Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 10:46 PM EDT

PDB ID	:	1G4S
Title	:	THIAMIN PHOSPHATE SYNTHASE
Authors	:	Peapus, D.H.; Chiu, H.-J.; Campobasso, N.; Reddick, J.J.; Begley, T.P.; Ealick, S.E.
Deposited on	:	2000-10-27
Resolution	:	1.70 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:

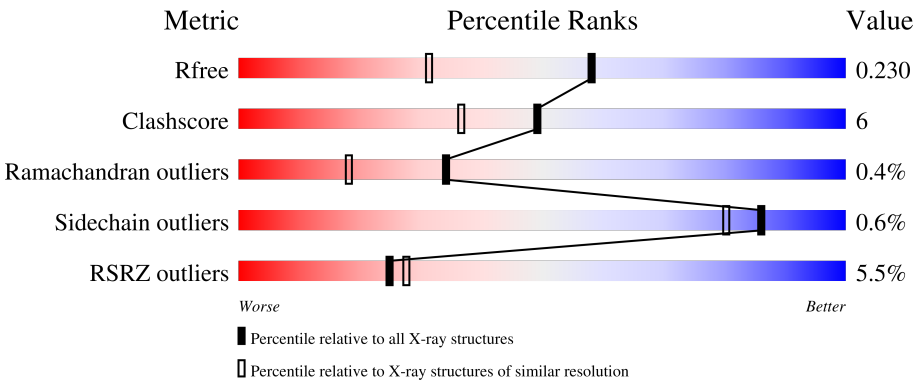
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	226	5% 81% 19%
1	B	226	6% 90% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3778 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 THIAMIN PHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1706	1057	306	334	9	0	5	0
1	B	226	1710	1059	309	333	9	0	5	0

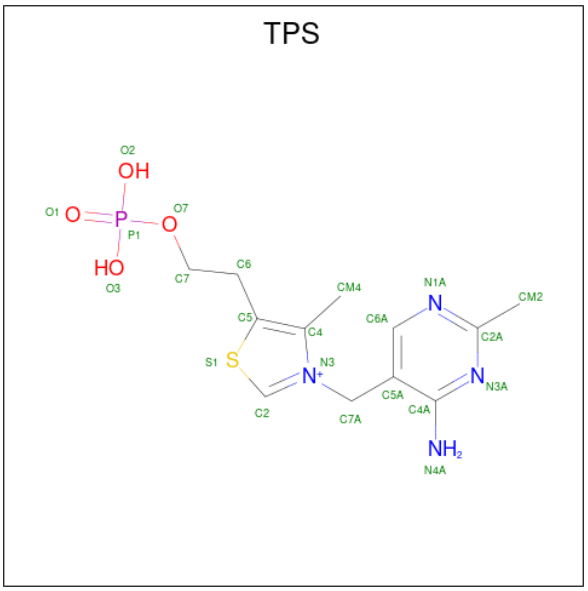
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	HIS	-	cloning artifact	UNP P39594
A	11	GLY	-	cloning artifact	UNP P39594
A	12	ILE	-	cloning artifact	UNP P39594
A	13	ARG	-	cloning artifact	UNP P39594
A	130	ALA	SER	engineered mutation	UNP P39594
B	1010	HIS	-	cloning artifact	UNP P39594
B	1011	GLY	-	cloning artifact	UNP P39594
B	1012	ILE	-	cloning artifact	UNP P39594
B	1013	ARG	-	cloning artifact	UNP P39594
B	1130	ALA	SER	engineered mutation	UNP P39594

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

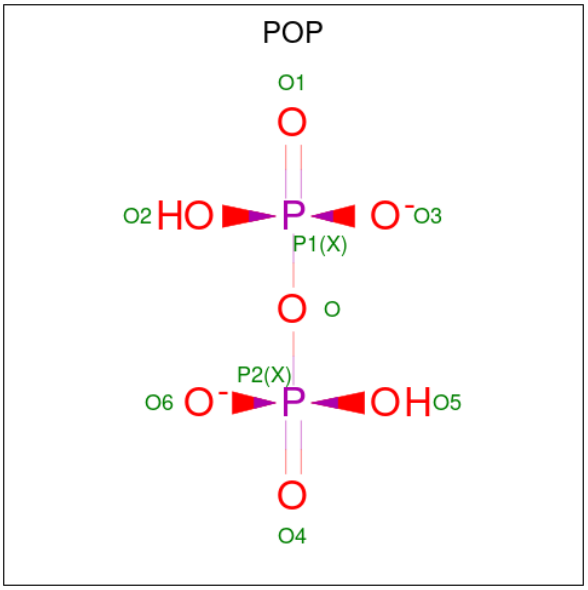
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is THIAMIN PHOSPHATE (three-letter code: TPS) (formula: $C_{12}H_{18}N_4O_4PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	22	12	4	4	1	1	0	0
			Total	C	N	O	P	S		
3	B	1	22	12	4	4	1	1	0	0

