



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:43 am BST

PDB ID : 6GUA  
Title : Xylulose 5-phosphate phosphoketolase from *Lactococcus lactis*  
Authors : Scheidig, A.J.; Szedlacsek, S.E.  
Deposited on : 2018-06-19  
Resolution : 1.95 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

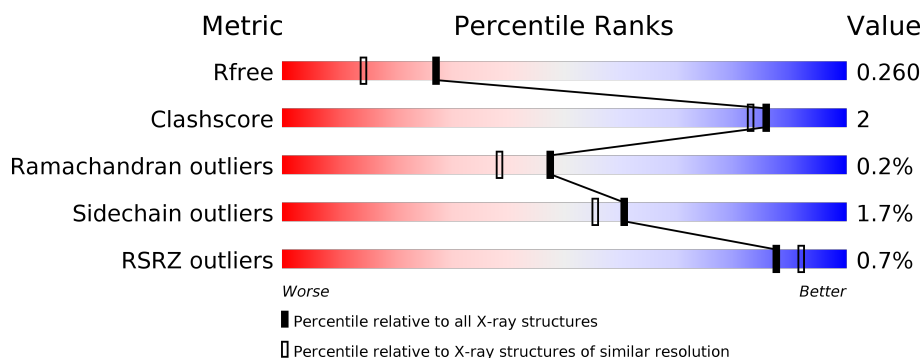
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION, SOLUTION SCATTERING*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	822	
1	B	822	
1	C	822	
1	D	822	
1	E	822	
1	F	822	

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Mol	Chain	Length	Quality of chain
1	G	822	<div><div></div><div>96%</div><div>.</div></div>
1	H	822	<div>%<div><div></div><div>91%</div><div>8%</div></div></div>

## 2 Entry composition

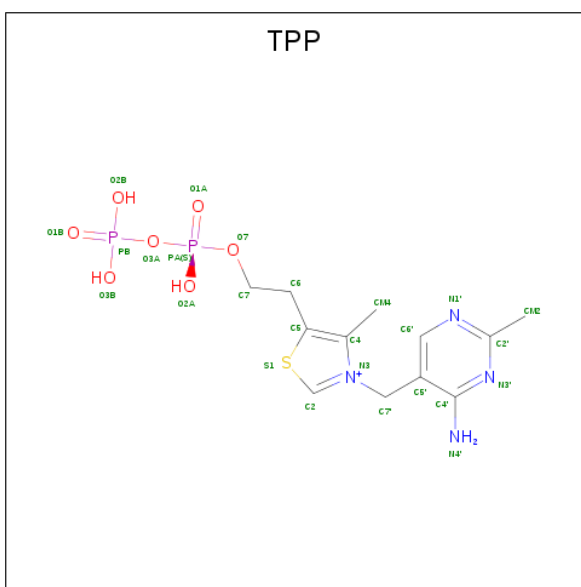
There are 5 unique types of molecules in this entry. The entry contains 110088 atoms, of which 51051 are hydrogens and 0 are deuteriums.

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 Probable phosphoketolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	821	Total	C	H	N	O	S	0	1	0
			12946	4202	6352	1129	1240	23			
1	B	818	Total	C	H	N	O	S	0	2	0
			12912	4191	6337	1127	1234	23			
1	C	820	Total	C	H	N	O	S	0	4	0
			12989	4212	6380	1135	1239	23			
1	D	820	Total	C	H	N	O	S	0	2	0
			12966	4205	6368	1134	1236	23			
1	E	820	Total	C	H	N	O	S	0	4	0
			12973	4208	6371	1131	1239	24			
1	F	820	Total	C	H	N	O	S	0	4	0
			12984	4212	6382	1130	1237	23			
1	G	820	Total	C	H	N	O	S	0	2	0
			12952	4203	6359	1129	1237	24			
1	H	819	Total	C	H	N	O	S	0	8	0
			12984	4212	6374	1132	1243	23			

- 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	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		

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

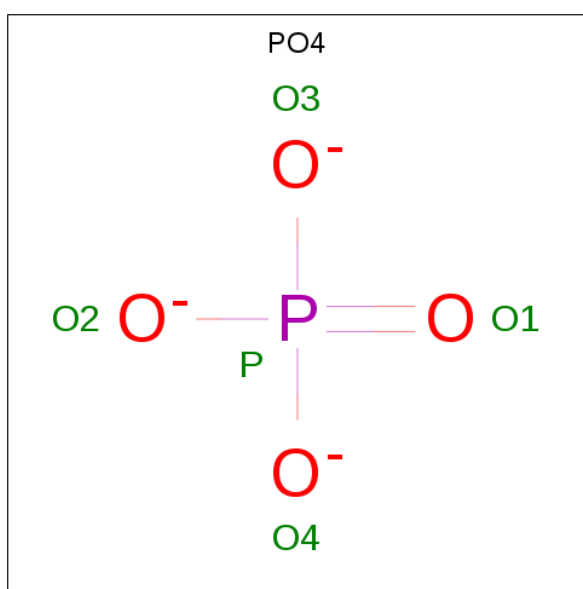
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	P	0	0
			5	4	1		

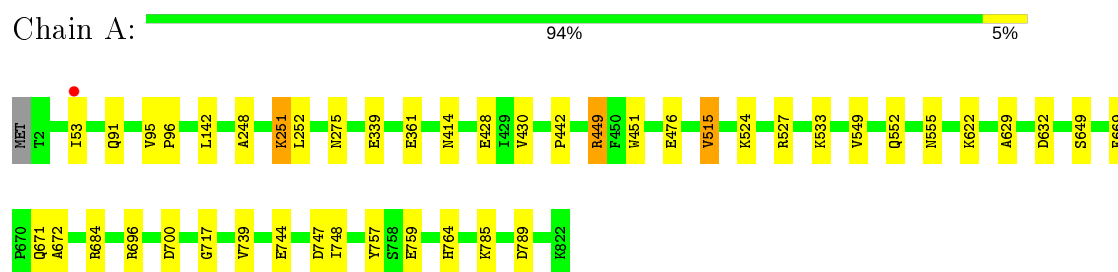
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	893	Total	O	0	0
			893	893		
5	B	683	Total	O	0	0
			683	683		
5	C	622	Total	O	0	0
			622	622		
5	D	818	Total	O	0	0
			818	818		
5	E	616	Total	O	0	0
			616	616		
5	F	821	Total	O	0	0
			821	821		
5	G	866	Total	O	0	0
			866	866		
5	H	679	Total	O	0	0
			679	679		

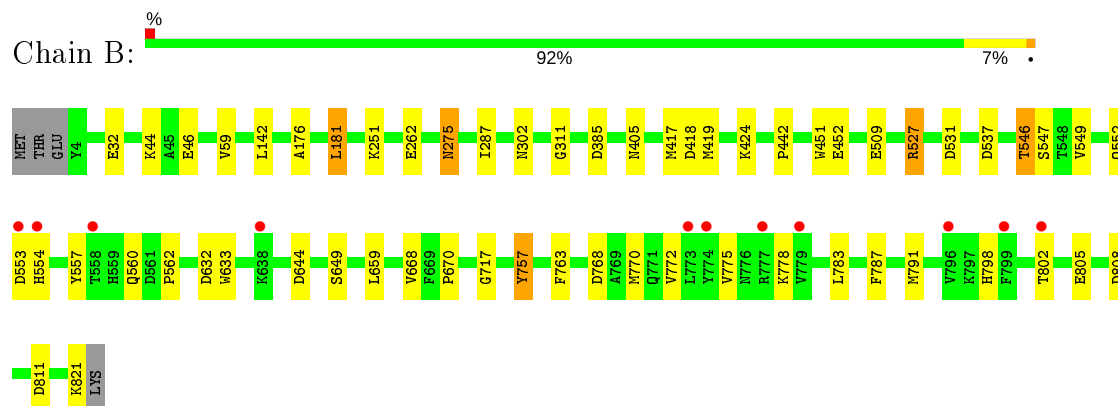
### 3 Residue-property plots [i](#)

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.

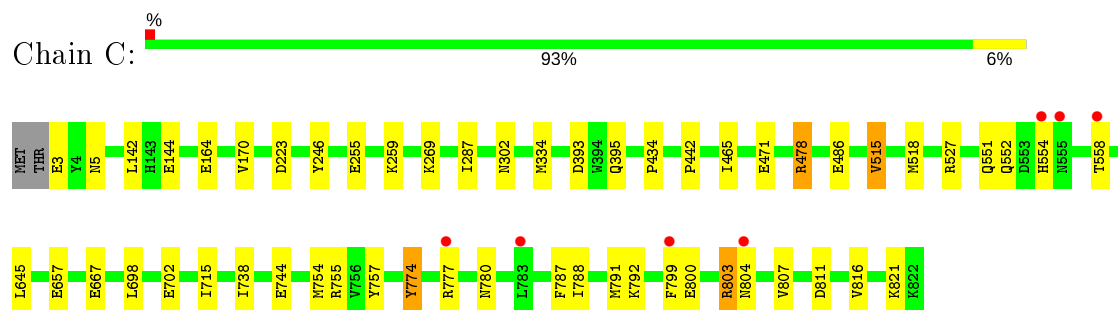
- Molecule 1: Probable phosphoketolase



- Molecule 1: Probable phosphoketolase



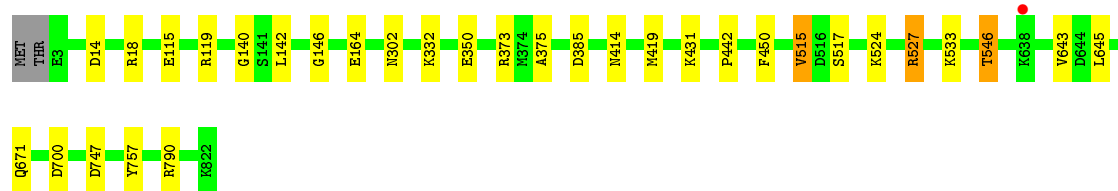
- Molecule 1: Probable phosphoketolase



- Molecule 1: Probable phosphoketolase

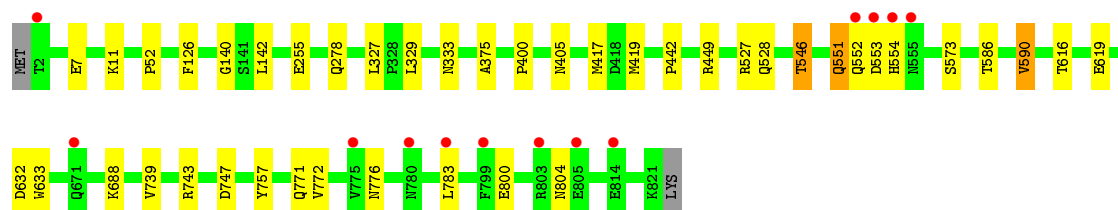






- Molecule 1: Probable phosphoketolase

Chain E:



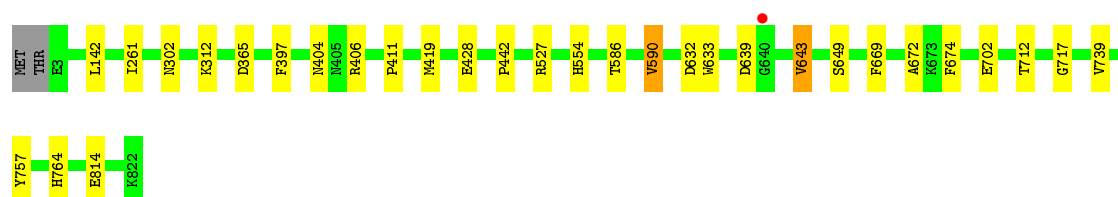
- Molecule 1: Probable phosphoketolase

Chain F:



