	8.26	125.74	118.30
1	A	200[B]	ASP	CB-CG-OD1	8.26	125.74	118.30
1	A	555	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	395[A]	ARG	NE-CZ-NH1	7.54	124.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	395[B]	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	486	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	617	ARG	CD-NE-CZ	7.21	133.70	123.60
1	A	23	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	497	LYS	CD-CE-NZ	7.19	128.24	111.70
1	A	121	ALA	CA-C-N	7.06	132.73	117.20
1	A	332	SER	N-CA-CB	-6.96	100.06	110.50
1	A	438	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	542	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	148	ARG	NH1-CZ-NH2	-6.69	112.04	119.40
1	A	268	GLU	OE1-CD-OE2	6.64	131.27	123.30
1	A	474	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	23	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	357	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	A	334	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	246	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	579	GLU	OE1-CD-OE2	-6.21	115.84	123.30
1	A	594	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	474	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	297[A]	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	297[B]	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	230[A]	GLN	CB-CG-CD	5.74	126.52	111.60
1	A	230[B]	GLN	CB-CG-CD	5.74	126.52	111.60
1	A	121	ALA	C-N-CA	5.58	135.64	121.70
1	A	273[A]	GLU	CG-CD-OE1	5.57	129.43	118.30
1	A	273[B]	GLU	CG-CD-OE1	5.57	129.43	118.30
1	A	358	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	309[A]	TYR	CB-CG-CD2	5.48	124.29	121.00
1	A	309[B]	TYR	CB-CG-CD2	5.48	124.29	121.00
1	A	64	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	333	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	389	PHE	CB-CG-CD1	5.30	124.51	120.80
1	A	229	GLY	O-C-N	-5.29	114.24	122.70
1	A	275[A]	TYR	CZ-CE2-CD2	-5.28	115.05	119.80
1	A	275[B]	TYR	CZ-CE2-CD2	-5.28	115.05	119.80
1	A	331	ALA	CB-CA-C	-5.26	102.20	110.10
1	A	333	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	A	550	ARG	CD-NE-CZ	5.10	130.74	123.60
1	A	101	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	ARG	Sidechain
1	A	148	ARG	Sidechain
1	A	23	ARG	Sidechain
1	A	302	ARG	Sidechain
1	A	358	ARG	Sidechain
1	A	395[A]	ARG	Sidechain

5.2 Too-close contacts (i)

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	5360	0	5290	40	0
2	A	52	0	73	10	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	16	0	12	2	0
6	A	26	0	15	1	0
7	A	871	0	0	22	1
All	All	6327	0	5390	47	1

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 4.

