Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2024 – 03:03 pm BST

PDB ID	:	8R3O
Title	:	Transketolase from Haemophilus influenzae in complex with thiamin pyrophosphate
Authors	:	Ballut, L.; Georges, R.N.; Aghajari, N.; Hecquet, L.; Charmantray, F.; Doumeche, B.
Deposited on	:	2023-11-10
Resolution	:	2.10 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:

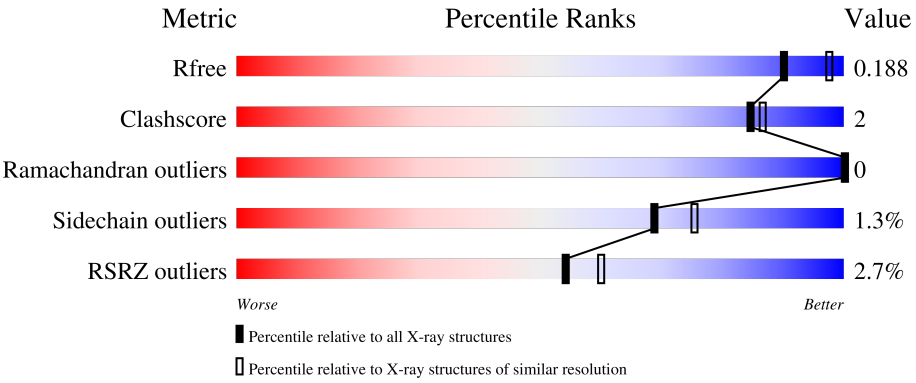
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	680	3% 91% 6%
1	B	680	3% 92% 6%
1	C	680	2% 94%
1	D	680	2% 93% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CIT	D	703	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 23000 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	664	Total	C	N	O	S	0	1	0
			5124	3246	889	970	19			
1	B	667	Total	C	N	O	S	0	0	0
			5146	3259	893	975	19			
1	C	666	Total	C	N	O	S	0	0	0
			5138	3253	892	974	19			
1	D	665	Total	C	N	O	S	0	0	0
			5126	3247	890	970	19			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	666	GLU	-	expression tag	UNP P43757
A	667	ASN	-	expression tag	UNP P43757
A	668	LEU	-	expression tag	UNP P43757
A	669	TYR	-	expression tag	UNP P43757
A	670	PHE	-	expression tag	UNP P43757
A	671	GLN	-	expression tag	UNP P43757
A	672	GLY	-	expression tag	UNP P43757
A	673	LEU	-	expression tag	UNP P43757
A	674	GLU	-	expression tag	UNP P43757
A	675	HIS	-	expression tag	UNP P43757
A	676	HIS	-	expression tag	UNP P43757
A	677	HIS	-	expression tag	UNP P43757
A	678	HIS	-	expression tag	UNP P43757
A	679	HIS	-	expression tag	UNP P43757
A	680	HIS	-	expression tag	UNP P43757
B	666	GLU	-	expression tag	UNP P43757
B	667	ASN	-	expression tag	UNP P43757
B	668	LEU	-	expression tag	UNP P43757
B	669	TYR	-	expression tag	UNP P43757
B	670	PHE	-	expression tag	UNP P43757
B	671	GLN	-	expression tag	UNP P43757

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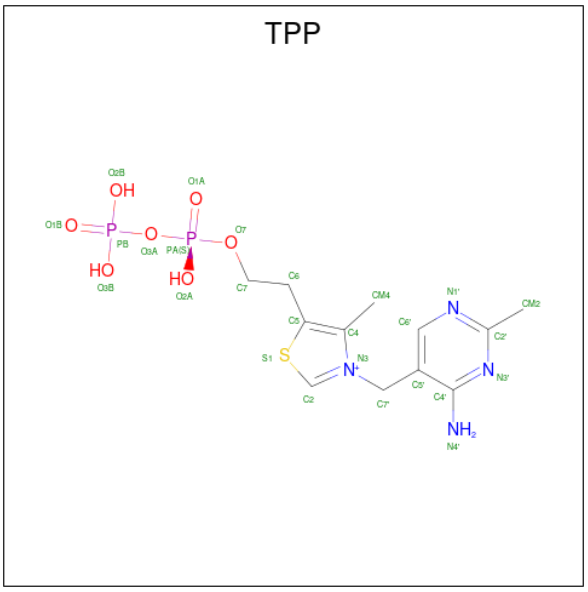
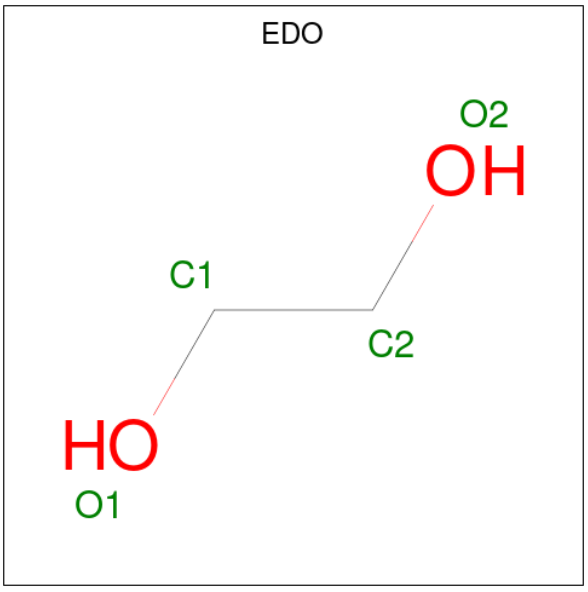
Chain	Residue	Modelled	Actual	Comment	Reference
B	672	GLY	-	expression tag	UNP P43757
B	673	LEU	-	expression tag	UNP P43757
B	674	GLU	-	expression tag	UNP P43757
B	675	HIS	-	expression tag	UNP P43757
B	676	HIS	-	expression tag	UNP P43757
B	677	HIS	-	expression tag	UNP P43757
B	678	HIS	-	expression tag	UNP P43757
B	679	HIS	-	expression tag	UNP P43757
B	680	HIS	-	expression tag	UNP P43757
C	666	GLU	-	expression tag	UNP P43757
C	667	ASN	-	expression tag	UNP P43757
C	668	LEU	-	expression tag	UNP P43757
C	669	TYR	-	expression tag	UNP P43757
C	670	PHE	-	expression tag	UNP P43757
C	671	GLN	-	expression tag	UNP P43757
C	672	GLY	-	expression tag	UNP P43757
C	673	LEU	-	expression tag	UNP P43757
C	674	GLU	-	expression tag	UNP P43757
C	675	HIS	-	expression tag	UNP P43757
C	676	HIS	-	expression tag	UNP P43757
C	677	HIS	-	expression tag	UNP P43757
C	678	HIS	-	expression tag	UNP P43757
C	679	HIS	-	expression tag	UNP P43757
C	680	HIS	-	expression tag	UNP P43757
D	666	GLU	-	expression tag	UNP P43757
D	667	ASN	-	expression tag	UNP P43757
D	668	LEU	-	expression tag	UNP P43757
D	669	TYR	-	expression tag	UNP P43757
D	670	PHE	-	expression tag	UNP P43757
D	671	GLN	-	expression tag	UNP P43757
D	672	GLY	-	expression tag	UNP P43757
D	673	LEU	-	expression tag	UNP P43757
D	674	GLU	-	expression tag	UNP P43757
D	675	HIS	-	expression tag	UNP P43757
D	676	HIS	-	expression tag	UNP P43757
D	677	HIS	-	expression tag	UNP P43757
D	678	HIS	-	expression tag	UNP P43757
D	679	HIS	-	expression tag	UNP P43757
D	680	HIS	-	expression tag	UNP P43757

