Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 03:08 am GMT

PDB ID	:	2VK8
Title	:	Crystal structure of the Saccharomyces cerevisiae pyruvate decarboxylase variant E477Q in complex with its substrate
Authors	:	Kutter, S.; Weik, M.; Weiss, M.S.; Konig, S.
Deposited on	:	2007-12-17
Resolution	:	1.42 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:

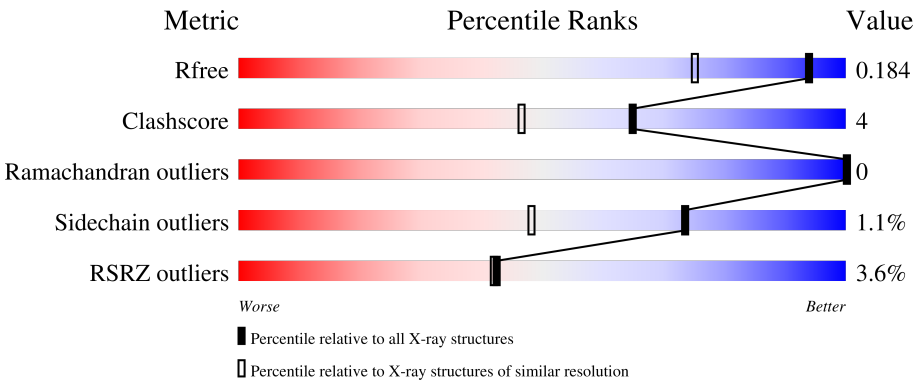
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.42 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	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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	563	5% 93% 7%
1	B	563	% 91% 8% •
1	C	563	4% 93% 7%
1	D	563	4% 92% 8%

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
4	2OP	A	1566	-	-	X	-
4	2OP	D	1566	X	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19242 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.

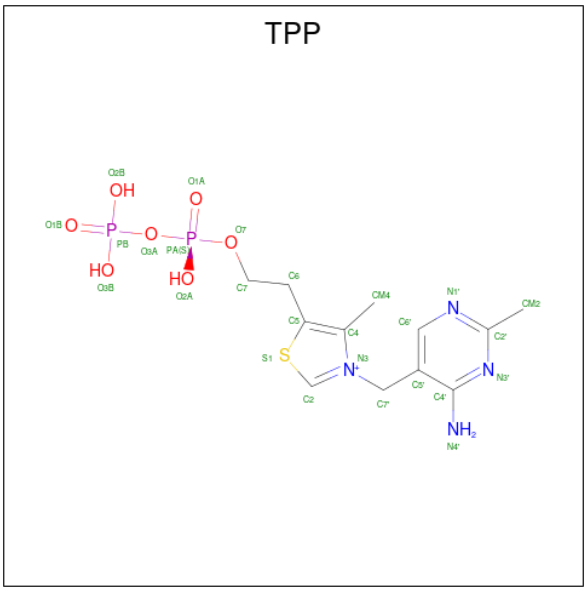
- Molecule 1 is a protein called PYRUVATE DECARBOXYLASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	562	4323	2760	725	822	16	0	0	0
1	B	562	4323	2760	725	822	16	0	0	0
1	C	562	4323	2760	725	822	16	0	0	0
1	D	562	4323	2760	725	822	16	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	477	GLN	GLU	engineered mutation	UNP P06169
B	477	GLN	GLU	engineered mutation	UNP P06169
C	477	GLN	GLU	engineered mutation	UNP P06169
D	477	GLN	GLU	engineered mutation	UNP P06169
A	206	VAL	ALA	conflict	UNP P06169
A	208	ASP	VAL	conflict	UNP P06169
A	538	VAL	ILE	conflict	UNP P06169
B	206	VAL	ALA	conflict	UNP P06169
B	208	ASP	VAL	conflict	UNP P06169
B	538	VAL	ILE	conflict	UNP P06169
C	206	VAL	ALA	conflict	UNP P06169
C	208	ASP	VAL	conflict	UNP P06169
C	538	VAL	ILE	conflict	UNP P06169
D	206	VAL	ALA	conflict	UNP P06169
D	208	ASP	VAL	conflict	UNP P06169
D	538	VAL	ILE	conflict	UNP P06169

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

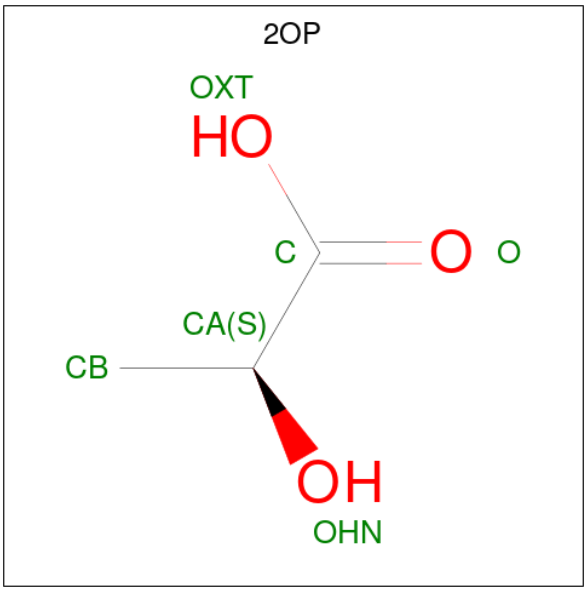


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	26	12	4	7	2	1	0	0
2	B	1	26	12	4	7	2	1	0	0
2	C	1	26	12	4	7	2	1	0	0
2	D	1	26	12	4	7	2	1	0	0

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

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

- Molecule 4 is (2S)-2-HYDROXYPROPANOIC ACID (three-letter code: 2OP) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	D	1	6	3	3	0	0

- Molecule 5 is water.

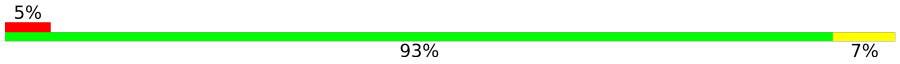
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	423	423	423	0	0
5	B	533	533	533	0	0
5	C	433	433	433	0	0
5	D	429	429	429	0	0

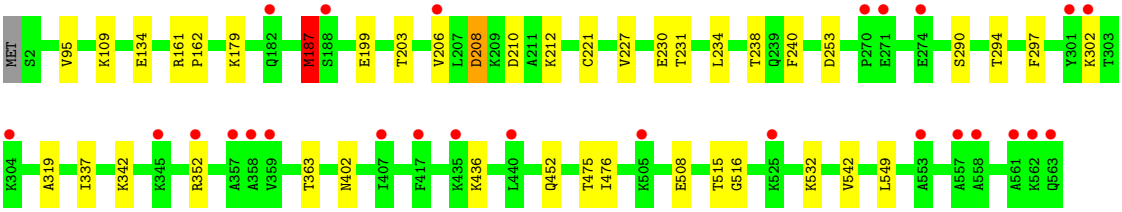
3 Residue-property plots (i)