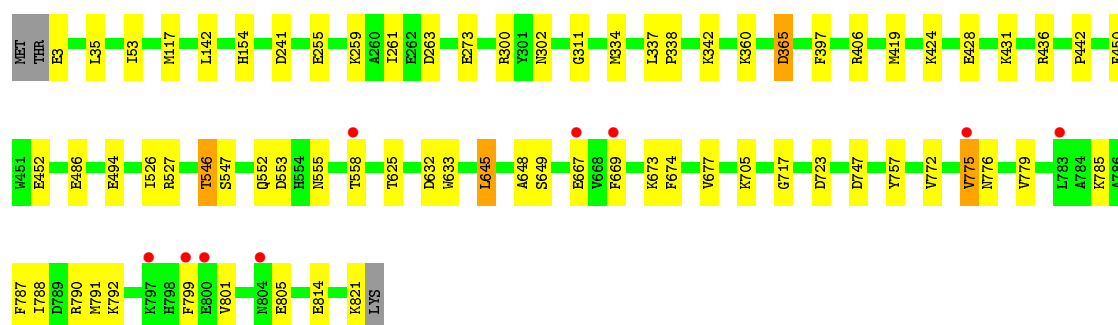
- Molecule 1: Probable phosphoketolase

Chain G:



- Molecule 1: Probable phosphoketolase

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.10Å 141.50Å 161.15Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	44.30 – 1.95 44.32 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.3 (44.30-1.95) 97.4 (44.32-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 1.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.212 , 0.261 0.212 , 0.260	Depositor DCC
$R_{free}$ test set	25030 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 35.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.56$ , $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.117 for h,-k,-l 0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	110088	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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 42.92 % 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 1.9021e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PO4, 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	0.30	0/6776	0.49	0/9182
1	B	0.29	0/6760	0.49	0/9161
1	C	0.29	0/6800	0.48	0/9212
1	D	0.29	0/6783	0.49	0/9189
1	E	0.29	0/6793	0.48	0/9204
1	F	0.29	0/6793	0.48	0/9204
1	G	0.30	0/6778	0.49	0/9183
1	H	0.31	1/6821 (0.0%)	0.49	0/9243
All	All	0.30	1/54304 (0.0%)	0.49	0/73578

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	775	VAL	CB-CG1	-5.11	1.42	1.52

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	6594	6352	6351	29	0
1	B	6575	6337	6335	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6609	6380	6378	35	0
1	D	6598	6368	6366	24	0
1	E	6602	6371	6369	26	0
1	F	6602	6382	6379	17	0
1	G	6593	6359	6357	15	0
1	H	6610	6374	6350	49	0
2	A	26	16	16	1	0
2	B	26	16	16	0	0
2	C	26	16	16	1	0
2	D	26	16	16	3	0
2	E	26	16	16	1	0
2	F	26	16	16	1	0
2	G	26	16	16	2	0
2	H	26	16	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	1	0
4	E	10	0	0	1	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	A	893	0	0	10	3
5	B	683	0	0	13	0
5	C	622	0	0	15	0
5	D	818	0	0	12	0
5	E	616	0	0	10	0
5	F	821	0	0	12	2
5	G	866	0	0	7	5
5	H	679	0	0	19	0
All	All	59037	51051	51013	231	5

