



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:13 AM UTC

PDB ID : 8R3R / pdb_00008r3r
Title : Transketolase from Streptococcus pneumoniae 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 : 2.35 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

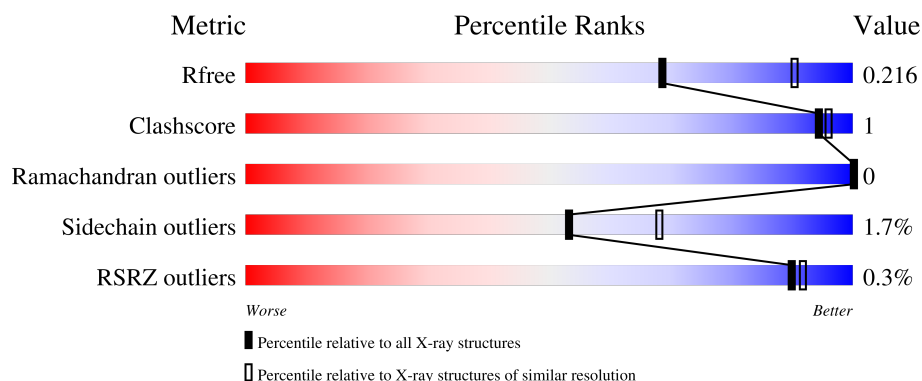
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

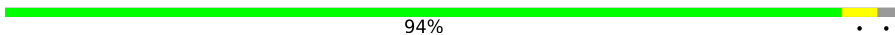
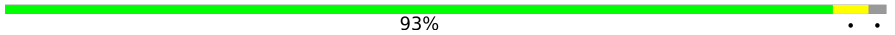
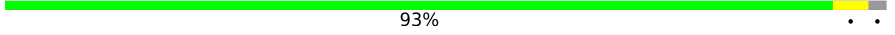
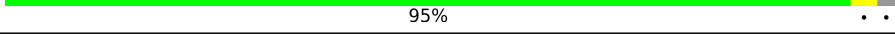
The reported resolution of this entry is 2.35 Å.

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	673	 94%
1	B	673	 93%
1	C	673	 93%
1	D	673	 95%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22537 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 Probable transketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	658	Total	C	N	O	S	0	1	0
			5023	3171	860	980	12			
1	B	658	Total	C	N	O	S	0	0	0
			5011	3164	857	978	12			
1	C	657	Total	C	N	O	S	0	0	0
			5006	3161	856	977	12			
1	D	658	Total	C	N	O	S	0	1	0
			5017	3167	858	980	12			

There are 60 discrepancies between the modelled and reference sequences:

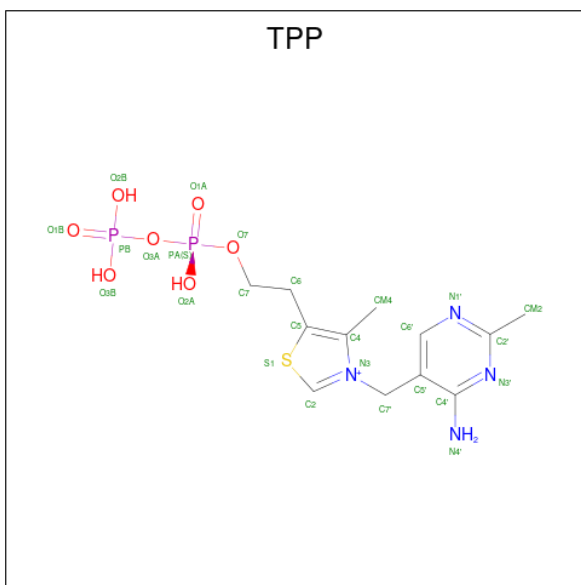
Chain	Residue	Modelled	Actual	Comment	Reference
A	659	GLU	-	expression tag	UNP P22976
A	660	ASN	-	expression tag	UNP P22976
A	661	LEU	-	expression tag	UNP P22976
A	662	TYR	-	expression tag	UNP P22976
A	663	PHE	-	expression tag	UNP P22976
A	664	GLN	-	expression tag	UNP P22976
A	665	GLY	-	expression tag	UNP P22976
A	666	LEU	-	expression tag	UNP P22976
A	667	GLU	-	expression tag	UNP P22976
A	668	HIS	-	expression tag	UNP P22976
A	669	HIS	-	expression tag	UNP P22976
A	670	HIS	-	expression tag	UNP P22976
A	671	HIS	-	expression tag	UNP P22976
A	672	HIS	-	expression tag	UNP P22976
A	673	HIS	-	expression tag	UNP P22976
B	659	GLU	-	expression tag	UNP P22976
B	660	ASN	-	expression tag	UNP P22976
B	661	LEU	-	expression tag	UNP P22976
B	662	TYR	-	expression tag	UNP P22976
B	663	PHE	-	expression tag	UNP P22976
B	664	GLN	-	expression tag	UNP P22976