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

• Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1

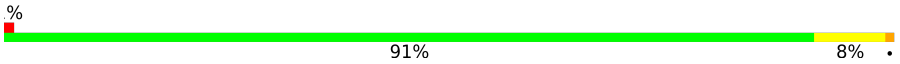
Chain A:

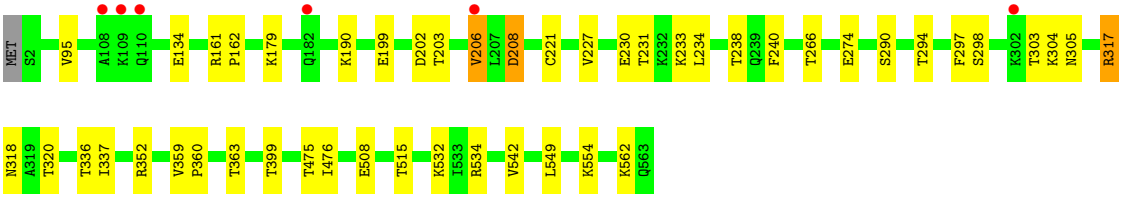




• Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1

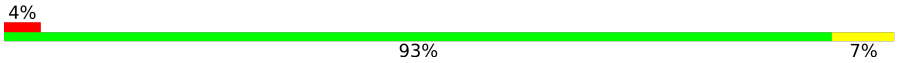
Chain B:

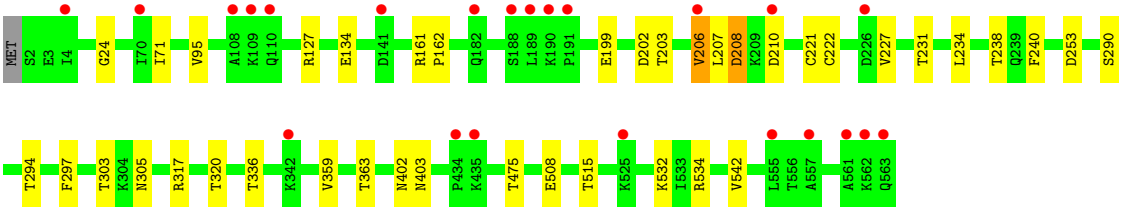




• Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1

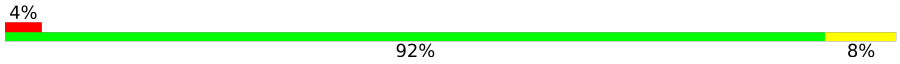
Chain C:

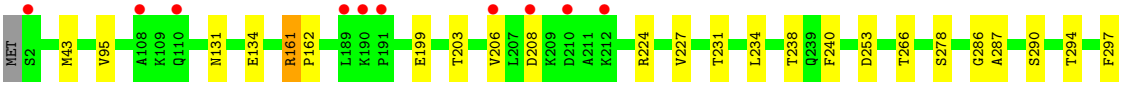




• Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1

Chain D:





S298
Y301
K302
T303
K304
N305
H310
A319
L330
L334
K345
V359
P360
T363
N402
E431
R459
T475
E508
T515
K525
K532
V542
Q547
K554
L555
T556
A557
A558
T559
N560
A561
K562
Q563

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.98Å 190.51Å 84.14Å 90.00° 113.01° 90.00°	Depositor
Resolution (Å)	95.35 – 1.42 33.22 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.6 (95.35-1.42) 99.6 (33.22-1.42)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.186 0.180 , 0.184	Depositor DCC
R_{free} test set	1068 reflections (0.25%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19242	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: 2OP, MG, TPP

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	0.58	3/4414 (0.1%)	0.62	6/6002 (0.1%)
1	B	0.60	4/4414 (0.1%)	0.64	3/6002 (0.0%)
1	C	0.56	1/4414 (0.0%)	0.60	2/6002 (0.0%)
1	D	0.54	1/4414 (0.0%)	0.63	4/6002 (0.1%)
All	All	0.57	9/17656 (0.1%)	0.62	15/24008 (0.1%)

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	7	0
1	B	8	0
1	C	9	0
1	D	8	0
All	All	32	0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	ASP	CB-CG	-14.63	1.21	1.51
1	A	208	ASP	CB-CG	-13.39	1.23	1.51
1	C	208	ASP	CB-CG	-13.35	1.23	1.51
1	A	230	GLU	CD-OE2	-6.42	1.18	1.25
1	B	208	ASP	CA-CB	-6.00	1.40	1.53
1	A	230	GLU	CD-OE1	-5.67	1.19	1.25
1	B	230	GLU	CD-OE2	-5.40	1.19	1.25
1	D	161	ARG	CG-CD	-5.04	1.39	1.51
1	B	230	GLU	CD-OE1	-5.03	1.20	1.25

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	161	ARG	NE-CZ-NH1	15.28	127.94	120.30
1	B	208	ASP	CB-CG-OD1	-9.78	109.50	118.30
1	D	161	ARG	NE-CZ-NH2	-9.63	115.48	120.30
1	C	208	ASP	CB-CG-OD1	-9.33	109.91	118.30
1	A	208	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	A	187	MET	CG-SD-CE	-7.47	88.24	100.20
1	D	161	ARG	CD-NE-CZ	6.64	132.90	123.60
1	A	208	ASP	OD1-CG-OD2	6.50	135.65	123.30
1	D	161	ARG	CG-CD-NE	6.42	125.28	111.80
1	B	208	ASP	N-CA-CB	-6.17	99.49	110.60
1	C	208	ASP	OD1-CG-OD2	6.02	134.74	123.30
1	B	208	ASP	OD1-CG-OD2	5.82	134.35	123.30
1	A	208	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	A	208	ASP	N-CA-CB	-5.16	101.31	110.60
1	A	436	LYS	CD-CE-NZ	5.11	123.44	111.70

All (32) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	203	THR	CB
1	A	231	THR	CB
1	A	238	THR	CB
1	A	266	THR	CB
1	A	294	THR	CB
1	A	475	THR	CB
1	A	515	THR	CB
1	B	203	THR	CB
1	B	231	THR	CB
1	B	238	THR	CB
1	B	294	THR	CB
1	B	303	THR	CB
1	B	363	THR	CB
1	B	475	THR	CB
1	B	515	THR	CB
1	C	203	THR	CB
1	C	231	THR	CB
1	C	238	THR	CB
1	C	266	THR	CB
1	C	294	THR	CB
1	C	303	THR	CB
1	C	320	THR	CB
1	C	475	THR	CB

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Mol	Chain	Res	Type	Atom
1	C	515	THR	CB
1	D	203	THR	CB
1	D	231	THR	CB
1	D	238	THR	CB
1	D	294	THR	CB
1	D	303	THR	CB
1	D	363	THR	CB
1	D	475	THR	CB
1	D	515	THR	CB

There are no planarity outliers.