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 (231) 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:G:406:ARG:NH2	5:G:1001:HOH:O	1.90	1.03
1:C:811:ASP:OD1	5:C:1001:HOH:O	1.79	0.99
1:H:558:THR:OG1	5:H:1001:HOH:O	1.82	0.96
1:B:670:PRO:O	5:B:1001:HOH:O	1.91	0.89
1:B:275:ASN:OD1	5:B:1002:HOH:O	1.94	0.85
1:H:436[A]:ARG:NH1	5:H:1006:HOH:O	2.08	0.84
1:E:333:ASN:OD1	5:E:1001:HOH:O	1.95	0.84
1:E:739:VAL:O	5:E:1002:HOH:O	1.96	0.83
1:F:53:ILE:O	5:F:1001:HOH:O	1.98	0.82
1:H:799:PHE:O	5:H:1002:HOH:O	1.96	0.82
1:C:471:GLU:OE1	5:C:1002:HOH:O	1.98	0.82
1:C:478[A]:ARG:NH1	5:C:1010:HOH:O	2.14	0.81
1:B:644:ASP:OD1	1:B:778:LYS:NZ	2.13	0.80
1:B:811:ASP:OD1	5:B:1003:HOH:O	2.00	0.80
1:D:414:ASN:OD1	5:D:1001:HOH:O	2.01	0.79
1:H:814:GLU:OE2	5:H:1003:HOH:O	2.01	0.78
1:C:754:MET:SD	5:C:1476:HOH:O	2.40	0.78
1:A:700:ASP:OD1	5:A:1001:HOH:O	2.01	0.78
1:E:551:GLN:O	5:E:1003:HOH:O	1.99	0.78
1:H:428:GLU:HA	1:H:431:LYS:HE3	1.66	0.77
1:H:790:ARG:NH2	5:H:1008:HOH:O	2.17	0.77
1:B:405[A]:ASN:OD1	5:B:1004:HOH:O	2.01	0.77
1:E:743:ARG:NH2	5:E:1002:HOH:O	2.11	0.77
4:C:903:PO4:O1	5:C:1003:HOH:O	2.02	0.77
1:C:164:GLU:OE1	5:C:1004:HOH:O	2.03	0.76
1:A:361:GLU:OE2	5:A:1002:HOH:O	2.03	0.75
1:B:531:ASP:OD2	5:B:1005:HOH:O	2.04	0.75
1:C:800:GLU:O	1:C:804:ASN:ND2	2.19	0.74
1:A:744:GLU:O	1:B:527:ARG:NH2	2.21	0.74
1:H:747:ASP:OD2	5:H:1004:HOH:O	2.06	0.73
1:B:768:ASP:OD1	5:B:1006:HOH:O	2.05	0.73
1:H:667:GLU:OE1	5:H:1007:HOH:O	2.08	0.72
1:H:821:LYS:O	5:H:1005:HOH:O	2.07	0.72
1:D:14:ASP:OD2	1:D:18[B]:ARG:NH1	2.23	0.70
1:E:800:GLU:OE2	1:E:804:ASN:ND2	2.23	0.70
1:G:404:ASN:ND2	5:G:1007:HOH:O	2.25	0.70
1:D:700:ASP:OD1	5:D:1002:HOH:O	2.10	0.69
1:C:551:GLN:O	5:C:1005:HOH:O	2.09	0.69
1:H:342:LYS:NZ	5:H:1011:HOH:O	2.23	0.68
1:B:452:GLU:OE1	5:B:1008:HOH:O	2.11	0.68
1:H:772:VAL:HA	1:H:775:VAL:HG12	1.75	0.68
1:D:350:GLU:OE2	5:D:1003:HOH:O	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:GLU:OE1	5:E:1004:HOH:O	2.12	0.68
1:C:246:TYR:OH	5:C:1006:HOH:O	2.09	0.67
1:C:465:ILE:O	5:C:1007:HOH:O	2.10	0.67
1:B:262:GLU:OE2	5:B:1007:HOH:O	2.11	0.67
1:B:547:SER:O	1:B:552:GLN:NE2	2.28	0.66
1:A:764:HIS:NE2	5:A:1008:HOH:O	2.27	0.66
1:H:632:ASP:OD1	1:H:633:TRP:N	2.28	0.66
1:G:312:LYS:NZ	5:G:1010:HOH:O	2.28	0.65
1:D:332:LYS:HG3	1:G:814:GLU:HB3	1.78	0.65
1:E:278:GLN:OE1	5:E:1005:HOH:O	2.15	0.65
1:C:223:ASP:OD1	5:C:1009:HOH:O	2.14	0.65
1:C:787:PHE:CZ	1:C:791:MET:HE2	2.31	0.65
1:B:821:LYS:O	5:B:1009:HOH:O	2.15	0.65
1:G:702:GLU:OE2	5:G:1002:HOH:O	2.15	0.65
1:H:406:ARG:NH2	5:H:1015:HOH:O	2.28	0.64
1:C:667:GLU:OE2	5:C:1008:HOH:O	2.14	0.64
1:H:397:PHE:HZ	1:H:428:GLU:HG3	1.63	0.64
1:C:5:ASN:ND2	5:C:1018:HOH:O	2.30	0.63
1:C:144:GLU:OE1	5:C:1011:HOH:O	2.16	0.63
1:F:638:LYS:NZ	5:F:1009:HOH:O	2.31	0.62
2:F:901:TPP:C2	2:F:901:TPP:HN42	2.13	0.61
1:C:3:GLU:N	5:C:1025:HOH:O	2.34	0.60
1:E:632:ASP:OD1	1:E:633:TRP:N	2.33	0.60
1:E:554:HIS:ND1	1:F:53:ILE:O	2.31	0.60
1:D:790:ARG:NE	5:D:1022:HOH:O	2.35	0.60
1:H:788:ILE:HG22	1:H:792:LYS:HE3	1.85	0.59
1:G:586:THR:O	1:G:590:VAL:HG13	2.02	0.59
1:D:385:ASP:OD2	5:D:1004:HOH:O	2.17	0.58
1:E:400:PRO:O	1:E:405:ASN:ND2	2.35	0.58
1:A:476:GLU:OE1	5:A:1003:HOH:O	2.17	0.58
1:F:355:ALA:O	5:F:1002:HOH:O	2.17	0.58
1:F:404:ASN:ND2	5:F:1013:HOH:O	2.34	0.58
1:A:251:LYS:HD2	1:A:252:LEU:N	2.18	0.58
1:D:790:ARG:NH2	5:D:1023:HOH:O	2.37	0.58
1:A:759:GLU:OE1	5:A:1004:HOH:O	2.17	0.57
2:D:901:TPP:HN42	2:D:901:TPP:C2	2.17	0.57
1:G:712:THR:OG1	5:G:1003:HOH:O	2.17	0.57
1:F:5:ASN:ND2	5:F:1018:HOH:O	2.36	0.57
1:E:586:THR:O	1:E:590:VAL:HG13	2.04	0.56
1:B:772:VAL:HA	1:B:775:VAL:HG12	1.87	0.55
1:A:515:VAL:CG1	1:A:515:VAL:O	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:VAL:O	1:C:515:VAL:HG13	2.07	0.55
1:C:788:ILE:HG22	1:C:792:LYS:HE3	1.88	0.55
1:B:419:MET:HG3	1:B:546:THR:HG21	1.88	0.55
1:D:515:VAL:O	1:D:515:VAL:CG1	2.55	0.55
1:H:431:LYS:NZ	5:H:1017:HOH:O	2.33	0.54
1:B:385:ASP:OD2	5:B:1010:HOH:O	2.19	0.54
1:D:533:LYS:N	1:D:533:LYS:HD2	2.22	0.54
1:G:764:HIS:NE2	5:G:1015:HOH:O	2.34	0.54
1:A:414:ASN:OD1	5:A:1005:HOH:O	2.18	0.53
1:H:788:ILE:CG2	1:H:792:LYS:HE3	2.38	0.53
1:C:774:TYR:O	1:C:777:ARG:NH1	2.41	0.53
1:D:747:ASP:OD1	5:D:1005:HOH:O	2.19	0.53
1:H:419:MET:HG3	1:H:546:THR:HG21	1.90	0.53
1:E:771:GLN:NE2	5:E:1027:HOH:O	2.39	0.53
1:C:558:THR:HA	1:D:524:LYS:HD3	1.92	0.53
2:G:901:TPP:HN42	2:G:901:TPP:C2	2.22	0.52
1:H:772:VAL:O	1:H:775:VAL:HG12	2.08	0.52
4:E:903:PO4:O2	5:E:1006:HOH:O	2.18	0.52
1:B:632:ASP:OD1	1:B:633:TRP:N	2.43	0.52
1:E:419:MET:HG3	1:E:546:THR:HG21	1.92	0.52
2:A:901:TPP:C2	2:A:901:TPP:HN42	2.22	0.52
1:E:554:HIS:CE1	1:F:53:ILE:HD13	2.45	0.52
1:B:549:VAL:HG21	1:B:562:PRO:HD3	1.91	0.52
1:B:417:MET:HE1	1:B:451:TRP:CZ3	2.46	0.51
1:F:204:ASP:OD2	5:F:1003:HOH:O	2.19	0.51
1:A:684:ARG:HD2	1:A:696:ARG:O	2.11	0.51
1:G:397:PHE:HZ	1:G:428:GLU:HG3	1.76	0.51
1:H:772:VAL:CA	1:H:775:VAL:HG12	2.41	0.51
1:D:533:LYS:NZ	5:D:1037:HOH:O	2.45	0.50
1:F:586:THR:O	1:F:590:VAL:HG13	2.10	0.50
1:H:772:VAL:HA	1:H:775:VAL:CG1	2.41	0.50
1:A:622:LYS:NZ	1:A:629:ALA:CB	2.75	0.50
1:E:7:GLU:HG2	1:E:11:LYS:HE3	1.94	0.50
1:C:698:LEU:HB3	1:C:702:GLU:HG3	1.93	0.49
1:C:269:LYS:NZ	5:C:1033:HOH:O	2.41	0.49
1:A:671:GLN:NE2	5:A:1014:HOH:O	2.35	0.49
1:B:787:PHE:O	1:B:791:MET:HG2	2.11	0.49
1:H:705:LYS:NZ	5:H:1033:HOH:O	2.45	0.49
1:C:515:VAL:HG22	1:C:518:MET:SD	2.53	0.49
1:D:419:MET:HG3	1:D:546:THR:HG21	1.95	0.49
1:H:555:ASN:ND2	5:H:1031:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LYS:HE2	5:A:1762:HOH:O	2.13	0.49
1:A:53:ILE:HD12	1:B:554:HIS:CD2	2.48	0.48
1:B:176:ALA:HA	1:B:181:LEU:HD22	1.94	0.48
1:H:365:ASP:OD1	1:H:365:ASP:N	2.45	0.48
1:C:393[B]:ASP:OD1	1:C:395:GLN:NE2	2.47	0.47
1:E:573[B]:SER:OG	1:E:688:LYS:NZ	2.41	0.47
1:C:799:PHE:O	1:C:803:ARG:HG2	2.14	0.47
2:G:901:TPP:N1'	1:H:486:GLU:OE2	2.47	0.47
1:A:552:GLN:O	1:A:555:ASN:O	2.33	0.47
1:H:428:GLU:HA	1:H:431:LYS:CE	2.42	0.47
1:H:397:PHE:CZ	1:H:428:GLU:HG3	2.46	0.47
1:C:715:ILE:HD13	1:C:738:ILE:HB	1.97	0.46
1:H:259:LYS:HE2	1:H:263:ASP:OD2	2.15	0.46
1:H:342:LYS:NZ	5:H:1028:HOH:O	2.42	0.46
1:E:528:GLN:NE2	5:E:1013:HOH:O	2.30	0.46
1:A:747:ASP:OD1	1:A:748:ILE:N	2.46	0.46
1:B:424:LYS:HG2	1:B:452:GLU:HG3	1.98	0.46
1:B:772:VAL:HA	1:B:775:VAL:CG1	2.46	0.46
1:C:486:GLU:OE2	2:D:901:TPP:N1'	2.49	0.46
1:C:515:VAL:CG1	1:C:515:VAL:O	2.63	0.46
1:C:657:GLU:OE2	1:C:755:ARG:NH1	2.40	0.46
1:A:428:GLU:OE2	5:A:1006:HOH:O	2.20	0.46
1:G:632:ASP:OD1	1:G:633:TRP:N	2.49	0.46
1:D:431:LYS:NZ	5:D:1050:HOH:O	2.48	0.45
1:F:802:THR:HG23	1:F:803:ARG:HD2	1.98	0.45
1:H:337:LEU:N	1:H:338:PRO:HD2	2.31	0.45
1:H:154:HIS:NE2	1:H:494:GLU:OE1	2.39	0.45
1:B:805:GLU:OE1	5:B:1011:HOH:O	2.21	0.45
1:E:573[A]:SER:HB3	1:E:688:LYS:HZ3	1.80	0.45
1:G:643:VAL:HG22	1:G:674:PHE:HA	1.99	0.45
1:D:517:SER:OG	5:D:1006:HOH:O	2.21	0.45
1:H:35:LEU:HG	1:H:117:MET:HE2	1.97	0.45
1:C:434:PRO:O	1:C:478[A]:ARG:NH1	2.50	0.45
1:H:772:VAL:C	1:H:775:VAL:HG12	2.37	0.45
1:H:419:MET:CE	1:H:450:PHE:CZ	3.01	0.44
1:H:787:PHE:HE1	5:H:1008:HOH:O	2.00	0.44
1:B:798:HIS:O	1:B:802:THR:HG22	2.18	0.44
1:D:146:GLY:O	2:D:901:TPP:N4'	2.51	0.44
1:B:649:SER:HA	1:B:717:GLY:O	2.17	0.44
1:F:112:GLN:NE2	5:F:1033:HOH:O	2.45	0.44
1:G:411:PRO:O	5:G:1004:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:360:LYS:NZ	5:H:1044:HOH:O	2.49	0.44
1:H:645:LEU:HD12	1:H:674:PHE:HB3	2.00	0.44
1:F:11:LYS:NZ	5:F:1053:HOH:O	2.51	0.44
1:B:670:PRO:HB3	1:B:821:LYS:HB2	1.99	0.43
1:D:164:GLU:HG2	5:D:1309:HOH:O	2.16	0.43
1:H:649:SER:HA	1:H:717:GLY:O	2.17	0.43
1:A:622:LYS:NZ	1:A:629:ALA:HB1	2.34	0.43
1:E:783:LEU:C	1:E:783:LEU:HD23	2.38	0.43
1:E:747:ASP:OD1	5:E:1007:HOH:O	2.21	0.43
2:H:901:TPP:HN42	2:H:901:TPP:C2	2.31	0.43
1:A:524:LYS:HD2	1:B:557:TYR:CD2	2.54	0.43
1:B:418:ASP:OD2	5:B:1013:HOH:O	2.21	0.43
1:B:668:VAL:HG12	1:B:783:LEU:HD21	1.99	0.43
1:A:449:ARG:HG3	1:A:451:TRP:CZ2	2.54	0.43
1:C:788:ILE:CG2	1:C:792:LYS:HE3	2.49	0.43
2:C:901:TPP:HN42	2:C:901:TPP:C2	2.32	0.43
1:F:12:LYS:HG3	1:F:363:LEU:HD23	2.00	0.43
1:A:669:PHE:CD2	1:A:672:ALA:HB2	2.54	0.43
1:G:554:HIS:HA	1:H:53:ILE:HG23	2.01	0.43
1:A:339:GLU:OE1	1:A:339:GLU:N	2.48	0.43
1:B:509:GLU:OE1	1:B:549:VAL:HG23	2.19	0.42
1:E:417:MET:SD	1:E:449:ARG:NH1	2.89	0.42
1:F:223:ASP:OD2	5:F:1004:HOH:O	2.21	0.42
1:A:91:GLN:O	1:A:95:VAL:HG13	2.19	0.42
1:H:273:GLU:OE1	5:H:1009:HOH:O	2.21	0.42
1:H:424:LYS:HG2	1:H:452:GLU:HG3	2.02	0.42
1:E:140:GLY:HA3	1:E:375:ALA:HA	2.02	0.42
1:F:749:THR:O	5:F:1005:HOH:O	2.22	0.42
1:A:785:LYS:HE3	1:A:789:ASP:OD2	2.20	0.42
1:H:625:THR:HG22	5:H:1559:HOH:O	2.19	0.42
1:E:52:PRO:HG2	1:E:329:LEU:O	2.20	0.42
1:H:547:SER:HB3	1:H:552:GLN:NE2	2.35	0.42
1:C:255:GLU:O	1:C:259:LYS:HG2	2.20	0.41
1:E:772:VAL:O	1:E:776:ASN:OD1	2.37	0.41
1:A:622:LYS:CE	5:A:1762:HOH:O	2.66	0.41
1:D:115:GLU:OE2	1:D:119:ARG:NH2	2.48	0.41
1:E:616:THR:HG23	1:E:619:GLU:H	1.85	0.41
1:C:800:GLU:O	1:C:804:ASN:CG	2.59	0.41
1:H:775:VAL:HG13	1:H:776:ASN:N	2.36	0.41
1:F:689:LYS:NZ	5:F:1070:HOH:O	2.54	0.41
1:H:300:ARG:NH1	5:H:1024:HOH:O	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:801:VAL:O	1:H:805:GLU:HB2	2.20	0.41
1:A:649:SER:HA	1:A:717:GLY:O	2.21	0.41
1:B:757:TYR:O	5:B:1012:HOH:O	2.21	0.41
1:F:54:GLY:C	5:F:1001:HOH:O	2.58	0.41
1:G:669:PHE:CD2	1:G:672:ALA:HB2	2.55	0.41
1:D:419:MET:CE	1:D:450:PHE:CZ	3.04	0.41
1:G:649:SER:HA	1:G:717:GLY:O	2.20	0.41
1:C:744:GLU:O	1:D:527:ARG:NH2	2.54	0.41
1:C:667:GLU:HG2	1:C:821:LYS:HE3	2.03	0.41
1:B:546:THR:HG22	1:B:547:SER:H	1.85	0.41
1:H:787:PHE:O	1:H:791:MET:HG2	2.21	0.41
1:D:373:ARG:NH1	5:D:1060:HOH:O	2.53	0.41
1:H:648:ALA:HA	1:H:677:VAL:O	2.21	0.41
1:B:44:LYS:HE3	1:B:46:GLU:CG	2.51	0.40
1:D:140:GLY:HA3	1:D:375:ALA:HA	2.04	0.40
2:E:901:TPP:HN42	2:E:901:TPP:C2	2.35	0.40
1:B:549:VAL:HG22	1:B:560:GLN:HA	2.02	0.40
1:C:554:HIS:N	1:C:554:HIS:CD2	2.90	0.40
1:E:552:GLN:O	1:E:553:ASP:HB2	2.20	0.40
1:A:515:VAL:HG13	1:A:515:VAL:O	2.20	0.40
1:B:763:PHE:HD1	1:B:791:MET:CE	2.33	0.40
1:D:533:LYS:CD	1:D:533:LYS:N	2.84	0.40
1:A:248:ALA:HA	1:A:251:LYS:HE3	2.03	0.40
1:A:95:VAL:HG22	1:A:96:PRO:HD3	2.03	0.40

All (5) 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:F:1285:HOH:O	5:G:1590:HOH:O[1_556]	2.00	0.20
5:A:1389:HOH:O	5:G:1442:HOH:O[1_656]	2.03	0.17
5:F:1562:HOH:O	5:G:1741:HOH:O[1_556]	2.09	0.11
5:A:1389:HOH:O	5:G:1135:HOH:O[1_656]	2.15	0.05
5:A:1629:HOH:O	5:G:1752:HOH:O[1_656]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	820/822 (100%)	794 (97%)	24 (3%)	2 (0%)	47	38
1	B	818/822 (100%)	792 (97%)	23 (3%)	3 (0%)	34	22
1	C	822/822 (100%)	798 (97%)	23 (3%)	1 (0%)	51	43
1	D	820/822 (100%)	795 (97%)	24 (3%)	1 (0%)	51	43
1	E	822/822 (100%)	799 (97%)	22 (3%)	1 (0%)	51	43
1	F	822/822 (100%)	797 (97%)	22 (3%)	3 (0%)	34	22
1	G	820/822 (100%)	795 (97%)	24 (3%)	1 (0%)	51	43
1	H	825/822 (100%)	802 (97%)	20 (2%)	3 (0%)	34	22
All	All	6569/6576 (100%)	6372 (97%)	182 (3%)	15 (0%)	47	38

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	553	ASP
1	A	275	ASN
1	B	275	ASN
1	F	54	GLY
1	G	442	PRO
1	H	442	PRO
1	A	442	PRO
1	B	442	PRO
1	C	442	PRO
1	D	442	PRO
1	E	442	PRO
1	F	275	ASN
1	F	442	PRO
1	H	311	GLY
1	B	311	GLY

### 5.3.2 Protein sidechains ⓘ

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	699/699 (100%)	688 (98%)	11 (2%)	62	58
1	B	697/699 (100%)	682 (98%)	15 (2%)	52	44
1	C	701/699 (100%)	684 (98%)	17 (2%)	49	40
1	D	699/699 (100%)	690 (99%)	9 (1%)	69	65
1	E	701/699 (100%)	693 (99%)	8 (1%)	73	71
1	F	701/699 (100%)	694 (99%)	7 (1%)	76	74
1	G	699/699 (100%)	688 (98%)	11 (2%)	62	58
1	H	704/699 (101%)	686 (97%)	18 (3%)	46	36
All	All	5601/5592 (100%)	5505 (98%)	96 (2%)	60	55

