



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2022 – 07:25 AM JST

PDB ID : 7WRT
Title : X-ray structure ofThermus thermophilus HB8 transketorase demonstrate in complex with TPP and D-erythrose-4-phosphate
Authors : Kamitori, S.; Yoshihara, A.
Deposited on : 2022-01-27
Resolution : 2.25 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 ⓘ 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 ⓘ](#)) 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	:	2.31.3
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)	:	2.31.3

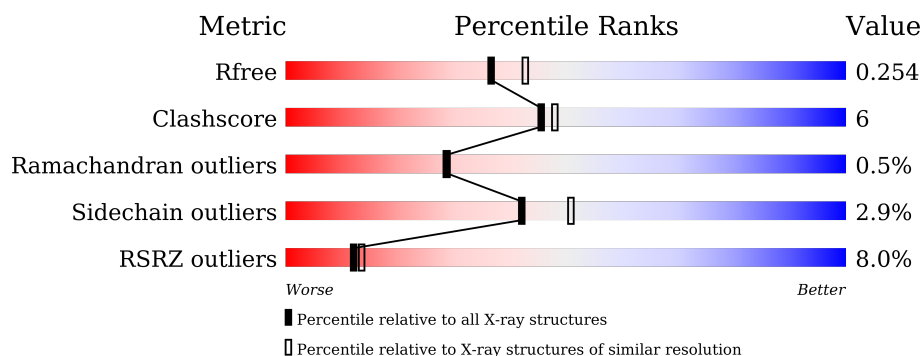
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 $\leq 5\%$. 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	672	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	B	672	<div> <div>2%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>
1	C	672	<div> <div>7%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
1	D	672	<div> <div>18%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20619 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	650	Total	C	N	O	S	0	0	0
			5070	3236	902	917	15			
1	B	650	Total	C	N	O	S	0	0	0
			5070	3236	902	917	15			
1	C	650	Total	C	N	O	S	0	0	0
			5070	3236	902	917	15			
1	D	650	Total	C	N	O	S	0	0	0
			5070	3236	902	917	15			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q5SM35
A	-19	GLY	-	expression tag	UNP Q5SM35
A	-18	SER	-	expression tag	UNP Q5SM35
A	-17	SER	-	expression tag	UNP Q5SM35
A	-16	HIS	-	expression tag	UNP Q5SM35
A	-15	HIS	-	expression tag	UNP Q5SM35
A	-14	HIS	-	expression tag	UNP Q5SM35
A	-13	HIS	-	expression tag	UNP Q5SM35
A	-12	HIS	-	expression tag	UNP Q5SM35
A	-11	HIS	-	expression tag	UNP Q5SM35
A	-10	SER	-	expression tag	UNP Q5SM35
A	-9	SER	-	expression tag	UNP Q5SM35
A	-8	GLY	-	expression tag	UNP Q5SM35
A	-7	LEU	-	expression tag	UNP Q5SM35
A	-6	VAL	-	expression tag	UNP Q5SM35
A	-5	PRO	-	expression tag	UNP Q5SM35
A	-4	ARG	-	expression tag	UNP Q5SM35
A	-3	GLY	-	expression tag	UNP Q5SM35
A	-2	SER	-	expression tag	UNP Q5SM35
A	-1	HIS	-	expression tag	UNP Q5SM35
A	0	SER	-	expression tag	UNP Q5SM35

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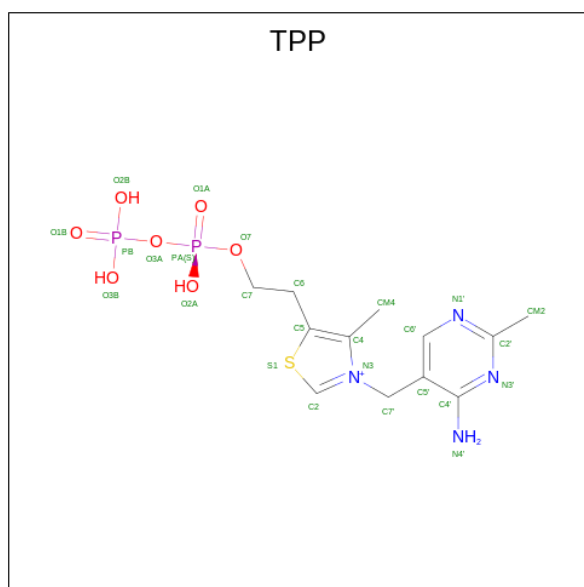
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP Q5SM35
B	-19	GLY	-	expression tag	UNP Q5SM35
B	-18	SER	-	expression tag	UNP Q5SM35
B	-17	SER	-	expression tag	UNP Q5SM35
B	-16	HIS	-	expression tag	UNP Q5SM35
B	-15	HIS	-	expression tag	UNP Q5SM35
B	-14	HIS	-	expression tag	UNP Q5SM35
B	-13	HIS	-	expression tag	UNP Q5SM35
B	-12	HIS	-	expression tag	UNP Q5SM35
B	-11	HIS	-	expression tag	UNP Q5SM35
B	-10	SER	-	expression tag	UNP Q5SM35
B	-9	SER	-	expression tag	UNP Q5SM35
B	-8	GLY	-	expression tag	UNP Q5SM35
B	-7	LEU	-	expression tag	UNP Q5SM35
B	-6	VAL	-	expression tag	UNP Q5SM35
B	-5	PRO	-	expression tag	UNP Q5SM35
B	-4	ARG	-	expression tag	UNP Q5SM35
B	-3	GLY	-	expression tag	UNP Q5SM35
B	-2	SER	-	expression tag	UNP Q5SM35
B	-1	HIS	-	expression tag	UNP Q5SM35
B	0	SER	-	expression tag	UNP Q5SM35
C	-20	MET	-	initiating methionine	UNP Q5SM35
C	-19	GLY	-	expression tag	UNP Q5SM35
C	-18	SER	-	expression tag	UNP Q5SM35
C	-17	SER	-	expression tag	UNP Q5SM35
C	-16	HIS	-	expression tag	UNP Q5SM35
C	-15	HIS	-	expression tag	UNP Q5SM35
C	-14	HIS	-	expression tag	UNP Q5SM35
C	-13	HIS	-	expression tag	UNP Q5SM35
C	-12	HIS	-	expression tag	UNP Q5SM35
C	-11	HIS	-	expression tag	UNP Q5SM35
C	-10	SER	-	expression tag	UNP Q5SM35
C	-9	SER	-	expression tag	UNP Q5SM35
C	-8	GLY	-	expression tag	UNP Q5SM35
C	-7	LEU	-	expression tag	UNP Q5SM35
C	-6	VAL	-	expression tag	UNP Q5SM35
C	-5	PRO	-	expression tag	UNP Q5SM35
C	-4	ARG	-	expression tag	UNP Q5SM35
C	-3	GLY	-	expression tag	UNP Q5SM35
C	-2	SER	-	expression tag	UNP Q5SM35
C	-1	HIS	-	expression tag	UNP Q5SM35
C	0	SER	-	expression tag	UNP Q5SM35

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	initiating methionine	UNP Q5SM35
D	-19	GLY	-	expression tag	UNP Q5SM35
D	-18	SER	-	expression tag	UNP Q5SM35
D	-17	SER	-	expression tag	UNP Q5SM35
D	-16	HIS	-	expression tag	UNP Q5SM35
D	-15	HIS	-	expression tag	UNP Q5SM35
D	-14	HIS	-	expression tag	UNP Q5SM35
D	-13	HIS	-	expression tag	UNP Q5SM35
D	-12	HIS	-	expression tag	UNP Q5SM35
D	-11	HIS	-	expression tag	UNP Q5SM35
D	-10	SER	-	expression tag	UNP Q5SM35
D	-9	SER	-	expression tag	UNP Q5SM35
D	-8	GLY	-	expression tag	UNP Q5SM35
D	-7	LEU	-	expression tag	UNP Q5SM35
D	-6	VAL	-	expression tag	UNP Q5SM35
D	-5	PRO	-	expression tag	UNP Q5SM35
D	-4	ARG	-	expression tag	UNP Q5SM35
D	-3	GLY	-	expression tag	UNP Q5SM35
D	-2	SER	-	expression tag	UNP Q5SM35
D	-1	HIS	-	expression tag	UNP Q5SM35
D	0	SER	-	expression tag	UNP Q5SM35

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



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

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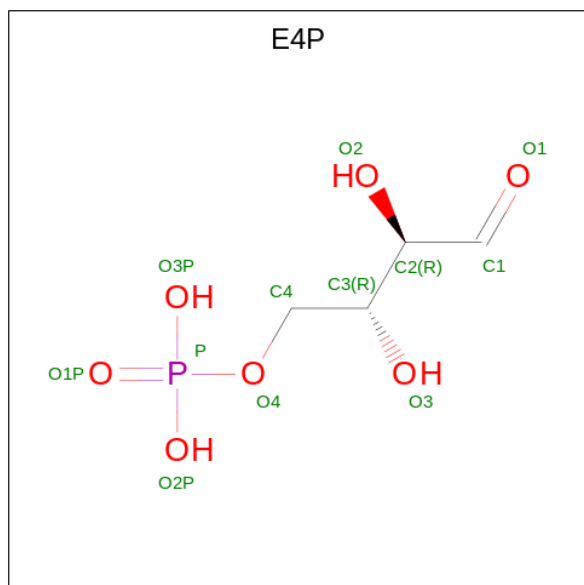
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is ERYTHROSE-4-PHOSPHATE (three-letter code: E4P) (formula: C₄H₉O₇P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			12	4	7	1		
4	B	1	Total	C	O	P	0	0
			12	4	7	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O	P	0	0
			12	4	7	1		
4	D	1	Total	C	O	P	0	0
			12	4	7	1		