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	4323	0	4328	35	0
1	B	4323	0	4327	39	0
1	C	4323	0	4327	36	0
1	D	4323	0	4327	38	0
2	A	26	0	16	0	0
2	B	26	0	16	0	0
2	C	26	0	16	0	0
2	D	26	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	5	5	0
4	B	6	0	4	2	0
4	C	6	0	4	3	0
4	D	6	0	4	4	0
5	A	423	0	0	3	0
5	B	533	0	0	6	0
5	C	433	0	0	6	0
5	D	429	0	0	7	0
All	All	19242	0	17390	142	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 4.

All (142) 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:221:CYS:SG	4:A:1566:2OP:HA	1.14	1.66
1:A:221:CYS:SG	4:A:1566:2OP:CA	2.11	1.37
1:A:187:MET:HA	1:A:187:MET:HE3	1.26	1.16
1:D:303:THR:HG22	1:D:305:ASN:H	1.09	1.13
1:A:294:THR:HG23	1:A:297:PHE:H	1.16	1.10
1:A:187:MET:HA	1:A:187:MET:CE	1.79	1.09
1:B:303:THR:HG22	1:B:305:ASN:H	1.17	1.08
1:B:294:THR:HG23	1:B:297:PHE:H	1.18	1.07
1:C:294:THR:HG23	1:C:297:PHE:H	1.23	1.00
1:C:303:THR:HG22	1:C:305:ASN:H	1.29	0.94
1:C:336:THR:CB	5:C:2228:HOH:O	2.16	0.93
1:D:294:THR:HG23	1:D:297:PHE:H	1.32	0.92
1:A:238:THR:HG23	1:A:240:PHE:H	1.35	0.91
1:B:238:THR:HG23	1:B:240:PHE:H	1.34	0.90
1:D:238:THR:HG23	1:D:240:PHE:H	1.33	0.90
1:C:238:THR:HG23	1:C:240:PHE:H	1.36	0.90
1:C:221:CYS:SG	4:C:1566:2OP:CB	2.63	0.86
1:D:290:SER:O	1:D:294:THR:HG22	1.77	0.84
1:D:360:PRO:O	1:D:363:THR:HG23	1.78	0.83
1:D:303:THR:HG22	1:D:305:ASN:N	1.94	0.83
1:B:203:THR:HG21	5:B:2190:HOH:O	1.79	0.82
1:C:290:SER:O	1:C:294:THR:HG22	1.84	0.78
1:A:187:MET:CE	1:A:187:MET:CA	2.46	0.77
1:B:303:THR:HG22	1:B:305:ASN:N	1.98	0.76
1:A:294:THR:CG2	1:A:297:PHE:H	1.97	0.74
1:B:290:SER:O	1:B:294:THR:HG22	1.88	0.74
1:A:187:MET:CA	1:A:187:MET:HE2	2.05	0.73
1:C:234:LEU:O	1:C:238:THR:HG22	1.89	0.73
1:A:234:LEU:O	1:A:238:THR:HG22	1.89	0.72
1:C:203:THR:HG21	5:C:2127:HOH:O	1.88	0.72
1:A:227:VAL:O	1:A:231:THR:HG23	1.90	0.71
1:D:199:GLU:O	1:D:203:THR:HG23	1.91	0.71
1:D:227:VAL:O	1:D:231:THR:HG23	1.90	0.71
1:D:310:HIS:ND1	4:D:1566:2OP:HB2	2.07	0.70
1:A:203:THR:HG21	5:A:2160:HOH:O	1.91	0.70
1:A:294:THR:HG23	1:A:297:PHE:N	2.00	0.70
1:B:360:PRO:O	1:B:363:THR:HG23	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:THR:HG23	5:C:2060:HOH:O	1.92	0.69
1:A:206:VAL:HG13	5:A:2162:HOH:O	1.93	0.69
1:B:221:CYS:SG	4:B:1566:2OP:C	2.81	0.68
1:B:294:THR:CG2	1:B:297:PHE:H	2.01	0.68
1:D:203:THR:HG21	5:D:2152:HOH:O	1.94	0.68
1:B:202:ASP:O	1:B:206:VAL:HG12	1.94	0.67
1:B:234:LEU:O	1:B:238:THR:HG22	1.94	0.67
1:C:227:VAL:O	1:C:231:THR:HG23	1.94	0.67
1:C:294:THR:CG2	1:C:297:PHE:H	2.05	0.67
1:D:234:LEU:O	1:D:238:THR:HG22	1.95	0.67
1:A:290:SER:O	1:A:294:THR:HG22	1.93	0.67
1:A:221:CYS:SG	4:A:1566:2OP:CB	2.83	0.65
1:C:199:GLU:O	1:C:203:THR:HG23	1.97	0.65
1:C:202:ASP:O	1:C:206:VAL:HG22	1.98	0.64
1:B:221:CYS:SG	4:B:1566:2OP:CB	2.85	0.64
1:B:227:VAL:O	1:B:231:THR:HG23	1.98	0.63
1:A:221:CYS:CB	4:A:1566:2OP:HA	2.23	0.63
1:A:206:VAL:HG23	5:A:2164:HOH:O	1.99	0.63
1:D:459:ARG:HD2	5:D:2052:HOH:O	1.97	0.63
1:A:475:THR:HG22	1:A:542:VAL:O	1.98	0.62
1:A:187:MET:HE3	1:A:187:MET:CA	2.10	0.62
1:A:221:CYS:SG	4:A:1566:2OP:C	2.85	0.62
1:B:475:THR:HG22	1:B:542:VAL:O	2.01	0.60
1:D:431:GLU:O	5:D:2317:HOH:O	2.16	0.60
1:D:206:VAL:CG1	5:D:2155:HOH:O	2.50	0.59
1:B:303:THR:HG23	5:B:2280:HOH:O	2.03	0.59
1:C:127:ARG:NH2	1:D:131:ASN:OD1	2.36	0.58
1:B:199:GLU:O	1:B:203:THR:HG23	2.03	0.58
1:B:266:THR:HG23	1:B:298:SER:HB2	1.85	0.58
1:D:363:THR:HB	1:D:515:THR:HG22	1.85	0.58
1:D:286:GLY:HA2	4:D:1566:2OP:HB3	1.84	0.57
1:D:363:THR:HB	1:D:515:THR:CG2	2.35	0.57
1:D:294:THR:CG2	1:D:297:PHE:H	2.12	0.56
1:B:234:LEU:CD1	1:B:337:ILE:HD13	2.35	0.56
1:A:508:GLU:HG3	1:A:532:LYS:HD2	1.85	0.56