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LEU
1	A	251	LYS
1	A	430	VAL
1	A	449	ARG
1	A	515	VAL
1	A	527	ARG
1	A	533	LYS
1	A	549	VAL
1	A	632	ASP
1	A	739	VAL
1	A	757	TYR
1	B	32	GLU
1	B	59	VAL
1	B	142	LEU
1	B	181	LEU
1	B	251	LYS
1	B	287	ILE
1	B	302	ASN
1	B	527	ARG

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Mol	Chain	Res	Type
1	B	537	ASP
1	B	546	THR
1	B	553	ASP
1	B	659	LEU
1	B	757	TYR
1	B	770	MET
1	B	808	ASP
1	C	142	LEU
1	C	170	VAL
1	C	287	ILE
1	C	302	ASN
1	C	334	MET
1	C	478[A]	ARG
1	C	478[B]	ARG
1	C	515	VAL
1	C	527	ARG
1	C	552	GLN
1	C	645	LEU
1	C	757	TYR
1	C	774	TYR
1	C	780	ASN
1	C	803	ARG
1	C	807	VAL
1	C	816	VAL
1	D	142	LEU
1	D	302	ASN
1	D	515	VAL
1	D	527	ARG
1	D	546	THR
1	D	643	VAL
1	D	645	LEU
1	D	671	GLN
1	D	757	TYR
1	E	126	PHE
1	E	142	LEU
1	E	327	LEU
1	E	527	ARG
1	E	546	THR
1	E	551	GLN
1	E	590	VAL
1	E	757	TYR
1	F	142	LEU

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Mol	Chain	Res	Type
1	F	287	ILE
1	F	527	ARG
1	F	533	LYS
1	F	739	VAL
1	F	757	TYR
1	F	822	LYS
1	G	142	LEU
1	G	261	ILE
1	G	302	ASN
1	G	365	ASP
1	G	419	MET
1	G	527	ARG
1	G	590	VAL
1	G	639	ASP
1	G	643	VAL
1	G	739	VAL
1	G	757	TYR
1	H	3	GLU
1	H	142	LEU
1	H	241	ASP
1	H	255	GLU
1	H	261	ILE
1	H	302	ASN
1	H	334	MET
1	H	365	ASP
1	H	526	ILE
1	H	527	ARG
1	H	546	THR
1	H	645	LEU
1	H	669	PHE
1	H	723[A]	ASP
1	H	723[B]	ASP
1	H	757	TYR
1	H	779	VAL
1	H	785	LYS

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

Mol	Chain	Res	Type
1	C	266	GLN
1	C	804	ASN
1	D	776	ASN

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Mol	Chain	Res	Type
1	F	112	GLN
1	H	554	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	PO4	A	903	-	4,4,4	0.91	0	6,6,6	0.52	0
4	PO4	H	903	-	4,4,4	0.86	0	6,6,6	0.45	0
4	PO4	E	904	-	4,4,4	0.91	0	6,6,6	0.53	0
4	PO4	G	903	-	4,4,4	0.86	0	6,6,6	0.56	0
2	TPP	A	901	3	22,27,27	1.74	5 (22%)	29,40,40	1.73	9 (31%)
2	TPP	G	901	3	22,27,27	1.64	5 (22%)	29,40,40	1.88	8 (27%)
4	PO4	C	903	-	4,4,4	0.88	0	6,6,6	0.44	0
4	PO4	B	901	-	4,4,4	0.88	0	6,6,6	0.55	0
4	PO4	E	903	-	4,4,4	0.89	0	6,6,6	0.47	0
2	TPP	E	901	3	22,27,27	1.72	6 (27%)	29,40,40	1.62	6 (20%)
2	TPP	H	901	3	22,27,27	1.66	6 (27%)	29,40,40	1.64	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPP	C	901	3	22,27,27	1.69	6 (27%)	29,40,40	1.77	7 (24%)
2	TPP	F	901	3	22,27,27	1.61	7 (31%)	29,40,40	1.75	7 (24%)
2	TPP	B	902	3	22,27,27	1.65	5 (22%)	29,40,40	1.74	7 (24%)
2	TPP	D	901	3	22,27,27	1.59	5 (22%)	29,40,40	1.79	6 (20%)
4	PO4	C	904	-	4,4,4	0.91	0	6,6,6	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	A	901	3	-	3/16/17/17	0/2/2/2
2	TPP	G	901	3	-	4/16/17/17	0/2/2/2
2	TPP	E	901	3	-	4/16/17/17	0/2/2/2
2	TPP	B	902	3	-	3/16/17/17	0/2/2/2
2	TPP	H	901	3	-	3/16/17/17	0/2/2/2
2	TPP	C	901	3	-	2/16/17/17	0/2/2/2
2	TPP	F	901	3	-	6/16/17/17	0/2/2/2
2	TPP	D	901	3	-	6/16/17/17	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	TPP	C4-N3	-5.31	1.35	1.39
2	E	901	TPP	C4-N3	-5.25	1.35	1.39
2	H	901	TPP	C4-N3	-5.10	1.35	1.39
2	C	901	TPP	C4-N3	-4.95	1.35	1.39
2	B	902	TPP	C4-N3	-4.84	1.35	1.39
2	D	901	TPP	C4-N3	-4.73	1.35	1.39
2	F	901	TPP	C4-N3	-4.49	1.35	1.39
2	G	901	TPP	C4-N3	-4.47	1.35	1.39
2	A	901	TPP	C2'-N1'	2.73	1.38	1.34
2	G	901	TPP	C2'-N1'	2.71	1.38	1.34
2	B	902	TPP	C4'-N3'	2.67	1.38	1.35
2	C	901	TPP	C4'-N3'	2.65	1.38	1.35
2	E	901	TPP	C4'-N3'	2.60	1.38	1.35
2	C	901	TPP	C2'-N1'	2.52	1.38	1.34
2	D	901	TPP	C2'-N1'	2.49	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	TPP	C2'-N3'	2.45	1.38	1.34
2	H	901	TPP	C2'-N1'	2.41	1.38	1.34
2	E	901	TPP	C2'-N1'	2.40	1.38	1.34
2	H	901	TPP	C2'-N3'	2.39	1.38	1.34
2	B	902	TPP	C2'-N3'	2.37	1.38	1.34
2	F	901	TPP	C2'-N1'	2.36	1.38	1.34
2	E	901	TPP	C2'-N3'	2.35	1.38	1.34
2	A	901	TPP	C6'-N1'	2.32	1.39	1.34
2	F	901	TPP	C4'-N3'	2.31	1.38	1.35
2	G	901	TPP	C6'-N1'	2.31	1.39	1.34
2	B	902	TPP	C2'-N1'	2.31	1.38	1.34
2	H	901	TPP	C4'-N3'	2.30	1.38	1.35
2	C	901	TPP	C2'-N3'	2.28	1.38	1.34
2	C	901	TPP	C6'-N1'	2.26	1.39	1.34
2	A	901	TPP	C4'-N3'	2.24	1.38	1.35
2	D	901	TPP	C6'-N1'	2.22	1.39	1.34
2	F	901	TPP	C6'-N1'	2.21	1.39	1.34
2	E	901	TPP	C6'-N1'	2.19	1.39	1.34
2	B	902	TPP	C6'-N1'	2.17	1.39	1.34
2	F	901	TPP	C7'-N3	-2.17	1.44	1.48
2	G	901	TPP	C2'-N3'	2.17	1.37	1.34
2	H	901	TPP	C7'-N3	-2.16	1.44	1.48
2	D	901	TPP	C2'-N3'	2.14	1.37	1.34
2	C	901	TPP	C7'-N3	-2.12	1.44	1.48
2	F	901	TPP	C2'-N3'	2.09	1.37	1.34
2	H	901	TPP	C6'-N1'	2.07	1.38	1.34
2	E	901	TPP	C7'-N3	-2.06	1.44	1.48
2	D	901	TPP	C4'-N3'	2.05	1.38	1.35
2	G	901	TPP	C4'-N3'	2.05	1.38	1.35
2	F	901	TPP	C5'-C4'	-2.01	1.39	1.42

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	TPP	C6-C5-C4	5.15	131.56	127.43
2	G	901	TPP	C6-C5-C4	5.04	131.48	127.43
2	G	901	TPP	CM2-C2'-N1'	4.66	122.26	117.14
2	B	902	TPP	C6-C5-C4	4.63	131.15	127.43
2	D	901	TPP	C6-C5-C4	4.59	131.12	127.43
2	D	901	TPP	CM2-C2'-N1'	4.24	121.81	117.14
2	A	901	TPP	C6-C5-C4	4.21	130.81	127.43
2	A	901	TPP	CM2-C2'-N1'	4.20	121.76	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	901	TPP	C6-C5-C4	4.18	130.79	127.43
2	F	901	TPP	CM2-C2'-N1'	4.02	121.56	117.14
2	E	901	TPP	C6-C5-C4	3.97	130.62	127.43
2	F	901	TPP	N1'-C2'-N3'	-3.79	119.02	125.54
2	F	901	TPP	C6-C5-C4	3.73	130.42	127.43
2	H	901	TPP	N1'-C2'-N3'	-3.61	119.32	125.54
2	C	901	TPP	N1'-C2'-N3'	-3.59	119.37	125.54
2	H	901	TPP	CM2-C2'-N1'	3.49	120.97	117.14
2	E	901	TPP	N1'-C2'-N3'	-3.43	119.64	125.54
2	A	901	TPP	N1'-C2'-N3'	-3.36	119.75	125.54
2	G	901	TPP	N1'-C2'-N3'	-3.36	119.76	125.54
2	D	901	TPP	N1'-C2'-N3'	-3.34	119.78	125.54
2	B	902	TPP	N1'-C2'-N3'	-3.34	119.80	125.54
2	C	901	TPP	CM2-C2'-N1'	3.24	120.70	117.14
2	E	901	TPP	CM2-C2'-N1'	3.24	120.70	117.14
2	B	902	TPP	CM2-C2'-N1'	3.19	120.65	117.14
2	F	901	TPP	CM4-C4-N3	3.10	126.48	122.53
2	G	901	TPP	CM4-C4-N3	2.93	126.27	122.53
2	D	901	TPP	CM4-C4-N3	2.76	126.05	122.53
2	B	902	TPP	CM4-C4-N3	2.73	126.01	122.53
2	F	901	TPP	C6'-N1'-C2'	2.64	120.46	115.96
2	C	901	TPP	C6'-N1'-C2'	2.57	120.33	115.96
2	H	901	TPP	C6'-N1'-C2'	2.55	120.30	115.96
2	B	902	TPP	C6'-N1'-C2'	2.51	120.23	115.96
2	B	902	TPP	PA-O3A-PB	-2.49	124.27	132.83
2	E	901	TPP	CM4-C4-N3	2.49	125.71	122.53
2	C	901	TPP	PA-O3A-PB	-2.45	124.40	132.83
2	G	901	TPP	C2'-N3'-C4'	2.45	121.91	118.08
2	E	901	TPP	PA-O3A-PB	-2.37	124.70	132.83
2	E	901	TPP	C6'-N1'-C2'	2.34	119.94	115.96
2	A	901	TPP	C6'-C5'-C4'	2.32	118.88	115.72
2	G	901	TPP	C6'-C5'-C4'	2.31	118.86	115.72
2	G	901	TPP	O3B-PB-O3A	2.27	112.25	104.64
2	D	901	TPP	C2'-N3'-C4'	2.26	121.61	118.08
2	F	901	TPP	PA-O3A-PB	-2.24	125.13	132.83
2	A	901	TPP	O2B-PB-O3A	2.24	112.15	104.64
2	A	901	TPP	CM4-C4-N3	2.24	125.38	122.53
2	A	901	TPP	PA-O3A-PB	-2.23	125.17	132.83
2	H	901	TPP	CM4-C4-N3	2.17	125.29	122.53
2	C	901	TPP	O3B-PB-O3A	2.13	111.77	104.64
2	C	901	TPP	CM4-C4-N3	2.13	125.24	122.53
2	A	901	TPP	C2'-N3'-C4'	2.12	121.39	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	TPP	C2'-N3'-C4'	2.12	121.38	118.08
2	B	902	TPP	O3B-PB-O3A	2.10	111.67	104.64
2	A	901	TPP	C6'-N1'-C2'	2.09	119.51	115.96
2	G	901	TPP	PA-O3A-PB	-2.07	125.72	132.83
2	D	901	TPP	C6'-N1'-C2'	2.06	119.46	115.96

There are no chirality outliers.