- 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		
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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

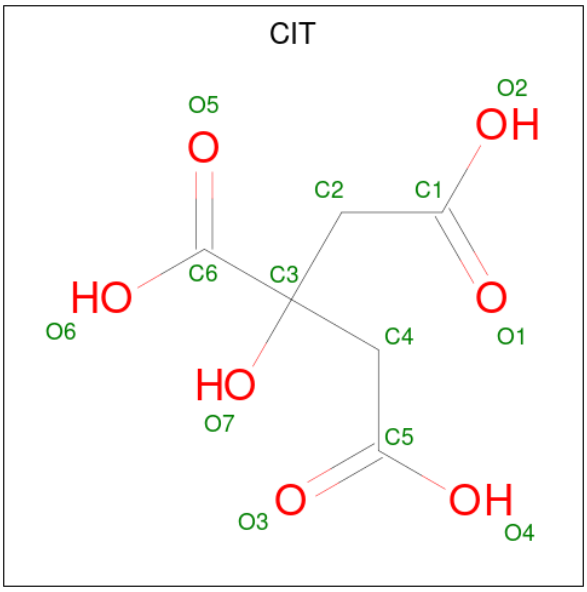


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0
5	D	1	Total C O 13 6 7	0	0

- Molecule 6 is water.

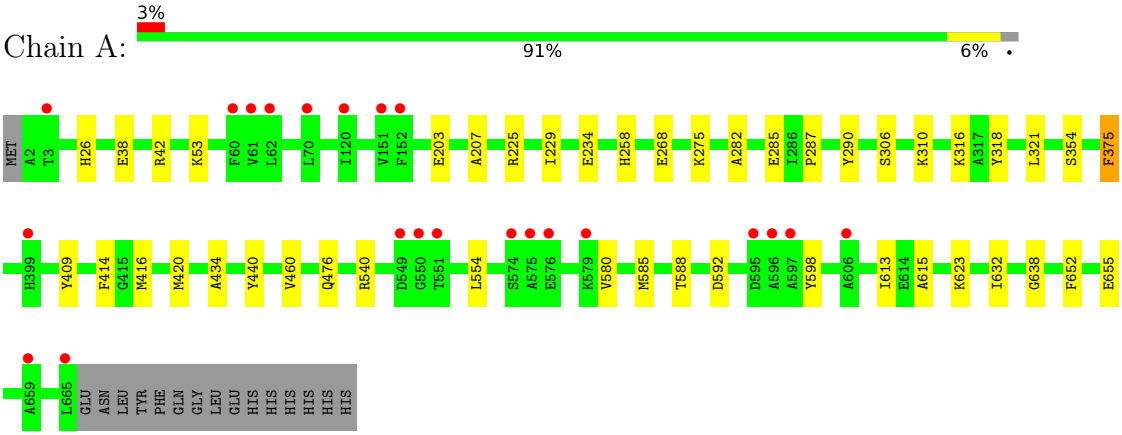
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	563	Total O 563 563	0	0
6	B	539	Total O 539 539	0	0
6	C	581	Total O 581 581	0	0
6	D	628	Total O 628 628	0	0

3 Residue-property plots (i)

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

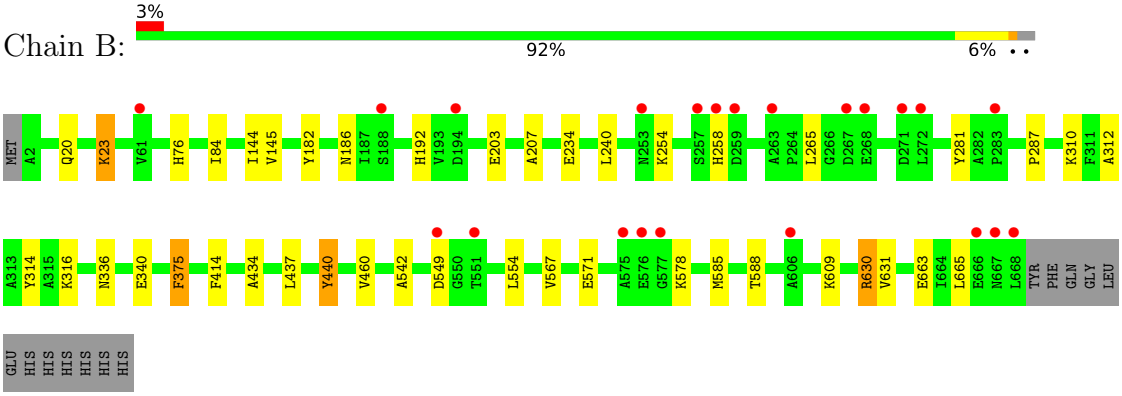
• Molecule 1: Transketolase

Chain A:



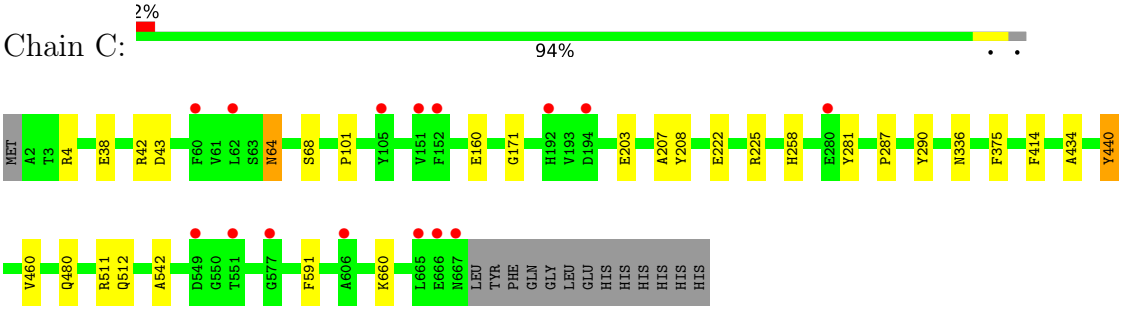
• Molecule 1: Transketolase

Chain B:



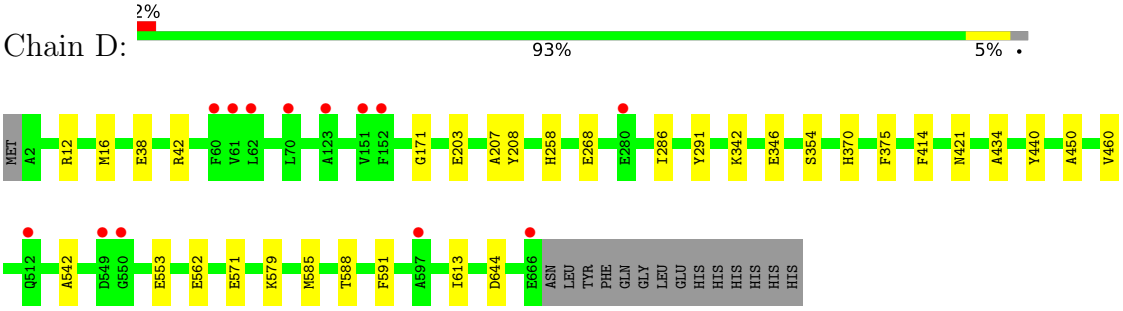
• Molecule 1: Transketolase

Chain C:



• Molecule 1: Transketolase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	110.25Å 90.67Å 155.25Å 90.00° 100.95° 90.00°	Depositor
Resolution (Å)	34.82 – 2.10 34.82 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (34.82-2.10) 96.3 (34.82-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.149 , 0.191 0.146 , 0.188	Depositor DCC
R_{free} test set	8437 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23000	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, MG, CIT, EDO

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	0.38	0/5249	0.57	0/7115
1	B	0.37	0/5268	0.57	0/7141
1	C	0.39	0/5260	0.56	0/7130
1	D	0.38	0/5248	0.58	0/7114
All	All	0.38	0/21025	0.57	0/28500

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5124	0	4988	29	0
1	B	5146	0	5006	27	0
1	C	5138	0	4995	16	0
1	D	5126	0	4985	19	0
2	A	26	0	16	1	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0
2	D	26	0	16	3	0
3	A	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	4	0	6	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	B	13	0	5	1	0
5	D	26	0	10	4	0
6	A	563	0	0	5	1
6	B	539	0	0	3	0
6	C	581	0	0	4	0
6	D	628	0	0	5	1
All	All	23000	0	20065	95	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (95) 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:C:207:ALA:HB2	1:D:203:GLU:HG2	1.54	0.88
1:C:203:GLU:HG2	1:D:207:ALA:HB2	1.61	0.81
1:B:310:LYS:NZ	6:B:801:HOH:O	2.15	0.76
2:A:701:TPP:H2	6:B:895:HOH:O	1.85	0.74
1:B:312:ALA:O	1:B:316:LYS:HD3	1.91	0.70
1:A:409:TYR:CG	1:A:416:MET:HG3	2.29	0.68
6:C:814:HOH:O	2:D:702:TPP:H2	1.92	0.68
1:A:409:TYR:CD2	1:A:416:MET:HG3	2.31	0.66
1:B:144:ILE:HD13	1:B:314:TYR:CE2	2.31	0.66
1:C:440:TYR:HE2	1:C:480:GLN:HG3	1.61	0.65
1:A:268:GLU:OE1	6:A:801:HOH:O	2.14	0.65
1:A:203:GLU:HG2	1:B:207:ALA:HB2	1.80	0.63
1:B:234:GLU:O	6:B:802:HOH:O	2.16	0.61
6:A:1007:HOH:O	2:B:702:TPP:H2	2.00	0.61
1:D:644:ASP:OD2	6:D:801:HOH:O	2.16	0.60
1:C:203:GLU:HG3	1:D:203:GLU:HG3	1.82	0.60
1:A:592:ASP:OD2	1:A:623:LYS:NZ	2.39	0.55
1:A:203:GLU:HG3	1:B:203:GLU:HG3	1.88	0.55
1:B:567:VAL:O	1:B:571:GLU:HG3	2.07	0.54
1:A:287:PRO:HG2	1:A:290:TYR:CD1	2.43	0.54
1:A:655:GLU:OE1	1:A:655:GLU:N	2.34	0.54
1:D:542:ALA:HB2	1:D:585:MET:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LYS:HD2	1:B:265:LEU:HD23	1.90	0.52
1:A:207:ALA:HB2	1:B:203:GLU:HG2	1.92	0.52
1:B:20:GLN:O	1:B:23:LYS:HD3	2.10	0.51
1:B:336:ASN:O	1:B:340:GLU:HG3	2.11	0.51
1:A:354:SER:OG	6:A:802:HOH:O	2.19	0.50
2:D:702:TPP:H2	2:D:702:TPP:HN42	1.75	0.50
1:B:316:LYS:N	1:B:316:LYS:HD2	2.25	0.50
1:B:585:MET:SD	1:B:588:THR:HG22	2.51	0.50
1:C:660:LYS:HG3	6:C:807:HOH:O	2.12	0.49
1:C:542:ALA:HB3	1:C:591:PHE:CD1	2.47	0.49
1:D:553:GLU:CG	1:D:579:LYS:HE2	2.43	0.49
1:C:64:ASN:OD1	1:C:64:ASN:N	2.46	0.48
1:A:275:LYS:HE3	6:A:949:HOH:O	2.14	0.48
1:B:542:ALA:HB2	1:B:585:MET:HG3	1.94	0.48
5:B:701:CIT:O4	5:B:701:CIT:O7	2.30	0.48
5:D:701:CIT:O1	5:D:701:CIT:O7	2.32	0.48
1:B:630:ARG:HG3	1:B:631:VAL:N	2.27	0.48
1:C:4:ARG:HH22	1:C:43:ASP:CG	2.17	0.48
1:A:318:TYR:HB3	1:A:321:LEU:HB2	1.97	0.47
1:C:336:ASN:OD1	6:C:801:HOH:O	2.20	0.47
1:D:542:ALA:HB3	1:D:591:PHE:CD1	2.49	0.47
1:D:421:ASN:OD1	1:D:450:ALA:HB2	2.14	0.47
1:D:434:ALA:HA	1:D:460:VAL:O	2.15	0.47
1:A:585:MET:SD	1:A:588:THR:HG22	2.55	0.46
1:A:234:GLU:O	6:A:803:HOH:O	2.20	0.46
1:C:160:GLU:OE2	2:C:701:TPP:HM23	2.15	0.46
1:B:182:TYR:HB2	1:B:240:LEU:HD11	1.97	0.46
1:C:38:GLU:OE2	1:C:42:ARG:HD3	2.15	0.46
1:C:287:PRO:HG2	1:C:290:TYR:CD1	2.51	0.46
1:C:434:ALA:HA	1:C:460:VAL:O	2.14	0.46
1:A:554:LEU:HB3	1:A:580:VAL:HG22	1.97	0.45
1:D:268:GLU:H	5:D:703:CIT:C5	2.28	0.45
5:D:703:CIT:C6	6:D:829:HOH:O	2.63	0.45
1:A:282:ALA:HB3	1:A:285:GLU:HG3	1.98	0.45
1:A:38:GLU:OE2	1:A:42:ARG:HD3	2.17	0.45
1:B:186:ASN:OD1	1:B:192:HIS:HD2	2.01	0.44
1:D:585:MET:SD	1:D:588:THR:HG22	2.57	0.44
1:A:434:ALA:HA	1:A:460:VAL:O	2.17	0.44
1:D:171:GLY:HA3	1:D:208:TYR:O	2.18	0.44
1:D:286:ILE:HB	1:D:291:TYR:CE2	2.52	0.44
1:D:38:GLU:OE2	1:D:42:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:ALA:HA	1:A:652:PHE:CZ	2.53	0.44
1:B:630:ARG:NH2	1:B:663:GLU:OE1	2.40	0.44
1:C:171:GLY:HA3	1:C:208:TYR:O	2.19	0.43
2:D:702:TPP:H2	6:D:1141:HOH:O	2.17	0.43
1:B:609:LYS:HZ3	1:B:609:LYS:HG2	1.54	0.43
1:D:342:LYS:HE2	1:D:346:GLU:OE2	2.19	0.43
1:B:310:LYS:HB3	1:B:310:LYS:HE3	1.65	0.43
1:D:12:ARG:O	1:D:16:MET:HG2	2.18	0.43
1:B:281:TYR:CZ	1:B:287:PRO:HG3	2.54	0.42
1:A:306:SER:O	1:A:310:LYS:HG3	2.19	0.42
1:A:416:MET:O	1:A:420:MET:HG3	2.20	0.42
1:B:375:PHE:HD1	1:B:375:PHE:HA	1.79	0.42
1:B:434:ALA:HA	1:B:460:VAL:O	2.19	0.42
1:A:540:ARG:HD3	1:A:598:TYR:CZ	2.54	0.42
1:D:562:GLU:HB3	1:D:613:ILE:HG22	2.02	0.41
1:A:476:GLN:OE1	1:A:638:GLY:HA3	2.20	0.41
1:D:370:HIS:NE2	6:D:809:HOH:O	2.36	0.41
1:A:375:PHE:HD1	1:A:375:PHE:HA	1.77	0.41
1:A:316:LYS:HB3	1:A:316:LYS:HE3	1.87	0.41
1:B:578:LYS:HD3	1:B:665:LEU:HD13	2.03	0.41
1:A:225:ARG:NH1	1:A:229:ILE:HD11	2.35	0.41
1:C:281:TYR:CZ	1:C:287:PRO:HG3	2.55	0.41
6:C:814:HOH:O	3:D:704:EDO:H11	2.20	0.41
1:A:310:LYS:HB3	1:A:310:LYS:HE3	1.92	0.41
1:B:76:HIS:CE1	1:B:84:ILE:HG12	2.55	0.41
1:C:68:SER:HB3	1:C:101:PRO:HD3	2.02	0.41
1:A:613:ILE:HG23	1:A:632:ILE:HB	2.03	0.40
1:B:144:ILE:HG13	1:B:145:VAL:HG23	2.02	0.40
1:D:571:GLU:OE2	6:D:802:HOH:O	2.22	0.40
1:B:437:LEU:O	1:B:440:TYR:HB3	2.20	0.40
5:D:703:CIT:C6	5:D:703:CIT:O2	2.69	0.40
1:A:26:HIS:NE2	3:A:702:EDO:H22	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1211:HOH:O	6:D:1375:HOH:O[1_655]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	663/680 (98%)	649 (98%)	14 (2%)	0	100	100
1	B	665/680 (98%)	653 (98%)	12 (2%)	0	100	100
1	C	664/680 (98%)	648 (98%)	16 (2%)	0	100	100
1	D	663/680 (98%)	648 (98%)	15 (2%)	0	100	100
All	All	2655/2720 (98%)	2598 (98%)	57 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	521/535 (97%)	516 (99%)	5 (1%)	76	82
1	B	523/535 (98%)	515 (98%)	8 (2%)	65	71
1	C	522/535 (98%)	513 (98%)	9 (2%)	60	67
1	D	520/535 (97%)	515 (99%)	5 (1%)	76	82
All	All	2086/2140 (98%)	2059 (99%)	27 (1%)	69	75