1:C:475:THR:HG22	1:C:542:VAL:O	2.05	0.56
1:B:317:ARG:HG3	5:B:2282:HOH:O	2.06	0.56
1:C:207:LEU:HD21	1:C:317:ARG:HH12	1.71	0.55
1:B:359:VAL:HB	1:B:363:THR:HG21	1.86	0.55
1:A:199:GLU:O	1:A:203:THR:HG23	2.07	0.55
1:C:221:CYS:CB	4:C:1566:2OP:CA	2.84	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:THR:HG22	1:D:542:VAL:O	2.08	0.54
1:C:207:LEU:HD21	1:C:317:ARG:NH1	2.23	0.54
1:C:221:CYS:SG	4:C:1566:2OP:C	2.89	0.54
1:B:294:THR:HG23	1:B:297:PHE:N	2.04	0.53
1:D:508:GLU:HG3	1:D:532:LYS:HD2	1.89	0.53
1:C:363:THR:HB	1:C:515:THR:HG22	1.91	0.53
1:B:363:THR:HB	1:B:515:THR:CG2	2.39	0.53
1:A:109:LYS:HZ2	1:B:562:LYS:HZ1	1.55	0.52
1:D:287:ALA:O	4:D:1566:2OP:HB1	2.11	0.51
1:C:363:THR:HB	1:C:515:THR:CG2	2.41	0.51
1:D:359:VAL:HB	1:D:363:THR:HG21	1.92	0.51
1:C:294:THR:HG23	1:C:297:PHE:N	2.08	0.51
1:B:508:GLU:HG3	1:B:532:LYS:HD2	1.93	0.50
1:B:363:THR:HB	1:B:515:THR:HG22	1.93	0.50
1:A:476:ILE:HG13	1:A:549:LEU:HD11	1.94	0.50
1:B:336:THR:CB	5:B:2307:HOH:O	2.60	0.50
1:A:134:GLU:HB2	1:A:161:ARG:HB2	1.95	0.49
1:B:352:ARG:HE	1:B:399:THR:HG21	1.77	0.49
1:B:476:ILE:HG13	1:B:549:LEU:HD11	1.96	0.48
1:C:508:GLU:HB2	1:C:534:ARG:HG2	1.96	0.48
1:A:475:THR:CG2	1:A:542:VAL:O	2.62	0.47
1:B:134:GLU:HB2	1:B:161:ARG:HB2	1.97	0.47
1:C:475:THR:CG2	1:C:542:VAL:O	2.63	0.47
1:A:253:ASP:HB3	1:A:402:ASN:OD1	2.14	0.47
1:D:203:THR:O	1:D:206:VAL:HG12	2.15	0.47
1:C:508:GLU:HG3	1:C:532:LYS:HD2	1.97	0.46
1:C:134:GLU:HB2	1:C:161:ARG:HB2	1.97	0.46
1:D:134:GLU:HB2	1:D:161:ARG:HB2	1.98	0.46
1:C:253:ASP:HB3	1:C:402:ASN:OD1	2.15	0.46
1:C:303:THR:HG22	1:C:305:ASN:N	2.12	0.46
1:A:109:LYS:NZ	1:B:562:LYS:NZ	2.63	0.46
1:B:274:GLU:HG3	5:B:2255:HOH:O	2.15	0.45
1:D:330:LEU:O	1:D:334:LEU:HG	2.17	0.45
1:C:359:VAL:HG23	1:C:515:THR:HG21	1.98	0.45
1:D:303:THR:HG21	1:D:305:ASN:HB3	1.99	0.45
1:B:508:GLU:HB2	1:B:534:ARG:HG2	1.98	0.44
1:B:233:LYS:HE3	5:B:2215:HOH:O	2.17	0.44
1:D:278:SER:HA	1:D:302:LYS:HE3	1.98	0.44
1:D:286:GLY:CA	4:D:1566:2OP:HB3	2.47	0.44
1:C:95:VAL:O	1:C:162:PRO:HA	2.17	0.44
1:A:109:LYS:NZ	1:B:562:LYS:HZ1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:VAL:O	1:A:162:PRO:HA	2.18	0.43
1:D:459:ARG:CD	5:D:2052:HOH:O	2.64	0.43
1:C:222:CYS:SG	1:C:231:THR:HG21	2.58	0.43
1:C:515:THR:HG23	5:C:2255:HOH:O	2.18	0.43
1:D:206:VAL:HG22	5:D:2158:HOH:O	2.19	0.43
1:C:403:ASN:HB2	5:C:2301:HOH:O	2.19	0.42
1:B:475:THR:CG2	1:B:542:VAL:O	2.67	0.42
1:D:266:THR:HG23	1:D:298:SER:HB2	2.02	0.42
1:D:515:THR:HG23	5:D:2266:HOH:O	2.20	0.42
1:A:212:LYS:HA	1:A:212:LYS:HE2	2.00	0.42
1:D:95:VAL:O	1:D:162:PRO:HA	2.19	0.42
1:A:515:THR:HG23	1:A:516:GLY:N	2.34	0.41
1:A:363:THR:HB	1:A:515:THR:CG2	2.51	0.41
1:B:95:VAL:O	1:B:162:PRO:HA	2.20	0.41
1:B:320:THR:O	1:C:320:THR:HG22	2.20	0.41
1:B:317:ARG:HB3	1:B:318:ASN:H	1.70	0.41
1:C:206:VAL:HG23	5:C:2134:HOH:O	2.20	0.41
1:B:303:THR:HG22	1:B:304:LYS:N	2.35	0.41
1:D:43:MET:HA	1:D:43:MET:HE2	2.02	0.41
1:D:224:ARG:CZ	1:D:224:ARG:HA	2.51	0.41
1:D:253:ASP:HB3	1:D:402:ASN:OD1	2.21	0.41
1:C:24:GLY:HA3	1:C:71:ILE:O	2.22	0.40
1:A:319:ALA:HB1	1:D:319:ALA:HB1	2.03	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	560/563 (100%)	551 (98%)	9 (2%)	0	100	100
1	B	560/563 (100%)	547 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	560/563 (100%)	551 (98%)	9 (2%)	0	100	100
1	D	560/563 (100%)	549 (98%)	11 (2%)	0	100	100
All	All	2240/2252 (100%)	2198 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	466/468 (100%)	457 (98%)	9 (2%)	57	24
1	B	466/468 (100%)	460 (99%)	6 (1%)	69	41
1	C	466/468 (100%)	463 (99%)	3 (1%)	86	69
1	D	466/468 (100%)	464 (100%)	2 (0%)	91	79
All	All	1864/1872 (100%)	1844 (99%)	20 (1%)	73	48

