



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:51 pm BST

PDB ID : 2XTA  
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis alpha-ketoglutarate decarboxylase in complex with acetyl-CoA (triclinic form)  
Authors : Wagner, T.; Bellinzoni, M.; Wehenkel, A.M.; O'Hare, H.M.; Alzari, P.M.  
Deposited on : 2010-10-05  
Resolution : 2.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

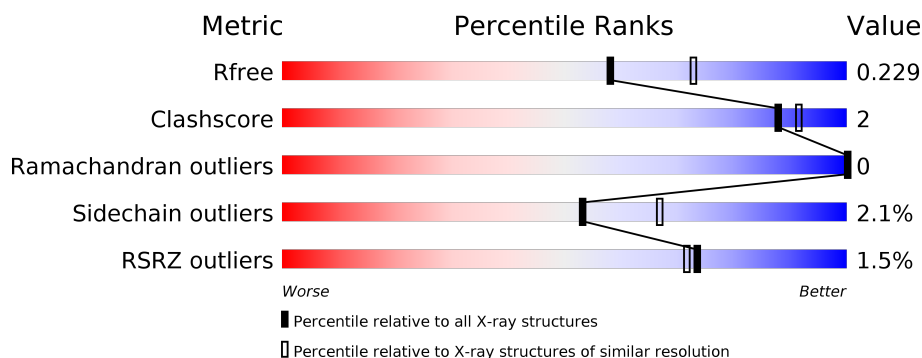
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	868	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	B	868	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
1	C	868	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>
1	D	868	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26097 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.

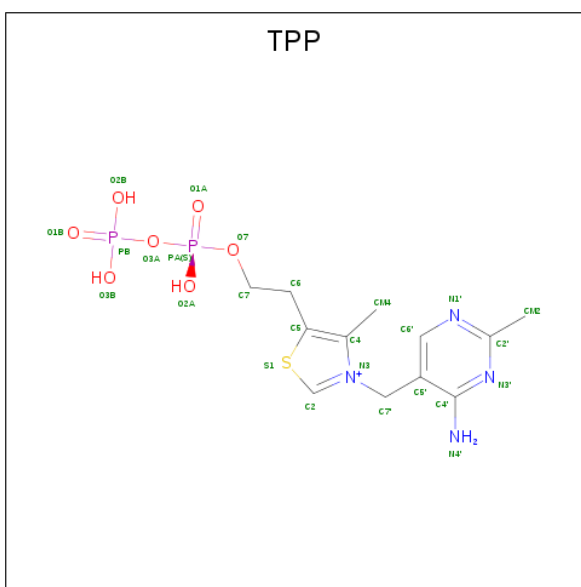
- Molecule 1 is a protein called 2-OXOGLUTARATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	826	Total	C	N	O	S	0	0	0
			6360	4007	1128	1202	23			
1	B	814	Total	C	N	O	S	0	0	0
			6223	3925	1105	1169	24			
1	C	817	Total	C	N	O	S	0	0	0
			6309	3980	1112	1193	24			
1	D	818	Total	C	N	O	S	0	0	0
			6252	3939	1105	1184	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	expression tag	UNP A0R2B1
B	360	GLY	-	expression tag	UNP A0R2B1
C	360	GLY	-	expression tag	UNP A0R2B1
D	360	GLY	-	expression tag	UNP A0R2B1

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



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

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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

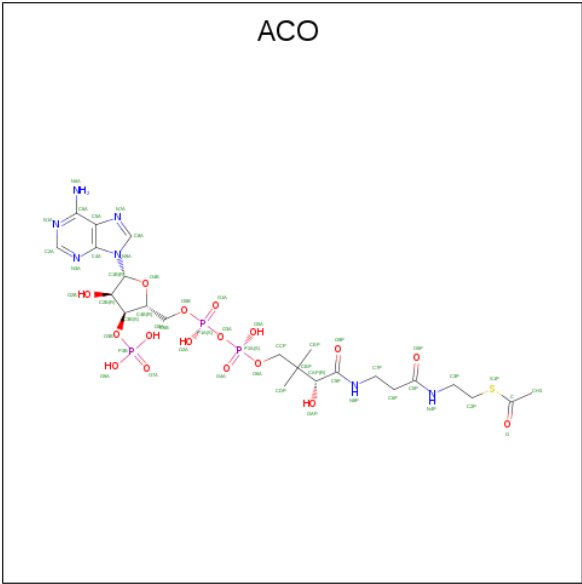
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is ACETYL COENZYME \*A (three-letter code: ACO) (formula: C<sub>23</sub>H<sub>38</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			33	12	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			33	12	5	13	3		
5	D	1	Total	C	N	O	P	0	0
			33	12	5	13	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	190	Total	O	0	0
			190	190		
6	B	186	Total	O	0	0
			186	186		
6	C	183	Total	O	0	0
			183	183		

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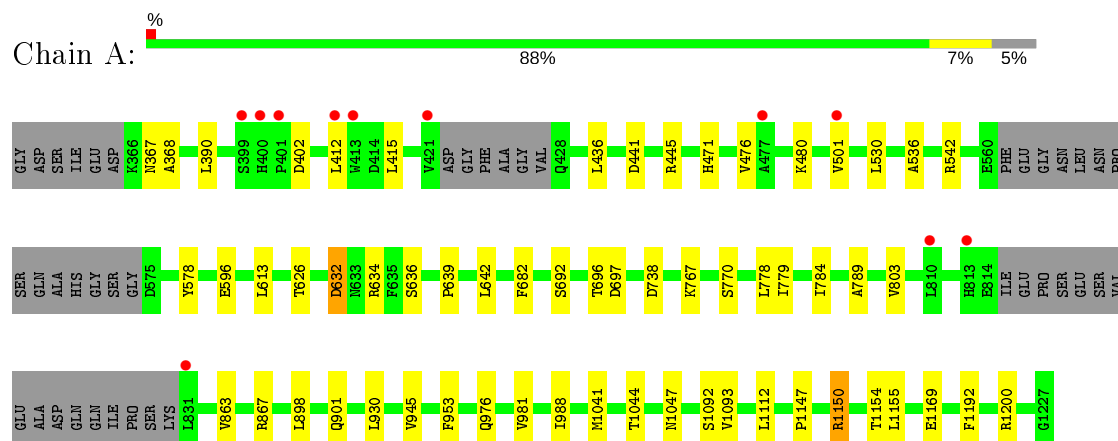
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	183	Total 183	O 183	0	0

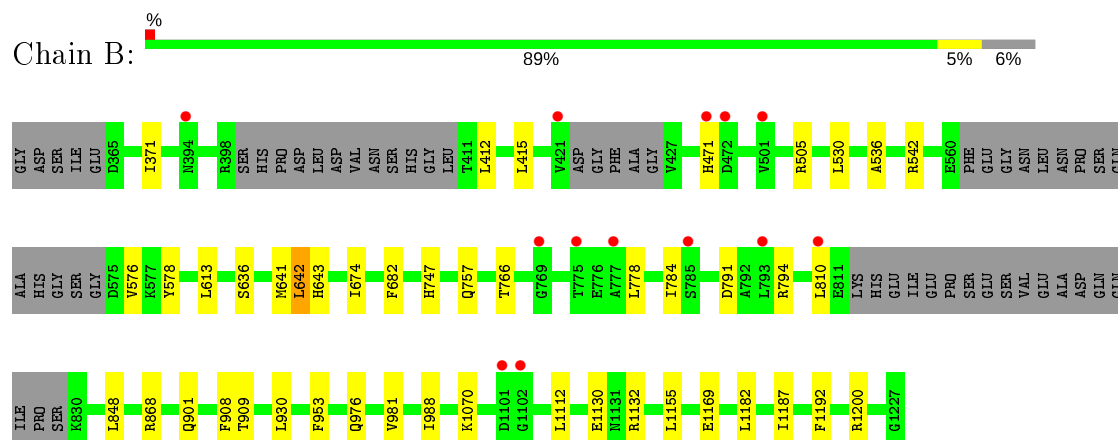
### 3 Residue-property plots [i](#)

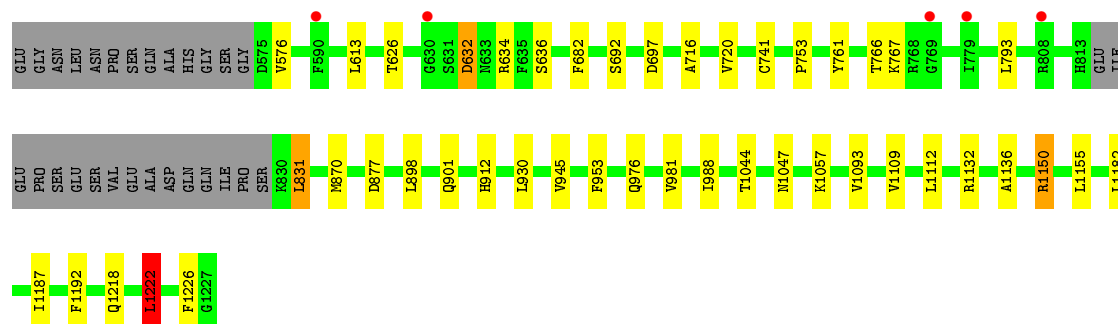
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE