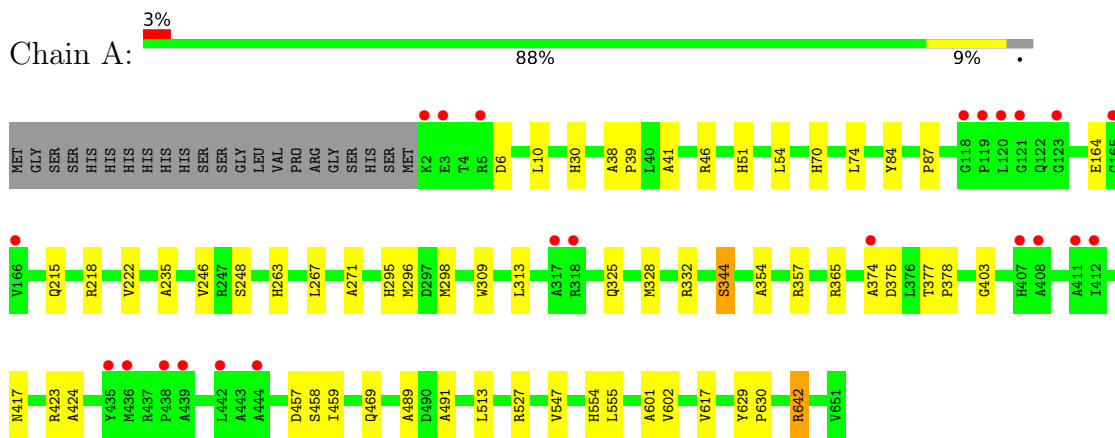
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	56	Total	O	0	0
			56	56		
5	B	61	Total	O	0	0
			61	61		
5	C	38	Total	O	0	0
			38	38		
5	D	28	Total	O	0	0
			28	28		

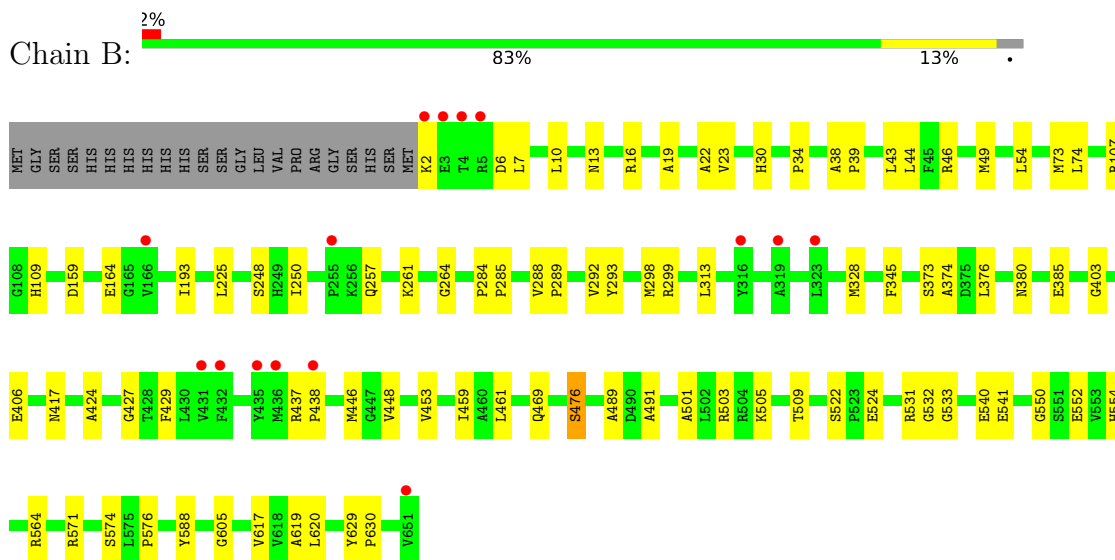
3 Residue-property plots

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

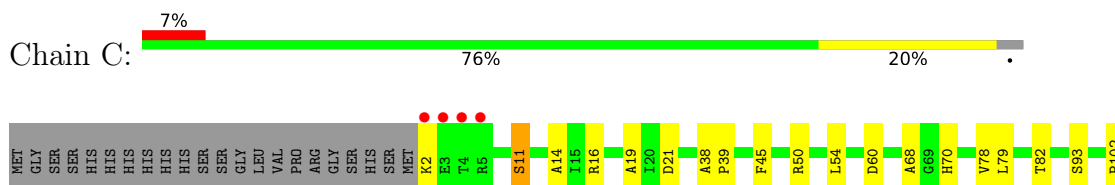
• Molecule 1: Transketolase

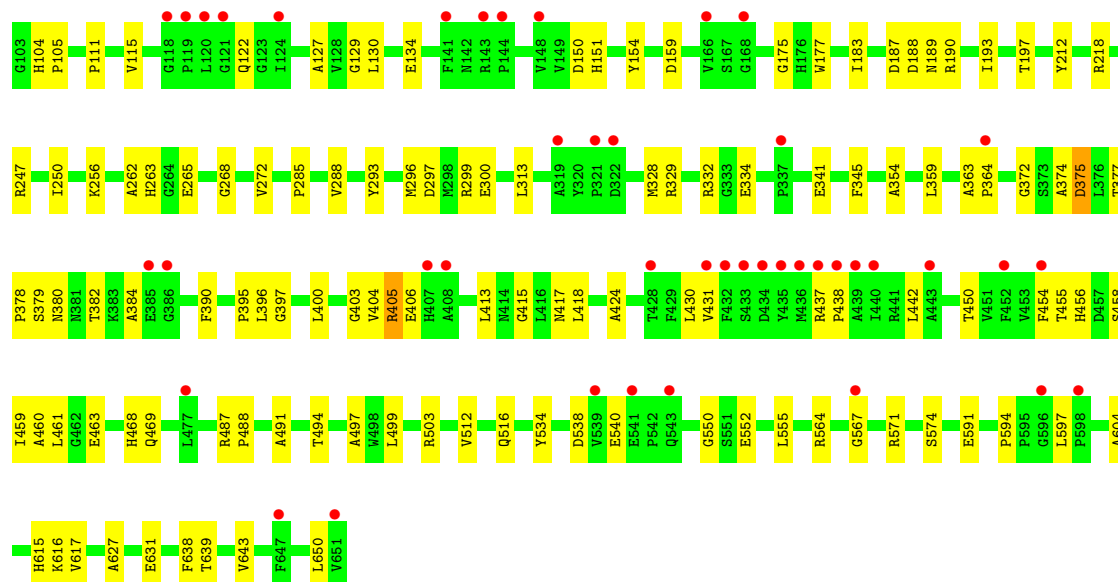


• Molecule 1: Transketolase

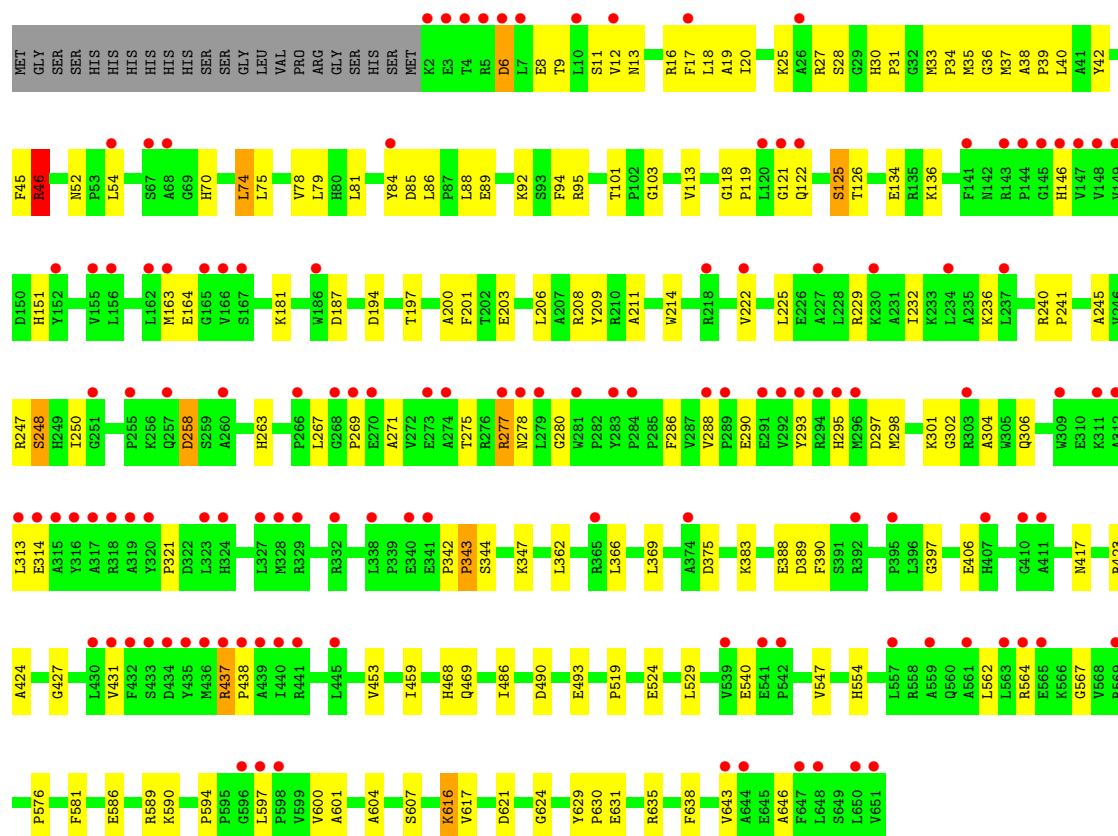
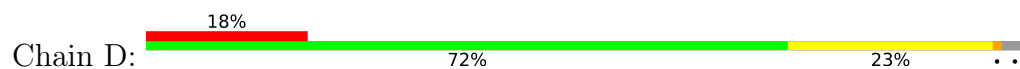


• Molecule 1: Transketolase





• Molecule 1: Transketolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.68Å 88.86Å 117.37Å 72.31° 88.70° 73.46°	Depositor
Resolution (Å)	41.86 – 2.25 41.86 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (41.86-2.25) 98.2 (41.86-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.202 , 0.254 0.207 , 0.254	Depositor DCC
R_{free} test set	6251 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20619	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: E4P, TPP, CA

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	0.77	0/5205	0.92	0/7080
1	B	0.77	1/5205 (0.0%)	0.89	0/7080
1	C	0.77	0/5205	0.88	0/7080
1	D	0.75	0/5205	0.86	0/7080
All	All	0.76	1/20820 (0.0%)	0.89	0/28320

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	552	GLU	CD-OE2	5.71	1.31	1.25

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	5070	0	5041	31	0
1	B	5070	0	5041	55	0
1	C	5070	0	5041	76	0
1	D	5070	0	5041	97	0
2	A	26	0	16	5	0
2	B	26	0	16	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	26	0	16	4	0
2	D	26	0	16	2	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	12	0	7	2	0
4	B	12	0	7	0	0
4	C	12	0	7	0	0
4	D	12	0	7	0	0
5	A	56	0	0	0	0
5	B	61	0	0	4	0
5	C	38	0	0	1	0
5	D	28	0	0	2	0
All	All	20619	0	20256	259	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 6.