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
4	A	1	9	7	2	0	0
			Total	O	P		
4	B	1	9	7	2	0	0

- Molecule 5 is water.

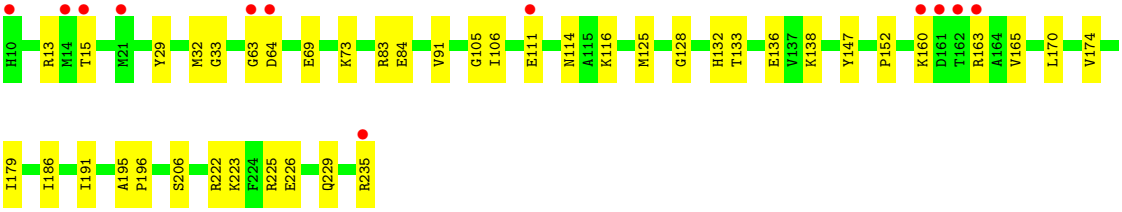
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	148	148	148	0	0
			Total	O		
5	B	150	150	150	0	0

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.

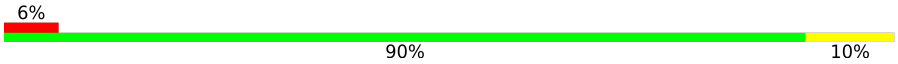
• Molecule 1: THIAMIN PHOSPHATE SYNTHASE

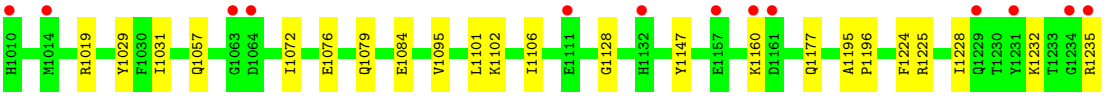
Chain A:



• Molecule 1: THIAMIN PHOSPHATE SYNTHASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	76.99Å 76.99Å 139.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.96 – 1.70 42.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.2 (42.96-1.70) 91.8 (42.96-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.68 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.239 0.196 , 0.230	Depositor DCC
R_{free} test set	2166 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3778	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4595e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: POP, TPS, MG

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	0.28	0/1752	0.54	0/2357
1	B	0.28	0/1757	0.55	0/2363
All	All	0.28	0/3509	0.55	0/4720

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 (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	1706	0	1727	28	0
1	B	1710	0	1731	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	22	0	16	0	0
3	B	22	0	16	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
5	A	148	0	0	1	1
5	B	150	0	0	4	0
All	All	3778	0	3490	41	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 6.