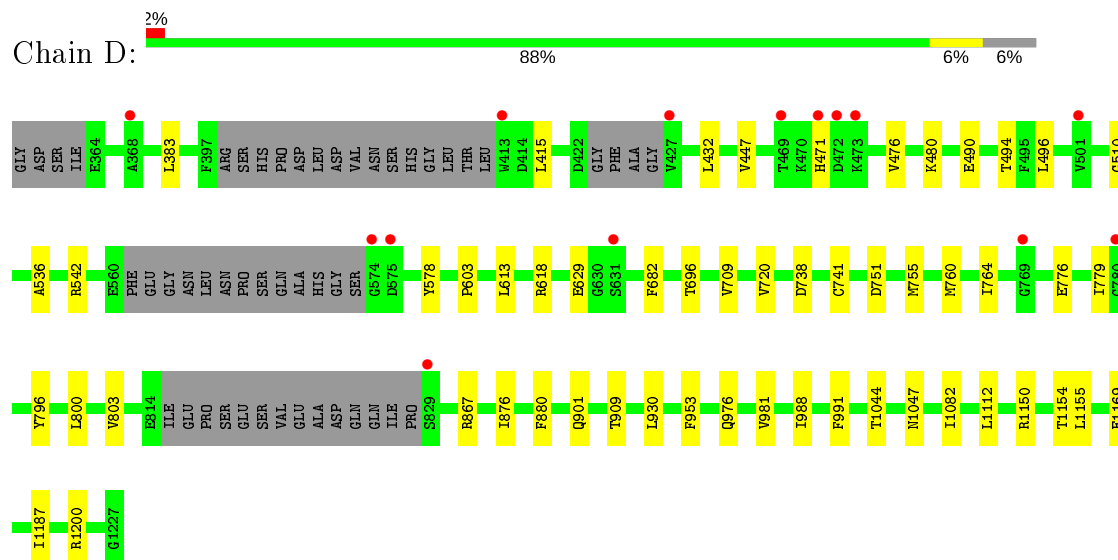


#### • Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE





- Molecule 1: 2-OXOGLUTARATE DECARBOXYLASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.55Å 83.58Å 160.07Å 99.59° 98.94° 100.68°	Depositor
Resolution (Å)	78.11 – 2.20 78.12 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.1 (78.11-2.20) 92.7 (78.12-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.9.3	Depositor
R, $R_{free}$	0.188 , 0.214 0.202 , 0.229	Depositor DCC
$R_{free}$ test set	9389 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	26097	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACO, 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	0.50	0/6492	0.62	0/8818
1	B	0.50	0/6349	0.63	0/8623
1	C	0.51	0/6438	0.63	1/8737 (0.0%)
1	D	0.51	0/6377	0.63	0/8656
All	All	0.51	0/25656	0.63	1/34834 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1222	LEU	CB-CG-CD1	5.12	119.70	111.00

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	6360	0	6105	27	0
1	B	6223	0	5967	23	0
1	C	6309	0	6084	25	0
1	D	6252	0	5998	27	0
2	A	26	0	16	2	0
2	B	26	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	26	0	16	1	0
2	D	26	0	16	1	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	33	0	13	0	0
5	C	33	0	13	0	0
5	D	33	0	13	0	0
6	A	190	0	0	1	0
6	B	186	0	0	0	0
6	C	183	0	0	0	0
6	D	183	0	0	1	0
All	All	26097	0	24257	100	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 2.

All (100) 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:B:641:MET:HE3	1:B:643:HIS:HE1	1.40	0.84
1:B:641:MET:CE	1:B:643:HIS:HE1	1.94	0.80
1:B:641:MET:CE	1:B:643:HIS:CE1	2.65	0.79
1:B:641:MET:HE2	1:B:643:HIS:CE1	2.21	0.75
1:A:1044:THR:HG22	1:A:1047:ASN:H	1.54	0.70
1:D:1044:THR:HG22	1:D:1047:ASN:H	1.57	0.68
1:C:716:ALA:O	1:C:720:VAL:HG12	1.93	0.68
1:C:1044:THR:HG22	1:C:1047:ASN:H	1.57	0.67
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	1.76	0.67
1:C:912:HIS:HE1	1:D:755:MET:HE1	1.60	0.66
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	1.78	0.66
1:B:848:LEU:HD12	1:B:868:ARG:HD2	1.76	0.65
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.78	0.64
1:D:494:THR:HG21	1:D:796:TYR:OH	1.96	0.64
1:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.78	0.64
1:A:368:ALA:HB1	1:B:371:ILE:HG13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:ASP:HA	1:C:445:ARG:HD3	1.81	0.61
1:C:912:HIS:HE1	1:D:755:MET:CE	2.13	0.61
1:C:870:MET:HE2	1:C:877:ASP:H	1.67	0.59
1:A:441:ASP:HA	1:A:445:ARG:HD3	1.86	0.57
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.87	0.56
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.88	0.56
1:B:641:MET:HE2	1:B:643:HIS:NE2	2.20	0.56
1:A:779:ILE:HD11	1:A:789:ALA:HB2	1.89	0.55
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.87	0.55
1:D:494:THR:HG23	1:D:800:LEU:HD13	1.91	0.53
1:D:876:ILE:HD11	1:D:1082:ILE:HD13	1.90	0.53
1:D:1169:GLU:O	1:D:1200:ARG:HD2	2.09	0.53
2:C:2001:TPP:H6'	1:D:901:GLN:OE1	2.10	0.51
1:C:1218:GLN:O	1:C:1222:LEU:HD13	2.11	0.50
1:B:641:MET:HE3	1:B:643:HIS:CE1	2.27	0.50
1:D:447:VAL:HG22	1:D:709:VAL:HG12	1.94	0.49
1:D:709:VAL:HG11	1:D:720:VAL:HG21	1.94	0.49
1:A:901:GLN:OE1	2:B:2001:TPP:H6'	2.13	0.49
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.13	0.49
1:A:412:LEU:HA	1:A:415:LEU:HD12	1.95	0.49
1:D:490:GLU:O	1:D:494:THR:HG22	2.13	0.49
1:B:505:ARG:HA	1:B:747:HIS:O	2.13	0.48
1:C:1132:ARG:NH1	1:C:1226:PHE:O	2.46	0.48
1:C:901:GLN:OE1	2:D:2001:TPP:H6'	2.13	0.48
1:B:1130:GLU:HG3	1:B:1132:ARG:HG3	1.94	0.48
1:D:618:ARG:HH21	1:D:629:GLU:HG2	1.79	0.48
1:C:510:GLY:O	1:C:741:CYS:HB2	2.15	0.47
1:D:776:GLU:HA	1:D:779:ILE:HD12	1.98	0.46
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.97	0.46
1:B:642:LEU:HD22	1:B:674:ILE:HB	1.98	0.46
1:B:1169:GLU:O	1:B:1200:ARG:HD2	2.16	0.46
1:D:1150:ARG:O	1:D:1154:THR:HG23	2.15	0.46
1:A:626:THR:HG21	1:A:636:SER:OG	2.17	0.45
1:C:412:LEU:HA	1:C:415:LEU:HD12	1.98	0.45
1:A:632:ASP:OD2	1:A:634:ARG:HB2	2.17	0.45
1:A:1150:ARG:O	1:A:1154:THR:HG23	2.16	0.44
1:D:510:GLY:O	1:D:741:CYS:HB2	2.16	0.44
1:B:412:LEU:HA	1:B:415:LEU:HD12	1.98	0.44
1:A:536:ALA:HB3	1:A:613:LEU:HD22	1.99	0.44
1:D:542:ARG:HD3	1:D:578:TYR:HA	2.00	0.43
1:D:751:ASP:HB2	6:D:3076:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:MET:HE1	6:A:3173:HOH:O	2.18	0.43
1:A:1093:VAL:HB	1:A:1150:ARG:HD3	2.00	0.43
1:A:778:LEU:HB3	1:A:784:ILE:HG12	2.00	0.43
1:A:1092:SER:HB2	1:A:1147:PRO:HG3	2.01	0.43
1:C:831:LEU:HD23	1:C:1057:LYS:HE3	2.00	0.43
1:C:536:ALA:HB3	1:C:613:LEU:HD22	2.01	0.43
1:A:863:VAL:O	1:A:867:ARG:HG3	2.19	0.42
1:A:476:VAL:HG12	1:A:480:LYS:HE3	2.01	0.42
1:D:476:VAL:HG12	1:D:480:LYS:HE2	2.00	0.42
1:B:778:LEU:HB3	1:B:784:ILE:HG12	2.01	0.42
1:B:1155:LEU:HD11	1:B:1192:PHE:CZ	2.55	0.42
1:D:760:MET:HG2	1:D:764:ILE:HD12	2.01	0.42
1:D:536:ALA:HB3	1:D:613:LEU:HD22	2.01	0.42
1:A:1155:LEU:HD11	1:A:1192:PHE:CZ	2.55	0.42
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.01	0.42
1:D:415:LEU:HA	1:D:432:LEU:HB3	2.02	0.42
1:D:696:THR:HG21	1:D:738:ASP:HB2	2.02	0.42
1:B:542:ARG:HD3	1:B:578:TYR:HA	2.02	0.41
1:C:1155:LEU:HD11	1:C:1192:PHE:CZ	2.55	0.41
1:C:626:THR:HG21	1:C:636:SER:OG	2.20	0.41
1:A:390:LEU:HD23	1:A:767:LYS:HD2	2.02	0.41
1:C:692:SER:HB2	1:C:697:ASP:OD2	2.19	0.41
1:A:898:LEU:O	1:A:945:VAL:HA	2.20	0.41
1:B:791:ASP:OD1	1:B:794:ARG:NH2	2.54	0.41
1:A:542:ARG:HD3	1:A:578:TYR:HA	2.02	0.41
1:C:476:VAL:HG12	1:C:480:LYS:HE3	2.02	0.41
1:A:530:LEU:HD22	1:A:636:SER:HA	2.02	0.41
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.55	0.41
1:C:632:ASP:OD2	1:C:634:ARG:HB2	2.20	0.41
1:C:753:PRO:HB2	1:C:761:TYR:CE2	2.56	0.41
1:A:1112:LEU:CD2	1:A:1155:LEU:HD22	2.50	0.41
1:A:692:SER:HB2	1:A:697:ASP:OD2	2.21	0.41
1:C:1109:VAL:HG21	1:C:1136:ALA:HB2	2.02	0.41
1:A:1169:GLU:O	1:A:1200:ARG:HD2	2.21	0.40
2:A:2001:TPP:H61	2:A:2001:TPP:HM41	1.96	0.40
1:B:536:ALA:HB3	1:B:613:LEU:HD22	2.03	0.40
1:C:455:LEU:HD13	1:D:383:LEU:HD21	2.03	0.40
1:B:530:LEU:HD22	1:B:636:SER:HA	2.03	0.40
1:C:1093:VAL:HB	1:C:1150:ARG:HD3	2.03	0.40
2:B:2001:TPP:H61	2:B:2001:TPP:HM41	1.94	0.40
1:C:898:LEU:O	1:C:945:VAL:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:603:PRO:HD3	1:D:991:PHE:CZ	2.56	0.40
1:D:867:ARG:HG2	1:D:880:PHE:CD1	2.55	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	818/868 (94%)	800 (98%)	18 (2%)	0	100	100
1	B	804/868 (93%)	786 (98%)	18 (2%)	0	100	100
1	C	805/868 (93%)	789 (98%)	16 (2%)	0	100	100
1	D	808/868 (93%)	792 (98%)	16 (2%)	0	100	100
All	All	3235/3472 (93%)	3167 (98%)	68 (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	649/726 (89%)	633 (98%)	16 (2%)	47	60
1	B	628/726 (86%)	615 (98%)	13 (2%)	53	67
1	C	648/726 (89%)	633 (98%)	15 (2%)	50	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	634/726 (87%)	625 (99%)	9 (1%)	67	80
All	All	2559/2904 (88%)	2506 (98%)	53 (2%)	53	67