All (259) 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:344:SER:O	1:A:357:ARG:NH1	2.03	0.92
1:B:417:ASN:HD21	1:B:424:ALA:H	1.24	0.81
1:A:417:ASN:HD21	1:A:424:ALA:H	1.32	0.77
1:B:503:ARG:HD3	5:B:956:HOH:O	1.88	0.74
1:D:52:ASN:ND2	1:D:306:GLN:OE1	2.21	0.72
1:D:607:SER:HB2	1:D:617:VAL:HG21	1.74	0.69
1:D:631:GLU:OE2	1:D:635:ARG:NH1	2.25	0.69
1:C:82:THR:HA	1:C:296:MET:O	1.93	0.69
1:C:332:ARG:NH1	1:C:334:GLU:OE1	2.27	0.68
1:D:250:ILE:HG22	1:D:258:ASP:HA	1.76	0.68
1:C:188:ASP:OD1	1:C:190:ARG:NE	2.23	0.67
1:B:34:PRO:HA	1:B:74:LEU:HD13	1.77	0.65
1:D:12:VAL:HG23	1:D:42:TYR:CD1	2.32	0.65
1:C:615:HIS:HB2	1:C:650:LEU:HD21	1.79	0.65
1:B:164:GLU:OE2	2:B:802:TPP:HM23	1.97	0.64
1:C:377:THR:OG1	1:D:194:ASP:OD2	2.16	0.64
1:C:461:LEU:C	1:C:461:LEU:HD12	2.18	0.64
1:B:193:ILE:HD12	2:B:802:TPP:C4	2.27	0.64
1:D:293:TYR:O	1:D:297:ASP:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:MET:HG3	5:B:948:HOH:O	1.98	0.64
1:D:134:GLU:OE1	1:D:181:LYS:HD3	1.98	0.63
1:A:489:ALA:O	1:A:554:HIS:HE1	1.81	0.63
1:B:38:ALA:HB3	1:B:39:PRO:HD3	1.80	0.62
1:C:188:ASP:O	1:C:247:ARG:HD2	2.00	0.62
1:B:376:LEU:HD13	1:B:429:PHE:CE1	2.35	0.62
5:C:830:HOH:O	2:D:802:TPP:H2	2.00	0.62
1:C:437:ARG:HB3	1:C:438:PRO:HD3	1.82	0.62
1:D:20:ILE:HG23	1:D:267:LEU:HD12	1.83	0.61
1:D:493:GLU:O	1:D:529:LEU:HD13	2.00	0.61
1:D:88:LEU:HD11	1:D:286:PHE:HB3	1.81	0.60
1:A:164:GLU:OE2	2:A:701:TPP:HM23	2.02	0.60
1:D:18:LEU:HD11	1:D:81:LEU:HD21	1.83	0.60
1:B:532:GLY:O	1:B:576:PRO:HD2	2.02	0.59
1:D:369:LEU:HA	1:D:423:ARG:O	2.02	0.59
1:C:115:VAL:HG22	1:C:418:LEU:HD13	1.83	0.59
1:C:390:PHE:HB2	1:C:397:GLY:O	2.02	0.58
1:D:30:HIS:HB2	1:D:70:HIS:O	2.03	0.58
1:B:159:ASP:HB2	2:B:802:TPP:O1A	2.03	0.58
1:D:547:VAL:O	1:D:601:ALA:HA	2.02	0.58
1:D:11:SER:HB2	1:D:42:TYR:HE1	1.68	0.58
1:D:271:ALA:O	1:D:275:THR:OG1	2.22	0.57
1:D:629:TYR:CD2	1:D:630:PRO:HA	2.38	0.57
1:D:13:ASN:O	1:D:17:PHE:HD1	1.87	0.57
2:A:701:TPP:H6'	5:B:911:HOH:O	2.02	0.57
1:D:8:GLU:HG2	1:D:42:TYR:OH	2.04	0.57
1:C:288:VAL:HB	1:C:293:TYR:CE2	2.39	0.56
2:C:701:TPP:HN42	2:C:701:TPP:C2	2.18	0.56
1:C:564:ARG:O	1:C:567:GLY:N	2.37	0.56
1:B:501:ALA:HB2	1:B:509:THR:HG21	1.87	0.56
1:A:417:ASN:HD21	1:A:424:ALA:N	2.02	0.56
1:D:203:GLU:OE1	1:D:208:ARG:NE	2.28	0.56
1:C:38:ALA:HB3	1:C:39:PRO:HD3	1.87	0.55
1:C:406:GLU:OE1	1:D:164:GLU:OE2	2.23	0.55
1:D:362:LEU:O	1:D:366:LEU:HD12	2.06	0.55
1:D:79:LEU:O	1:D:84:TYR:HB2	2.06	0.55
1:C:177:TRP:CD1	1:C:390:PHE:HE2	2.24	0.55
1:B:289:PRO:HG2	1:B:292:VAL:HG23	1.90	0.55
1:D:45:PHE:CD1	1:D:78:VAL:HG21	2.42	0.54
1:B:417:ASN:ND2	1:B:424:ALA:H	1.99	0.54
1:B:489:ALA:O	1:B:554:HIS:HE1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:MET:O	1:A:332:ARG:HG3	2.07	0.53
1:C:79:LEU:HD13	1:C:111:PRO:O	2.08	0.53
1:D:225:LEU:O	1:D:229:ARG:HG3	2.09	0.53
1:C:50:ARG:NH2	1:C:150:ASP:O	2.43	0.53
1:C:413:LEU:O	1:C:417:ASN:OD1	2.27	0.52
1:C:405:ARG:HG2	1:D:163:MET:O	2.08	0.52
1:D:16:ARG:C	1:D:20:ILE:HD12	2.30	0.52
1:D:208:ARG:O	1:D:211:ALA:HB3	2.10	0.52
1:D:36:GLY:O	1:D:222:VAL:HG11	2.10	0.52
1:C:359:LEU:HB3	1:C:384:ALA:HB2	1.91	0.52
1:C:455:THR:O	1:C:456:HIS:HB2	2.10	0.51
1:D:209:TYR:O	1:D:214:TRP:HB2	2.11	0.51
1:B:193:ILE:HG13	2:B:802:TPP:H71	1.93	0.51
1:A:6:ASP:O	1:A:10:LEU:HB2	2.12	0.50
1:D:46:ARG:NH1	1:D:295:HIS:O	2.44	0.50
1:C:390:PHE:CD1	1:C:395:PRO:HA	2.45	0.50
1:D:232:ILE:O	1:D:236:LYS:HG3	2.12	0.50
1:B:459:ILE:HA	1:B:469:GLN:HG2	1.94	0.50
1:D:247:ARG:HD2	1:D:248:SER:H	1.75	0.50
1:C:571:ARG:NH1	1:C:591:GLU:O	2.45	0.50
1:C:354:ALA:HB1	1:C:491:ALA:HA	1.93	0.50
1:A:30:HIS:HB2	1:A:70:HIS:O	2.12	0.49
2:A:701:TPP:N1'	1:B:406:GLU:OE2	2.45	0.49
1:B:19:ALA:O	1:B:23:VAL:HG23	2.11	0.49
1:C:594:PRO:HG2	1:C:597:LEU:HD12	1.94	0.49
1:C:134:GLU:HG3	1:C:151:HIS:CD2	2.47	0.49
1:C:390:PHE:CE1	1:C:395:PRO:HA	2.48	0.49
1:D:6:ASP:HA	1:D:9:THR:HB	1.95	0.49
1:D:16:ARG:O	1:D:20:ILE:HD12	2.12	0.48
1:B:437:ARG:NH1	1:B:476:SER:O	2.40	0.48
1:C:571:ARG:HH11	1:C:594:PRO:HD3	1.77	0.48
1:D:37:MET:CE	1:D:40:LEU:HD23	2.43	0.48
1:B:193:ILE:HD12	2:B:802:TPP:CM4	2.43	0.48
1:B:446:MET:HB3	1:B:448:VAL:HG23	1.95	0.48
1:D:134:GLU:HG3	1:D:151:HIS:O	2.14	0.48
1:D:342:PRO:O	1:D:343:PRO:O	2.30	0.48
1:D:431:VAL:HG11	1:D:468:HIS:HA	1.94	0.48
1:B:427:GLY:HA2	1:B:453:VAL:O	2.13	0.48
1:B:328:MET:CG	5:B:948:HOH:O	2.59	0.48
1:A:41:ALA:HB2	1:A:74:LEU:HD11	1.96	0.48
1:B:328:MET:HE2	1:B:328:MET:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASN:OD1	1:B:16:ARG:NH2	2.47	0.47
1:C:377:THR:N	1:C:378:PRO:CD	2.78	0.47
2:C:701:TPP:HN42	2:C:701:TPP:H2	1.78	0.47
1:D:187:ASP:OD1	1:D:187:ASP:C	2.51	0.47
1:D:581:PHE:CZ	1:D:589:ARG:HG2	2.49	0.47
1:B:373:SER:OG	1:B:380:ASN:ND2	2.46	0.47
1:C:21:ASP:OD2	1:C:285:PRO:HA	2.14	0.47
1:C:154:TYR:HA	1:C:183:ILE:O	2.14	0.47
1:C:354:ALA:CB	1:C:491:ALA:HA	2.44	0.47
1:C:431:VAL:HG11	1:C:468:HIS:HA	1.95	0.47
1:C:187:ASP:OD1	1:C:189:ASN:HB3	2.14	0.47
1:C:488:PRO:HD2	1:C:512:VAL:O	2.14	0.47
1:D:209:TYR:HD2	1:D:214:TRP:CD2	2.31	0.47
1:A:51:HIS:ND1	1:A:84:TYR:OH	2.32	0.47
1:A:267:LEU:O	1:A:271:ALA:HB3	2.14	0.47
1:D:469:GLN:OE1	1:D:624:GLY:HA3	2.15	0.47
2:C:701:TPP:H62	1:D:375:ASP:OD2	2.15	0.47
1:A:374:ALA:HA	1:A:403:GLY:O	2.15	0.47
1:C:459:ILE:HA	1:C:469:GLN:HG2	1.97	0.47
1:D:25:LYS:NZ	1:D:92:LYS:O	2.48	0.46
1:B:524:GLU:OE1	1:B:524:GLU:HA	2.15	0.46
1:A:222:VAL:HG23	1:A:246:VAL:HG11	1.97	0.46
1:A:459:ILE:HA	1:A:469:GLN:HG2	1.95	0.46
1:C:16:ARG:O	1:C:19:ALA:HB3	2.15	0.46
1:D:121:GLY:O	1:D:125:SER:OG	2.26	0.46
1:D:604:ALA:HA	1:D:638:PHE:CZ	2.50	0.46
1:C:534:TYR:CE2	1:C:574:SER:HB3	2.51	0.46
1:D:17:PHE:HA	1:D:20:ILE:HD12	1.96	0.46