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	LYS
1	A	187	MET
1	A	208	ASP
1	A	210	ASP
1	A	302	LYS
1	A	337	ILE
1	A	342	LYS
1	A	352	ARG
1	A	452	GLN
1	B	179	LYS
1	B	190	LYS
1	B	206	VAL
1	B	208	ASP
1	B	317	ARG

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Mol	Chain	Res	Type
1	B	554	LYS
1	C	206	VAL
1	C	208	ASP
1	C	210	ASP
1	D	208	ASP
1	D	525	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	2OP	D	1566	1	5,5,5	1.60	1 (20%)	4,6,6	1.10	0
2	TPP	C	1564	3	22,27,27	1.70	6 (27%)	29,40,40	1.35	5 (17%)
4	2OP	A	1566	-	5,5,5	1.14	1 (20%)	4,6,6	1.27	1 (25%)
4	2OP	C	1566	1	5,5,5	1.37	1 (20%)	4,6,6	1.74	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	2OP	B	1566	1	5,5,5	1.48	1 (20%)	4,6,6	0.95	0
2	TPP	D	1564	3	22,27,27	1.79	5 (22%)	29,40,40	1.34	3 (10%)
2	TPP	B	1564	3	22,27,27	1.56	2 (9%)	29,40,40	1.56	6 (20%)
2	TPP	A	1564	3	22,27,27	1.64	4 (18%)	29,40,40	1.44	5 (17%)