All (41) 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:105:GLY:HA2	1:A:125[A]:MET:HG2	1.64	0.79
1:B:1232:LYS:O	1:B:1235:ARG:HG2	1.86	0.75
1:A:83:ARG:HH12	1:B:1079:GLN:HE22	1.42	0.65
1:B:1195:ALA:HB3	1:B:1196:PRO:HD3	1.79	0.65
1:A:83:ARG:HH12	1:B:1079:GLN:NE2	1.95	0.65
1:A:132[B]:HIS:CG	1:A:163:ARG:HD2	2.36	0.60
1:A:133:THR:OG1	1:A:136:GLU:HG3	2.02	0.59
1:A:69:GLU:O	1:A:73:LYS:HG2	2.05	0.57
1:A:195:ALA:HB3	1:A:196:PRO:HD3	1.87	0.55
1:A:222:ARG:O	1:A:226:GLU:HG3	2.06	0.55
1:A:63:GLY:O	1:A:64:ASP:HB2	2.07	0.54
1:A:128:GLY:HA3	1:A:147:TYR:CZ	2.43	0.54
1:A:186:ILE:HB	1:A:206[B]:SER:OG	2.08	0.54
1:A:225:ARG:O	1:A:229:GLN:HG3	2.10	0.52
1:B:1095:VAL:HG22	1:B:1106:ILE:CD1	2.38	0.52
1:B:1095:VAL:HA	1:B:1106:ILE:HD12	1.93	0.51
1:B:1031:ILE:HG12	1:B:1057:GLN:HB3	1.93	0.51
1:B:1072:ILE:O	1:B:1076:GLU:HG3	2.11	0.51
1:A:91:VAL:O	1:A:106:ILE:HD12	2.11	0.50
1:A:132[A]:HIS:HB3	1:A:163:ARG:HH11	1.77	0.50
1:A:138:LYS:NZ	1:A:179:ILE:HD11	2.26	0.50
1:A:13[B]:ARG:HH21	1:A:15:THR:HG23	1.77	0.50
1:B:1128:GLY:HA3	1:B:1147:TYR:CZ	2.48	0.49
1:A:132[B]:HIS:HB2	1:A:163:ARG:HH11	1.78	0.48
1:A:138:LYS:HZ3	1:A:179:ILE:HD11	1.78	0.48
1:A:132[B]:HIS:CD2	1:A:163:ARG:HD2	2.50	0.47
1:A:235:ARG:HH11	1:A:235:ARG:HG3	1.80	0.47
1:A:111:GLU:HG2	1:A:111:GLU:O	2.15	0.47
1:A:152:PRO:HG2	1:A:165:VAL:HA	1.97	0.47
1:A:114:ASN:ND2	1:A:116:LYS:HB2	2.29	0.46
1:B:1084:GLU:HG3	5:B:3140:HOH:O	2.15	0.45
1:B:1177:GLN:HG3	5:B:3097:HOH:O	2.15	0.45
1:A:105:GLY:HA2	1:A:125[A]:MET:CG	2.39	0.44
1:A:84:GLU:HG2	5:A:3222:HOH:O	2.18	0.43
1:B:1225:ARG:HD2	5:B:3298:HOH:O	2.19	0.42
1:B:1224:PHE:O	1:B:1228:ILE:HG12	2.18	0.42
1:A:170:LEU:O	1:A:174:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ILE:HD12	1:A:223:LYS:HB3	2.02	0.41
1:A:32:MET:HG2	1:A:33:GLY:N	2.36	0.41
1:B:1019:ARG:HG2	5:B:3042:HOH:O	2.20	0.40
1:B:1101:LEU:O	1:B:1102:LYS:HB2	2.20	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)
5:A:3206:HOH:O	5:A:3206:HOH:O[8_665]	2.08	0.12

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	229/226 (101%)	219 (96%)	9 (4%)	1 (0%)	34	18
1	B	229/226 (101%)	221 (96%)	7 (3%)	1 (0%)	34	18
All	All	458/452 (101%)	440 (96%)	16 (4%)	2 (0%)	34	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	LYS
1	B	1160	LYS

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	178/173 (103%)	177 (99%)	1 (1%)	86	80
1	B	178/173 (103%)	177 (99%)	1 (1%)	86	80
All	All	356/346 (103%)	354 (99%)	2 (1%)	86	80

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	TYR
1	B	1029	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	114	ASN
1	B	1079	GLN
1	B	1139	GLN
1	B	1166	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	POP	A	2003	2	6,8,8	1.49	0	13,13,13	1.27	1 (7%)
3	TPS	A	2001	-	20,23,23	1.85	6 (30%)	25,33,33	1.21	3 (12%)
4	POP	B	2004	2	6,8,8	1.43	0	13,13,13	1.38	2 (15%)
3	TPS	B	2002	-	20,23,23	1.85	6 (30%)	25,33,33	1.20	2 (8%)