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	A	402	ASP
1	A	436	LEU
1	A	471	HIS
1	A	501	VAL
1	A	596	GLU
1	A	632	ASP
1	A	639	PRO
1	A	642	LEU
1	A	682	PHE
1	A	770	SER
1	A	803	VAL
1	A	930	LEU
1	A	953	PHE
1	A	976	GLN
1	A	1150	ARG
1	B	471	HIS
1	B	576	VAL
1	B	642	LEU
1	B	682	PHE
1	B	757	GLN
1	B	766	THR
1	B	810	LEU
1	B	909	THR
1	B	930	LEU
1	B	953	PHE
1	B	976	GLN
1	B	1182	LEU
1	B	1187	ILE
1	C	471	HIS
1	C	576	VAL
1	C	632	ASP
1	C	682	PHE
1	C	766	THR
1	C	767	LYS
1	C	793	LEU

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Mol	Chain	Res	Type
1	C	831	LEU
1	C	930	LEU
1	C	953	PHE
1	C	976	GLN
1	C	1150	ARG
1	C	1182	LEU
1	C	1187	ILE
1	C	1222	LEU
1	D	471	HIS
1	D	496	LEU
1	D	682	PHE
1	D	803	VAL
1	D	909	THR
1	D	930	LEU
1	D	953	PHE
1	D	976	GLN
1	D	1187	ILE

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

Mol	Chain	Res	Type
1	C	912	HIS
1	C	1030	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPP	C	2001	3	22,27,27	2.21	3 (13%)	29,40,40	1.98	9 (31%)
2	TPP	A	2001	3	22,27,27	2.08	4 (18%)	29,40,40	2.04	10 (34%)
2	TPP	D	2001	3	22,27,27	2.27	3 (13%)	29,40,40	1.76	7 (24%)
2	TPP	B	2001	3	22,27,27	1.98	3 (13%)	29,40,40	1.91	10 (34%)
5	ACO	A	2004	-	30,35,53	1.78	6 (20%)	34,54,79	1.48	2 (5%)
5	ACO	C	2004	-	30,35,53	1.57	7 (23%)	34,54,79	1.40	3 (8%)
5	ACO	D	2004	-	30,35,53	1.62	6 (20%)	34,54,79	1.48	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	C	2001	3	-	3/16/17/17	0/2/2/2
2	TPP	A	2001	3	-	3/16/17/17	0/2/2/2
2	TPP	D	2001	3	-	3/16/17/17	0/2/2/2
2	TPP	B	2001	3	-	3/16/17/17	0/2/2/2
5	ACO	A	2004	-	-	5/21/41/67	0/3/3/3
5	ACO	C	2004	-	-	6/21/41/67	0/3/3/3
5	ACO	D	2004	-	-	5/21/41/67	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TPP	C4-N3	-9.08	1.31	1.39
2	C	2001	TPP	C4-N3	-8.59	1.32	1.39
2	A	2001	TPP	C4-N3	-7.40	1.33	1.39
2	B	2001	TPP	C4-N3	-6.97	1.33	1.39
5	A	2004	ACO	O4B-C1B	4.05	1.46	1.41
5	A	2004	ACO	P3B-O7A	4.00	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2004	ACO	P3B-O7A	3.85	1.63	1.50
2	B	2001	TPP	PB-O1B	3.73	1.62	1.50
5	D	2004	ACO	O4B-C1B	3.54	1.46	1.41
5	D	2004	ACO	P3B-O7A	3.51	1.61	1.50
5	A	2004	ACO	P1A-O1A	3.42	1.63	1.50
5	A	2004	ACO	P3B-O3B	3.30	1.65	1.59
2	D	2001	TPP	PB-O1B	3.22	1.60	1.50
5	C	2004	ACO	P1A-O1A	3.17	1.62	1.50
2	C	2001	TPP	PB-O1B	3.13	1.60	1.50
5	D	2004	ACO	P1A-O1A	3.06	1.61	1.50
2	A	2001	TPP	PB-O1B	2.96	1.60	1.50
5	A	2004	ACO	P2A-O4A	2.92	1.61	1.50
2	A	2001	TPP	C2-N3	-2.89	1.29	1.36
2	C	2001	TPP	C2-N3	-2.84	1.30	1.36
5	C	2004	ACO	O4B-C1B	2.84	1.45	1.41
5	C	2004	ACO	P2A-O4A	2.72	1.60	1.50
2	B	2001	TPP	C2-N3	-2.70	1.30	1.36
5	D	2004	ACO	P3B-O8A	2.59	1.64	1.54
5	D	2004	ACO	P2A-O4A	2.47	1.59	1.50
2	D	2001	TPP	C2-N3	-2.38	1.31	1.36
5	C	2004	ACO	P3B-O8A	2.27	1.63	1.54
5	A	2004	ACO	P2A-O6A	2.25	1.68	1.59
5	D	2004	ACO	C8A-N7A	-2.25	1.30	1.34
5	C	2004	ACO	C8A-N7A	-2.22	1.30	1.34
2	A	2001	TPP	C6-C5	2.16	1.51	1.50
5	C	2004	ACO	P3B-O3B	2.11	1.63	1.59