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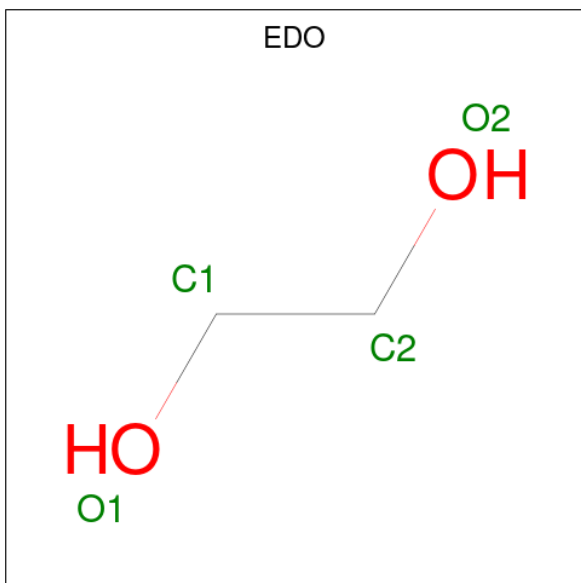
Chain	Residue	Modelled	Actual	Comment	Reference
B	665	GLY	-	expression tag	UNP P22976
B	666	LEU	-	expression tag	UNP P22976
B	667	GLU	-	expression tag	UNP P22976
B	668	HIS	-	expression tag	UNP P22976
B	669	HIS	-	expression tag	UNP P22976
B	670	HIS	-	expression tag	UNP P22976
B	671	HIS	-	expression tag	UNP P22976
B	672	HIS	-	expression tag	UNP P22976
B	673	HIS	-	expression tag	UNP P22976
C	659	GLU	-	expression tag	UNP P22976
C	660	ASN	-	expression tag	UNP P22976
C	661	LEU	-	expression tag	UNP P22976
C	662	TYR	-	expression tag	UNP P22976
C	663	PHE	-	expression tag	UNP P22976
C	664	GLN	-	expression tag	UNP P22976
C	665	GLY	-	expression tag	UNP P22976
C	666	LEU	-	expression tag	UNP P22976
C	667	GLU	-	expression tag	UNP P22976
C	668	HIS	-	expression tag	UNP P22976
C	669	HIS	-	expression tag	UNP P22976
C	670	HIS	-	expression tag	UNP P22976
C	671	HIS	-	expression tag	UNP P22976
C	672	HIS	-	expression tag	UNP P22976
C	673	HIS	-	expression tag	UNP P22976
D	659	GLU	-	expression tag	UNP P22976
D	660	ASN	-	expression tag	UNP P22976
D	661	LEU	-	expression tag	UNP P22976
D	662	TYR	-	expression tag	UNP P22976
D	663	PHE	-	expression tag	UNP P22976
D	664	GLN	-	expression tag	UNP P22976
D	665	GLY	-	expression tag	UNP P22976
D	666	LEU	-	expression tag	UNP P22976
D	667	GLU	-	expression tag	UNP P22976
D	668	HIS	-	expression tag	UNP P22976
D	669	HIS	-	expression tag	UNP P22976
D	670	HIS	-	expression tag	UNP P22976
D	671	HIS	-	expression tag	UNP P22976
D	672	HIS	-	expression tag	UNP P22976
D	673	HIS	-	expression tag	UNP P22976