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	258	HIS

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Mol	Chain	Res	Type
1	A	375	PHE
1	A	414	PHE
1	A	440	TYR
1	B	23	LYS
1	B	258	HIS
1	B	375	PHE
1	B	414	PHE
1	B	440	TYR
1	B	549	ASP
1	B	554	LEU
1	B	630	ARG
1	C	64	ASN
1	C	222	GLU
1	C	225	ARG
1	C	258	HIS
1	C	375	PHE
1	C	414	PHE
1	C	440	TYR
1	C	511	ARG
1	C	512	GLN
1	D	258	HIS
1	D	354	SER
1	D	375	PHE
1	D	414	PHE
1	D	440	TYR

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

Mol	Chain	Res	Type
1	A	94	HIS
1	A	628	ASN
1	B	192	HIS
1	B	667	ASN
1	D	94	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TPP	C	701	4	22,27,27	0.44	0	29,40,40	0.72	1 (3%)
5	CIT	D	701	-	12,12,12	1.04	0	17,17,17	1.37	2 (11%)
2	TPP	D	702	4	22,27,27	0.54	0	29,40,40	0.81	0
3	EDO	D	704	-	3,3,3	0.44	0	2,2,2	0.41	0
2	TPP	B	702	4	22,27,27	0.48	0	29,40,40	0.73	2 (6%)
5	CIT	D	703	-	12,12,12	1.14	0	17,17,17	2.18	8 (47%)
5	CIT	B	701	-	12,12,12	1.03	0	17,17,17	1.83	7 (41%)
2	TPP	A	701	4	22,27,27	0.60	0	29,40,40	0.72	0
3	EDO	A	702	-	3,3,3	0.46	0	2,2,2	0.43	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	C	701	4	-	4/16/17/17	0/2/2/2
5	CIT	D	701	-	-	10/16/16/16	-
2	TPP	D	702	4	-	7/16/17/17	0/2/2/2
3	EDO	D	704	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	B	702	4	-	4/16/17/17	0/2/2/2
5	CIT	D	703	-	-	11/16/16/16	-
5	CIT	B	701	-	-	8/16/16/16	-
2	TPP	A	701	4	-	4/16/17/17	0/2/2/2
3	EDO	A	702	-	-	0/1/1/1	-

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	701	CIT	O6-C6-C3	4.50	120.86	113.05
5	D	703	CIT	O6-C6-C3	3.97	119.94	113.05
5	D	703	CIT	O7-C3-C2	-3.87	100.34	109.40
5	D	701	CIT	O6-C6-C3	3.22	118.64	113.05
5	D	703	CIT	C2-C3-C6	3.19	116.97	110.11
5	D	703	CIT	O4-C5-O3	-3.12	115.51	123.30
5	B	701	CIT	O2-C1-O1	-2.50	117.07	123.30
5	B	701	CIT	O4-C5-O3	-2.46	117.17	123.30
5	D	703	CIT	O2-C1-C2	2.43	122.15	114.35
5	D	703	CIT	O6-C6-O5	-2.30	116.49	123.82
5	B	701	CIT	C4-C3-C2	2.26	115.07	109.16
5	B	701	CIT	O2-C1-C2	2.21	121.44	114.35
5	D	703	CIT	O4-C5-C4	2.19	121.37	114.35
5	D	703	CIT	O2-C1-O1	-2.13	117.99	123.30
5	B	701	CIT	O6-C6-O5	-2.12	117.06	123.82
2	B	702	TPP	PA-O3A-PB	2.06	139.90	132.83
5	D	701	CIT	O4-C5-C4	2.05	120.93	114.35
2	B	702	TPP	C5-C4-N3	2.05	111.67	107.57
5	B	701	CIT	O4-C5-C4	2.01	120.82	114.35
2	C	701	TPP	C5-C4-N3	2.00	111.58	107.57