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2004	ACO	N3A-C2A-N1A	-5.75	119.69	128.68
5	D	2004	ACO	N3A-C2A-N1A	-5.45	120.15	128.68
5	C	2004	ACO	N3A-C2A-N1A	-5.42	120.21	128.68
2	B	2001	TPP	C5-C4-N3	4.41	116.40	107.57
2	B	2001	TPP	CM4-C4-C5	-4.24	118.33	127.60
2	D	2001	TPP	C5-C4-N3	4.23	116.03	107.57
2	A	2001	TPP	C5-C4-N3	4.18	115.93	107.57
2	A	2001	TPP	C6-C5-C4	4.17	130.78	127.43
2	A	2001	TPP	CM4-C4-C5	-4.17	118.49	127.60
2	C	2001	TPP	C5-C4-N3	4.12	115.82	107.57
2	C	2001	TPP	CM4-C4-C5	-4.06	118.72	127.60
2	C	2001	TPP	C6'-N1'-C2'	3.86	122.53	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TPP	C6-C5-C4	3.76	130.45	127.43
2	D	2001	TPP	CM4-C4-C5	-3.69	119.53	127.60
2	A	2001	TPP	C6'-N1'-C2'	3.66	122.18	115.96
2	D	2001	TPP	C6'-N1'-C2'	3.61	122.10	115.96
2	B	2001	TPP	C6-C5-C4	3.52	130.25	127.43
5	D	2004	ACO	P2A-O3A-P1A	-3.43	121.06	132.83
2	A	2001	TPP	N1'-C2'-N3'	-3.27	119.91	125.54
5	A	2004	ACO	P2A-O3A-P1A	-3.26	121.64	132.83
5	C	2004	ACO	P2A-O3A-P1A	-3.22	121.78	132.83
2	B	2001	TPP	C6'-N1'-C2'	3.16	121.34	115.96
2	C	2001	TPP	N1'-C2'-N3'	-3.06	120.27	125.54
2	D	2001	TPP	N1'-C2'-N3'	-2.94	120.49	125.54
2	B	2001	TPP	N1'-C2'-N3'	-2.90	120.55	125.54
2	A	2001	TPP	CM2-C2'-N1'	2.78	120.19	117.14
2	C	2001	TPP	C5'-C6'-N1'	-2.76	119.22	123.82
2	A	2001	TPP	C7'-N3-C2	-2.62	120.61	125.35
2	C	2001	TPP	CM2-C2'-N1'	2.57	119.96	117.14
2	B	2001	TPP	C7'-N3-C2	-2.46	120.91	125.35
2	A	2001	TPP	CM4-C4-N3	2.39	125.57	122.53
2	B	2001	TPP	CM2-C2'-N1'	2.38	119.75	117.14
2	D	2001	TPP	C6-C5-C4	2.26	129.25	127.43
2	C	2001	TPP	CM4-C4-N3	2.26	125.41	122.53
2	D	2001	TPP	C5'-C6'-N1'	-2.22	120.12	123.82
2	A	2001	TPP	N4'-C4'-N3'	2.20	120.14	117.03
2	B	2001	TPP	C2'-N3'-C4'	2.19	121.50	118.08
2	D	2001	TPP	CM2-C2'-N1'	2.13	119.48	117.14
2	B	2001	TPP	CM4-C4-N3	2.12	125.23	122.53
2	A	2001	TPP	C5'-C6'-N1'	-2.08	120.35	123.82
2	C	2001	TPP	C7'-N3-C2	-2.07	121.61	125.35
2	B	2001	TPP	C5'-C6'-N1'	-2.07	120.38	123.82
5	C	2004	ACO	C4A-C5A-N7A	-2.04	107.27	109.40

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	TPP	PA-O3A-PB-O3B
2	A	2001	TPP	PA-O3A-PB-O3B
2	D	2001	TPP	PA-O3A-PB-O2B
2	D	2001	TPP	PA-O3A-PB-O3B
5	A	2004	ACO	C5B-O5B-P1A-O1A
5	A	2004	ACO	CCP-O6A-P2A-O3A

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Mol	Chain	Res	Type	Atoms
5	C	2004	ACO	C5B-O5B-P1A-O1A
5	C	2004	ACO	CCP-O6A-P2A-O3A
5	D	2004	ACO	C5B-O5B-P1A-O1A
5	D	2004	ACO	CCP-O6A-P2A-O3A
5	A	2004	ACO	P2A-O3A-P1A-O5B
5	C	2004	ACO	P2A-O3A-P1A-O5B
5	D	2004	ACO	P2A-O3A-P1A-O5B
2	C	2001	TPP	PA-O3A-PB-O2B
2	A	2001	TPP	PA-O3A-PB-O2B
2	B	2001	TPP	PA-O3A-PB-O2B
2	B	2001	TPP	PA-O3A-PB-O3B
5	A	2004	ACO	C5B-O5B-P1A-O3A
5	C	2004	ACO	C5B-O5B-P1A-O3A
5	D	2004	ACO	C5B-O5B-P1A-O3A
5	A	2004	ACO	C5B-O5B-P1A-O2A
5	C	2004	ACO	C5B-O5B-P1A-O2A
5	D	2004	ACO	C5B-O5B-P1A-O2A
2	C	2001	TPP	C7-O7-PA-O1A
2	A	2001	TPP	C7-O7-PA-O1A
2	D	2001	TPP	C7-O7-PA-O1A
2	B	2001	TPP	C7-O7-PA-O1A
5	C	2004	ACO	CCP-O6A-P2A-O5A

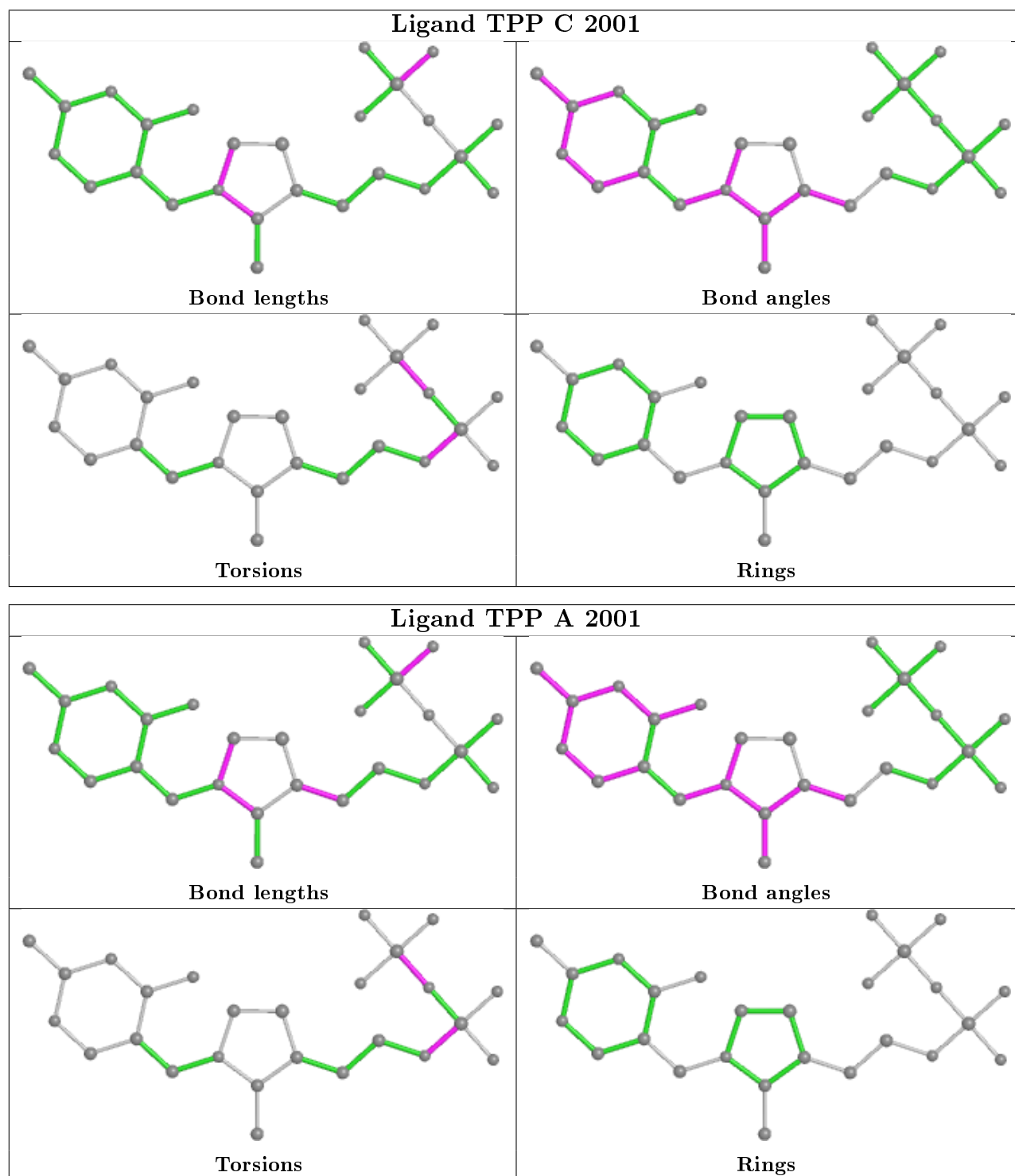
There are no ring outliers.