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: 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

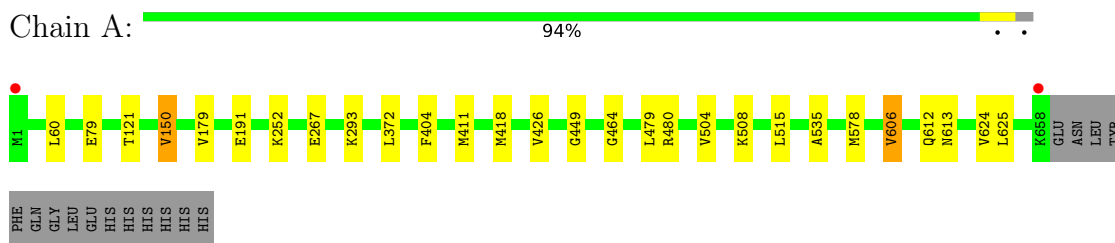
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	610	Total O 610 610	0	0
5	B	568	Total O 568 568	0	0
5	C	539	Total O 539 539	0	0
5	D	647	Total O 647 647	0	0

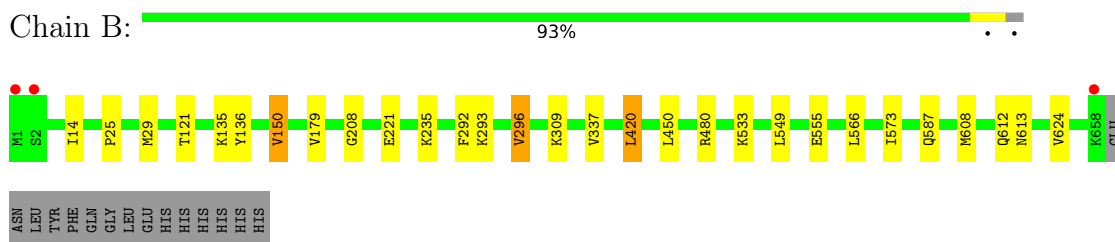
3 Residue-property plots [i](#)

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.

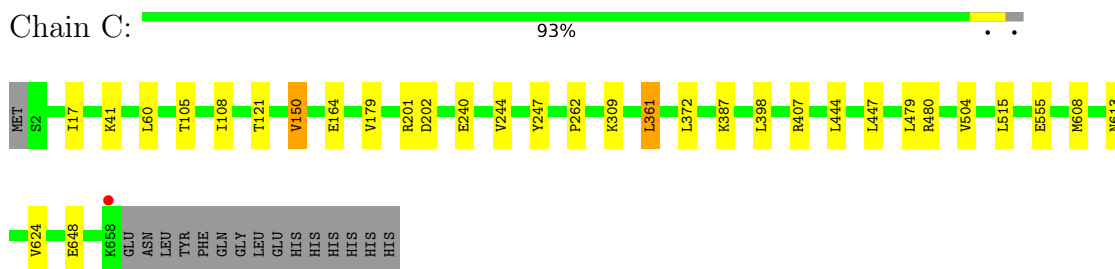
- Molecule 1: Probable transketolase



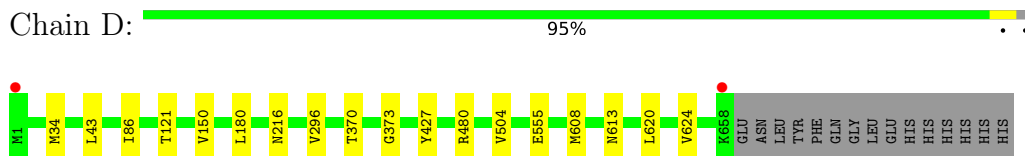
- Molecule 1: Probable transketolase



- Molecule 1: Probable transketolase



- Molecule 1: Probable transketolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.76Å 119.13Å 136.68Å 90.00° 106.46° 90.00°	Depositor
Resolution (Å)	34.05 – 2.35 34.05 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (34.05-2.35) 98.5 (34.05-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.154 , 0.216 0.154 , 0.216	Depositor DCC
R_{free} test set	5905 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.4	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	0.94	EDS
Total number of atoms	22537	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.54% 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: EDO, TPP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/5133	0.58	1/6982 (0.0%)
1	B	0.52	0/5121	0.57	0/6967
1	C	0.50	0/5116	0.56	1/6960 (0.0%)
1	D	0.52	0/5127	0.57	0/6975
All	All	0.52	0/20497	0.57	2/27884 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	361	LEU	CA-CB-CG	6.21	138.02	116.30
1	A	464	GLY	N-CA-C	5.23	116.48	111.67