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	POP	A	2003	2	-	4/6/6/6	-
3	TPS	A	2001	-	-	2/10/11/11	0/2/2/2
4	POP	B	2004	2	-	2/6/6/6	-
3	TPS	B	2002	-	-	2/10/11/11	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2002	TPS	C7A-N3	4.95	1.57	1.48
3	A	2001	TPS	C7A-N3	4.88	1.57	1.48
3	A	2001	TPS	C6-C5	2.98	1.52	1.50
3	B	2002	TPS	C2A-N1A	2.80	1.38	1.34
3	A	2001	TPS	C2A-N1A	2.68	1.38	1.34
3	B	2002	TPS	C4-N3	-2.66	1.37	1.39
3	A	2001	TPS	C4-N3	-2.49	1.37	1.39
3	A	2001	TPS	C4A-N3A	2.48	1.38	1.35
3	B	2002	TPS	C4A-N3A	2.43	1.38	1.35
3	B	2002	TPS	C6-C5	2.31	1.51	1.50
3	A	2001	TPS	C5A-C4A	2.21	1.46	1.42
3	B	2002	TPS	C5A-C4A	2.20	1.46	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2004	POP	O3-P1-O	2.53	113.11	104.64
3	A	2001	TPS	C5A-C7A-N3	-2.43	109.24	113.28
3	B	2002	TPS	C5-C4-N3	2.15	111.86	107.57
3	A	2001	TPS	CM2-C2A-N3A	2.14	120.49	117.15
3	A	2001	TPS	C5-C4-N3	2.13	111.83	107.57
3	B	2002	TPS	C5A-C7A-N3	-2.07	109.83	113.28
4	B	2004	POP	P2-O-P1	2.04	139.83	132.83
4	A	2003	POP	O3-P1-O1	-2.01	102.82	110.68

There are no chirality outliers.

All (10) torsion outliers are listed below:

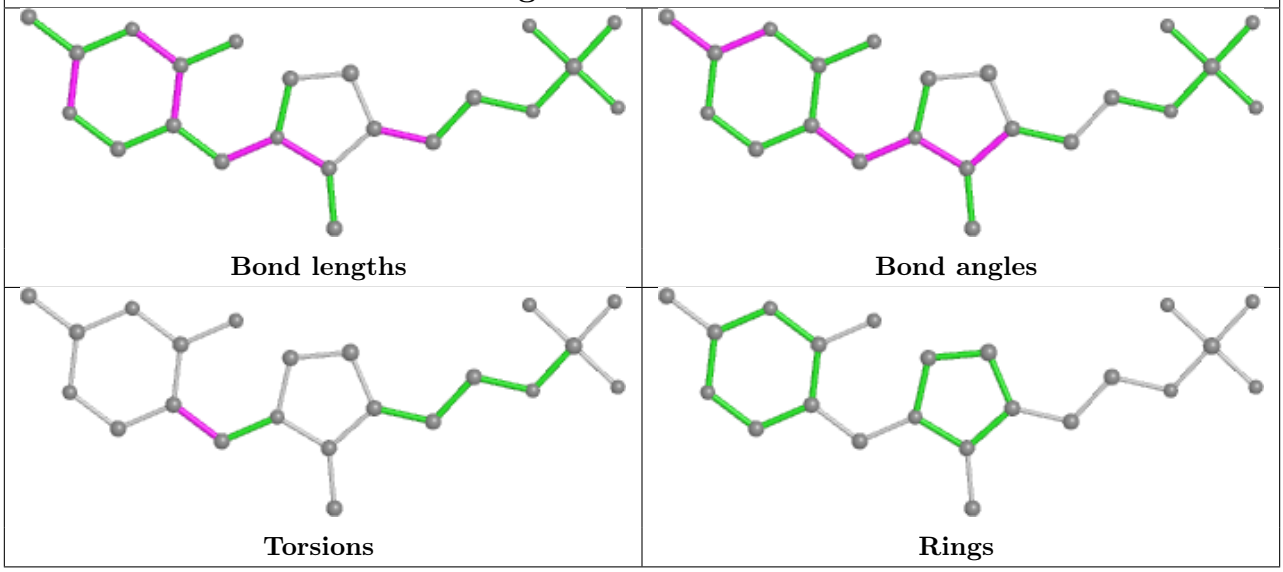
Mol	Chain	Res	Type	Atoms
3	A	2001	TPS	C6A-C5A-C7A-N3
3	B	2002	TPS	C6A-C5A-C7A-N3
4	A	2003	POP	P2-O-P1-O2
4	A	2003	POP	P1-O-P2-O5
3	A	2001	TPS	C4A-C5A-C7A-N3
3	B	2002	TPS	C4A-C5A-C7A-N3
4	A	2003	POP	P2-O-P1-O1
4	B	2004	POP	P1-O-P2-O4
4	A	2003	POP	P1-O-P2-O4
4	B	2004	POP	P2-O-P1-O1

There are no ring outliers.