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
4	2OP	D	1566	1	1/1/2/2	3/4/4/4	-
2	TPP	C	1564	3	-	3/16/17/17	0/2/2/2
4	2OP	A	1566	-	-	2/4/4/4	-
4	2OP	C	1566	1	-	3/4/4/4	-
4	2OP	B	1566	1	-	2/4/4/4	-
2	TPP	D	1564	3	-	3/16/17/17	0/2/2/2
2	TPP	B	1564	3	-	3/16/17/17	0/2/2/2
2	TPP	A	1564	3	-	4/16/17/17	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1564	TPP	C4-N3	-5.40	1.35	1.39
2	A	1564	TPP	C4-N3	-4.92	1.35	1.39
2	B	1564	TPP	C4-N3	-4.65	1.35	1.39
2	C	1564	TPP	C4-N3	-4.23	1.36	1.39
2	C	1564	TPP	C6-C5	3.58	1.52	1.50
4	D	1566	2OP	OXT-C	-3.38	1.19	1.30
2	B	1564	TPP	C6-C5	3.04	1.52	1.50
4	B	1566	2OP	OXT-C	-3.02	1.20	1.30
2	A	1564	TPP	C6-C5	2.75	1.52	1.50
2	D	1564	TPP	C4'-N3'	2.70	1.38	1.35
2	D	1564	TPP	C2'-N1'	2.66	1.38	1.34
2	C	1564	TPP	C4'-N3'	2.61	1.38	1.35
2	D	1564	TPP	C6-C5	2.47	1.52	1.50
2	C	1564	TPP	C6'-N1'	2.42	1.39	1.34
4	C	1566	2OP	OXT-C	-2.40	1.22	1.30
2	D	1564	TPP	C6'-N1'	2.31	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1564	TPP	C2'-N1'	2.24	1.38	1.34
2	A	1564	TPP	C6'-N1'	2.14	1.38	1.34
2	C	1564	TPP	C2'-N3'	2.14	1.37	1.34
4	A	1566	2OP	OXT-C	-2.13	1.23	1.30
2	A	1564	TPP	C2'-N1'	2.12	1.37	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1564	TPP	CM2-C2'-N1'	3.64	121.14	117.14
4	C	1566	2OP	CB-CA-C	3.43	118.39	110.63
2	B	1564	TPP	N1'-C2'-N3'	-3.42	119.66	125.54
2	B	1564	TPP	CM2-C2'-N1'	3.21	120.67	117.14
2	B	1564	TPP	C6-C5-C4	-3.11	124.93	127.43
2	A	1564	TPP	N1'-C2'-N3'	-3.04	120.31	125.54
2	D	1564	TPP	CM2-C2'-N1'	2.85	120.28	117.14
2	A	1564	TPP	C6'-N1'-C2'	2.79	120.71	115.96
2	D	1564	TPP	N1'-C2'-N3'	-2.79	120.74	125.54
2	C	1564	TPP	N1'-C2'-N3'	-2.78	120.75	125.54
2	A	1564	TPP	C5'-C6'-N1'	-2.68	119.35	123.82
2	B	1564	TPP	C2'-N3'-C4'	2.55	122.06	118.08
2	C	1564	TPP	C6'-C5'-C4'	2.35	118.92	115.72
2	A	1564	TPP	C6'-C5'-C4'	2.30	118.86	115.72
4	A	1566	2OP	CB-CA-C	2.25	115.73	110.63
2	D	1564	TPP	C6'-N1'-C2'	2.17	119.65	115.96
2	C	1564	TPP	C6'-N1'-C2'	2.14	119.60	115.96
2	B	1564	TPP	C6'-N1'-C2'	2.13	119.59	115.96
2	B	1564	TPP	O3B-PB-O2B	2.12	115.73	107.64
2	C	1564	TPP	C6-C5-C4	-2.06	125.78	127.43
2	C	1564	TPP	C5'-C6'-N1'	-2.06	120.39	123.82

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	1566	2OP	CA

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1564	TPP	PA-O3A-PB-O3B
2	B	1564	TPP	C4-C5-C6-C7
2	B	1564	TPP	PA-O3A-PB-O3B

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Mol	Chain	Res	Type	Atoms
2	C	1564	TPP	C4-C5-C6-C7
2	C	1564	TPP	PA-O3A-PB-O3B
2	D	1564	TPP	C4-C5-C6-C7
2	D	1564	TPP	PA-O3A-PB-O3B
4	D	1566	2OP	OXT-C-CA-OHN
4	C	1566	2OP	O-C-CA-CB
4	D	1566	2OP	O-C-CA-CB
4	D	1566	2OP	OXT-C-CA-CB
4	A	1566	2OP	O-C-CA-CB
2	A	1564	TPP	C4-C5-C6-C7
4	C	1566	2OP	OXT-C-CA-CB
4	A	1566	2OP	OXT-C-CA-CB
4	B	1566	2OP	O-C-CA-CB
2	A	1564	TPP	PA-O3A-PB-O2B
2	B	1564	TPP	PA-O3A-PB-O2B
2	C	1564	TPP	PA-O3A-PB-O2B
2	D	1564	TPP	PA-O3A-PB-O2B
4	C	1566	2OP	OXT-C-CA-OHN
2	A	1564	TPP	PA-O3A-PB-O1B
4	B	1566	2OP	OXT-C-CA-CB

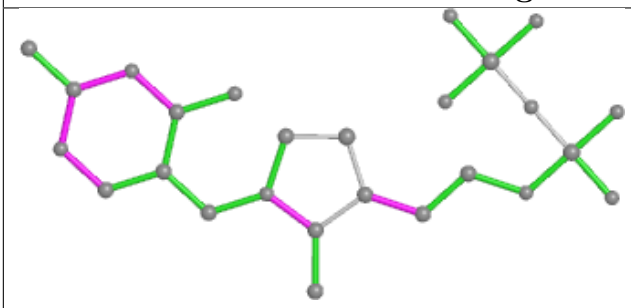
There are no ring outliers.

4 monomers are involved in 14 short contacts:

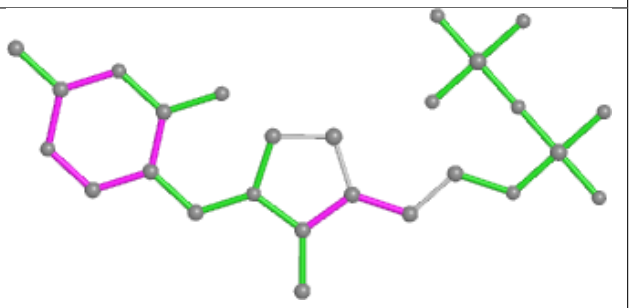
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1566	2OP	4	0
4	A	1566	2OP	5	0
4	C	1566	2OP	3	0
4	B	1566	2OP	2	0

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.