1:D:607:SER:HB3	1:D:621:ASP:OD1	2.16	0.46
1:C:494:THR:O	1:C:497:ALA:HB3	2.16	0.46
1:B:6:ASP:O	1:B:10:LEU:HB2	2.16	0.45
1:B:489:ALA:O	1:B:554:HIS:CE1	2.69	0.45
1:C:159:ASP:OD2	1:C:197:THR:HG21	2.16	0.45
1:B:54:LEU:HD21	1:B:299:ARG:HG2	1.97	0.45
1:C:430:LEU:HA	1:C:454:PHE:HB3	1.97	0.45
1:C:639:THR:O	1:C:643:VAL:HG23	2.16	0.45
1:B:531:ARG:NH2	1:B:588:TYR:CD1	2.85	0.45
1:C:313:LEU:HD21	1:C:328:MET:CE	2.47	0.45
1:D:581:PHE:CE2	1:D:589:ARG:HG2	2.52	0.45
1:B:437:ARG:HB3	1:B:438:PRO:HD3	1.99	0.45
1:C:375:ASP:OD2	2:D:802:TPP:H62	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:TYR:CD2	1:A:630:PRO:HA	2.51	0.45
1:D:383:LYS:NZ	1:D:389:ASP:OD1	2.50	0.45
1:D:437:ARG:N	1:D:438:PRO:CD	2.80	0.45
1:B:459:ILE:HD13	1:B:620:LEU:HD22	1.99	0.44
1:B:533:GLY:HA2	1:B:574:SER:O	2.17	0.44
1:C:102:PRO:HA	5:D:924:HOH:O	2.16	0.44
1:D:11:SER:HB2	1:D:42:TYR:CE1	2.52	0.44
1:D:30:HIS:O	1:D:34:PRO:HG2	2.17	0.44
1:A:377:THR:N	1:A:378:PRO:HD2	2.32	0.44
1:B:30:HIS:CD2	1:B:264:GLY:HA2	2.52	0.44
1:C:458:SER:OG	1:C:460:ALA:HB3	2.17	0.44
1:D:122:GLN:O	1:D:126:THR:OG1	2.25	0.44
1:D:643:VAL:O	1:D:646:ALA:HB3	2.17	0.44
1:A:263:HIS:CE1	2:A:701:TPP:H71	2.52	0.44
1:B:605:GLY:O	1:B:619:ALA:HB1	2.18	0.44
1:C:555:LEU:HD11	1:C:639:THR:C	2.38	0.44
1:C:129:GLY:HA3	1:C:415:GLY:HA3	2.00	0.44
1:A:41:ALA:CB	1:A:74:LEU:HD11	2.47	0.44
1:D:437:ARG:N	1:D:438:PRO:HD3	2.33	0.44
1:B:288:VAL:HB	1:B:293:TYR:CE2	2.52	0.43
1:B:461:LEU:HD12	1:B:461:LEU:C	2.39	0.43
1:C:256:LYS:O	1:C:262:ALA:HB2	2.18	0.43
1:C:413:LEU:HB3	1:C:450:THR:HG23	2.00	0.43
1:D:35:MET:CE	1:D:267:LEU:HD11	2.49	0.43
2:A:701:TPP:C2	2:A:701:TPP:HN42	2.30	0.43
1:B:44:LEU:O	1:B:49:MET:HB2	2.19	0.43
1:C:372:GLY:HA2	1:C:400:LEU:O	2.19	0.43
1:C:122:GLN:HB3	1:C:442:LEU:HD22	1.99	0.43
1:D:46:ARG:HA	1:D:298:MET:CE	2.49	0.43
1:D:594:PRO:HB2	1:D:597:LEU:HD12	2.00	0.43
1:B:43:LEU:HD13	1:B:225:LEU:HD22	2.01	0.43
1:D:519:PRO:O	1:D:554:HIS:NE2	2.51	0.43
1:C:45:PHE:CD1	1:C:78:VAL:HG11	2.54	0.43
1:A:555:LEU:HD23	1:A:602:VAL:HG11	2.01	0.43
1:B:328:MET:HA	1:B:328:MET:CE	2.48	0.43
1:B:540:GLU:O	1:B:541:GLU:C	2.57	0.43
1:D:84:TYR:O	1:D:86:LEU:N	2.51	0.43
1:A:215:GLN:OE1	1:A:235:ALA:HA	2.19	0.43
1:B:629:TYR:CD2	1:B:630:PRO:HA	2.54	0.43
1:D:390:PHE:HB2	1:D:397:GLY:O	2.19	0.43
1:C:68:ALA:HB1	1:C:70:HIS:CE1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:ARG:O	1:D:19:ALA:HB3	2.19	0.42
1:C:104:HIS:HA	1:C:105:PRO:HD3	1.93	0.42
1:C:297:ASP:OD1	1:C:299:ARG:HG3	2.18	0.42
1:C:487:ARG:HG2	1:C:550:GLY:HA3	2.01	0.42
1:D:301:LYS:O	1:D:304:ALA:HB3	2.19	0.42
4:A:703:E4P:H1	1:B:193:ILE:HD11	2.01	0.42
1:C:193:ILE:HG12	1:C:263:HIS:CD2	2.55	0.42
1:D:79:LEU:HD23	1:D:84:TYR:CD1	2.55	0.42
1:D:417:ASN:HD21	1:D:424:ALA:H	1.66	0.42
1:D:459:ILE:HG23	5:D:922:HOH:O	2.19	0.42
1:B:374:ALA:HA	1:B:403:GLY:O	2.20	0.42
1:C:345:PHE:CE2	1:C:491:ALA:HB1	2.54	0.42
1:C:516:GLN:O	1:C:516:GLN:HG2	2.19	0.42
1:A:642:ARG:HE	1:A:642:ARG:HB3	1.65	0.42
1:C:404:VAL:HG12	1:D:164:GLU:HG2	2.02	0.42
1:D:38:ALA:HB3	1:D:39:PRO:HD3	2.02	0.42
1:D:277:ARG:O	1:D:280:GLY:N	2.51	0.42
1:C:499:LEU:O	1:C:503:ARG:HG3	2.19	0.42
1:D:250:ILE:CG2	1:D:258:ASP:HA	2.48	0.42
1:D:288:VAL:CG1	1:D:293:TYR:CE2	3.03	0.42
1:C:329:ARG:NH1	1:C:334:GLU:O	2.53	0.42
1:C:627:ALA:HA	1:D:95:ARG:O	2.19	0.42
1:D:39:PRO:HB3	1:D:225:LEU:CD2	2.50	0.42
1:A:375:ASP:OD2	2:B:802:TPP:H62	2.20	0.42
1:C:363:ALA:O	1:C:364:PRO:C	2.56	0.42
1:C:604:ALA:HA	1:C:638:PHE:CZ	2.55	0.42
1:B:22:ALA:HB3	1:B:73:MET:HG3	2.02	0.41
1:A:309:TRP:CH2	1:A:313:LEU:HD11	2.55	0.41
4:A:703:E4P:H1	2:B:802:TPP:C2	2.50	0.41
1:B:284:PRO:HB2	1:B:285:PRO:HD2	2.02	0.41
1:B:489:ALA:HA	1:B:550:GLY:HA2	2.02	0.41
1:D:89:GLU:O	1:D:92:LYS:HB2	2.21	0.41
1:D:564:ARG:O	1:D:567:GLY:N	2.51	0.41
1:A:38:ALA:HB3	1:A:39:PRO:HD3	2.02	0.41
1:A:457:ASP:HB3	1:A:513:LEU:O	2.21	0.41
1:B:505:LYS:HA	1:B:505:LYS:HD3	1.87	0.41
1:C:417:ASN:HD21	1:C:424:ALA:H	1.66	0.41
1:C:60:ASP:O	1:C:151:HIS:HB3	2.20	0.41
2:C:701:TPP:N1'	1:D:406:GLU:OE2	2.54	0.41
1:D:33:MET:HB3	1:D:34:PRO:HD3	2.02	0.41
1:D:38:ALA:N	1:D:39:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:VAL:HA	1:D:616:LYS:O	2.20	0.41
1:C:11:SER:O	1:C:14:ALA:HB3	2.21	0.41
1:C:175:GLY:HA3	1:C:212:TYR:O	2.21	0.41
1:D:486:ILE:HA	1:D:576:PRO:O	2.19	0.41
1:A:547:VAL:HG13	1:A:601:ALA:HA	2.02	0.41
1:B:7:LEU:HD12	1:B:7:LEU:HA	1.86	0.41
1:D:70:HIS:CD2	1:D:263:HIS:CE1	3.09	0.41
1:D:197:THR:HB	1:D:201:PHE:HB3	2.01	0.41
1:C:380:ASN:HB3	1:C:382:THR:HG23	2.03	0.41
1:B:250:ILE:O	1:B:257:GLN:HA	2.20	0.41
1:C:374:ALA:HA	1:C:403:GLY:O	2.21	0.41
1:D:94:PHE:HA	1:D:101:THR:OG1	2.21	0.41
1:D:427:GLY:HA2	1:D:453:VAL:O	2.21	0.41
1:D:586:GLU:O	1:D:590:LYS:HG3	2.21	0.41
1:A:296:MET:O	1:A:298:MET:HG2	2.21	0.41
1:C:127:ALA:O	1:C:130:LEU:HB2	2.21	0.41
1:D:206:LEU:HD21	1:D:245:ALA:HB2	2.02	0.41
1:B:345:PHE:CE2	1:B:491:ALA:HB1	2.57	0.40
1:C:463:GLU:HB3	1:D:95:ARG:HD3	2.03	0.40
1:D:75:LEU:HD21	1:D:113:VAL:HG22	2.03	0.40
1:D:240:ARG:C	1:D:241:PRO:O	2.58	0.40
1:B:501:ALA:CB	1:B:509:THR:HG21	2.49	0.40
1:D:39:PRO:O	1:D:42:TYR:HB3	2.21	0.40
1:A:417:ASN:ND2	1:A:423:ARG:HA	2.37	0.40
1:C:268:GLY:O	1:C:272:VAL:HG23	2.22	0.40
1:D:31:PRO:C	1:D:34:PRO:HD2	2.41	0.40
1:A:38:ALA:N	1:A:39:PRO:CD	2.85	0.40
1:A:46:ARG:HE	1:A:295:HIS:CE1	2.40	0.40
1:A:354:ALA:CB	1:A:491:ALA:HA	2.51	0.40
1:B:46:ARG:HD2	1:B:298:MET:CE	2.51	0.40
1:B:617:VAL:HG22	1:B:619:ALA:HB2	2.02	0.40
1:D:118:GLY:N	1:D:119:PRO:CD	2.84	0.40
1:D:459:ILE:HA	1:D:469:GLN:HG2	2.03	0.40
1:C:538:ASP:OD1	1:C:571:ARG:HD3	2.21	0.40
1:D:34:PRO:HA	1:D:74:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