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TPP	C5-C6-C7-O7
2	A	701	TPP	C7-O7-PA-O1A
2	B	702	TPP	C5-C6-C7-O7
2	B	702	TPP	C7-O7-PA-O1A
2	C	701	TPP	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
2	C	701	TPP	C7-O7-PA-O1A
2	D	702	TPP	C5-C6-C7-O7
2	D	702	TPP	C7-O7-PA-O1A
5	B	701	CIT	C2-C3-C4-C5
5	B	701	CIT	O7-C3-C4-C5
5	B	701	CIT	C6-C3-C4-C5
5	D	703	CIT	O7-C3-C6-O6
5	D	703	CIT	C4-C3-C6-O6
5	B	701	CIT	C1-C2-C3-C6
5	B	701	CIT	C1-C2-C3-C4
5	D	701	CIT	C1-C2-C3-O7
5	D	701	CIT	C1-C2-C3-C6
5	D	703	CIT	C2-C3-C4-C5
5	D	701	CIT	C4-C3-C6-O6
5	D	703	CIT	C4-C3-C6-O5
5	D	701	CIT	C1-C2-C3-C4
5	D	703	CIT	C1-C2-C3-O7
5	D	703	CIT	C2-C3-C6-O5
5	D	703	CIT	C2-C3-C6-O6
5	B	701	CIT	C1-C2-C3-O7
2	B	702	TPP	C7-O7-PA-O3A
2	D	702	TPP	C7-O7-PA-O3A
2	A	701	TPP	C7-O7-PA-O2A
2	B	702	TPP	C7-O7-PA-O2A
2	C	701	TPP	C7-O7-PA-O2A
2	D	702	TPP	C7-O7-PA-O2A
5	D	701	CIT	C2-C3-C6-O6
5	D	701	CIT	C4-C3-C6-O5
5	D	703	CIT	C1-C2-C3-C4
5	D	703	CIT	O2-C1-C2-C3
5	D	701	CIT	O7-C3-C6-O6
5	D	703	CIT	O7-C3-C6-O5
2	D	702	TPP	PA-O3A-PB-O1B
5	D	703	CIT	O1-C1-C2-C3
5	D	701	CIT	C2-C3-C4-C5
5	D	701	CIT	C2-C3-C6-O5
5	B	701	CIT	C3-C4-C5-O3
2	A	701	TPP	C7-O7-PA-O3A
2	C	701	TPP	C7-O7-PA-O3A
2	D	702	TPP	PB-O3A-PA-O1A
2	D	702	TPP	PB-O3A-PA-O2A
5	D	701	CIT	C6-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
5	B	701	CIT	C3-C4-C5-O4

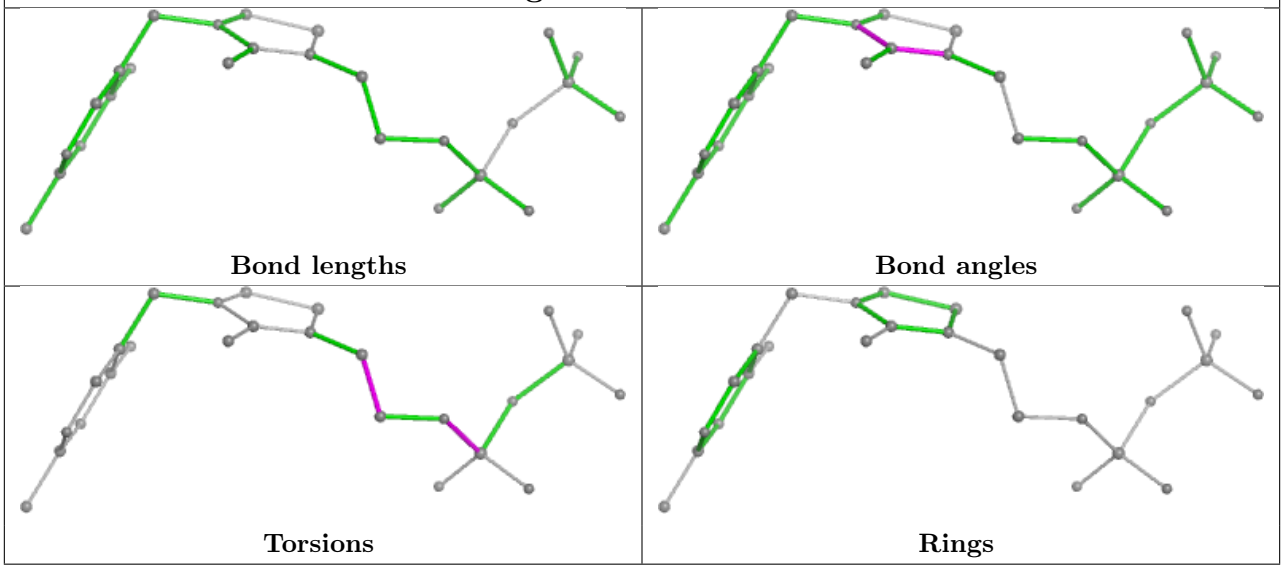
There are no ring outliers.

9 monomers are involved in 13 short contacts:

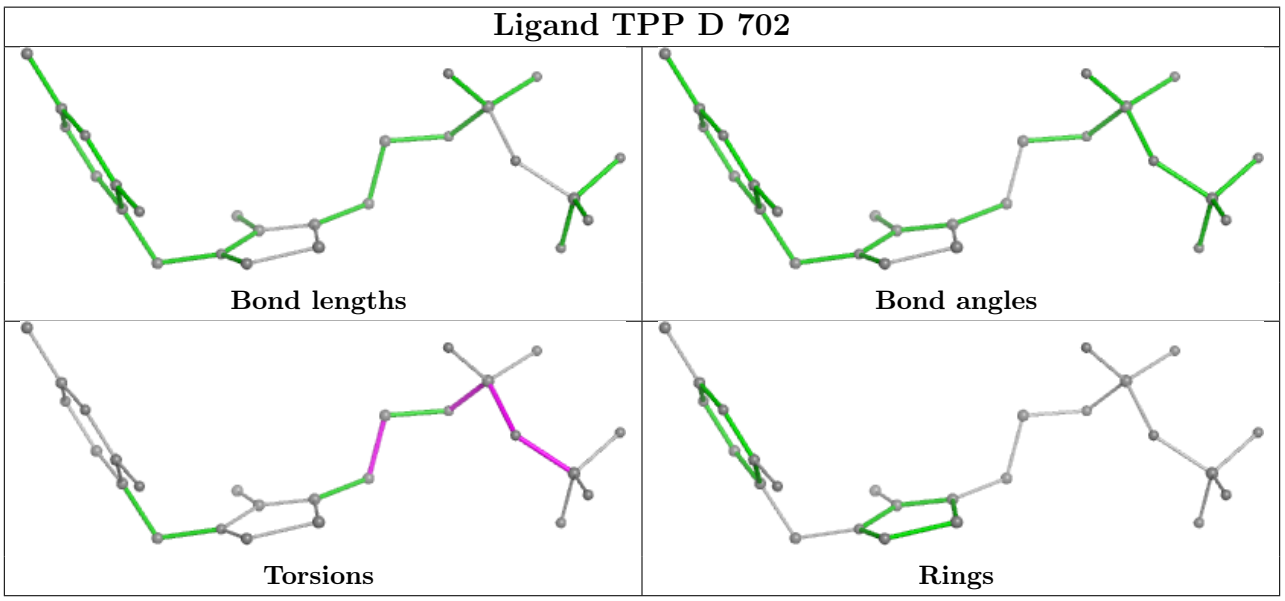
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	TPP	1	0
5	D	701	CIT	1	0
2	D	702	TPP	3	0
3	D	704	EDO	1	0
2	B	702	TPP	1	0
5	D	703	CIT	3	0
5	B	701	CIT	1	0
2	A	701	TPP	1	0
3	A	702	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