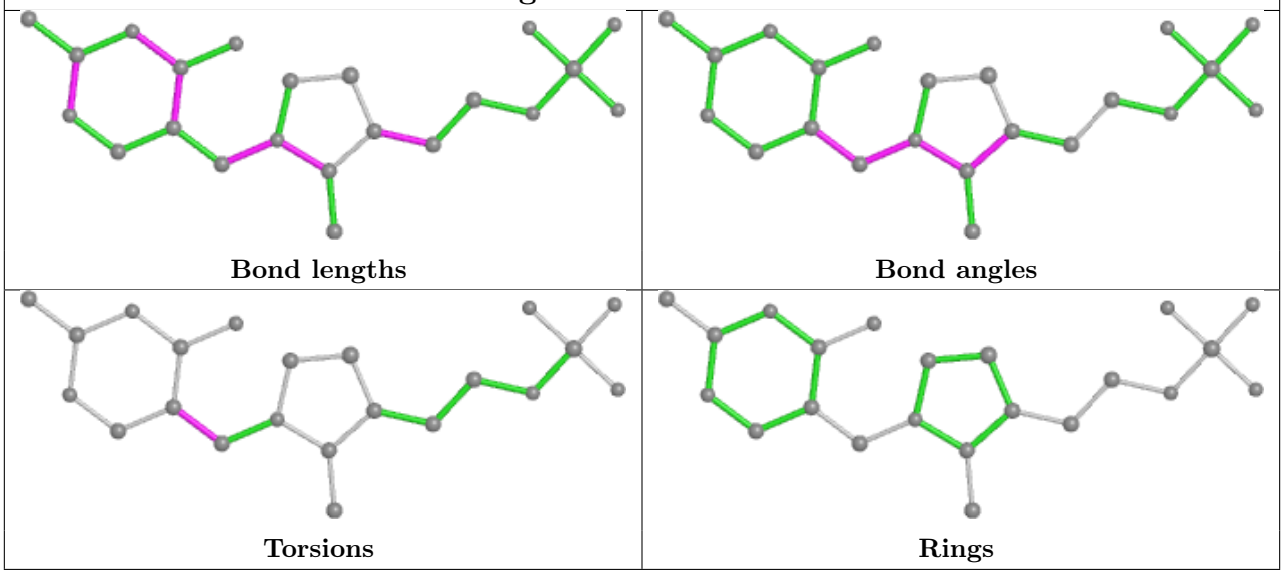
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 TPS A 2001



Ligand TPS B 2002



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	226/226 (100%)	0.36	12 (5%)	26	29	9, 16, 30, 47	0
1	B	226/226 (100%)	0.32	13 (5%)	23	25	10, 16, 30, 54	0
All	All	452/452 (100%)	0.34	25 (5%)	25	27	9, 16, 30, 54	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1063	GLY	7.0
1	B	1010	HIS	6.2
1	A	160	LYS	6.1
1	A	10	HIS	5.5
1	A	161	ASP	5.4
1	B	1161	ASP	5.1
1	B	1235	ARG	5.1
1	B	1160	LYS	4.4
1	A	63	GLY	4.3
1	A	235	ARG	3.3
1	A	111	GLU	3.0
1	A	14	MET	2.9
1	A	64	ASP	2.7
1	B	1111	GLU	2.6
1	B	1229	GLN	2.6
1	B	1157	GLU	2.6
1	A	162	THR	2.5
1	B	1064	ASP	2.4
1	B	1234	GLY	2.4
1	A	163	ARG	2.3
1	A	15	THR	2.3
1	B	1014	MET	2.1
1	A	21	MET	2.1
1	B	1132[A]	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1231	TYR	2.1

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)