All (31) torsion outliers are listed below:

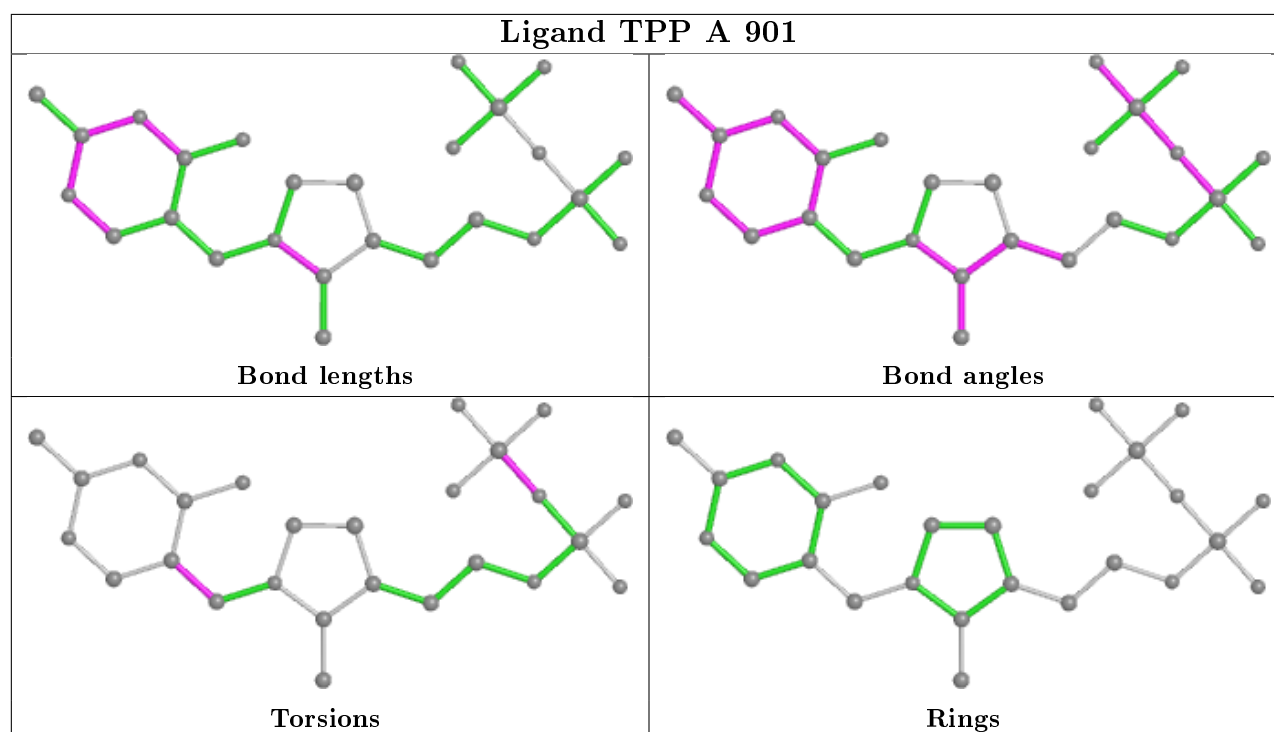
Mol	Chain	Res	Type	Atoms
2	G	901	TPP	C4'-C5'-C7'-N3
2	A	901	TPP	C4'-C5'-C7'-N3
2	A	901	TPP	PA-O3A-PB-O2B
2	H	901	TPP	C4'-C5'-C7'-N3
2	C	901	TPP	PA-O3A-PB-O2B
2	F	901	TPP	C4'-C5'-C7'-N3
2	B	902	TPP	PA-O3A-PB-O3B
2	D	901	TPP	C4'-C5'-C7'-N3
2	D	901	TPP	PA-O3A-PB-O2B
2	D	901	TPP	PB-O3A-PA-O1A
2	G	901	TPP	PA-O3A-PB-O1B
2	F	901	TPP	PA-O3A-PB-O1B
2	E	901	TPP	PA-O3A-PB-O1B
2	B	902	TPP	PA-O3A-PB-O2B
2	F	901	TPP	C4-C5-C6-C7
2	E	901	TPP	C4-C5-C6-C7
2	B	902	TPP	PA-O3A-PB-O1B
2	D	901	TPP	PA-O3A-PB-O1B
2	G	901	TPP	PA-O3A-PB-O2B
2	G	901	TPP	PA-O3A-PB-O3B
2	A	901	TPP	PA-O3A-PB-O3B
2	H	901	TPP	PA-O3A-PB-O2B
2	H	901	TPP	PA-O3A-PB-O3B
2	C	901	TPP	PA-O3A-PB-O3B
2	F	901	TPP	PA-O3A-PB-O2B
2	F	901	TPP	PA-O3A-PB-O3B
2	E	901	TPP	PA-O3A-PB-O2B
2	E	901	TPP	PA-O3A-PB-O3B
2	D	901	TPP	PB-O3A-PA-O2A
2	F	901	TPP	C6'-C5'-C7'-N3
2	D	901	TPP	C6'-C5'-C7'-N3

There are no ring outliers.

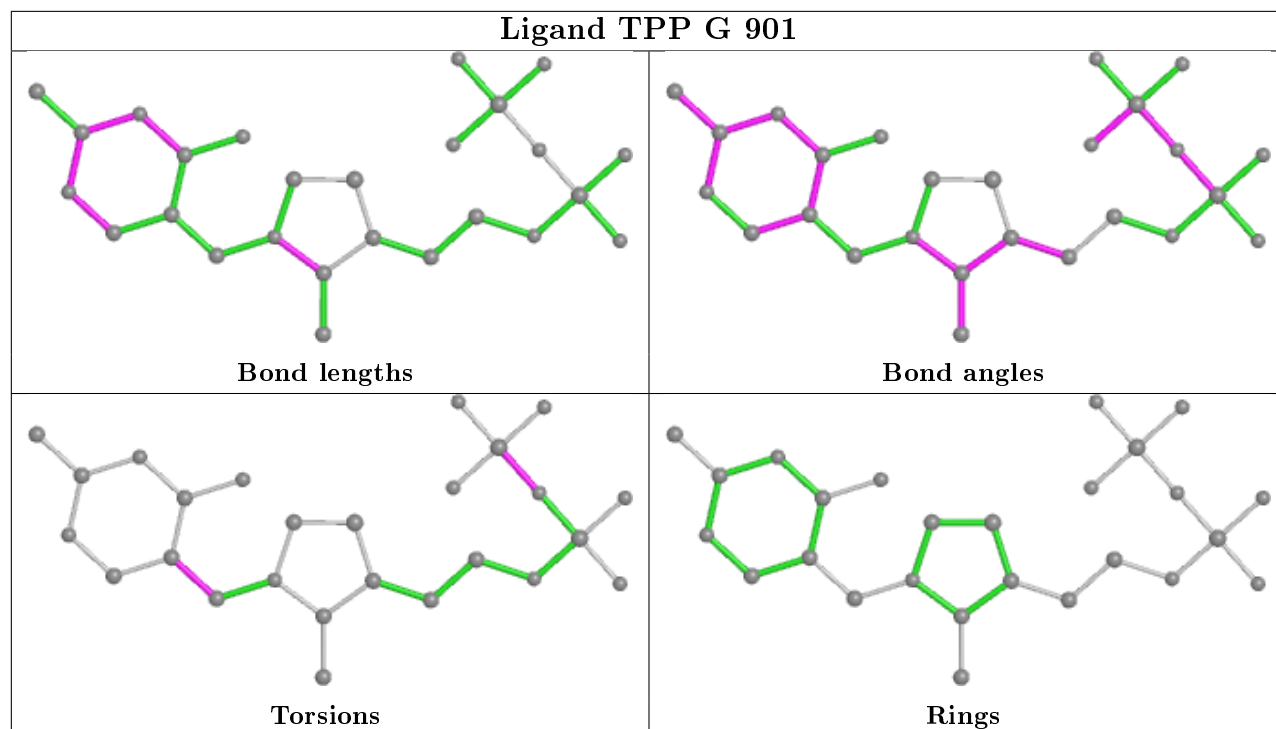
9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	TPP	1	0
2	G	901	TPP	2	0
4	C	903	PO4	1	0
4	E	903	PO4	1	0
2	E	901	TPP	1	0
2	H	901	TPP	1	0
2	C	901	TPP	1	0
2	F	901	TPP	1	0
2	D	901	TPP	3	0

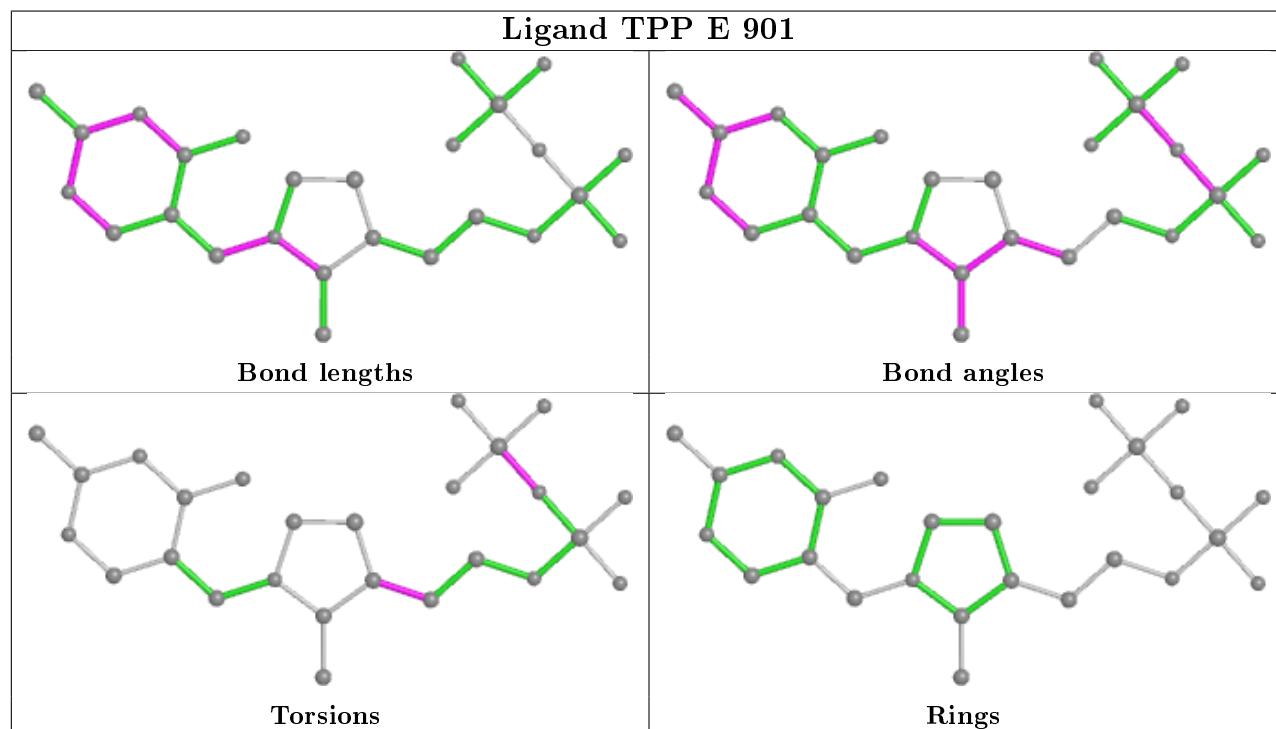
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