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	648/672 (96%)	629 (97%)	19 (3%)	0	100	100
1	B	648/672 (96%)	618 (95%)	30 (5%)	0	100	100
1	C	648/672 (96%)	605 (93%)	41 (6%)	2 (0%)	41	46
1	D	648/672 (96%)	564 (87%)	73 (11%)	11 (2%)	9	4
All	All	2592/2688 (96%)	2416 (93%)	163 (6%)	13 (0%)	29	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	269	PRO
1	D	343	PRO
1	D	46	ARG
1	D	302	GLY
1	C	375	ASP
1	D	103	GLY
1	D	200	ALA
1	D	277	ARG
1	C	631	GLU
1	D	85	ASP
1	D	74	LEU
1	D	321	PRO
1	D	28	SER

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	521/540 (96%)	510 (98%)	11 (2%)	53	62
1	B	521/540 (96%)	510 (98%)	11 (2%)	53	62
1	C	521/540 (96%)	505 (97%)	16 (3%)	40	49
1	D	521/540 (96%)	499 (96%)	22 (4%)	30	34
All	All	2084/2160 (96%)	2024 (97%)	60 (3%)	42	51

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LEU
1	A	87	PRO
1	A	218	ARG
1	A	248	SER
1	A	325	GLN
1	A	344	SER
1	A	365	ARG
1	A	458	SER
1	A	527	ARG
1	A	617	VAL
1	A	642	ARG
1	B	2	LYS
1	B	107	ARG
1	B	109	HIS
1	B	248	SER
1	B	261	LYS
1	B	313	LEU
1	B	385	GLU
1	B	476	SER
1	B	522	SER
1	B	564	ARG
1	B	571	ARG
1	C	2	LYS
1	C	11	SER
1	C	54	LEU
1	C	93	SER
1	C	218	ARG
1	C	250	ILE
1	C	265	GLU
1	C	300	GLU
1	C	341	GLU
1	C	379	SER
1	C	396	LEU

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Mol	Chain	Res	Type
1	C	405	ARG
1	C	540	GLU
1	C	552	GLU
1	C	616	LYS
1	C	617	VAL
1	D	6	ASP
1	D	27	ARG
1	D	46	ARG
1	D	54	LEU
1	D	125	SER
1	D	136	LYS
1	D	146	HIS
1	D	248	SER
1	D	258	ASP
1	D	278	ASN
1	D	290	GLU
1	D	313	LEU
1	D	314	GLU
1	D	344	SER
1	D	347	LYS
1	D	388	GLU
1	D	437	ARG
1	D	490	ASP
1	D	524	GLU
1	D	540	GLU
1	D	562	LEU
1	D	616	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	380	ASN
1	A	417	ASN
1	A	554	HIS
1	A	560	GLN
1	B	380	ASN
1	B	394	ASN
1	B	417	ASN
1	B	554	HIS
1	B	560	GLN
1	C	146	HIS

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Mol	Chain	Res	Type
1	C	263	HIS
1	C	380	ASN
1	C	394	ASN
1	C	417	ASN
1	D	263	HIS
1	D	417	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	E4P	B	801	-	9,11,11	0.70	0	12,15,15	1.11	1 (8%)
4	E4P	C	703	-	9,11,11	0.54	0	12,15,15	2.09	4 (33%)
4	E4P	A	703	-	9,11,11	1.40	1 (11%)	12,15,15	2.70	6 (50%)
2	TPP	D	802	3	22,27,27	0.64	0	29,40,40	0.91	1 (3%)
2	TPP	C	701	3	22,27,27	0.66	0	29,40,40	0.90	1 (3%)
4	E4P	D	801	-	9,11,11	0.74	0	12,15,15	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TPP	A	701	3	22,27,27	0.73	1 (4%)	29,40,40	0.84	0
2	TPP	B	802	3	22,27,27	0.63	0	29,40,40	0.79	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
4	E4P	B	801	-	-	3/10/12/12	-
4	E4P	C	703	-	-	6/10/12/12	-
4	E4P	A	703	-	-	2/10/12/12	-
2	TPP	D	802	3	-	4/16/17/17	0/2/2/2
2	TPP	C	701	3	-	2/16/17/17	0/2/2/2
4	E4P	D	801	-	-	7/10/12/12	-
2	TPP	A	701	3	-	2/16/17/17	0/2/2/2
2	TPP	B	802	3	-	1/16/17/17	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	E4P	C4-C3	3.68	1.57	1.51
2	A	701	TPP	C7'-N3	-2.17	1.44	1.48

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	E4P	P-O4-C4	5.05	132.21	118.30
4	A	703	E4P	O4-P-O1P	-4.88	92.78	106.47
4	C	703	E4P	O4-P-O1P	-4.38	94.20	106.47
4	A	703	E4P	O3-C3-C4	3.86	118.60	109.92
4	C	703	E4P	O2-C2-C1	-3.15	102.64	110.08
4	A	703	E4P	O2P-P-O4	2.85	114.33	106.73
4	B	801	E4P	P-O4-C4	2.49	125.14	118.30
2	D	802	TPP	PA-O3A-PB	2.39	141.04	132.83
4	C	703	E4P	O3-C3-C4	-2.31	104.72	109.92
4	C	703	E4P	P-O4-C4	2.30	124.63	118.30
2	C	701	TPP	C5-C4-N3	2.16	111.89	107.57
4	A	703	E4P	O4-C4-C3	2.11	115.00	109.36
4	A	703	E4P	O3P-P-O1P	2.05	118.72	110.68

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	802	TPP	C4-C5-C6-C7
2	D	802	TPP	C4-C5-C6-C7
2	D	802	TPP	C5-C6-C7-O7
4	A	703	E4P	O3-C3-C4-O4
4	B	801	E4P	C4-O4-P-O1P
4	B	801	E4P	C4-O4-P-O2P
4	B	801	E4P	C4-O4-P-O3P
4	C	703	E4P	C2-C3-C4-O4
4	C	703	E4P	O3-C3-C4-O4
4	C	703	E4P	C4-O4-P-O1P
4	D	801	E4P	C1-C2-C3-O3
4	D	801	E4P	C1-C2-C3-C4
4	D	801	E4P	C4-O4-P-O1P
4	D	801	E4P	C4-O4-P-O2P
4	D	801	E4P	C4-O4-P-O3P
4	A	703	E4P	C2-C3-C4-O4
4	D	801	E4P	O2-C2-C3-O3
4	C	703	E4P	C3-C4-O4-P
4	C	703	E4P	C4-O4-P-O2P
2	C	701	TPP	C5-C6-C7-O7
2	A	701	TPP	PB-O3A-PA-O2A
4	D	801	E4P	O2-C2-C3-C4
4	C	703	E4P	C4-O4-P-O3P
2	D	802	TPP	PB-O3A-PA-O1A
2	D	802	TPP	PB-O3A-PA-O2A
2	A	701	TPP	C4-C5-C6-C7
2	C	701	TPP	C4-C5-C6-C7