4 monomers are involved in 6 short contacts:

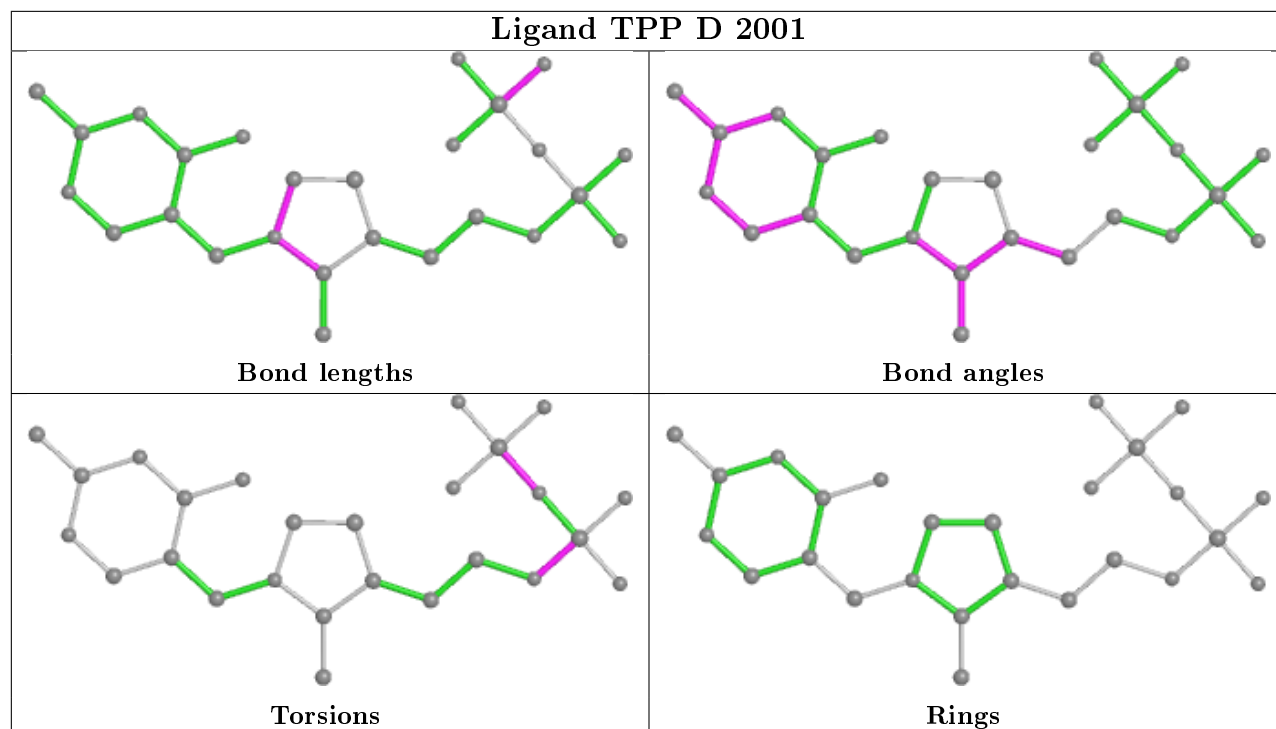
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	TPP	1	0
2	A	2001	TPP	2	0
2	D	2001	TPP	1	0
2	B	2001	TPP	2	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

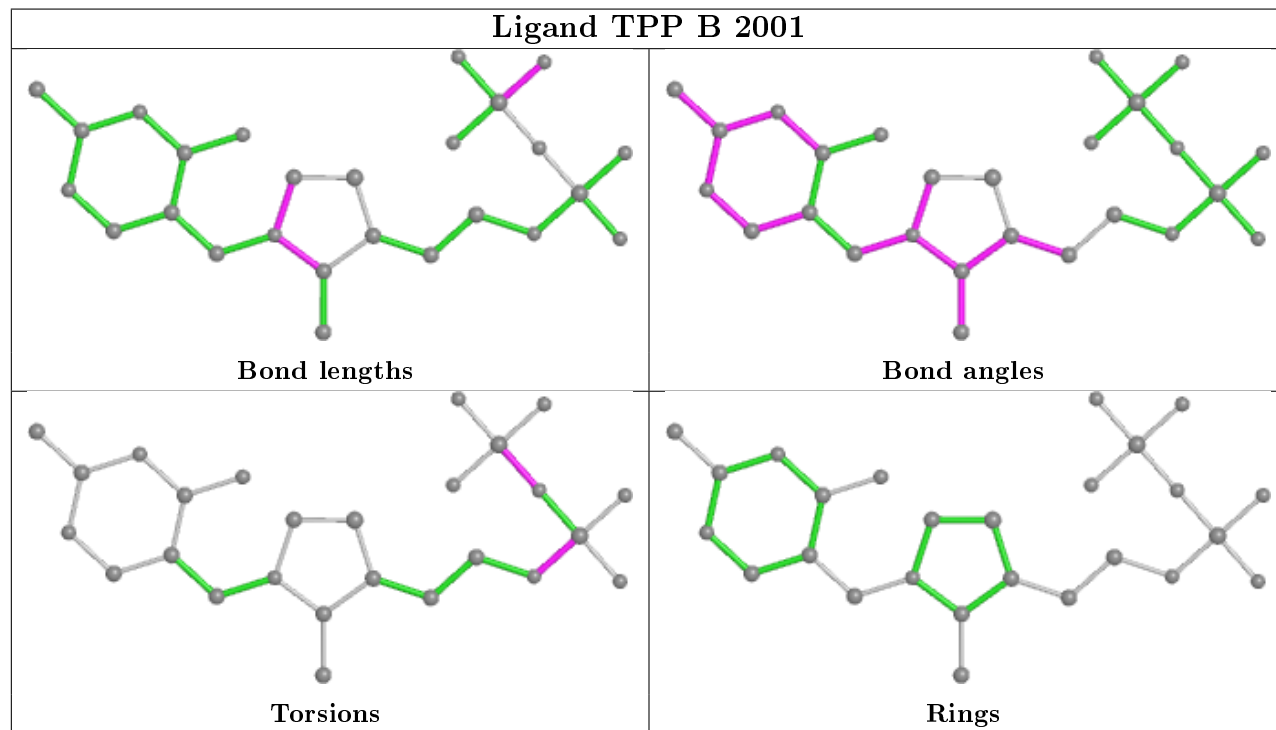
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