All (47) 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)
2:A:1005:EDO:C1	2:A:1005:EDO:C2	1.85	1.55
2:A:1013[B]:EDO:C1	2:A:1013[B]:EDO:C2	1.83	1.52
2:A:1010:EDO:O2	2:A:1010:EDO:C2	1.66	1.41
1:A:275[B]:TYR:CE1	7:A:7764:HOH:O	2.01	1.12
2:A:1013[A]:EDO:C1	2:A:1013[A]:EDO:C2	2.31	1.07
1:A:297[B]:ASP:OD1	7:A:7606:HOH:O	2.02	0.78
1:A:264[A]:LYS:HG3	7:A:7724[A]:HOH:O	1.86	0.76
1:A:277[B]:GLN:OE1	7:A:7549:HOH:O	2.11	0.68
1:A:233[B]:HIS:HB2	7:A:7751:HOH:O	1.97	0.63
1:A:369:MET:CE	1:A:386[B]:CYS:HG	2.13	0.62
1:A:268:GLU:HG3	7:A:7632[A]:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275[B]:TYR:CZ	7:A:7764:HOH:O	2.34	0.61
1:A:297[B]:ASP:CG	7:A:7606:HOH:O	2.38	0.60
1:A:441[B]:PRO:HB3	7:A:7774:HOH:O	2.03	0.58
1:A:275[B]:TYR:HE1	7:A:7764:HOH:O	1.62	0.57
1:A:189:GLN:HE22	5:A:1014[A]:S6P:H3	1.70	0.57
1:A:193:ALA:HB1	7:A:7799[A]:HOH:O	2.05	0.56
1:A:603:LYS:HE3	7:A:7486:HOH:O	2.06	0.56
1:A:195:LEU:H	2:A:1013[A]:EDO:C2	2.19	0.55
1:A:12:LEU:HD13	1:A:222[B]:GLU:OE1	2.09	0.53
2:A:1013[B]:EDO:C2	2:A:1013[B]:EDO:O1	2.55	0.52
1:A:222[B]:GLU:HG2	7:A:7140[B]:HOH:O	2.09	0.52
1:A:499:LYS:HD3	7:A:7692[B]:HOH:O	2.10	0.52
1:A:297[B]:ASP:OD2	7:A:7606:HOH:O	2.19	0.51
1:A:94[B]:GLU:HG3	7:A:7485:HOH:O	2.10	0.50
1:A:212:HIS:CD2	1:A:232[A]:LYS:HD3	2.47	0.50
1:A:232[B]:LYS:NZ	7:A:7728:HOH:O	2.44	0.50
1:A:255[B]:GLU:OE1	7:A:7210:HOH:O	2.20	0.50
2:A:1010:EDO:C2	2:A:1010:EDO:HO2	2.10	0.50
1:A:194:PRO:HB2	2:A:1013[A]:EDO:H22	1.93	0.49
1:A:369:MET:HG2	1:A:386[B]:CYS:SG	2.53	0.49
1:A:314:LYS:N	1:A:314:LYS:HD3	2.28	0.49
1:A:415[B]:SER:O	1:A:416:HIS:HB2	2.11	0.49
1:A:195:LEU:HG	2:A:1013[A]:EDO:H21	1.95	0.47
1:A:13:GLN:NE2	1:A:279[A]:GLN:HG3	2.30	0.47
1:A:222[B]:GLU:HG3	7:A:7543:HOH:O	2.16	0.46
1:A:523:LYS:NZ	7:A:7699:HOH:O	2.50	0.45
1:A:429:MET:SD	1:A:593[B]:PRO:HG2	2.58	0.44
1:A:226:LYS:HE3	7:A:7120[B]:HOH:O	2.19	0.43
5:A:1014[A]:S6P:O2	6:A:1015:TPP:H7'2	2.18	0.43
1:A:232[A]:LYS:HG3	7:A:7751:HOH:O	2.19	0.42
1:A:373:ALA:HB2	1:A:386[A]:CYS:SG	2.59	0.42
1:A:274:ILE:O	1:A:277[B]:GLN:HB2	2.21	0.41
1:A:443:SER:HA	1:A:467[A]:ILE:O	2.20	0.41
1:A:417:CYS:HB2	1:A:471:ARG:CZ	2.51	0.41
1:A:338:LEU:HB2	1:A:386[B]:CYS:HB2	2.03	0.40
1:A:36:GLY:H	2:A:1001:EDO:C1	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:7768:HOH:O	7:A:7768:HOH:O[2_556]	2.17	0.03

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	697/637 (109%)	672 (96%)	23 (3%)	2 (0%)	41 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	593[A]	PRO
1	A	593[B]	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	579/518 (112%)	560 (97%)	19 (3%)	38 8

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	VAL
1	A	230[A]	GLN
1	A	230[B]	GLN
1	A	232[A]	LYS

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Mol	Chain	Res	Type
1	A	232[B]	LYS
1	A	281	LYS
1	A	282	LYS
1	A	300[A]	ASN
1	A	300[B]	ASN
1	A	314	LYS
1	A	412[A]	LEU
1	A	412[B]	LEU
1	A	432	GLU
1	A	447	TYR
1	A	500	ASP
1	A	523	LYS
1	A	525	GLU
1	A	553	LYS
1	A	594	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	189	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\#\|Z\| > 2$
6	TPP	A	1015	5,3	22,27,27	1.22	3 (13%)	29,40,40	1.08	3 (10%)
2	EDO	A	1002	-	3,3,3	3.14	2 (66%)	2,2,2	0.60	0
2	EDO	A	1012	-	3,3,3	2.41	2 (66%)	2,2,2	1.97	1 (50%)
2	EDO	A	1013[A]	-	3,3,3	12.88	2 (66%)	2,2,2	2.11	1 (50%)
2	EDO	A	1005	-	3,3,3	3.64	2 (66%)	2,2,2	1.04	0
5	S6P	A	1014[A]	6	15,15,15	1.45	3 (20%)	21,21,21	1.18	1 (4%)
2	EDO	A	1004[B]	-	3,3,3	15.44	1 (33%)	2,2,2	3.17	1 (50%)
2	EDO	A	1001	-	3,3,3	0.84	0	2,2,2	1.08	0
2	EDO	A	1010	-	3,3,3	2.89	1 (33%)	2,2,2	1.70	0
2	EDO	A	1007	-	3,3,3	0.47	0	2,2,2	0.43	0
2	EDO	A	1011	-	3,3,3	1.69	1 (33%)	2,2,2	3.88	2 (100%)
2	EDO	A	1013[B]	-	3,3,3	3.49	3 (100%)	2,2,2	1.33	0
2	EDO	A	1008	-	3,3,3	2.57	2 (66%)	2,2,2	2.24	2 (100%)
2	EDO	A	1004[A]	-	3,3,3	2.55	2 (66%)	2,2,2	1.78	1 (50%)
2	EDO	A	1003	-	3,3,3	0.93	0	2,2,2	0.38	0