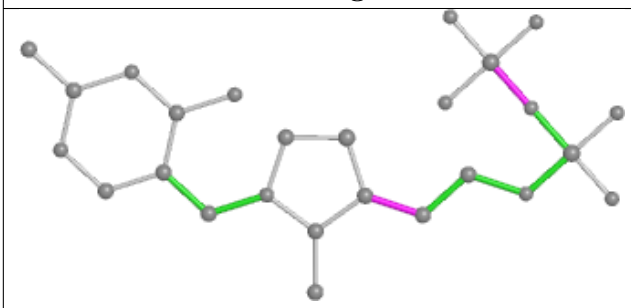
Ligand TPP C 1564



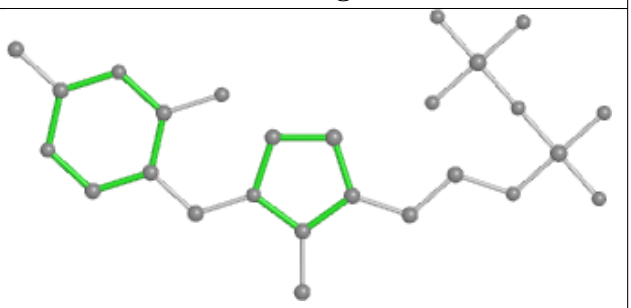
Bond lengths



Bond angles

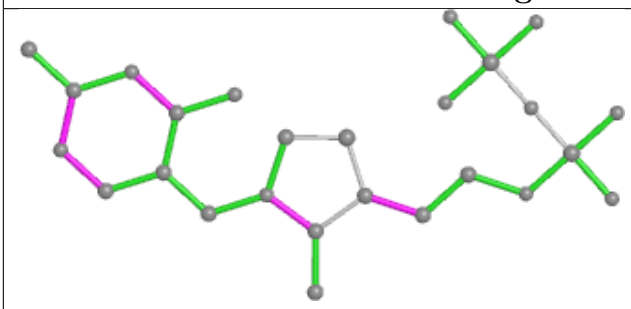


Torsions

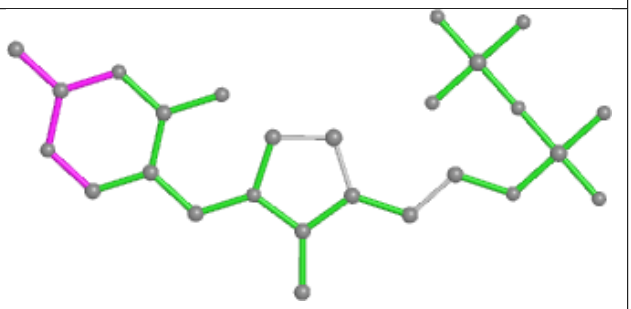


Rings

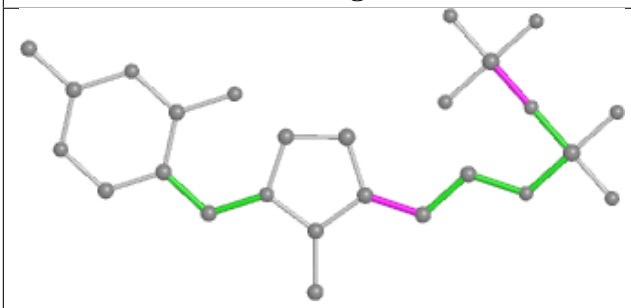
Ligand TPP D 1564



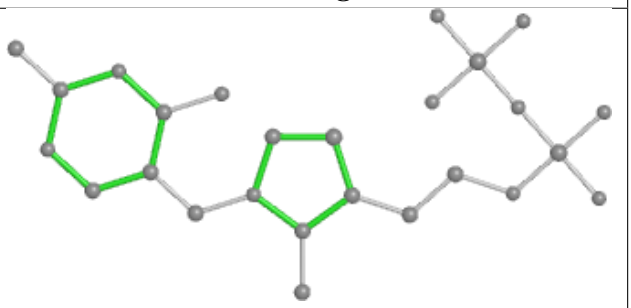
Bond lengths



Bond angles

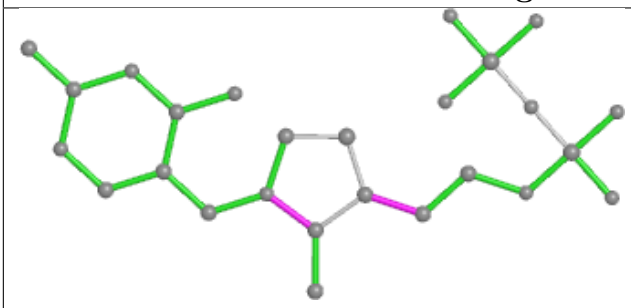


Torsions

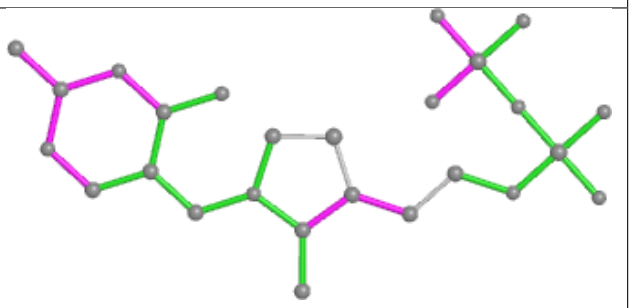


Rings

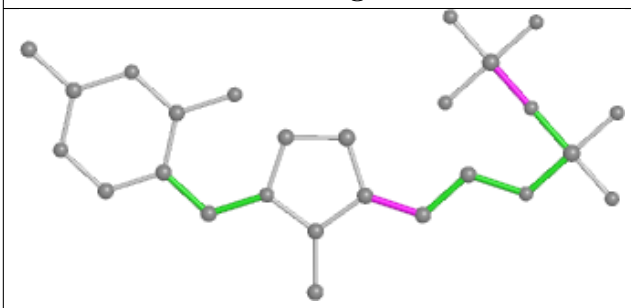
Ligand TPP B 1564



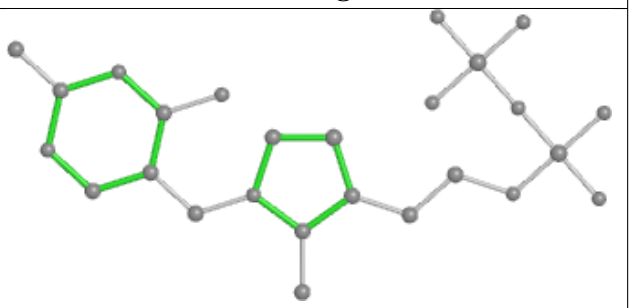
Bond lengths



Bond angles

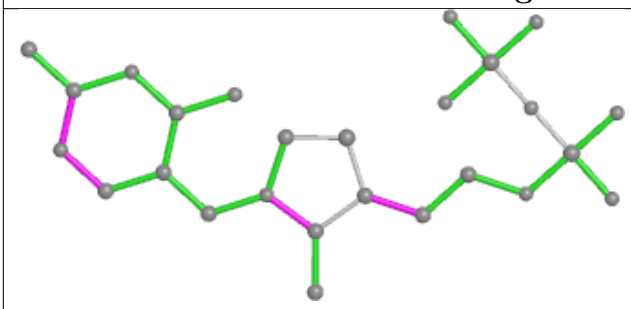


Torsions

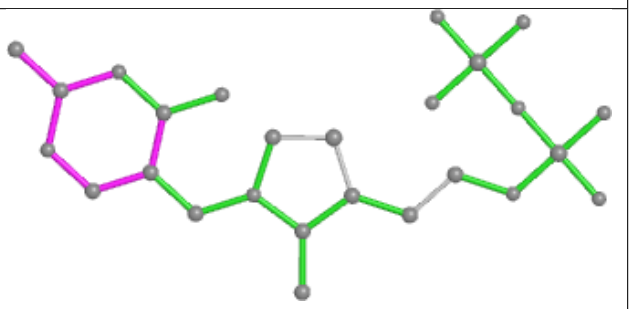


Rings

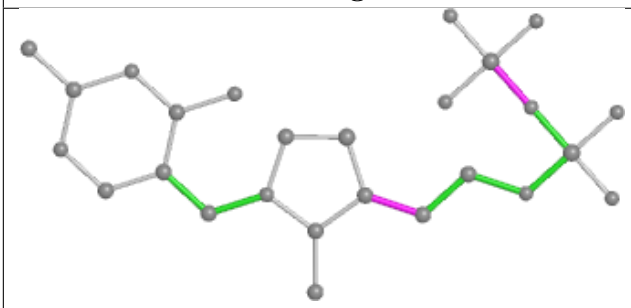
Ligand TPP A 1564



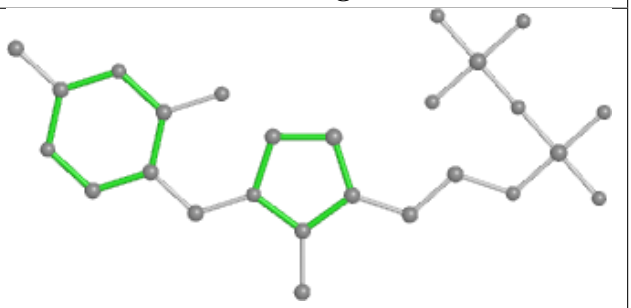
Bond lengths



Bond angles



Torsions



Rings

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	562/563 (99%)	0.20	26 (4%)	32	31	10, 18, 28, 35	0
1	B	562/563 (99%)	-0.05	6 (1%)	80	79	9, 15, 24, 34	0
1	C	562/563 (99%)	0.19	23 (4%)	37	37	10, 18, 30, 37	0
1	D	562/563 (99%)	0.17	25 (4%)	34	34	10, 18, 28, 35	0
All	All	2248/2252 (99%)	0.13	80 (3%)	42	42	9, 17, 28, 37	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	358	ALA	5.0
1	A	357	ALA	4.2
1	D	302	LYS	3.9
1	A	302	LYS	3.8
1	C	108	ALA	3.8
1	D	108	ALA	3.6
1	D	563	GLN	3.6
1	A	206	VAL	3.6
1	C	206	VAL	3.6
1	D	562	LYS	3.4
1	C	182	GLN	3.4
1	C	4	ILE	3.3
1	C	110	GLN	3.3
1	C	563	GLN	3.3
1	D	558	ALA	3.3
1	B	206	VAL	3.2
1	C	109	LYS	3.2
1	B	108	ALA	3.1
1	A	270	PRO	3.1
1	A	558	ALA	3.1
1	D	301	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	557	ALA	3.1
1	B	110	GLN	3.0
1	D	189	LEU	3.0
1	A	407	ILE	3.0
1	A	359	VAL	2.9
1	C	435	LYS	2.8
1	C	434	PRO	2.8
1	C	188	SER	2.8
1	C	562	LYS	2.7
1	A	562	LYS	2.7
1	B	302	LYS	2.7
1	A	561	ALA	2.7
1	D	212	LYS	2.7
1	C	191	PRO	2.7
1	A	301	TYR	2.6
1	C	210	ASP	2.5
1	D	559	THR	2.5
1	D	208	ASP	2.5
1	A	304	LYS	2.5
1	C	525	LYS	2.5
1	D	547	GLN	2.4
1	C	189	LEU	2.4
1	A	435	LYS	2.4
1	C	190	LYS	2.4
1	A	352	ARG	2.4
1	A	274	GLU	2.4
1	D	191	PRO	2.4
1	C	555	LEU	2.4
1	D	555	LEU	2.4
1	D	525	LYS	2.3
1	A	440	LEU	2.3
1	C	561	ALA	2.3
1	D	556	THR	2.3
1	D	304	LYS	2.3
1	D	206	VAL	2.3
1	A	182	GLN	2.2
1	D	345	LYS	2.2
1	D	554	LYS	2.2
1	C	141	ASP	2.2
1	C	342	LYS	2.2
1	A	417	PHE	2.1
1	D	210	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	271	GLU	2.1
1	D	2	SER	2.1
1	B	109	LYS	2.1
1	A	525	LYS	2.1
1	D	110	GLN	2.1
1	A	553	ALA	2.1
1	C	226	ASP	2.1
1	D	190	LYS	2.1
1	A	563	GLN	2.1
1	A	345	LYS	2.1
1	C	557	ALA	2.1
1	D	561	ALA	2.1
1	B	182	GLN	2.0
1	C	70	ILE	2.0
1	A	557	ALA	2.0
1	A	505	LYS	2.0
1	A	188	SER	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
4	2OP	D	1566	6/6	0.88	0.14	22,25,26,27	0
4	2OP	A	1566	6/6	0.89	0.14	22,24,25,26	0
4	2OP	C	1566	6/6	0.91	0.12	22,24,25,25	0
4	2OP	B	1566	6/6	0.94	0.12	18,19,19,21	0
2	TPP	D	1564	26/26	0.97	0.09	12,14,16,19	1
2	TPP	B	1564	26/26	0.98	0.09	9,10,12,17	1