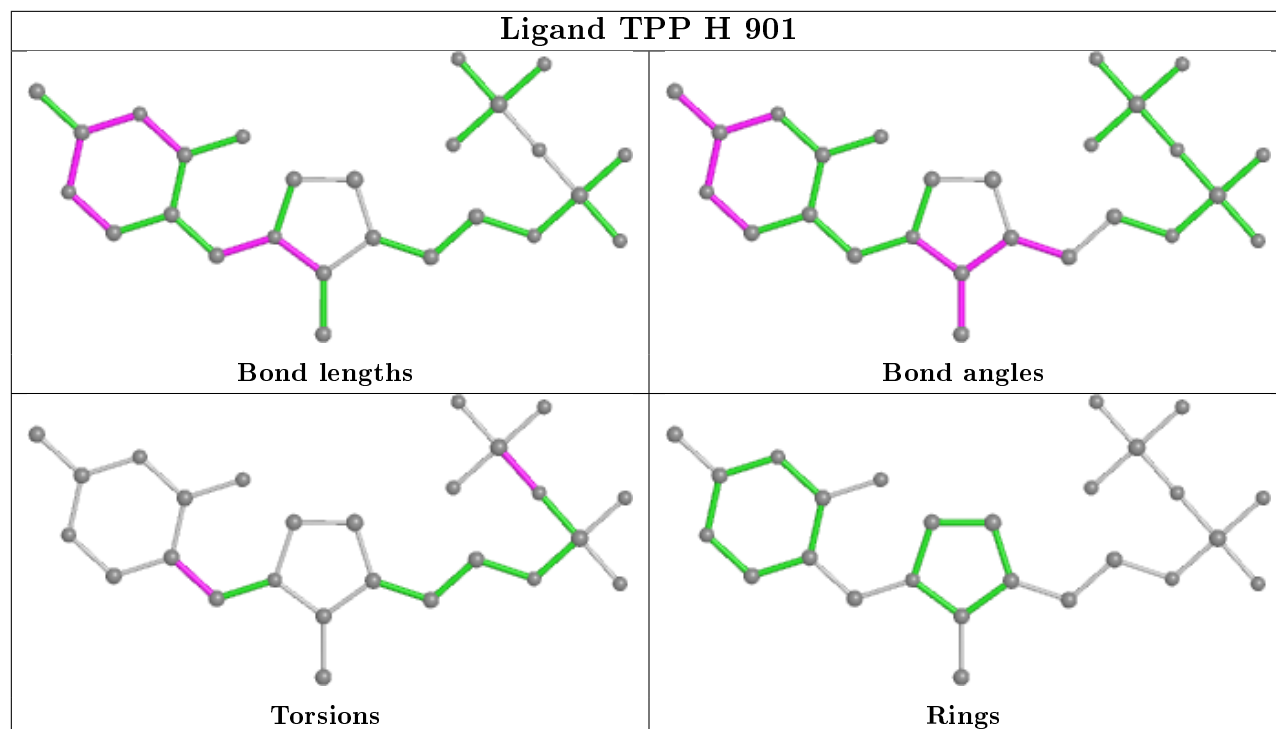
## Ligand TPP G 901



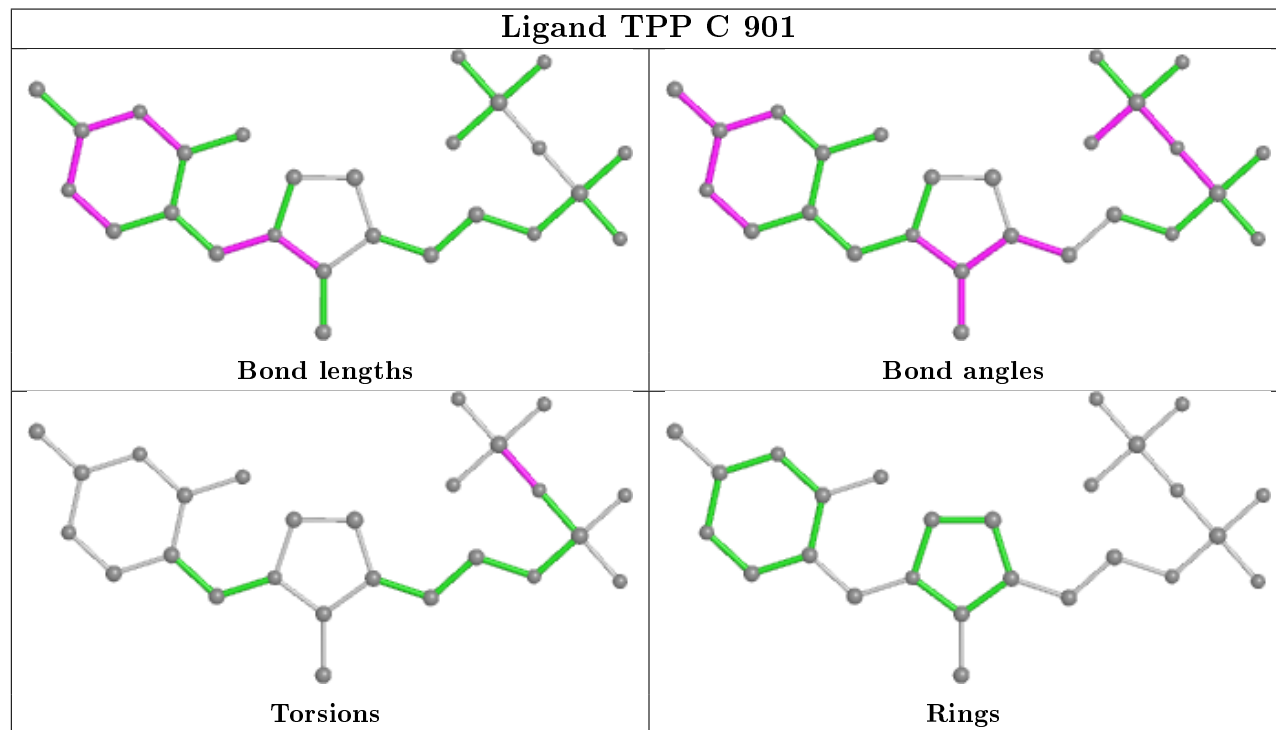
## Ligand TPP E 901



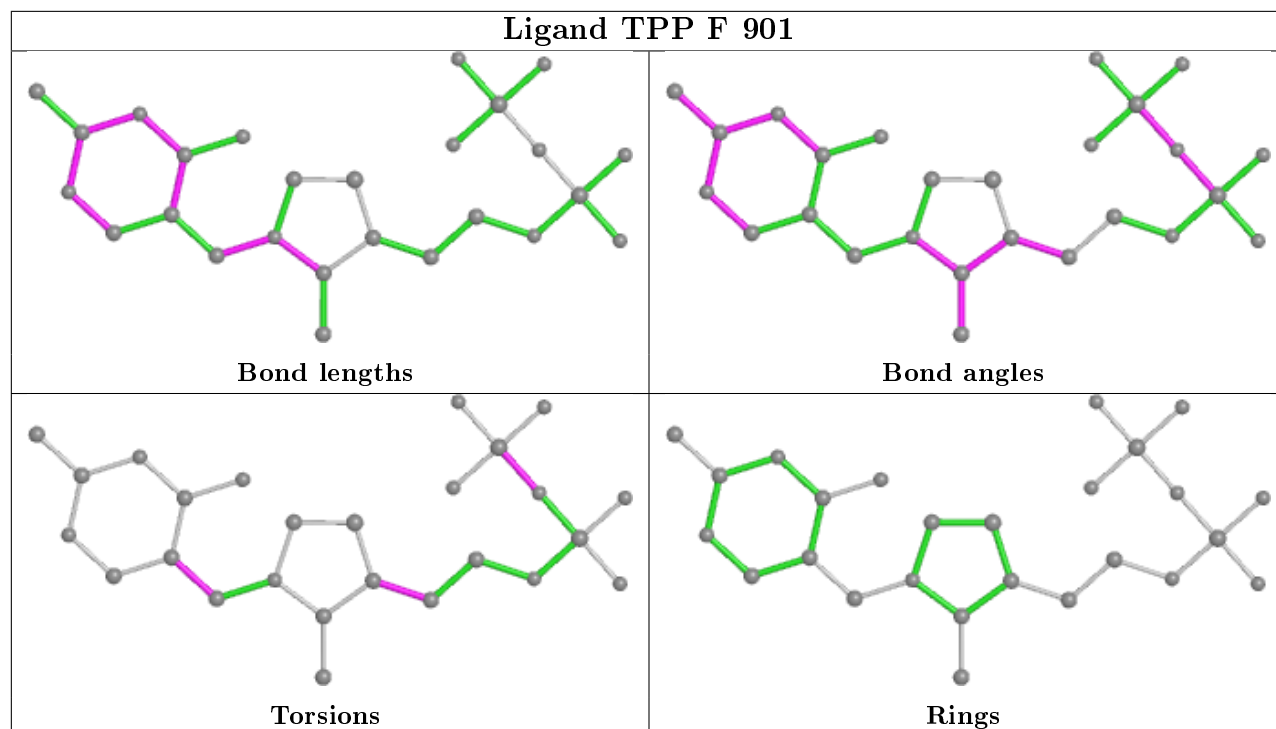
## Ligand TPP H 901



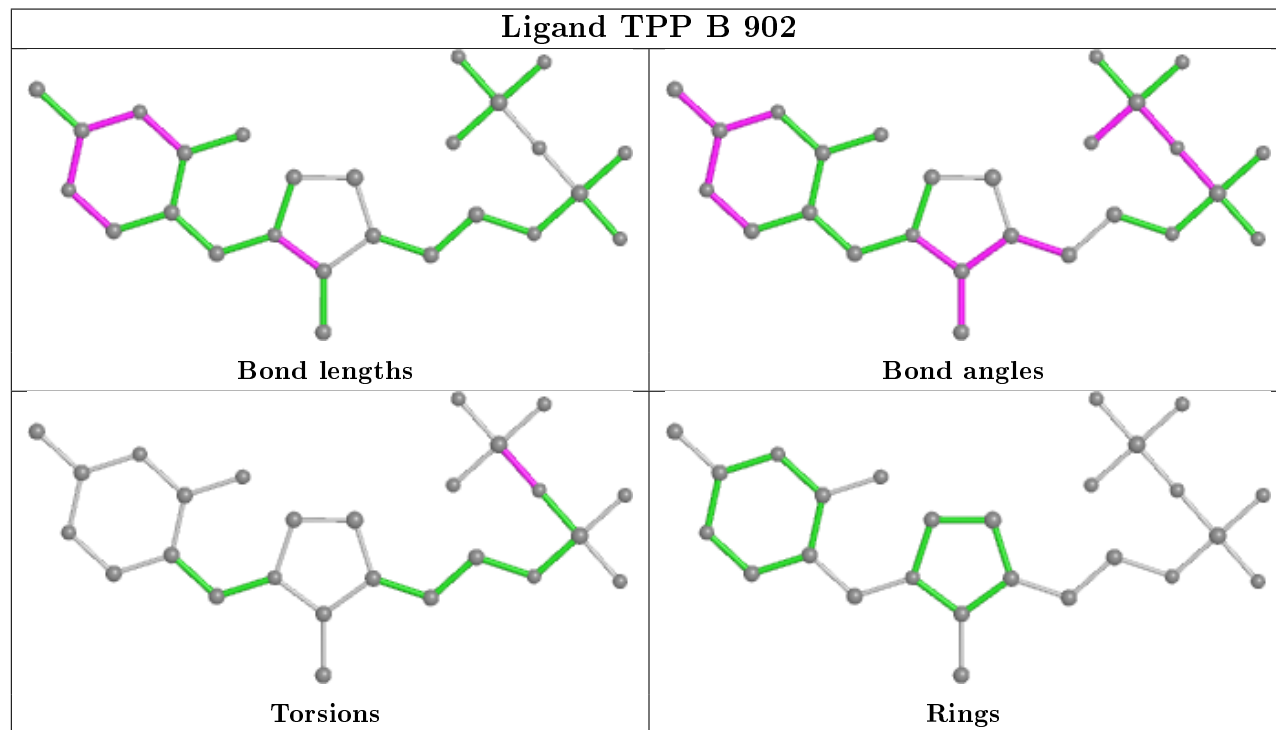
## Ligand TPP C 901

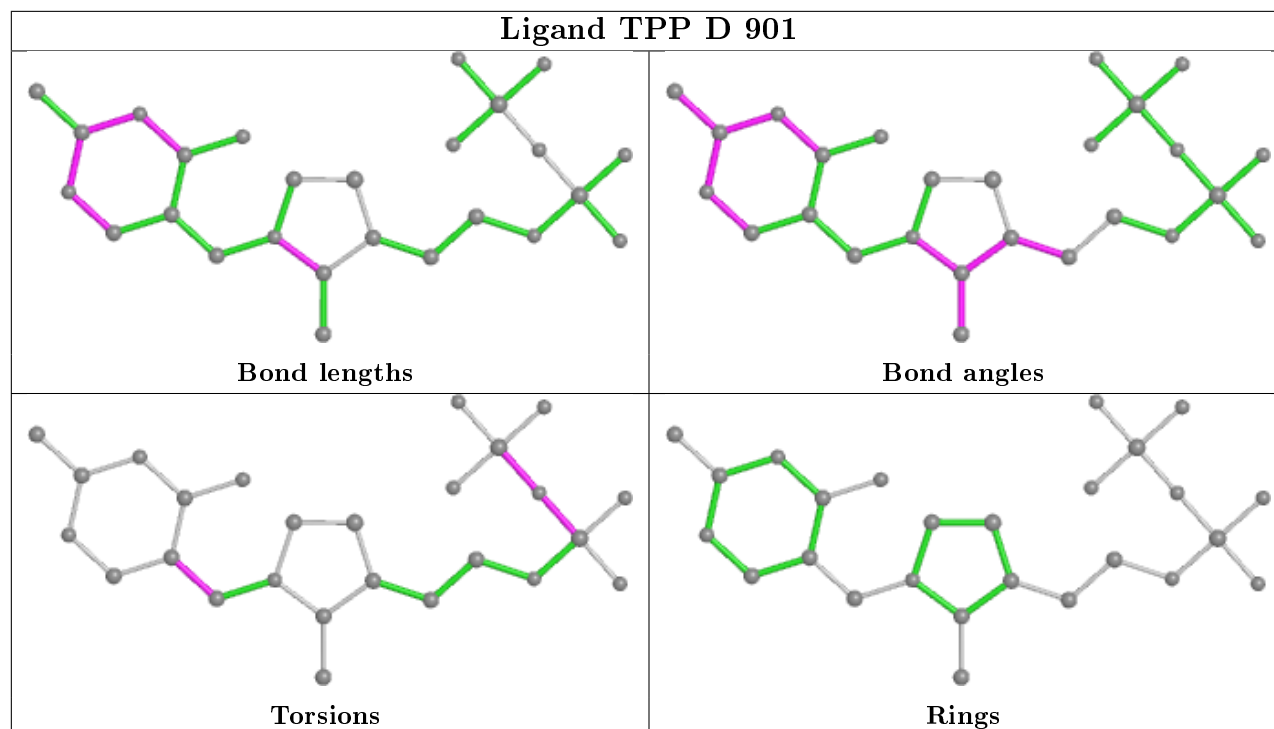


## Ligand TPP F 901



## Ligand TPP B 902





## 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	821/822 (99%)	-0.46	1 (0%) 95 97	13, 22, 35, 69	0
1	B	818/822 (99%)	-0.29	11 (1%) 77 83	15, 27, 59, 80	0
1	C	820/822 (99%)	-0.24	7 (0%) 84 89	17, 30, 54, 75	0
1	D	820/822 (99%)	-0.42	1 (0%) 95 97	15, 24, 38, 60	0
1	E	820/822 (99%)	-0.22	13 (1%) 72 79	17, 31, 55, 82	0
1	F	820/822 (99%)	-0.44	0 100 100	15, 25, 38, 55	0
1	G	820/822 (99%)	-0.46	1 (0%) 95 97	13, 22, 36, 59	0
1	H	819/822 (99%)	-0.31	9 (1%) 80 85	13, 25, 53, 81	0
All	All	6558/6576 (99%)	-0.36	43 (0%) 87 92	13, 26, 49, 82	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	799	PHE	5.7
1	E	554	HIS	5.1
1	B	799	PHE	3.8
1	C	799	PHE	3.7
1	B	774	TYR	3.7
1	H	669	PHE	3.6
1	E	799	PHE	3.5
1	E	552	GLN	3.1
1	B	558	THR	3.1
1	H	800	GLU	3.1
1	C	554	HIS	3.1
1	E	555	ASN	2.8
1	E	2	THR	2.7
1	H	558	THR	2.7
1	E	814	GLU	2.6
1	E	783	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	671[A]	GLN	2.6
1	H	667	GLU	2.6
1	B	796	VAL	2.6
1	E	780	ASN	2.5
1	C	558	THR	2.5
1	B	638	LYS	2.5
1	H	775	VAL	2.5
1	B	554	HIS	2.4
1	B	779	VAL	2.4
1	H	804	ASN	2.4
1	E	803	ARG	2.4
1	H	783	LEU	2.4
1	E	553	ASP	2.3
1	B	773	LEU	2.3
1	C	777	ARG	2.3
1	C	555	ASN	2.3
1	B	802	THR	2.3
1	D	638	LYS	2.3
1	H	797	LYS	2.2
1	E	805	GLU	2.2
1	C	783	LEU	2.2
1	B	553	ASP	2.1
1	C	804	ASN	2.1
1	A	53	ILE	2.1
1	E	775	VAL	2.1