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
6	TPP	A	1015	5,3	-	2/16/17/17	0/2/2/2
2	EDO	A	1002	-	-	0/1/1/1	-
2	EDO	A	1012	-	-	0/1/1/1	-
2	EDO	A	1013[A]	-	-	0/1/1/1	-
2	EDO	A	1005	-	-	1/1/1/1	-
5	S6P	A	1014[A]	6	-	3/20/20/20	-
2	EDO	A	1004[B]	-	-	0/1/1/1	-
2	EDO	A	1001	-	-	0/1/1/1	-
2	EDO	A	1010	-	-	0/1/1/1	-
2	EDO	A	1007	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	1011	-	-	1/1/1/1	-
2	EDO	A	1013[B]	-	-	0/1/1/1	-
2	EDO	A	1008	-	-	0/1/1/1	-
2	EDO	A	1004[A]	-	-	0/1/1/1	-
2	EDO	A	1003	-	-	0/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004[B]	EDO	O2-C2	26.74	2.80	1.42
2	A	1013[A]	EDO	O2-C2	-18.83	0.44	1.42
2	A	1013[A]	EDO	C2-C1	11.87	2.31	1.48
2	A	1005	EDO	C2-C1	5.35	1.85	1.48
2	A	1013[B]	EDO	C2-C1	5.02	1.83	1.48
2	A	1010	EDO	O2-C2	4.80	1.66	1.42
2	A	1002	EDO	O1-C1	-4.73	1.17	1.42
2	A	1012	EDO	O2-C2	3.38	1.59	1.42
2	A	1005	EDO	O1-C1	3.31	1.59	1.42
2	A	1004[A]	EDO	C2-C1	3.20	1.70	1.48
2	A	1008	EDO	C2-C1	3.15	1.70	1.48
6	A	1015	TPP	C4'-N3'	3.08	1.39	1.35
5	A	1014[A]	S6P	C2-C3	3.01	1.59	1.53
2	A	1008	EDO	O2-C2	-2.76	1.27	1.42
2	A	1002	EDO	C2-C1	2.62	1.66	1.48
2	A	1013[B]	EDO	O2-C2	-2.60	1.28	1.42
2	A	1011	EDO	O2-C2	2.57	1.55	1.42
5	A	1014[A]	S6P	O3-C3	-2.41	1.37	1.43
2	A	1004[A]	EDO	O1-C1	2.40	1.54	1.42
6	A	1015	TPP	C2'-N1'	2.37	1.38	1.34
5	A	1014[A]	S6P	C5-C4	2.33	1.57	1.53
6	A	1015	TPP	C4-N3	2.15	1.41	1.39
2	A	1013[B]	EDO	O1-C1	2.13	1.53	1.42
2	A	1012	EDO	C2-C1	2.03	1.62	1.48

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1004[B]	EDO	O2-C2-C1	-4.16	82.01	111.91
2	A	1011	EDO	O2-C2-C1	-3.89	83.94	111.91
2	A	1011	EDO	O1-C1-C2	3.87	139.78	111.91
2	A	1013[A]	EDO	O1-C1-C2	-2.93	90.80	111.91
5	A	1014[A]	S6P	P-O6-C6	2.82	126.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1008	EDO	O1-C1-C2	-2.31	95.32	111.91
6	A	1015	TPP	CM2-C2'-N3'	2.26	120.69	117.15
6	A	1015	TPP	CM4-C4-N3	-2.25	119.67	122.53
2	A	1008	EDO	O2-C2-C1	2.17	127.55	111.91
6	A	1015	TPP	C5-C4-N3	2.16	111.89	107.57
2	A	1004[A]	EDO	O1-C1-C2	-2.11	96.74	111.91
2	A	1012	EDO	O1-C1-C2	2.08	126.86	111.91