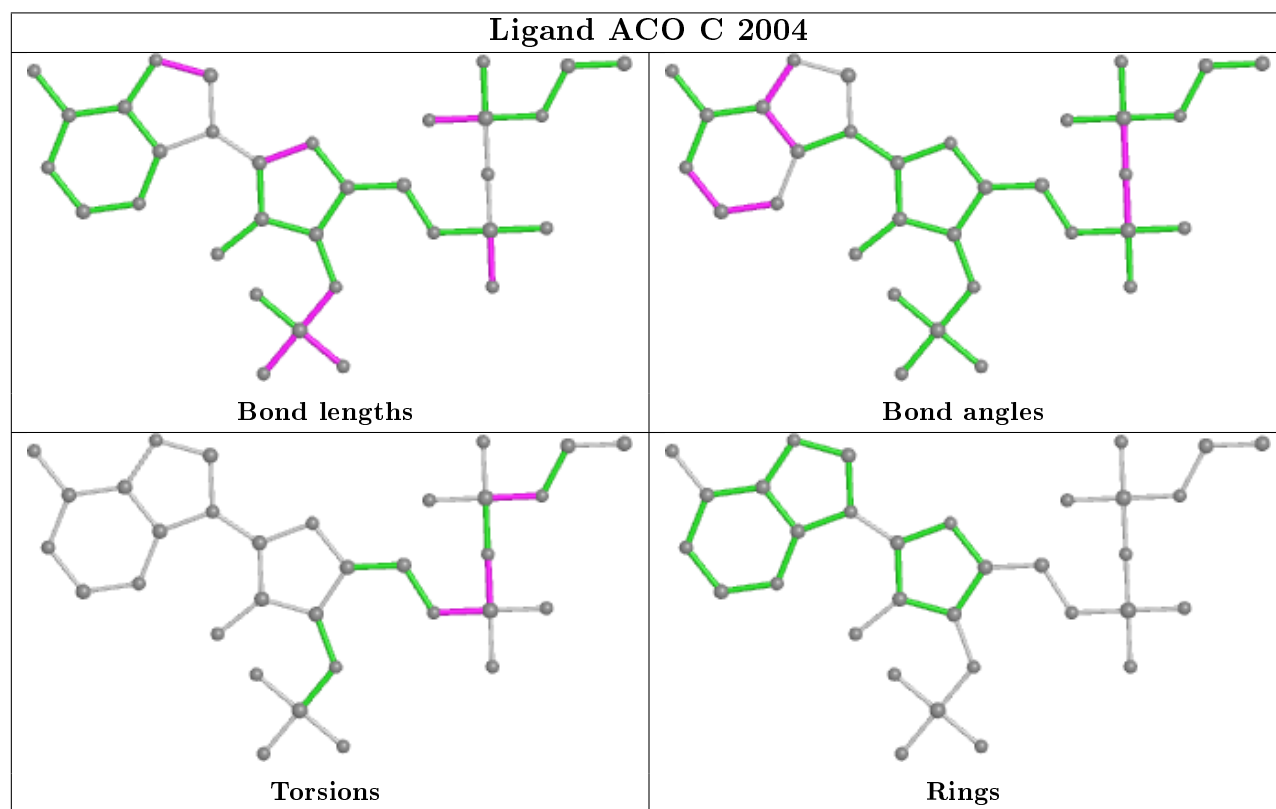
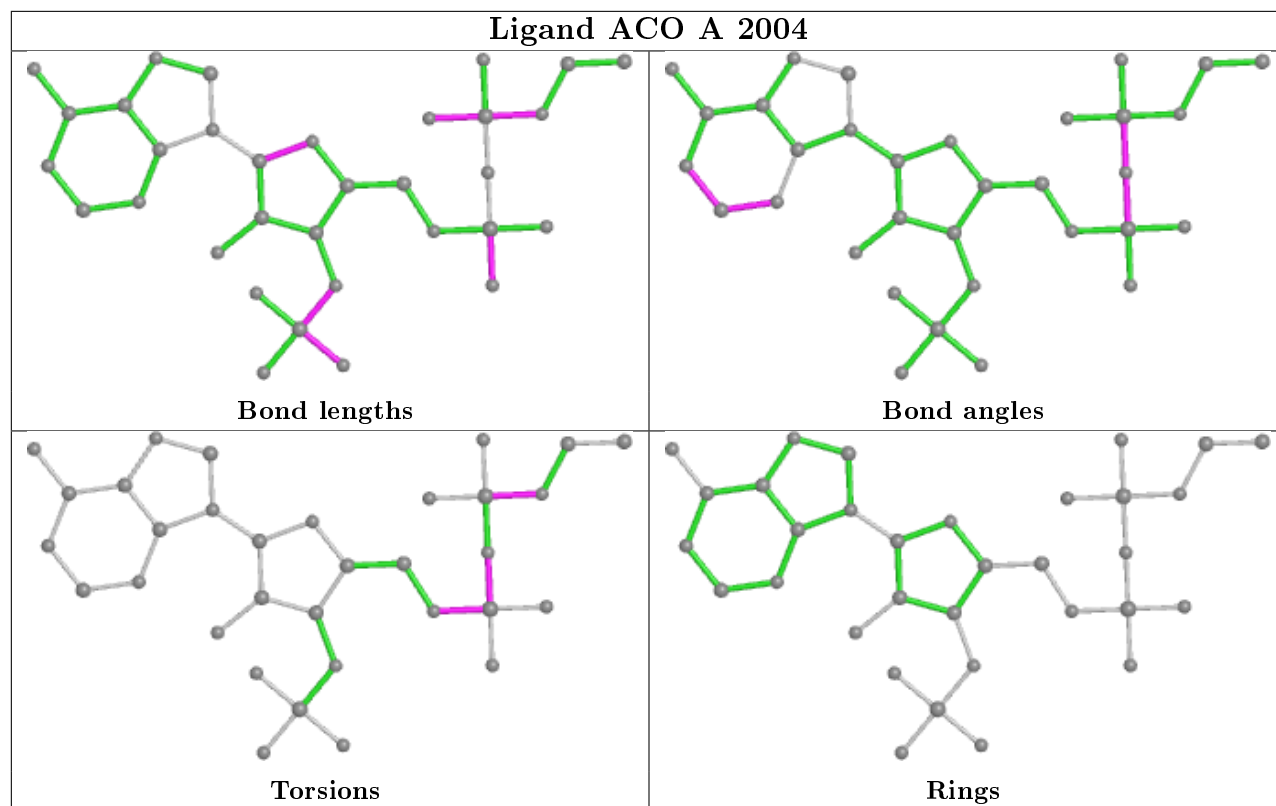


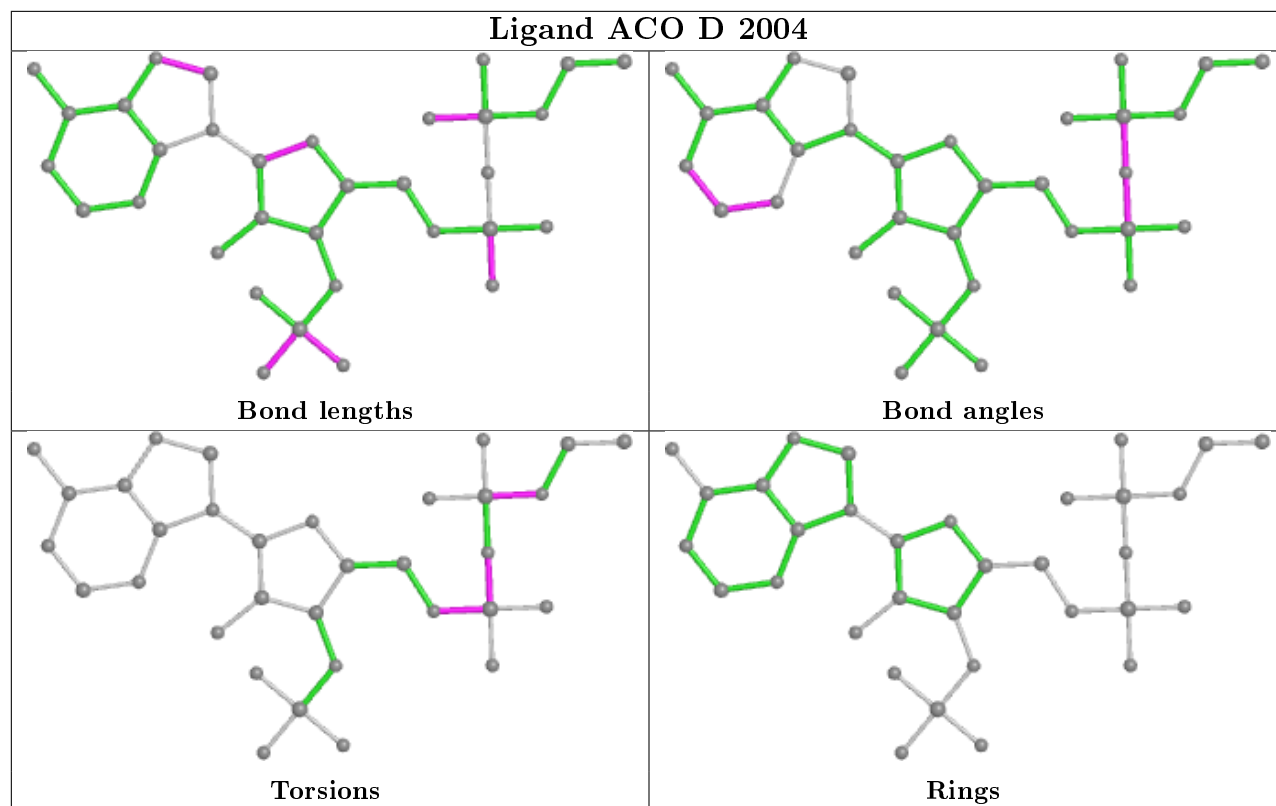
## Ligand TPP D 2001



## Ligand TPP B 2001







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	826/868 (95%)	-0.16	11 (1%) 77 75	23, 40, 81, 111	0
1	B	814/868 (93%)	-0.17	13 (1%) 72 70	21, 41, 80, 108	0
1	C	817/868 (94%)	-0.18	12 (1%) 73 72	20, 39, 78, 105	0
1	D	818/868 (94%)	-0.17	14 (1%) 70 68	18, 39, 78, 107	0
All	All	3275/3472 (94%)	-0.17	50 (1%) 73 72	18, 40, 79, 111	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	472	ASP	8.3
1	A	813	HIS	4.9
1	C	401	PRO	4.0
1	B	472	ASP	3.9
1	D	829	SER	3.8
1	D	413	TRP	3.6
1	A	413	TRP	3.5
1	D	471	HIS	3.3
1	C	413	TRP	3.3
1	C	779	ILE	3.2
1	B	421	VAL	3.2
1	C	769	GLY	3.2
1	D	574	GLY	3.0
1	B	793	LEU	3.0
1	C	402	ASP	3.0
1	D	427	VAL	2.9
1	C	590	PHE	2.9
1	C	472	ASP	2.9
1	D	501	VAL	2.9
1	B	775	THR	2.8
1	B	1102	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	399	SER	2.7
1	C	400	HIS	2.7
1	C	395	THR	2.7
1	D	769	GLY	2.7
1	C	808	ARG	2.6
1	B	501	VAL	2.6
1	A	400	HIS	2.6
1	B	777	ALA	2.6
1	A	401	PRO	2.6
1	A	412	LEU	2.6
1	B	810	LEU	2.6
1	D	631	SER	2.5
1	D	368	ALA	2.5
1	D	780	GLY	2.5
1	C	630	GLY	2.4
1	A	477	ALA	2.4
1	C	429	ARG	2.3
1	A	810	LEU	2.3
1	B	394	ASN	2.3
1	B	785	SER	2.3
1	A	421	VAL	2.3
1	D	473	LYS	2.3
1	B	1101	ASP	2.2
1	A	831	LEU	2.1
1	D	469	THR	2.1
1	B	769	GLY	2.1
1	B	471	HIS	2.0
1	A	501	VAL	2.0
1	D	575	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