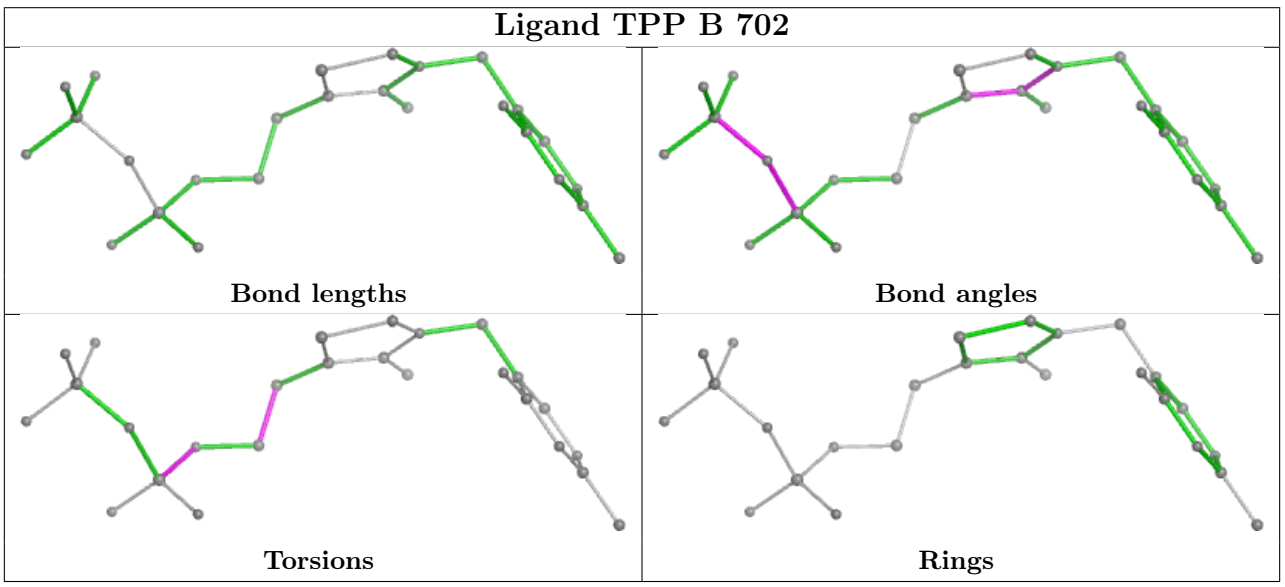
Ligand TPP C 701

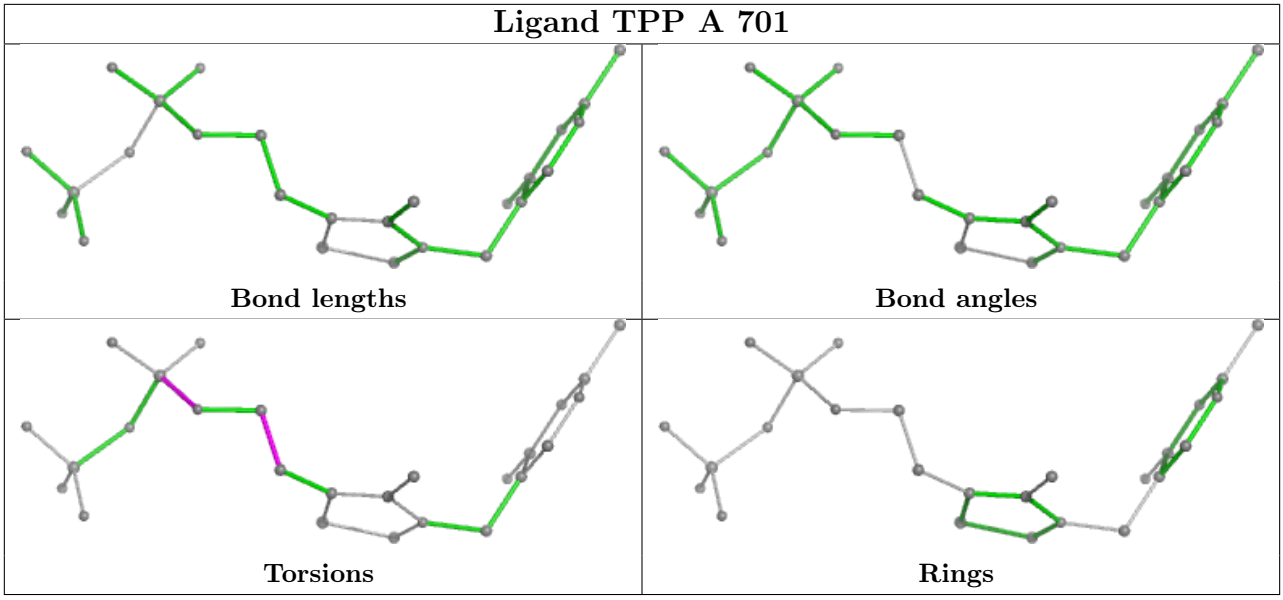


Ligand TPP D 702



Ligand TPP B 702





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	664/680 (97%)	-0.03	22 (3%)	46	53	15, 25, 41, 58	0
1	B	667/680 (98%)	-0.04	22 (3%)	46	53	15, 25, 42, 57	0
1	C	666/680 (97%)	0.01	15 (2%)	60	65	15, 24, 38, 69	0
1	D	665/680 (97%)	-0.08	13 (1%)	65	69	15, 23, 35, 58	0
All	All	2662/2720 (97%)	-0.03	72 (2%)	54	60	15, 24, 40, 69	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	667	ASN	5.3
1	A	549	ASP	4.5
1	B	549	ASP	4.5
1	C	666	GLU	4.0
1	A	550	GLY	3.9
1	C	105	TYR	3.5
1	B	575	ALA	3.4
1	D	666	GLU	3.4
1	B	268	GLU	3.4
1	C	549	ASP	3.3
1	A	575	ALA	3.3
1	C	551	THR	3.2
1	C	577	GLY	3.2
1	A	579	LYS	3.2
1	B	668	LEU	3.1
1	D	61	VAL	3.1
1	B	667	ASN	3.1
1	A	606	ALA	3.1
1	D	62	LEU	3.1
1	A	61	VAL	3.0
1	A	665	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	271	ASP	2.8
1	B	272	LEU	2.8
1	C	192	HIS	2.8
1	A	62	LEU	2.8
1	A	597	ALA	2.7
1	C	62	LEU	2.7
1	A	151	VAL	2.6
1	B	577	GLY	2.6
1	A	152	PHE	2.6
1	B	61	VAL	2.6
1	D	151	VAL	2.6
1	A	551	THR	2.6
1	C	151	VAL	2.5
1	B	259	ASP	2.5
1	C	60	PHE	2.5
1	A	574	SER	2.5
1	C	280	GLU	2.5
1	A	659	ALA	2.5
1	B	551	THR	2.4
1	D	512	GLN	2.4
1	B	258	HIS	2.4
1	A	595	ASP	2.4
1	C	194	ASP	2.3
1	D	152	PHE	2.3
1	D	549	ASP	2.3
1	D	60	PHE	2.3
1	A	399	HIS	2.3
1	A	576	GLU	2.2
1	A	60	PHE	2.2
1	D	70	LEU	2.2
1	B	253	ASN	2.1
1	B	606	ALA	2.1
1	D	597	ALA	2.1
1	C	152	PHE	2.1
1	A	596	ALA	2.1
1	B	576	GLU	2.1
1	D	280	GLU	2.1
1	B	194	ASP	2.1
1	B	263	ALA	2.1
1	D	550	GLY	2.1
1	B	188	SER	2.1
1	C	606	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	665	LEU	2.0
1	B	666	GLU	2.0
1	B	257	SER	2.0
1	B	283	PRO	2.0
1	A	70	LEU	2.0
1	A	120	ILE	2.0
1	B	267	ASP	2.0
1	A	3	THR	2.0
1	D	123	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)