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1014[A]	S6P	C6-O6-P-O1P
5	A	1014[A]	S6P	C6-O6-P-O2P
2	A	1011	EDO	O1-C1-C2-O2
5	A	1014[A]	S6P	C6-O6-P-O3P
6	A	1015	TPP	PA-O3A-PB-O2B
6	A	1015	TPP	C4-C5-C6-C7
2	A	1007	EDO	O1-C1-C2-O2
2	A	1005	EDO	O1-C1-C2-O2

There are no ring outliers.

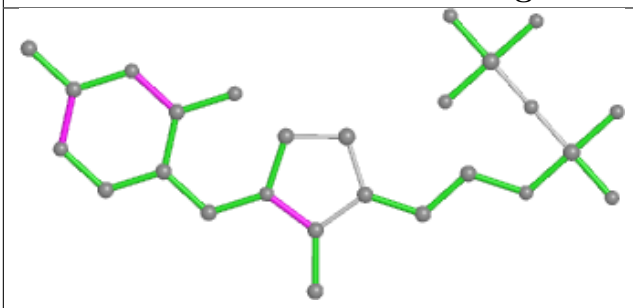
7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1015	TPP	1	0
2	A	1013[A]	EDO	4	0
2	A	1005	EDO	1	0
5	A	1014[A]	S6P	2	0
2	A	1001	EDO	1	0
2	A	1010	EDO	2	0
2	A	1013[B]	EDO	2	0

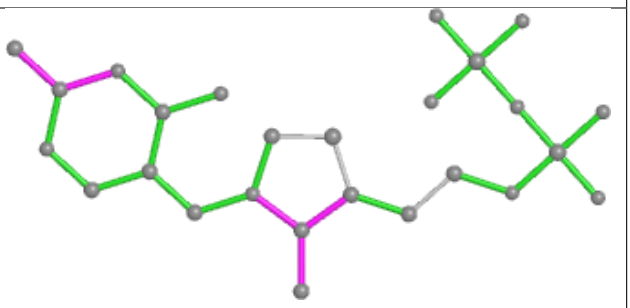
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