1	G	640	GLY	2.0
1	B	777	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

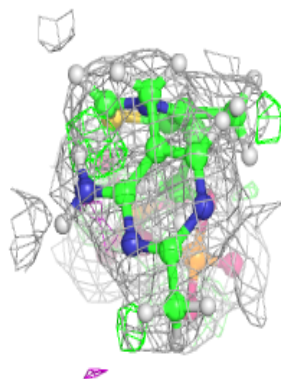
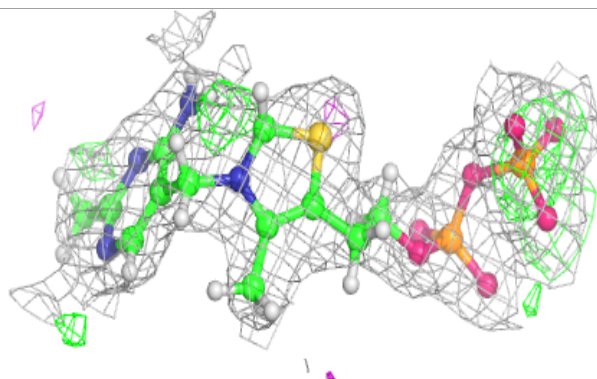
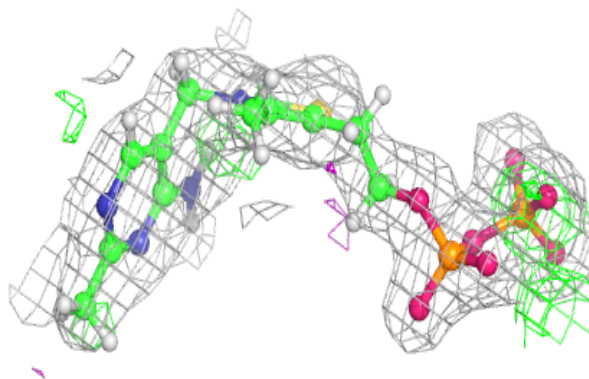
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PO4	H	903	5/5	0.73	0.26	45,59,91,99	0
4	PO4	E	903	5/5	0.77	0.17	51,67,77,91	0
4	PO4	C	903	5/5	0.79	0.30	72,72,85,103	0
4	PO4	A	903	5/5	0.83	0.20	50,52,76,88	0
4	PO4	C	904	5/5	0.95	0.12	34,37,46,53	0
4	PO4	E	904	5/5	0.96	0.11	34,50,58,63	0
2	TPP	G	901	26/26	0.96	0.10	9,22,32,45	0
3	MG	F	902	1/1	0.97	0.07	26,26,26,26	0
3	MG	H	902	1/1	0.97	0.09	24,24,24,24	0
2	TPP	A	901	26/26	0.97	0.10	11,24,33,39	0
3	MG	G	902	1/1	0.97	0.08	22,22,22,22	0
3	MG	E	902	1/1	0.98	0.08	25,25,25,25	0
2	TPP	C	901	26/26	0.98	0.09	16,25,34,37	0
2	TPP	F	901	26/26	0.98	0.09	10,21,35,42	0
2	TPP	H	901	26/26	0.98	0.09	11,20,31,37	0
4	PO4	G	903	5/5	0.98	0.08	35,37,44,53	0
2	TPP	E	901	26/26	0.98	0.10	13,25,36,40	0
2	TPP	B	902	26/26	0.98	0.09	12,22,33,34	0
2	TPP	D	901	26/26	0.98	0.10	14,23,35,42	0
4	PO4	B	901	5/5	0.98	0.10	30,37,44,45	0
3	MG	D	902	1/1	0.99	0.07	16,16,16,16	0
3	MG	A	902	1/1	0.99	0.06	15,15,15,15	0
3	MG	B	903	1/1	0.99	0.09	20,20,20,20	0
3	MG	C	902	1/1	0.99	0.09	27,27,27,27	0

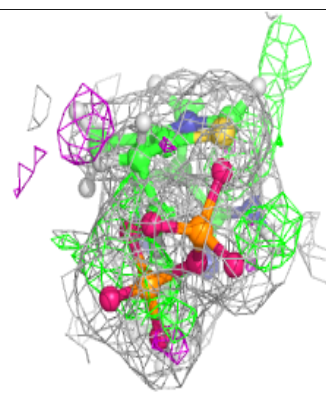
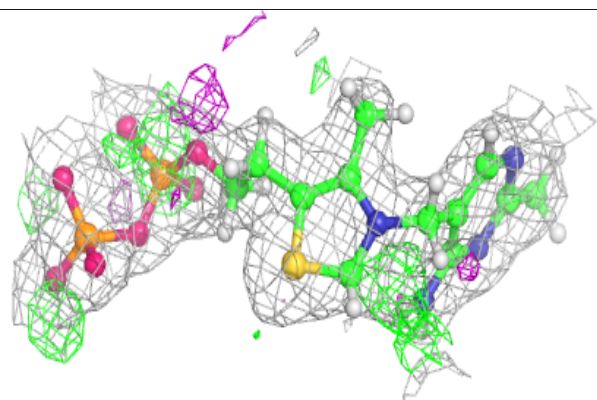
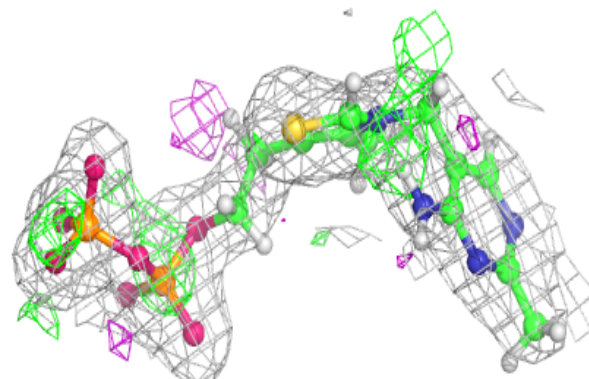
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around TPP G 901:**

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

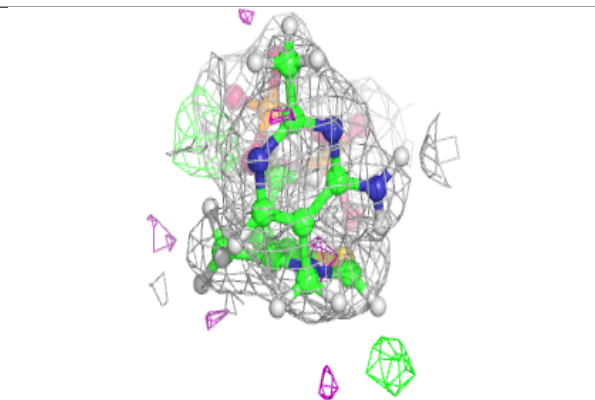
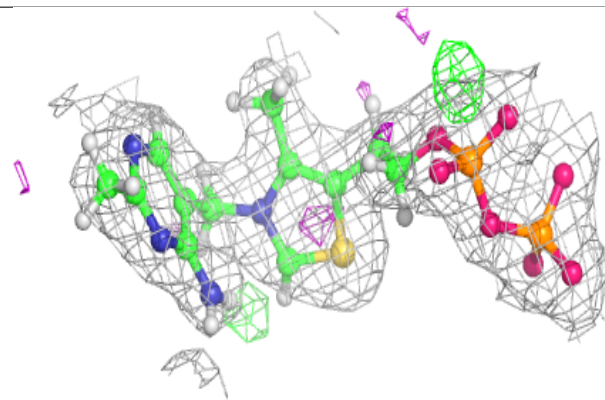
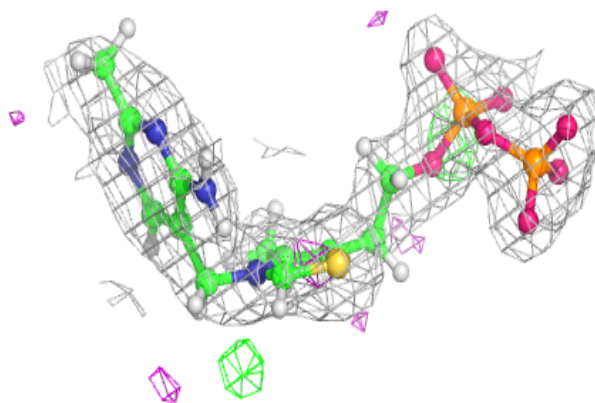
**Electron density around TPP A 901:**