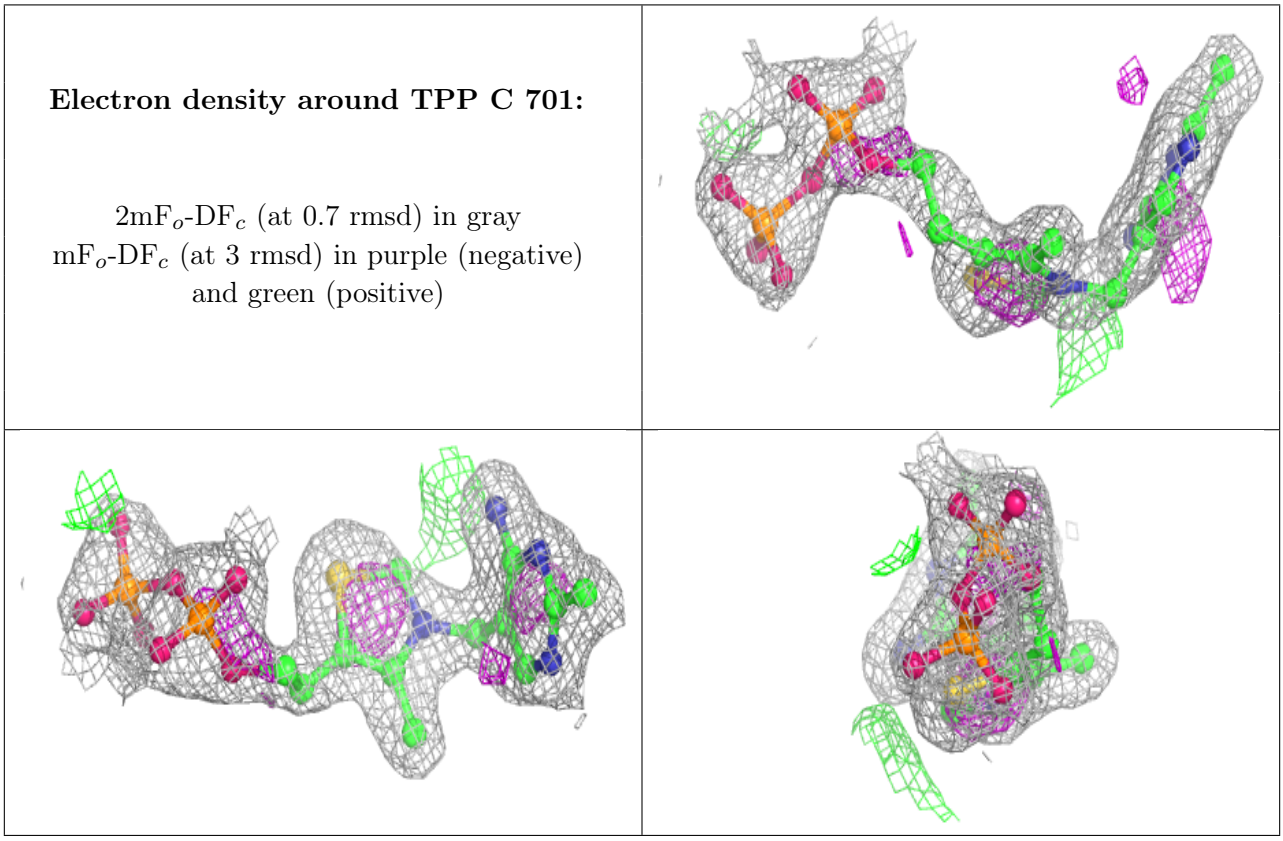
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	CIT	B	701	13/13	0.71	0.26	32,38,43,44	13
5	CIT	D	703	13/13	0.75	0.22	30,36,46,51	0
5	CIT	D	701	13/13	0.77	0.27	34,41,45,50	13
3	EDO	A	702	4/4	0.90	0.19	31,33,33,42	0
3	EDO	D	704	4/4	0.92	0.13	32,37,40,41	0
2	TPP	C	701	26/26	0.93	0.15	23,33,43,44	0
2	TPP	B	702	26/26	0.93	0.12	23,35,42,44	0
2	TPP	D	702	26/26	0.95	0.11	19,24,32,39	0
2	TPP	A	701	26/26	0.95	0.11	18,24,31,40	0
4	MG	C	702	1/1	0.96	0.14	29,29,29,29	0
4	MG	B	703	1/1	0.97	0.10	25,25,25,25	0
4	MG	D	705	1/1	0.98	0.10	21,21,21,21	0
4	MG	A	703	1/1	0.98	0.03	21,21,21,21	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.

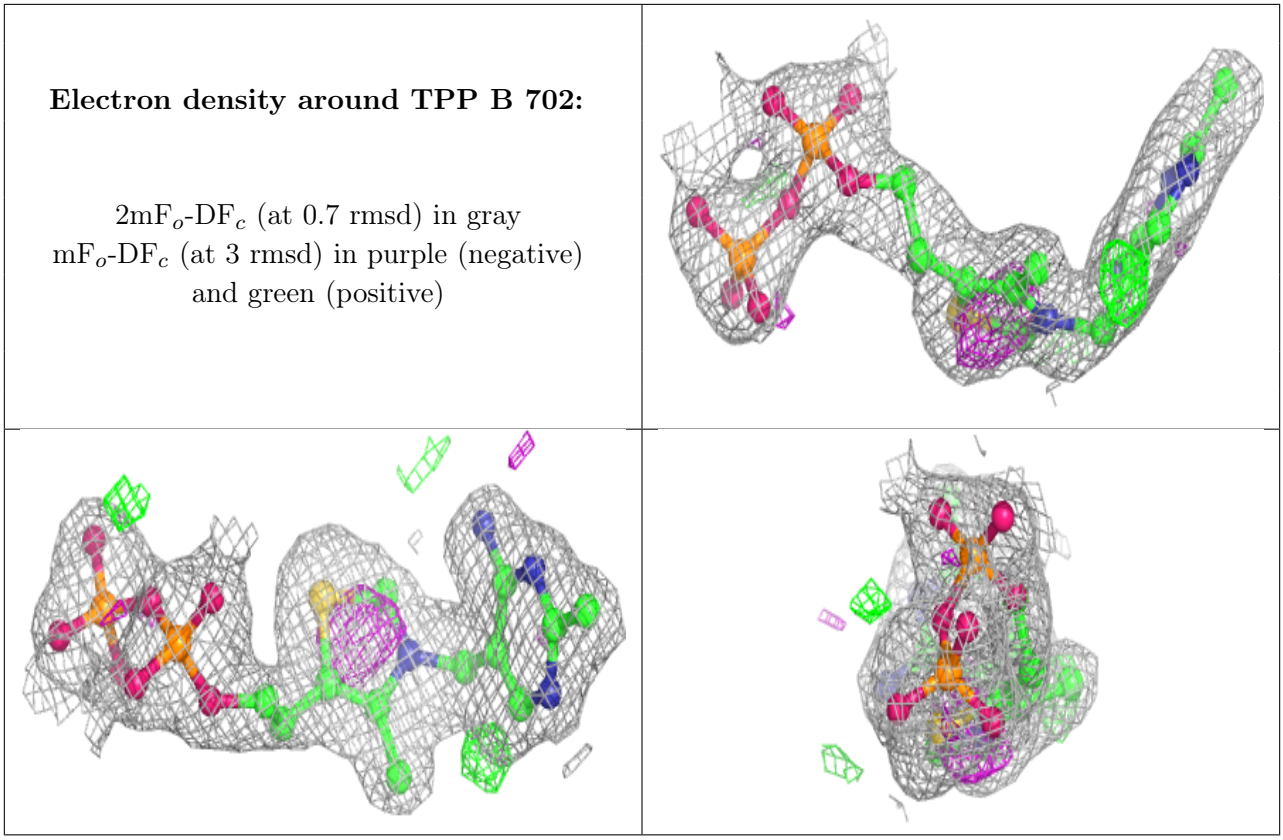
Electron density around TPP C 701:

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



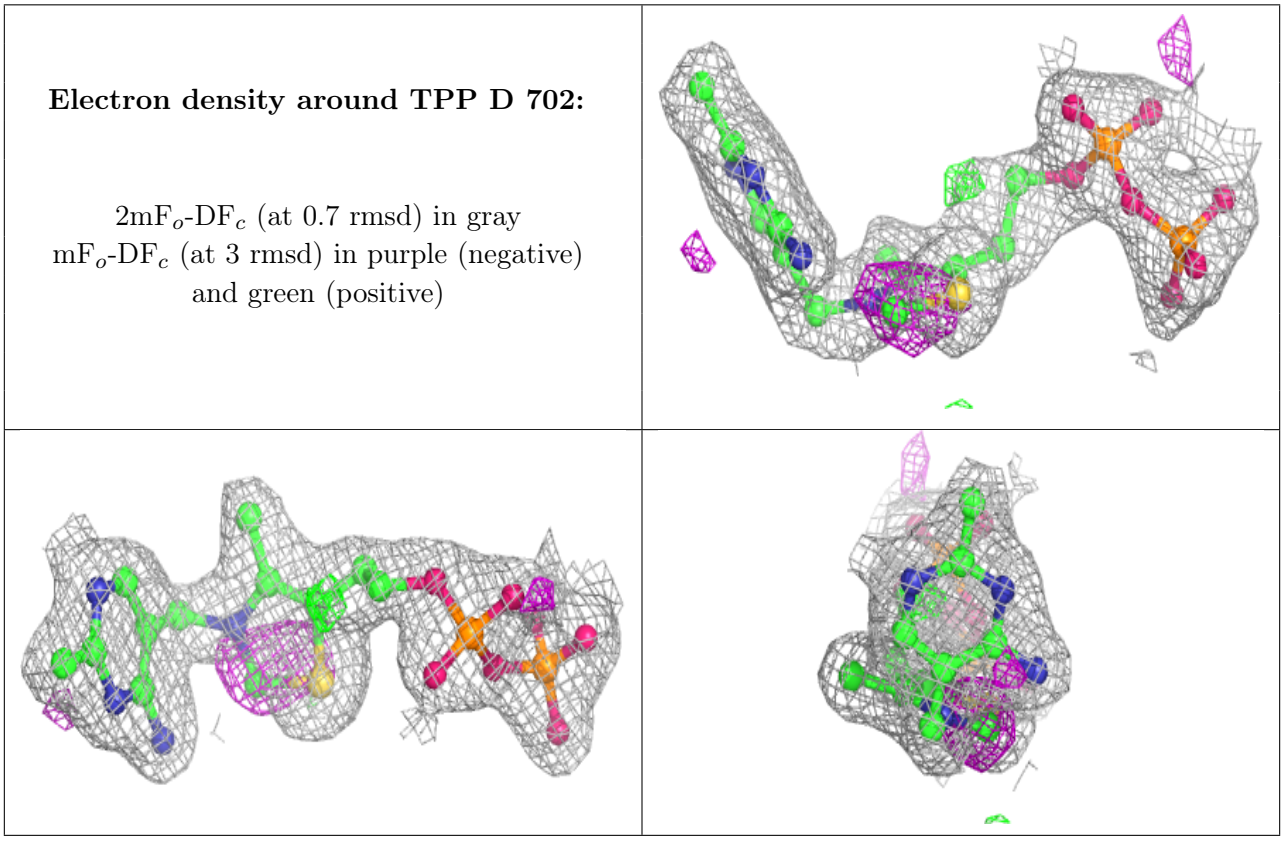
Electron density around TPP B 702:

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



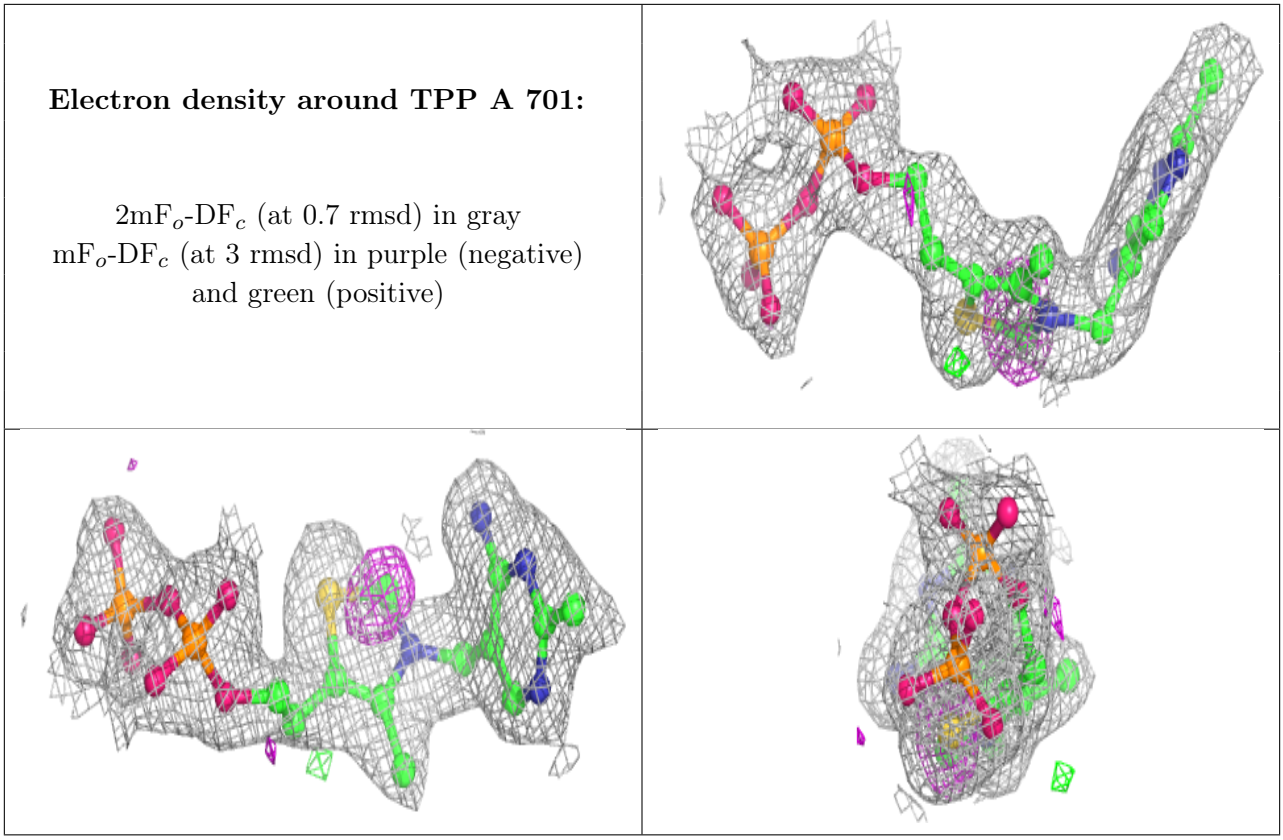
Electron density around TPP D 702:

$2mF_o$-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 701:

$2mF_o$-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.