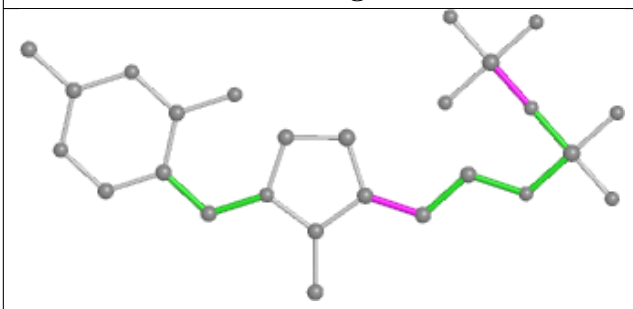
Ligand TPP A 1015



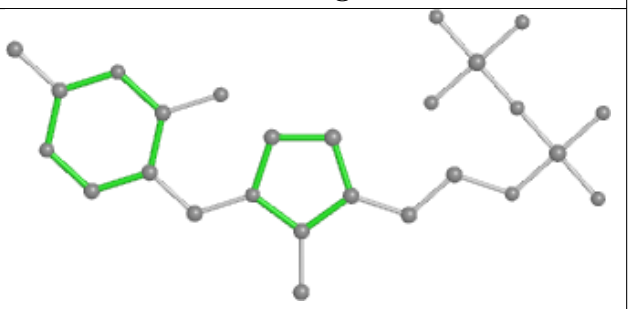
Bond lengths



Bond angles

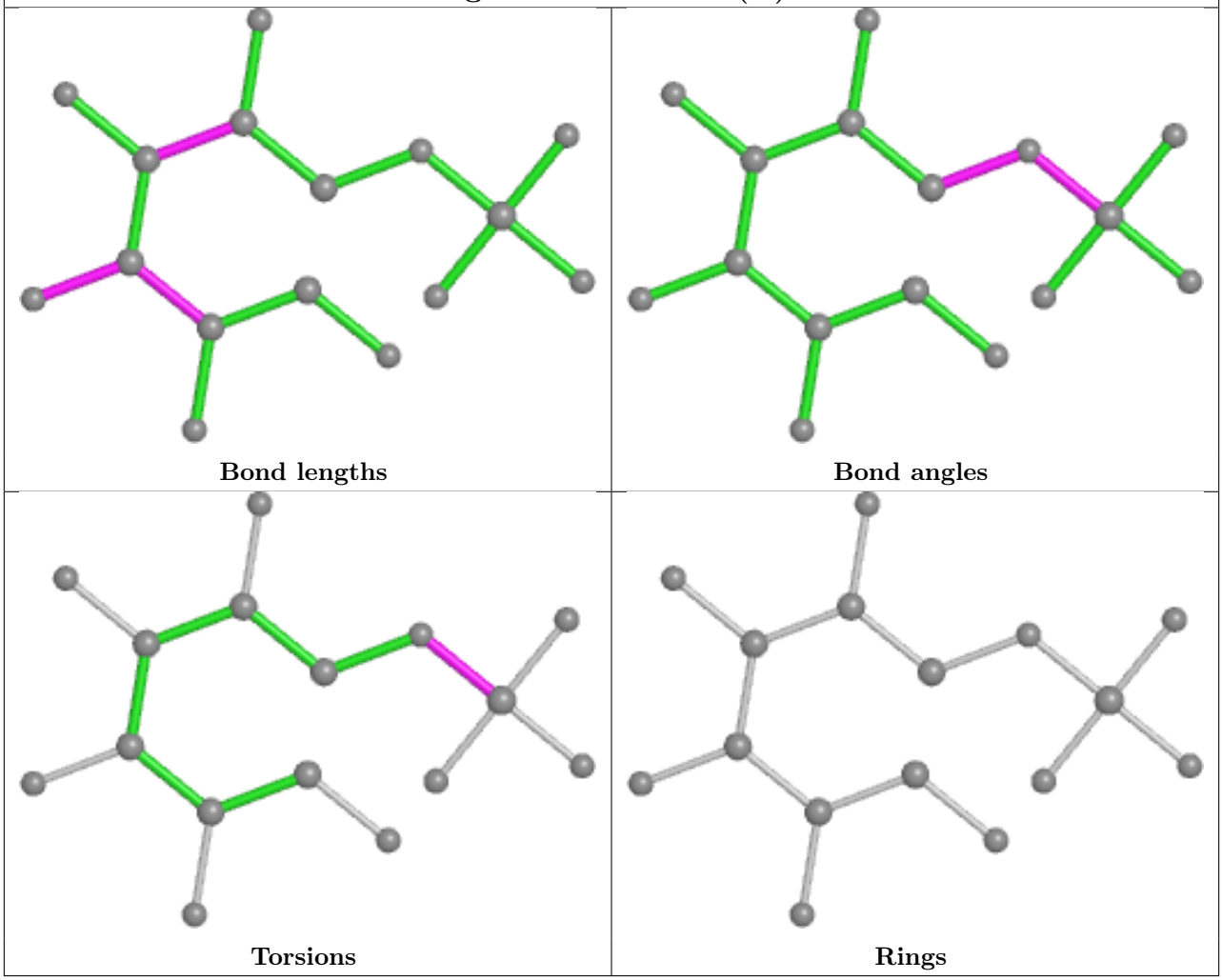


Torsions



Rings

Ligand S6P A 1014 (A)



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	620/637 (97%)	-0.59	3 (0%)	91	84	4, 7, 29, 90	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298	ILE	3.7
1	A	297[A]	ASP	2.2
1	A	296	VAL	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 monosaccharides 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(Å^2)	Q<0.9
2	EDO	A	1007	4/4	0.77	0.21	17,18,41,59	0
2	EDO	A	1012	4/4	0.84	0.10	29,34,40,41	0
2	EDO	A	1011	4/4	0.91	0.09	21,22,38,39	0
2	EDO	A	1008	4/4	0.94	0.10	15,21,23,25	0