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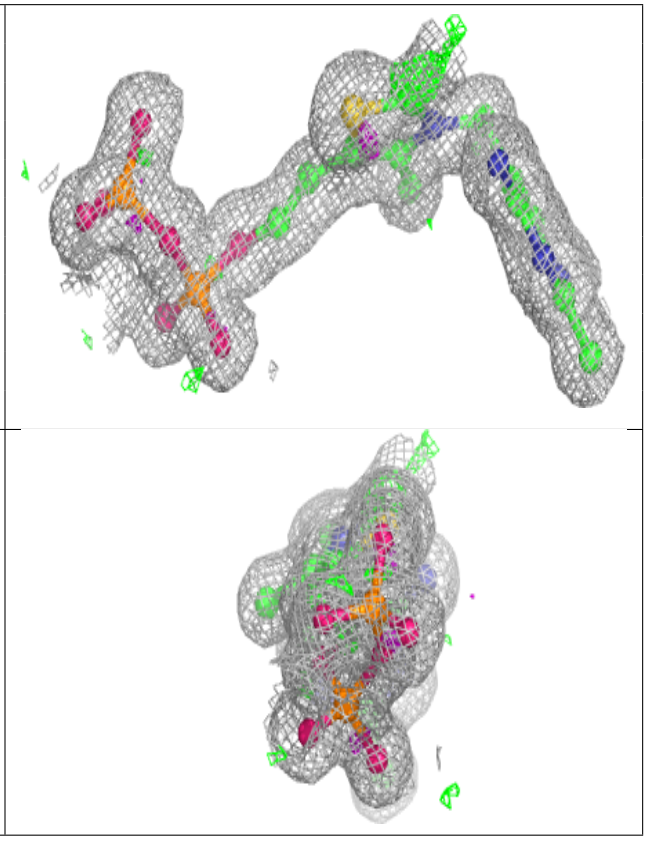
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TPP	C	1564	26/26	0.98	0.08	9,12,14,18	1
2	TPP	A	1564	26/26	0.98	0.09	11,13,15,19	1
3	MG	D	1565	1/1	0.98	0.06	14,14,14,14	0
3	MG	A	1565	1/1	0.99	0.05	13,13,13,13	0
3	MG	C	1565	1/1	1.00	0.06	11,11,11,11	0
3	MG	B	1565	1/1	1.00	0.04	10,10,10,10	0

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.

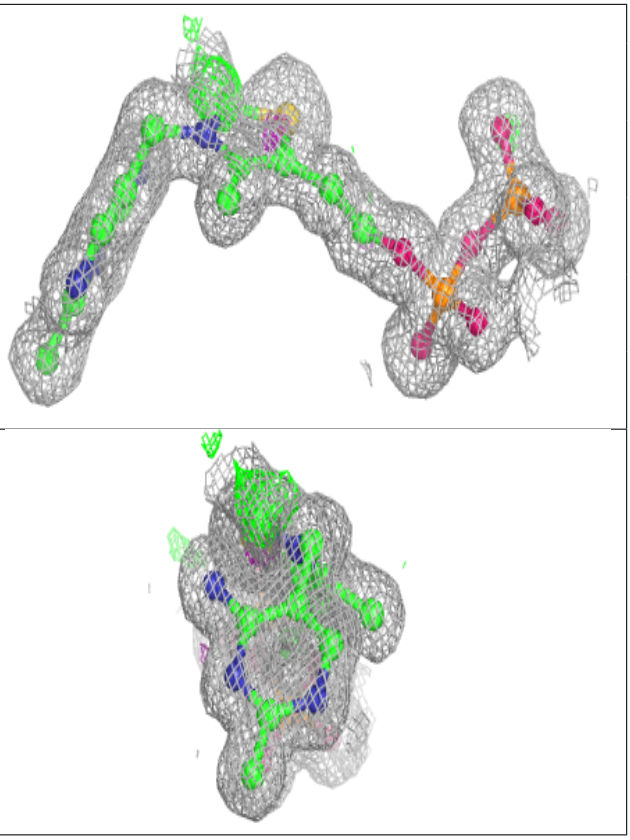
Electron density around TPP D 1564:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



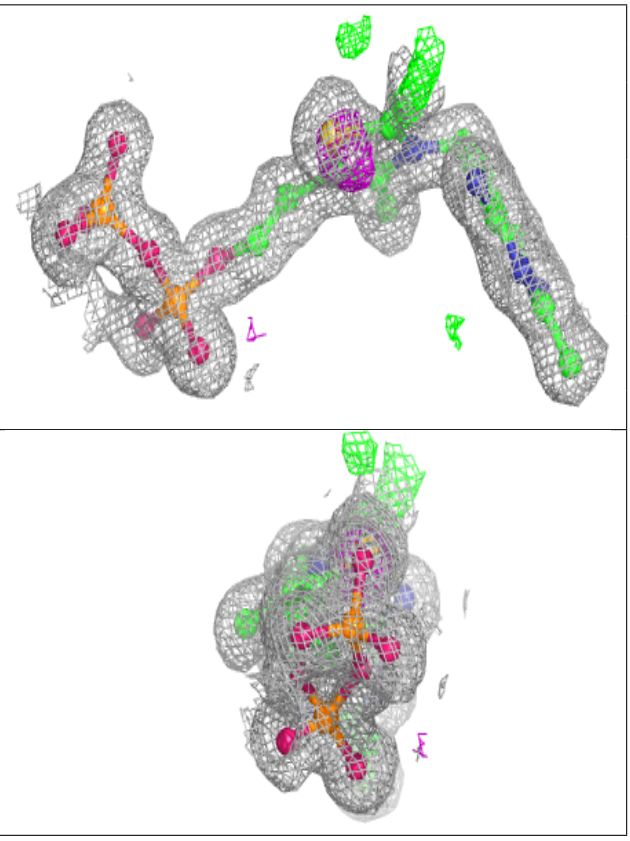
Electron density around TPP B 1564:

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



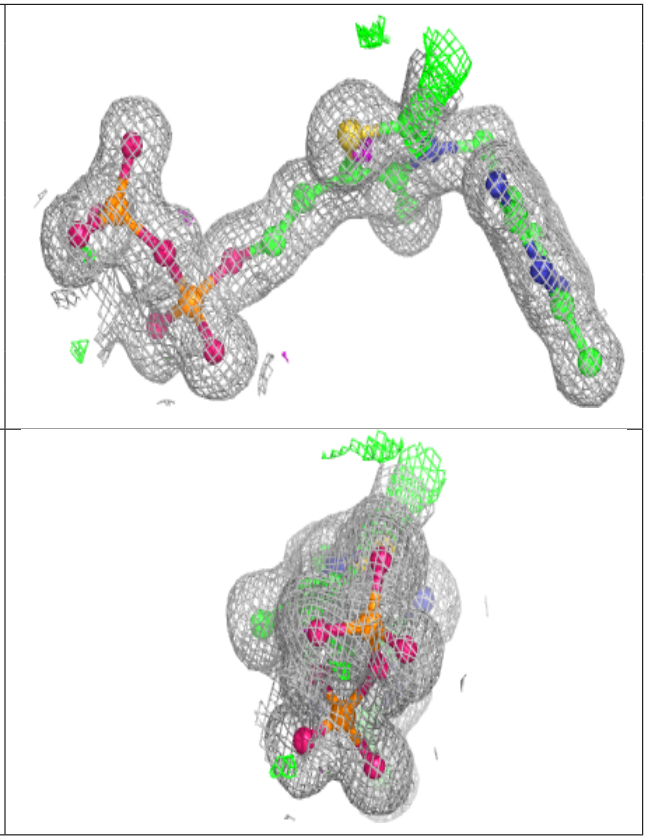
Electron density around TPP C 1564:

$2mF_o$-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 1564:

$2mF_o$-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.