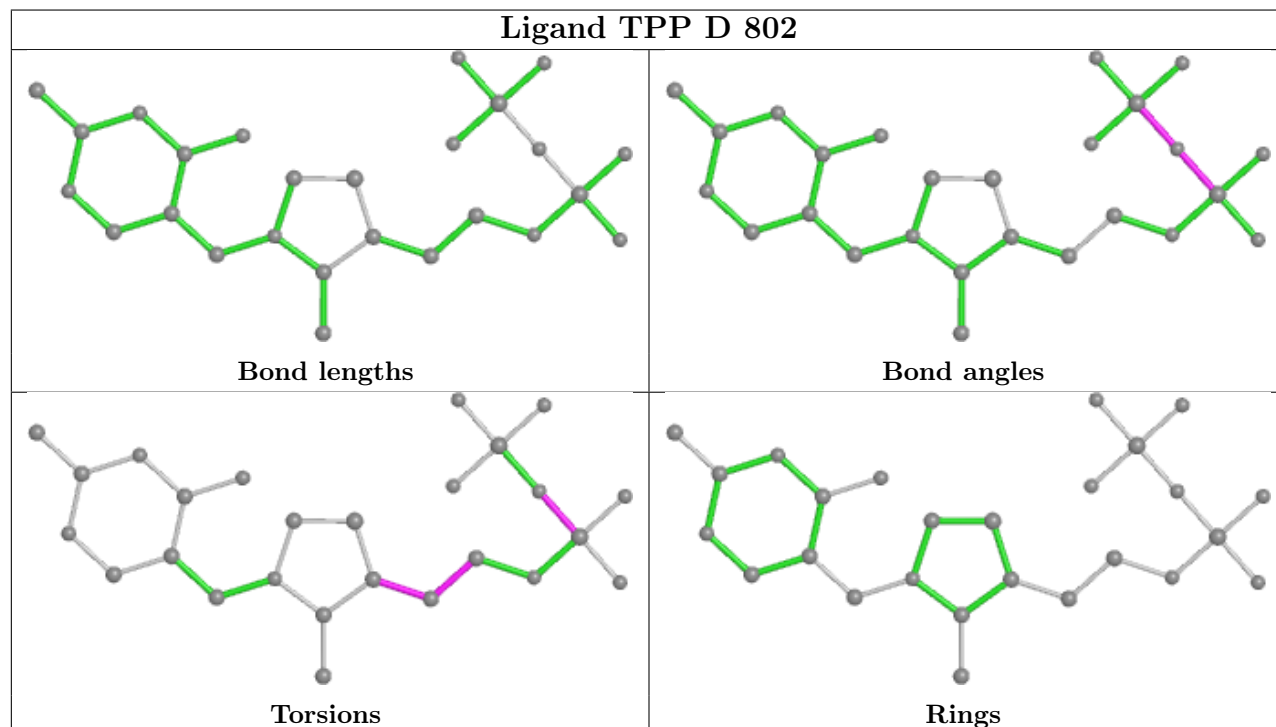
There are no ring outliers.

5 monomers are involved in 19 short contacts:

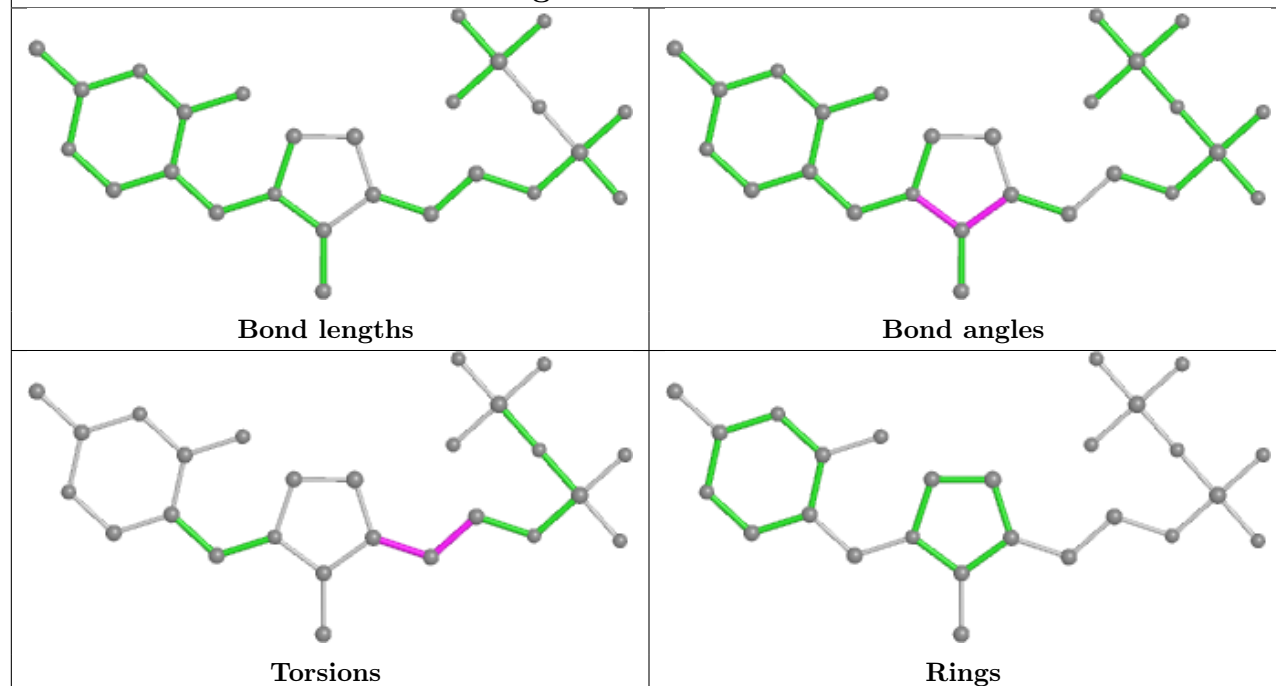
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	E4P	2	0
2	D	802	TPP	2	0
2	C	701	TPP	4	0
2	A	701	TPP	5	0
2	B	802	TPP	7	0

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

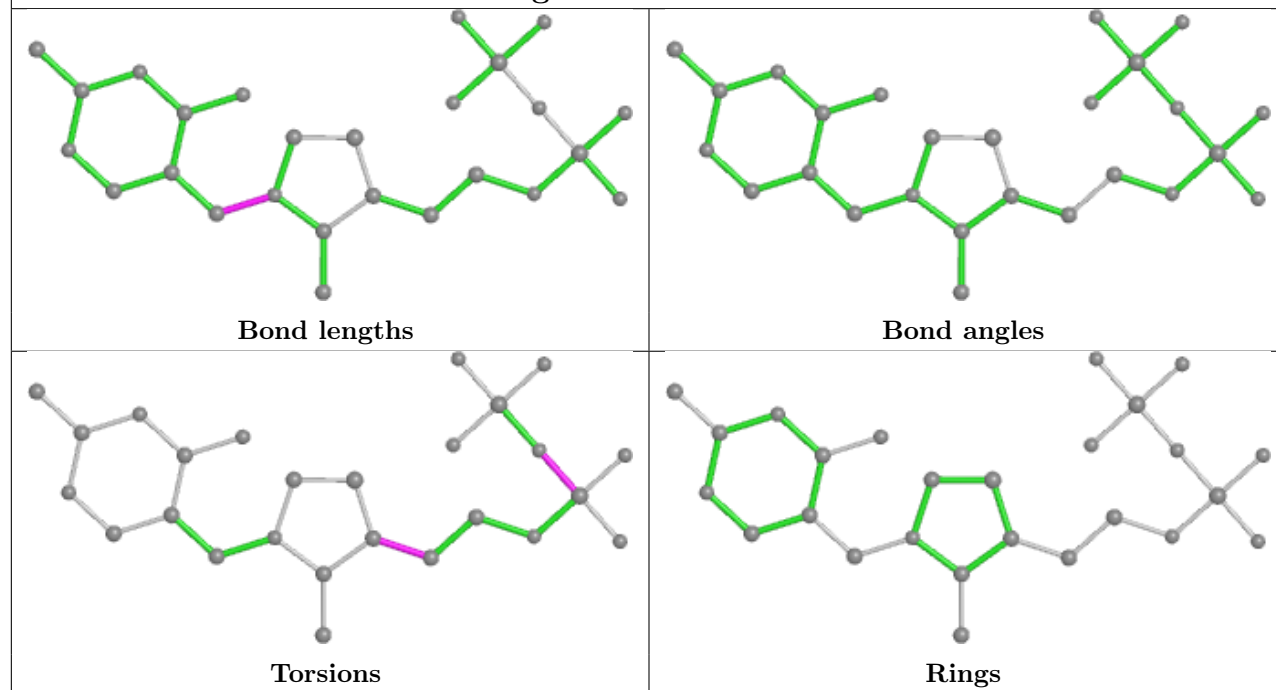
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