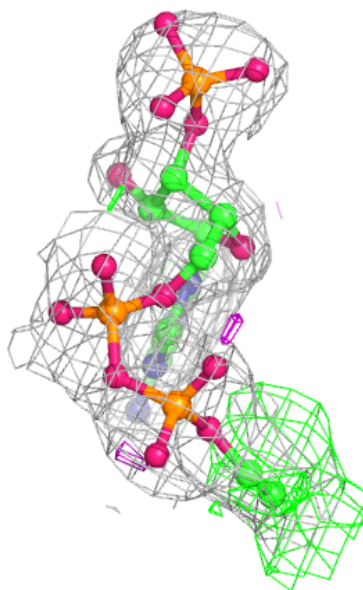
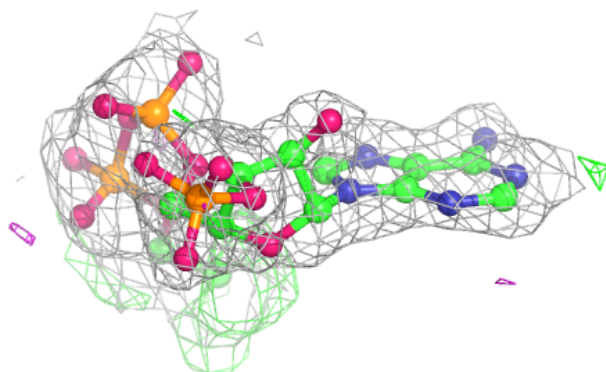
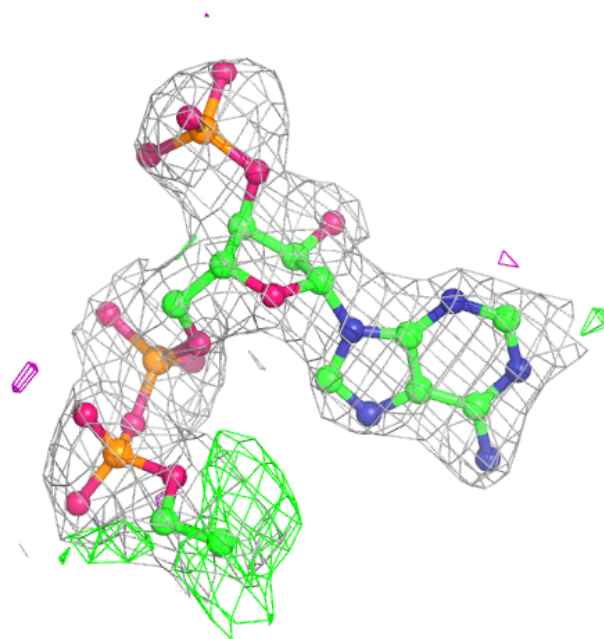
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACO	D	2004	33/51	0.87	0.16	53,75,91,92	0
4	CA	A	2003	1/1	0.89	0.05	75,75,75,75	0
5	ACO	A	2004	33/51	0.92	0.13	47,60,77,77	0
4	CA	D	2003	1/1	0.93	0.10	57,57,57,57	0
4	CA	B	2003	1/1	0.94	0.09	74,74,74,74	0
4	CA	C	2003	1/1	0.94	0.07	55,55,55,55	0
5	ACO	C	2004	33/51	0.95	0.11	43,54,78,82	0
3	MG	B	2002	1/1	0.98	0.05	23,23,23,23	0
3	MG	D	2002	1/1	0.98	0.06	23,23,23,23	0
2	TPP	D	2001	26/26	0.98	0.13	18,27,40,55	0
2	TPP	B	2001	26/26	0.98	0.13	18,30,44,50	0
3	MG	A	2002	1/1	0.98	0.13	18,18,18,18	0
3	MG	C	2002	1/1	0.99	0.09	18,18,18,18	0
2	TPP	A	2001	26/26	0.99	0.12	19,28,38,50	0
2	TPP	C	2001	26/26	0.99	0.12	18,30,43,49	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.

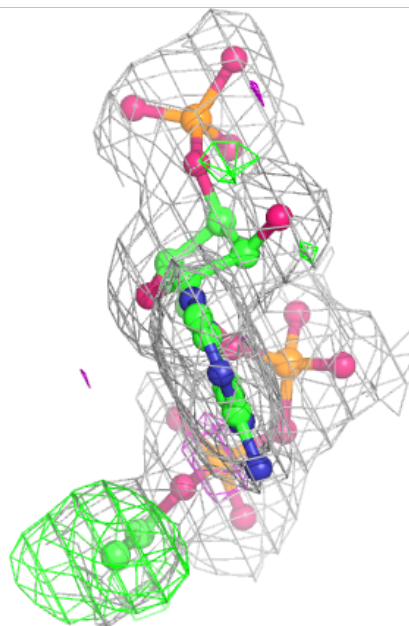
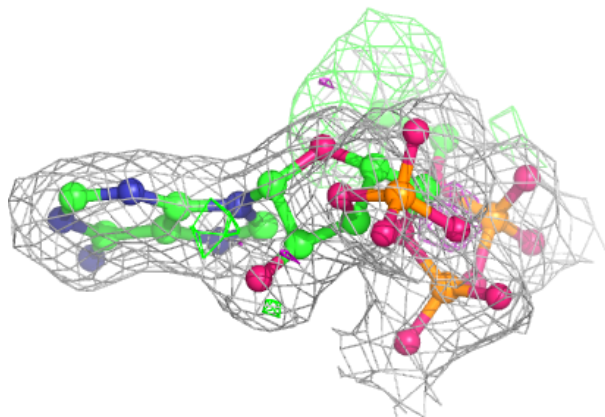
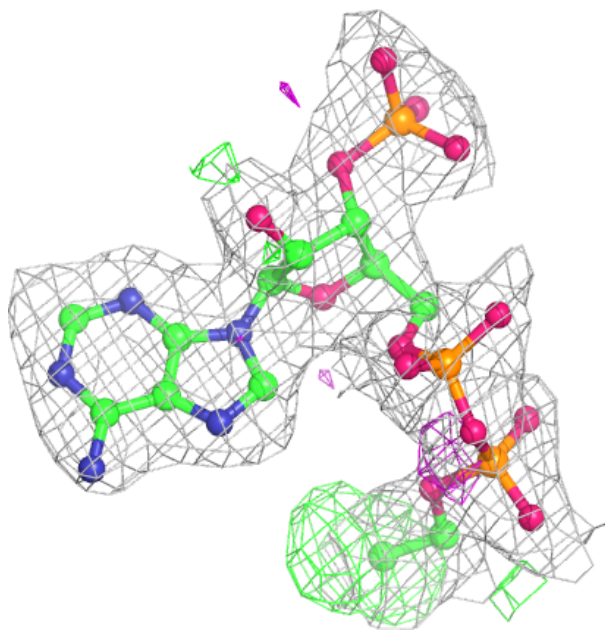
**Electron density around ACO D 2004:**

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



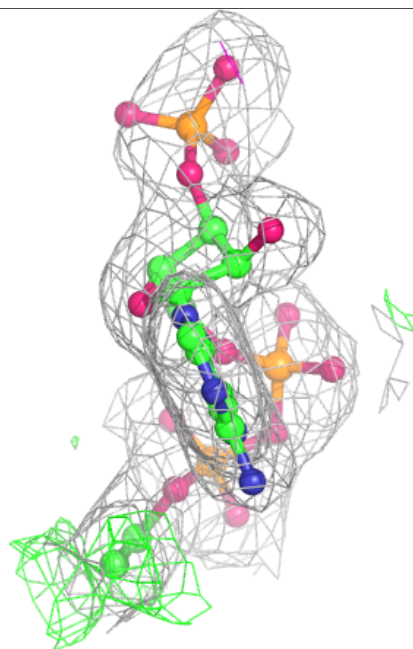
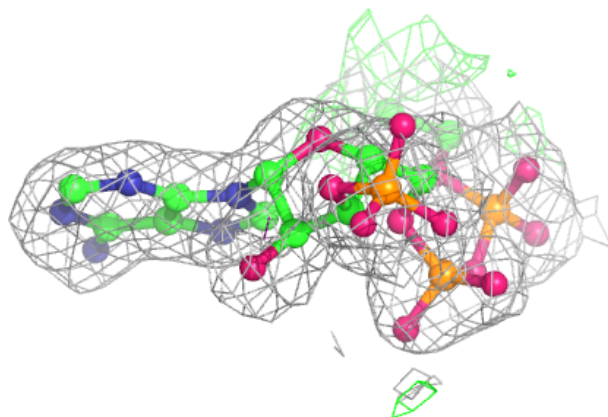
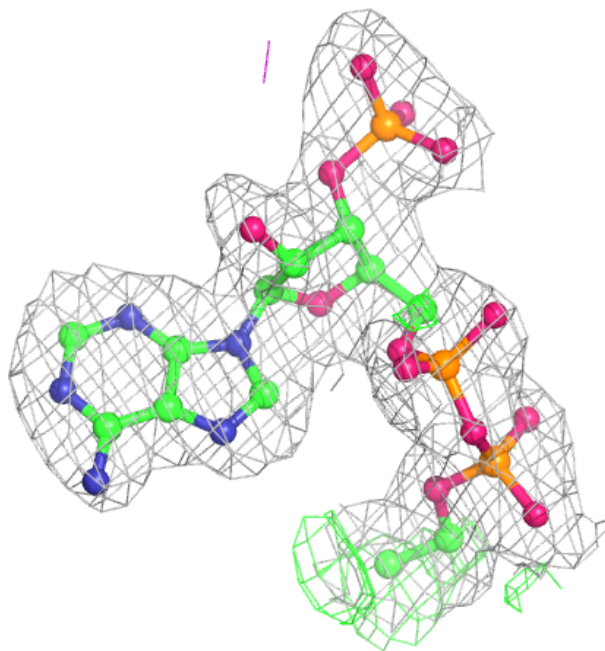
**Electron density around ACO A 2004:**