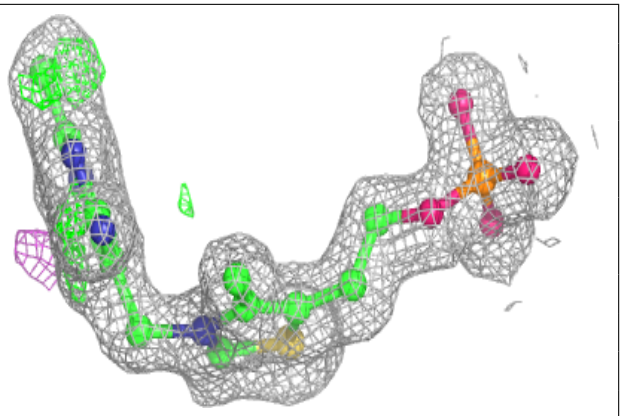
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

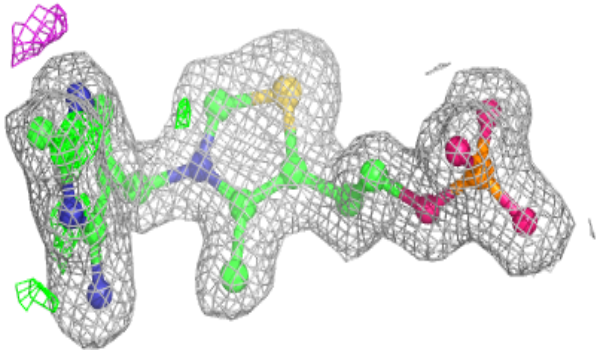
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TPS	B	2002	22/22	0.94	0.11	10,15,17,19	0
3	TPS	A	2001	22/22	0.95	0.11	10,13,15,17	0
4	POP	A	2003	9/9	0.97	0.08	12,15,20,21	0
4	POP	B	2004	9/9	0.97	0.08	13,15,22,23	0
2	MG	A	2005	1/1	0.98	0.08	15,15,15,15	0
2	MG	B	2006	1/1	0.99	0.05	15,15,15,15	0

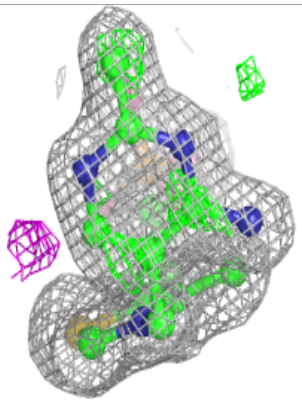
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPS B 2002:

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

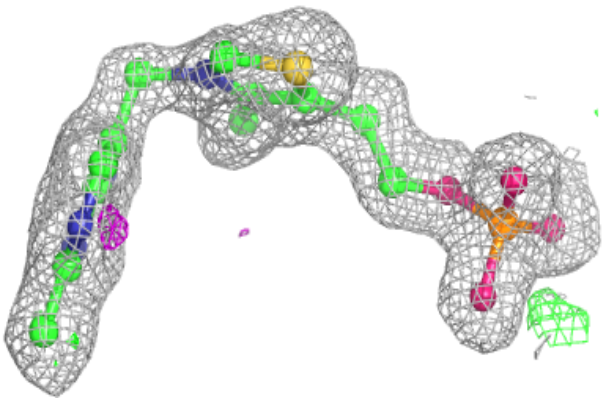


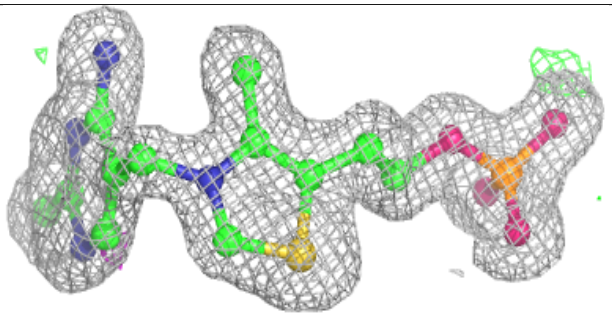


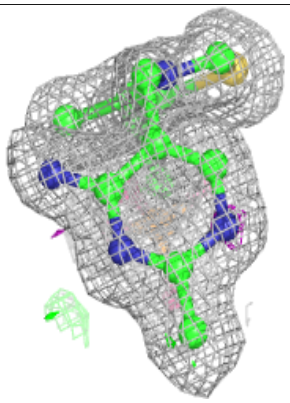


Electron density around TPS A 2001:

$2mF_o$-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.