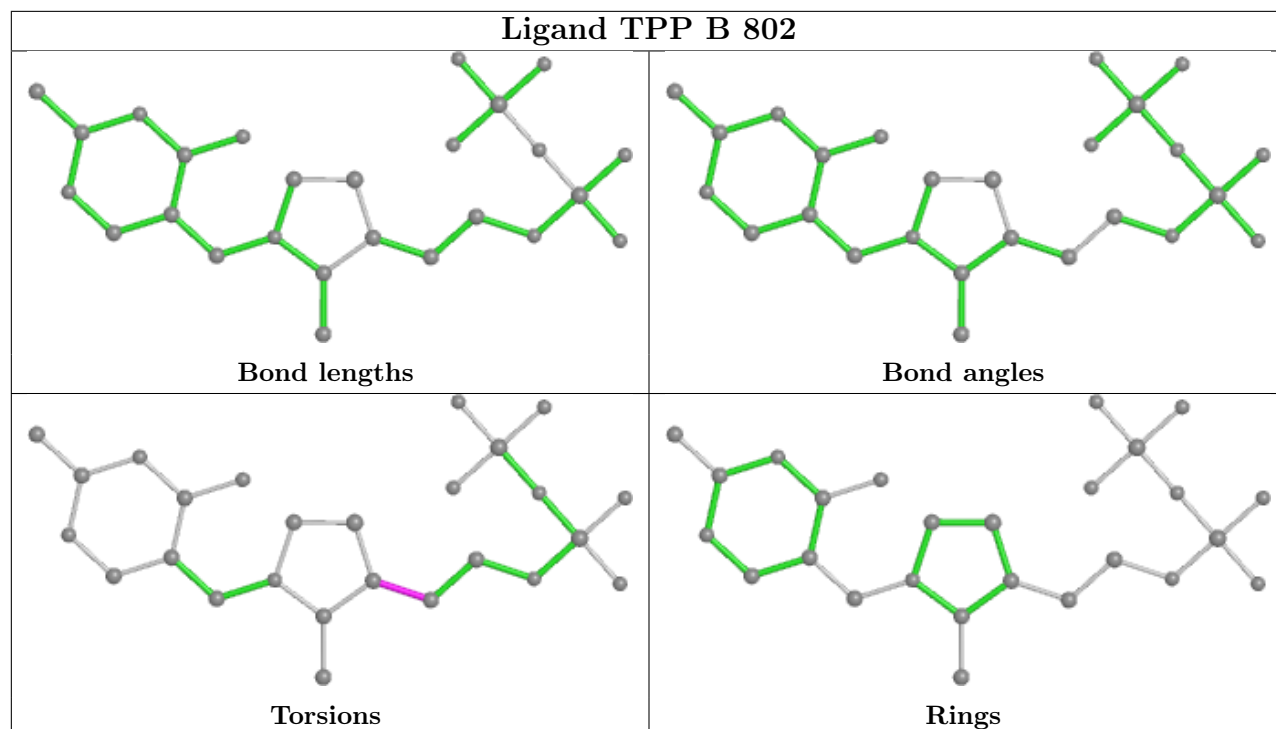


Ligand TPP C 701



Ligand TPP A 701





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, 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	650/672 (96%)	-0.04	23 (3%)	44	46	24, 42, 65, 149	0
1	B	650/672 (96%)	0.01	15 (2%)	60	63	28, 46, 71, 120	0
1	C	650/672 (96%)	0.33	47 (7%)	15	16	44, 61, 87, 133	0
1	D	650/672 (96%)	0.99	124 (19%)	1	1	44, 75, 111, 160	0
All	All	2600/2688 (96%)	0.32	209 (8%)	12	13	24, 55, 96, 160	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	GLU	7.9
1	D	2	LYS	7.9
1	A	2	LYS	7.5
1	D	316	TYR	6.9
1	D	5	ARG	6.6
1	D	4	THR	6.4
1	C	2	LYS	6.3
1	B	651	VAL	6.1
1	D	10	LEU	5.7
1	D	320	TYR	5.6
1	D	144	PRO	5.4
1	D	319	ALA	5.3
1	D	148	VAL	5.0
1	D	313	LEU	5.0
1	C	435	TYR	4.7
1	D	435	TYR	4.6
1	D	439	ALA	4.4
1	D	436	MET	4.4
1	C	436	MET	4.4
1	C	168	GLY	4.3
1	D	152	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	438	PRO	4.2
1	D	141	PHE	4.1
1	C	4	THR	4.1
1	D	166	VAL	4.1
1	C	322	ASP	4.1
1	D	651	VAL	4.0
1	D	296	MET	4.0
1	B	4	THR	4.0
1	C	440	ILE	3.9
1	D	227	ALA	3.9
1	D	432	PHE	3.9
1	D	341	GLU	3.9
1	C	386	GLY	3.9
1	B	5	ARG	3.9
1	D	437	ARG	3.8
1	D	564	ARG	3.8
1	D	318	ARG	3.6
1	C	431	VAL	3.6
1	D	162	LEU	3.6
1	D	146	HIS	3.6
1	C	319	ALA	3.6
1	B	2	LYS	3.6
1	C	567	GLY	3.6
1	D	294	ARG	3.6
1	D	288	VAL	3.5
1	C	3	GLU	3.5
1	C	148	VAL	3.5
1	C	433	SER	3.5
1	D	407	HIS	3.4
1	C	5	ARG	3.4
1	C	166	VAL	3.4
1	C	438	PRO	3.4
1	D	338	LEU	3.4
1	A	166	VAL	3.4
1	D	237	LEU	3.3
1	D	563	LEU	3.3
1	D	222	VAL	3.3
1	D	283	TYR	3.3
1	C	541	GLU	3.3
1	D	644	ALA	3.2
1	C	432	PHE	3.2
1	D	278	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	3	GLU	3.2
1	C	407	HIS	3.2
1	D	291	GLU	3.2
1	D	650	LEU	3.2
1	D	284	PRO	3.2
1	B	435	TYR	3.2
1	B	166	VAL	3.2
1	C	596	GLY	3.2
1	D	255	PRO	3.1
1	D	295	HIS	3.1
1	D	303	ARG	3.1
1	D	434	ASP	3.1
1	A	438	PRO	3.1
1	D	147	VAL	3.0
1	A	436	MET	3.0
1	D	279	LEU	3.0
1	D	565	GLU	3.0
1	D	277	ARG	3.0
1	D	167	SER	3.0
1	D	598	PRO	3.0
1	D	273	GLU	3.0
1	B	432	PHE	2.9
1	D	26	ALA	2.9
1	D	292	VAL	2.9
1	D	281	TRP	2.9
1	D	411	ALA	2.9
1	B	3	GLU	2.9
1	D	121	GLY	2.9
1	C	439	ALA	2.9
1	C	143	ARG	2.9
1	D	332	ARG	2.9
1	C	428	THR	2.8
1	D	145	GLY	2.8
1	C	437	ARG	2.8
1	D	54	LEU	2.8
1	D	542	PRO	2.8
1	A	407	HIS	2.8
1	D	324	HIS	2.8
1	C	408	ALA	2.8
1	B	319	ALA	2.8
1	C	651	VAL	2.8
1	C	443	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	312	ALA	2.7
1	D	647	PHE	2.7
1	D	269	PRO	2.7
1	A	318	ARG	2.7
1	D	365	ARG	2.7
1	D	559	ALA	2.7
1	A	121	GLY	2.7
1	D	440	ILE	2.7
1	D	260	ALA	2.7
1	D	557	LEU	2.7
1	D	433	SER	2.7
1	D	643	VAL	2.7
1	C	120	LEU	2.6
1	D	156	LEU	2.6
1	D	597	LEU	2.6
1	D	17	PHE	2.6
1	D	6	ASP	2.6
1	D	328	MET	2.6
1	B	323	LEU	2.6
1	D	234	LEU	2.6
1	D	323	LEU	2.6
1	A	435	TYR	2.6
1	D	309	TRP	2.6
1	C	385	GLU	2.6
1	D	410	GLY	2.6
1	D	314	GLU	2.6
1	A	120	LEU	2.5
1	A	442	LEU	2.5
1	D	315	ALA	2.5
1	D	317	ALA	2.5
1	D	67	SER	2.5
1	D	165	GLY	2.5
1	C	144	PRO	2.5
1	A	165	GLY	2.5
1	D	251	GLY	2.5
1	D	311	LYS	2.5
1	C	118	GLY	2.5
1	D	430	LEU	2.5
1	D	68	ALA	2.5
1	C	321	PRO	2.5
1	C	364	PRO	2.5
1	C	598	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	434	ASP	2.5
1	D	431	VAL	2.5
1	B	438	PRO	2.4
1	A	411	ALA	2.4
1	C	337	PRO	2.4
1	D	445	LEU	2.4
1	D	268	GLY	2.4
1	C	454	PHE	2.4
1	D	274	ALA	2.3
1	D	289	PRO	2.3
1	A	439	ALA	2.3
1	C	539	VAL	2.3
1	D	270	GLU	2.3
1	A	123	GLY	2.3
1	C	119	PRO	2.3
1	B	436	MET	2.3
1	D	149	VAL	2.3
1	C	121	GLY	2.3
1	D	329	ARG	2.3
1	D	374	ALA	2.3
1	D	561	ALA	2.3
1	D	218	ARG	2.3
1	D	395	PRO	2.3
1	B	316	TYR	2.3
1	D	340	GLU	2.3
1	A	412	ILE	2.3
1	D	596	GLY	2.2
1	D	293	TYR	2.2
1	B	431	VAL	2.2
1	A	317	ALA	2.2
1	D	539	VAL	2.2
1	A	118	GLY	2.2
1	D	648	LEU	2.2
1	D	541	GLU	2.2
1	C	452	PHE	2.2
1	A	408	ALA	2.2
1	C	124	ILE	2.2
1	C	477	LEU	2.2
1	D	120	LEU	2.2
1	D	155	VAL	2.2
1	D	186	TRP	2.2
1	D	569	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	392	ARG	2.1
1	D	441	ARG	2.1
1	D	163	MET	2.1
1	C	141	PHE	2.1
1	A	119	PRO	2.1
1	A	444	ALA	2.1
1	D	257	GLN	2.1
1	A	5	ARG	2.1
1	D	143	ARG	2.1
1	D	7	LEU	2.1
1	D	122	GLN	2.1
1	B	255	PRO	2.1
1	D	84	TYR	2.1
1	C	543	GLN	2.0
1	D	230	LYS	2.0
1	C	647	PHE	2.0
1	D	327	LEU	2.0
1	D	266	PRO	2.0
1	D	12	VAL	2.0
1	A	374	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