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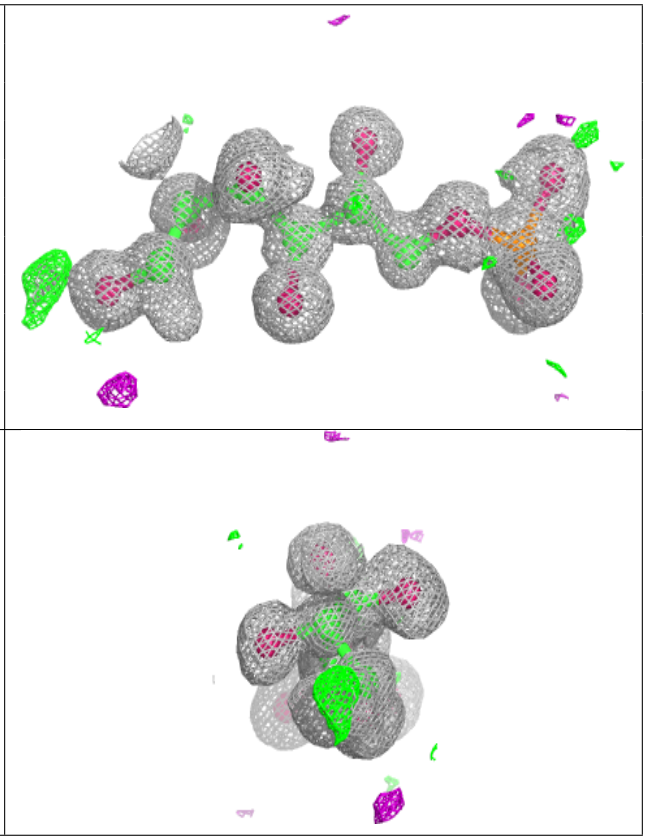
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	A	1004[B]	4/4	0.97	0.10	8,18,25,52	4
2	EDO	A	1010	4/4	0.97	0.12	11,22,24,26	0
2	EDO	A	1005	4/4	0.97	0.07	7,12,12,14	0
2	EDO	A	1004[A]	4/4	0.97	0.10	11,13,14,19	4
2	EDO	A	1001	4/4	0.98	0.07	9,14,14,24	0
2	EDO	A	1002	4/4	0.98	0.06	7,12,12,13	0
2	EDO	A	1013[A]	4/4	0.98	0.13	4,6,7,18	4
2	EDO	A	1013[B]	4/4	0.98	0.13	6,7,8,9	4
2	EDO	A	1003	4/4	0.99	0.05	8,12,12,13	0
5	S6P	A	1014[A]	16/16	0.99	0.04	5,6,9,9	16
4	NA	A	1009	1/1	1.00	0.02	6,6,6,6	0
3	MG	A	1006	1/1	1.00	0.02	3,3,3,3	0
6	TPP	A	1015	26/26	1.00	0.04	3,4,5,6	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.

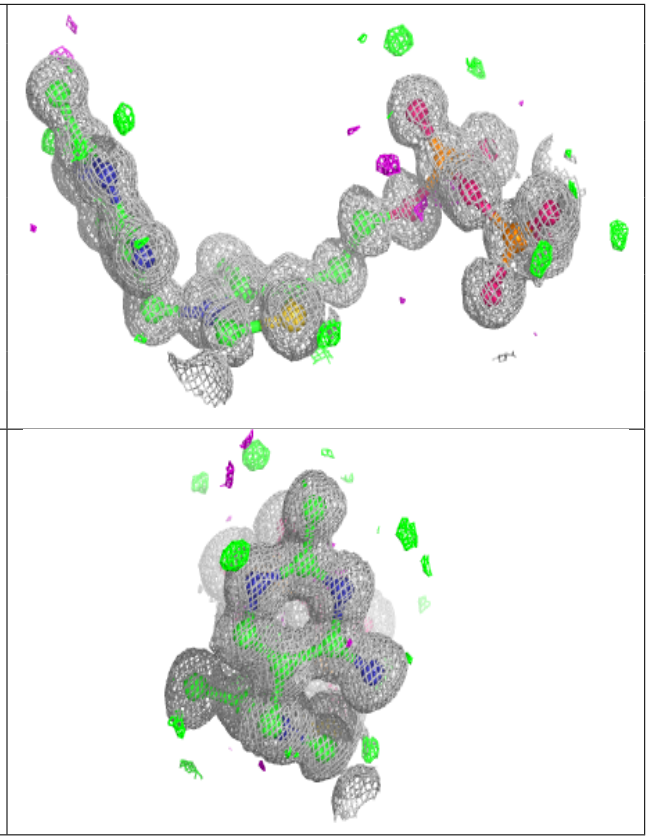
Electron density around S6P A 1014 (A):

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 TPP A 1015:

$2mF_o$-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.