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



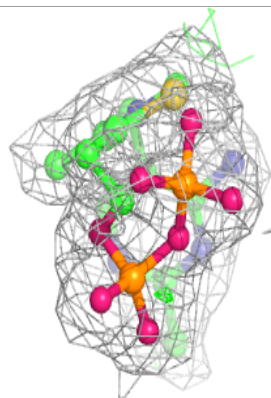
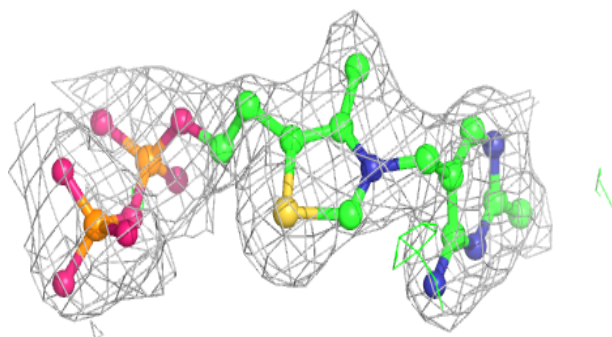
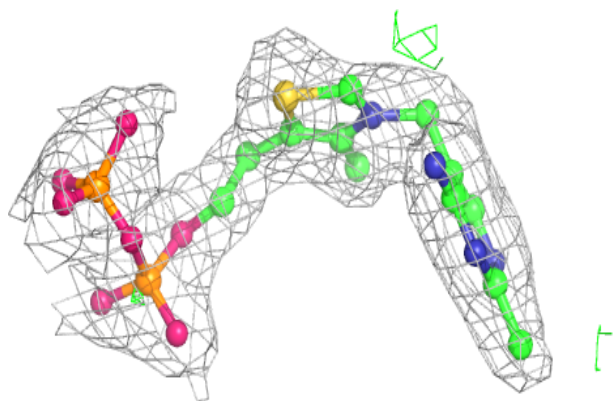
**Electron density around ACO C 2004:**

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

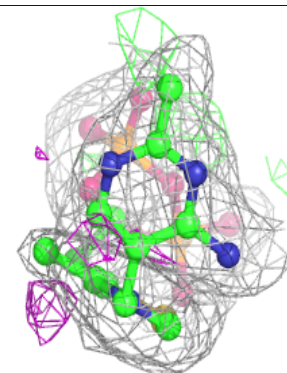
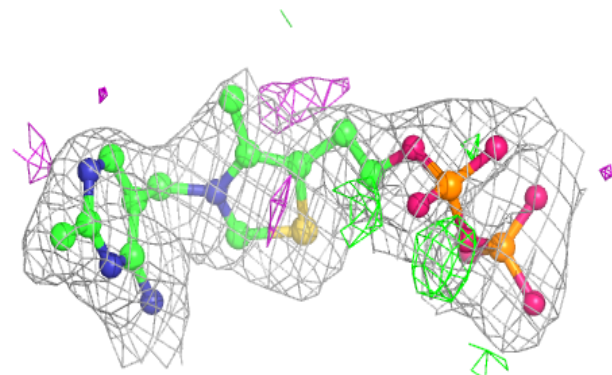
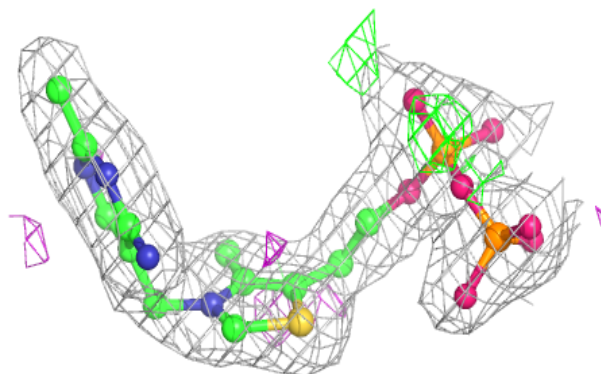


**Electron density around TPP D 2001:**

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

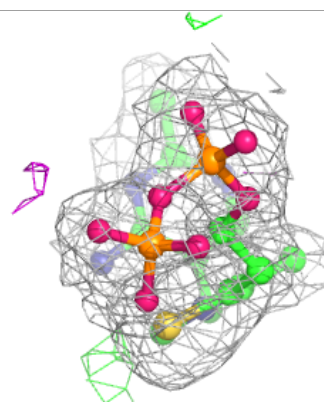
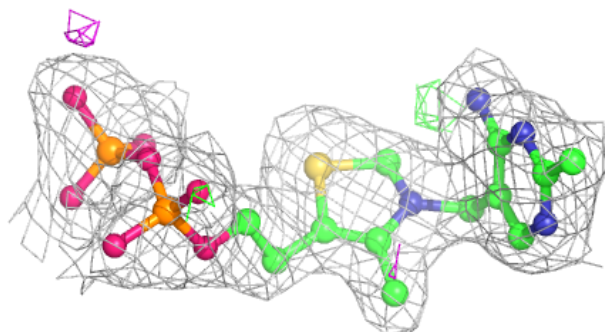
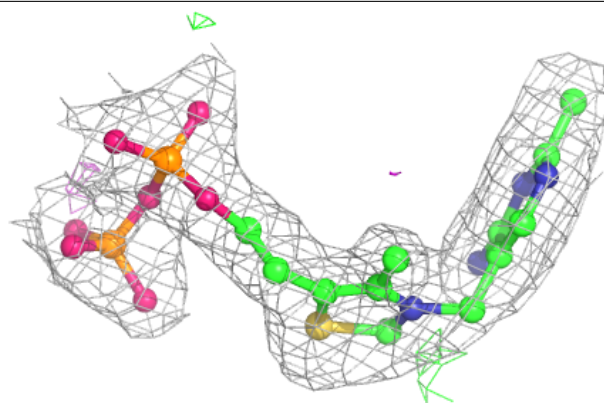
**Electron density around TPP B 2001:**

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

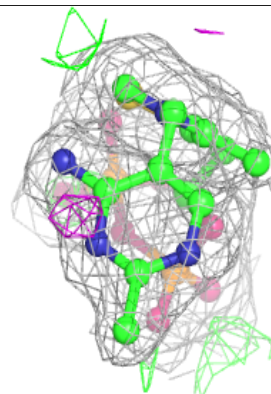
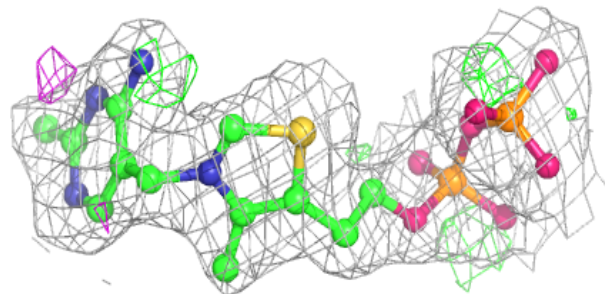
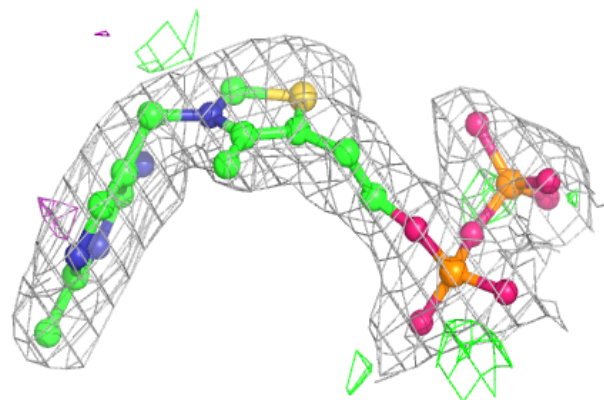


**Electron density around TPP A 2001:**

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

**Electron density around TPP C 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

There are no such residues in this entry.