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

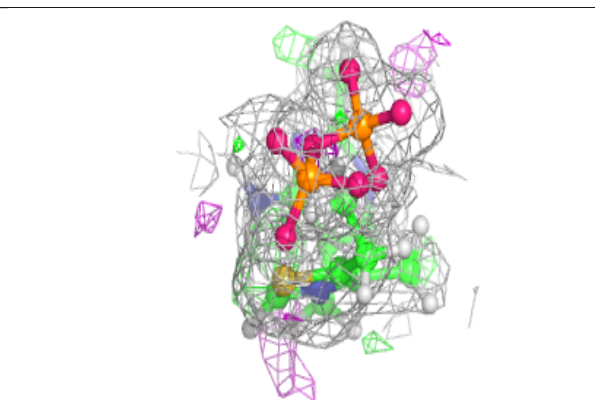
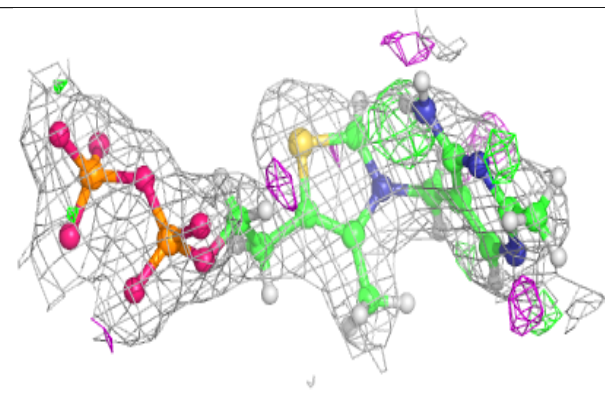
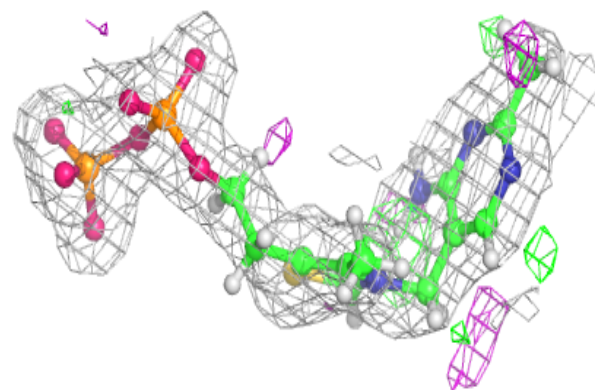


**Electron density around TPP C 901:**

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

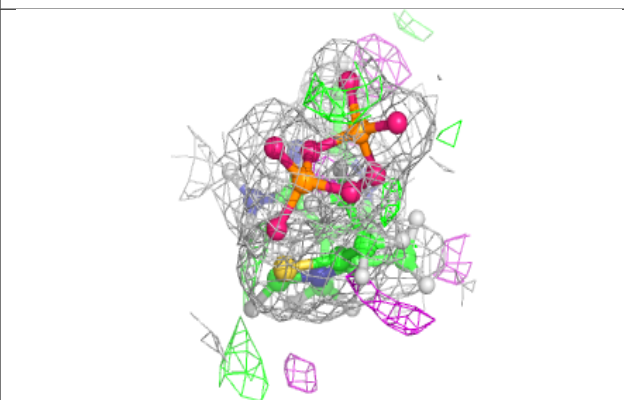
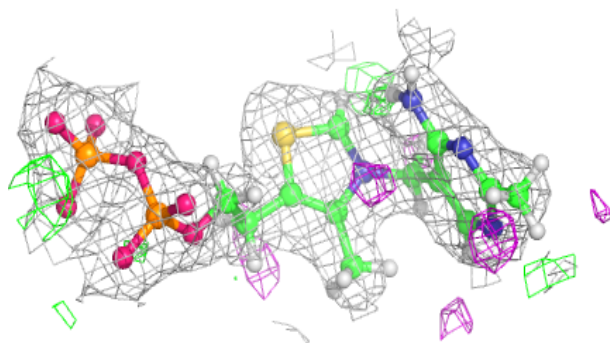
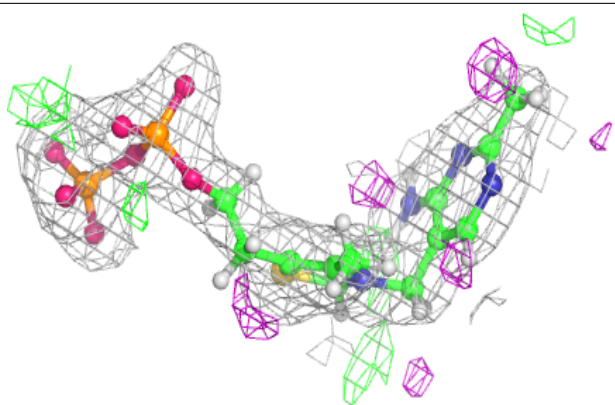
**Electron density around TPP F 901:**

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

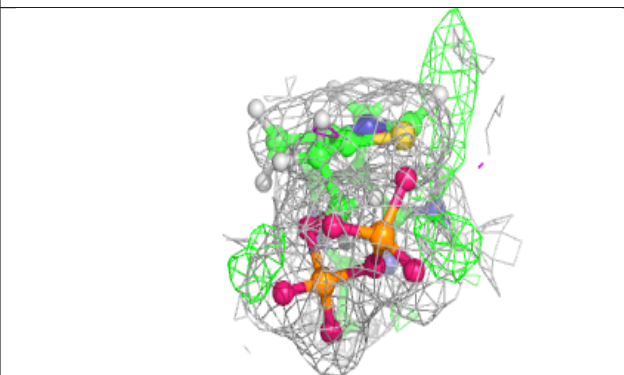
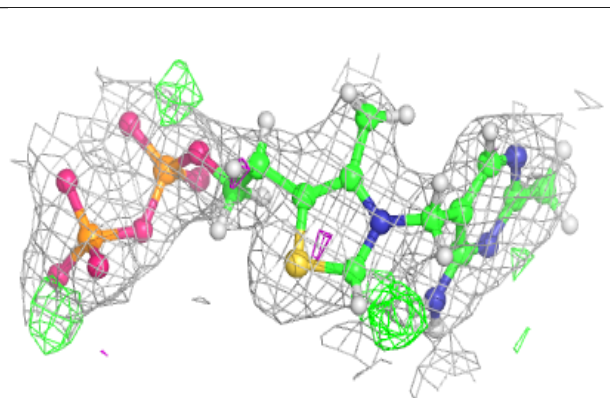
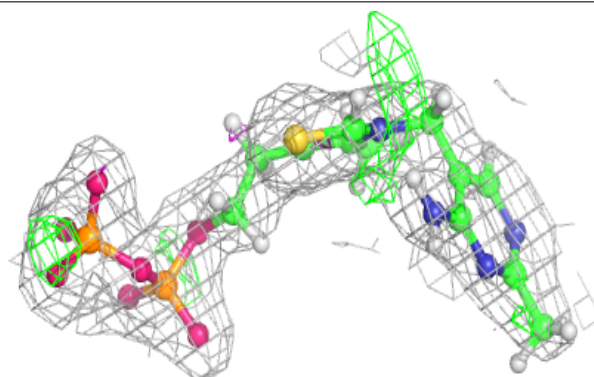


**Electron density around TPP H 901:**

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

**Electron density around TPP E 901:**

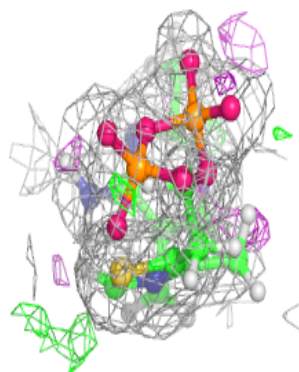
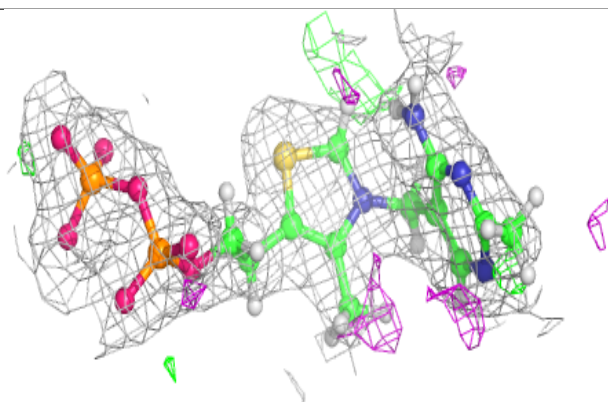
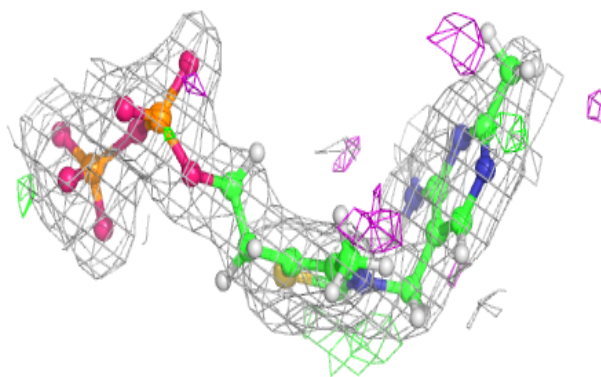
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



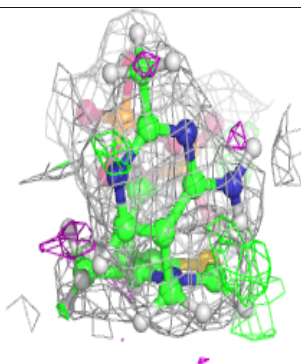
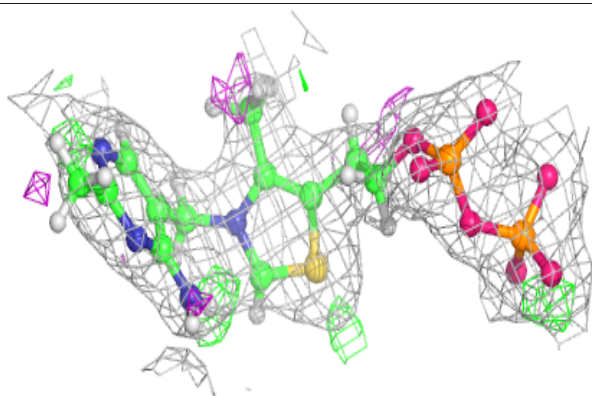
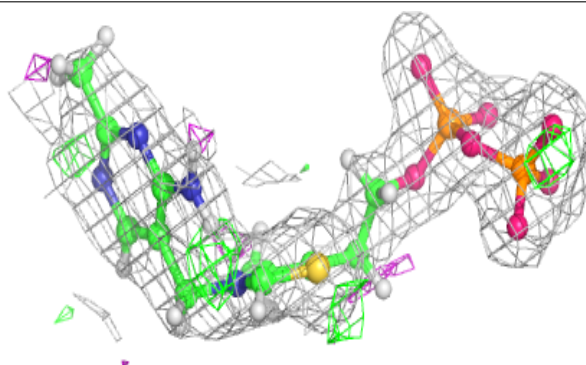


**Electron density around TPP B 902:**

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

**Electron density around TPP D 901:**

$2mF_o-DF_c$  (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.