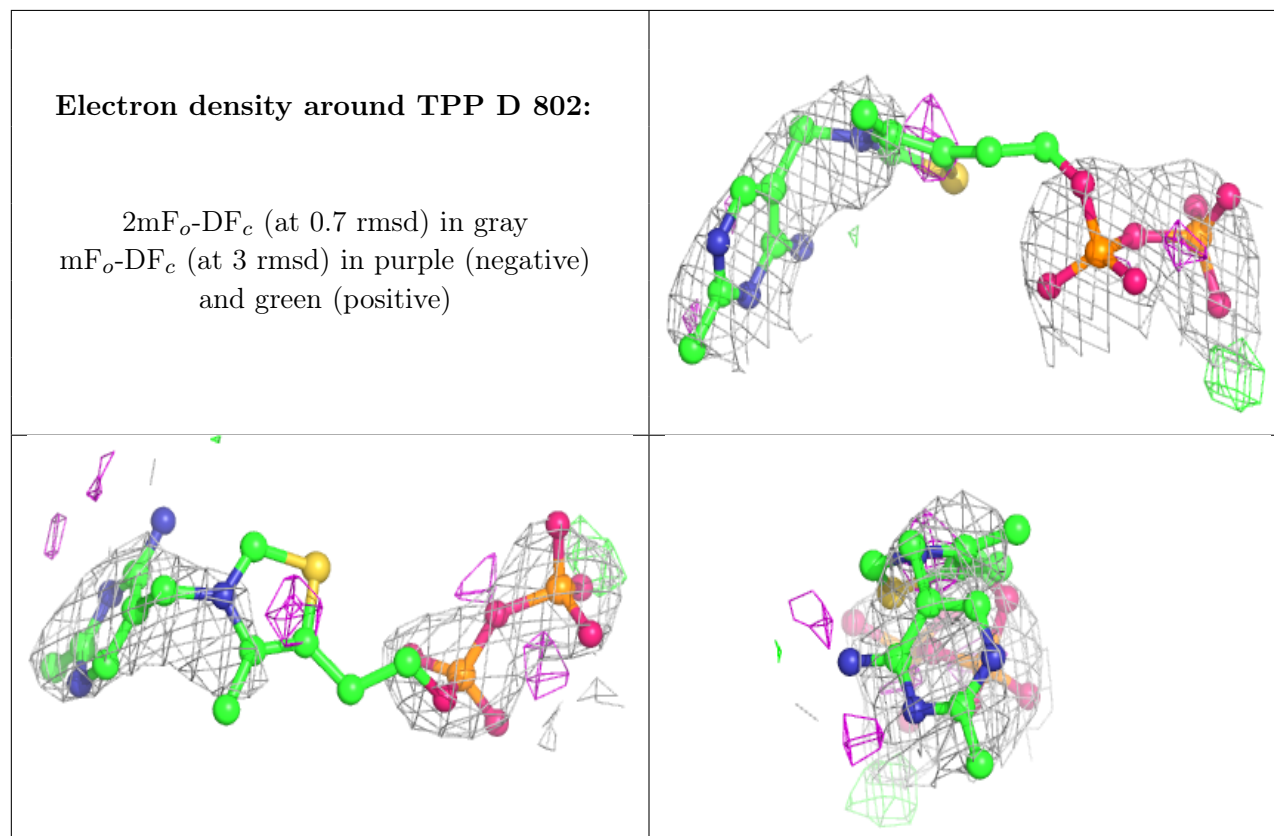
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	TPP	D	802	26/26	0.81	0.29	80,110,142,159	0
2	TPP	C	701	26/26	0.87	0.20	69,101,131,161	0
2	TPP	B	802	26/26	0.91	0.17	56,77,92,98	0

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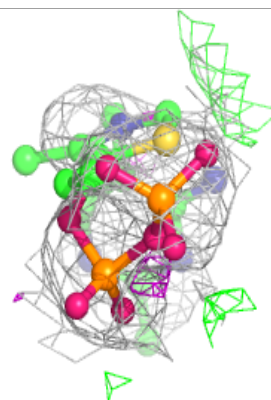
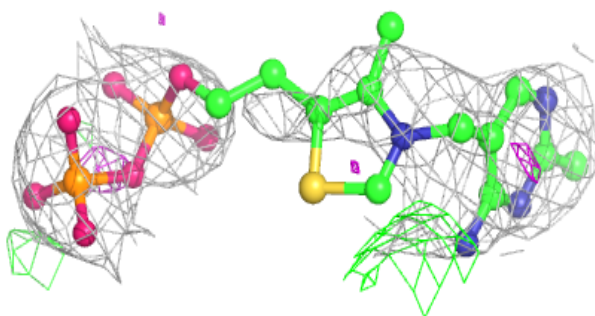
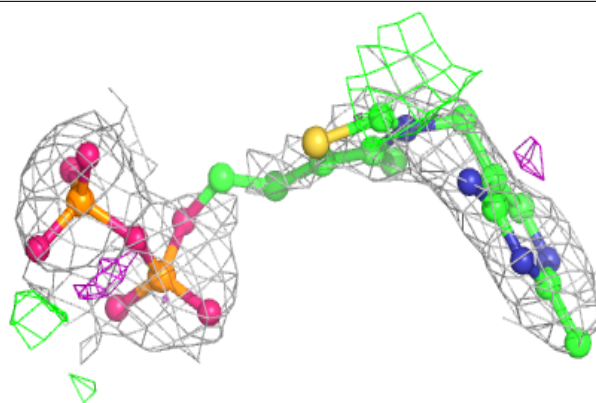
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TPP	A	701	26/26	0.92	0.18	41,73,87,100	0
4	E4P	C	703	12/12	0.93	0.15	72,84,88,89	0
4	E4P	D	801	12/12	0.93	0.16	68,74,78,85	0
4	E4P	A	703	12/12	0.96	0.18	51,69,82,85	0
3	CA	A	702	1/1	0.97	0.04	59,59,59,59	0
3	CA	C	702	1/1	0.97	0.07	73,73,73,73	0
3	CA	D	803	1/1	0.97	0.08	73,73,73,73	0
3	CA	B	803	1/1	0.98	0.04	58,58,58,58	0
4	E4P	B	801	12/12	0.98	0.10	48,54,69,69	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.

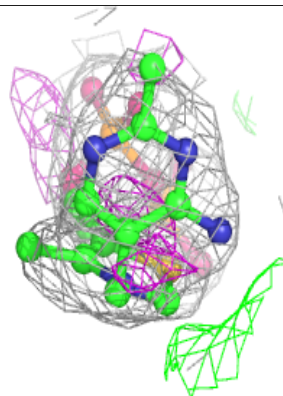
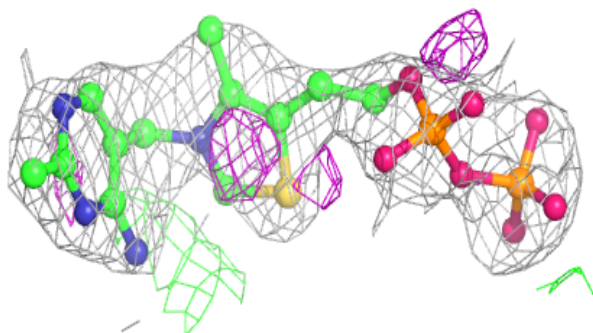
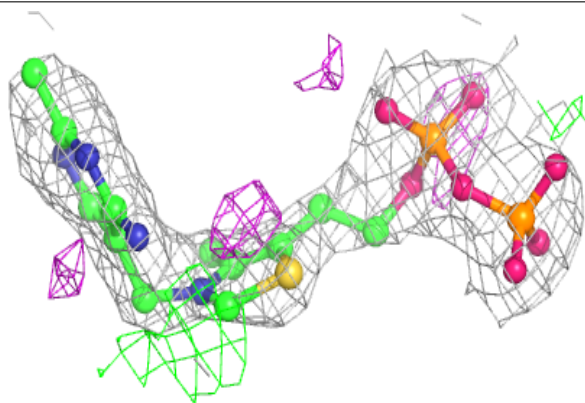


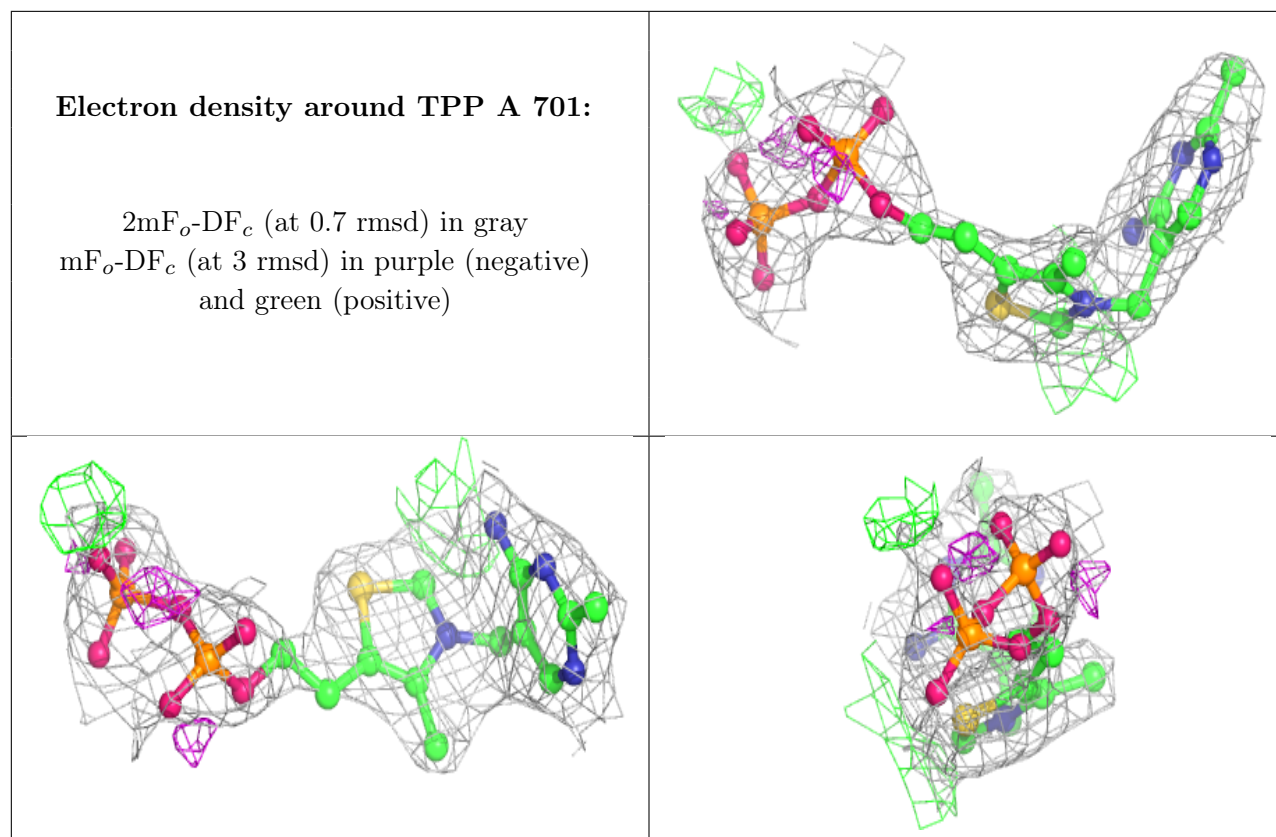
Electron density around TPP C 701:

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

**Electron density around TPP B 802:**

$2mF_o-DF_c$ (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.