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	5023	0	4869	14	0
1	B	5011	0	4853	17	0
1	C	5006	0	4848	12	0
1	D	5017	0	4857	7	0
2	A	26	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	26	0	16	0	0
2	C	26	0	16	1	0
2	D	26	0	16	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	610	0	0	2	0
5	B	568	0	0	3	0
5	C	539	0	0	2	0
5	D	647	0	0	0	0
All	All	22537	0	19503	52	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 1.

All (52) 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:79:GLU:H	1:A:79:GLU:CD	1.96	0.74
1:A:449:GLY:O	1:A:508:LYS:HD3	1.91	0.71
1:A:480:ARG:HH11	1:A:613:ASN:HD21	1.42	0.67
1:B:221:GLU:OE1	5:B:801:HOH:O	2.13	0.66
1:C:480:ARG:HH11	1:C:613:ASN:HD21	1.43	0.66
1:D:34:MET:CE	1:D:180:LEU:HB3	2.25	0.66
1:C:41:LYS:NZ	5:C:802:HOH:O	2.28	0.64
1:D:34:MET:HE2	1:D:180:LEU:HB3	1.80	0.64
2:A:701:TPP:H2	2:A:701:TPP:HN42	1.69	0.58
1:D:480:ARG:HH11	1:D:613:ASN:HD21	1.52	0.56
1:B:25:PRO:O	1:B:29:MET:HG3	2.08	0.52
1:C:105:THR:HB	1:C:108:ILE:HD12	1.92	0.52
1:B:150:VAL:CG1	1:B:179:VAL:HG22	2.41	0.51
1:C:244:VAL:HG13	1:C:247:TYR:HB2	1.93	0.50
2:C:701:TPP:HN42	2:C:701:TPP:H2	1.75	0.50
1:D:216:ASN:C	1:D:216:ASN:HD22	2.19	0.50
1:C:17:ILE:HG22	1:C:262:PRO:HB3	1.94	0.50
1:B:420:LEU:HD13	1:B:450:LEU:HD21	1.93	0.50
1:B:208:GLY:O	1:B:235:LYS:HD2	2.13	0.49
1:A:150:VAL:HG13	1:A:179:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:VAL:HG12	5:B:1076:HOH:O	2.12	0.49
1:A:191:GLU:HG3	5:A:943:HOH:O	2.12	0.48
1:A:252:LYS:HE2	1:A:267:GLU:HG2	1.94	0.48
1:C:201:ARG:NH1	1:C:240:GLU:OE1	2.44	0.48
1:B:14:ILE:HD11	1:B:29:MET:HE3	1.96	0.48
1:A:612:GLN:NE2	1:B:612:GLN:OE1	2.47	0.47
2:A:701:TPP:HN42	2:A:701:TPP:C2	2.29	0.46
1:C:648:GLU:OE1	1:C:648:GLU:N	2.31	0.45
1:D:555:GLU:CD	1:D:608:MET:HG3	2.42	0.44
1:B:533:LYS:HD3	1:B:587:GLN:OE1	2.17	0.44
1:D:480:ARG:NH1	1:D:613:ASN:HD21	2.15	0.44
1:A:293:LYS:HD3	5:A:1274:HOH:O	2.17	0.44
1:C:202:ASP:OD2	5:C:801:HOH:O	2.21	0.44
1:B:135:LYS:HG2	1:B:136:TYR:CD2	2.52	0.44
1:D:373:GLY:HA3	1:D:427:TYR:CE1	2.53	0.44
1:C:309:LYS:O	1:C:309:LYS:HD3	2.18	0.43
1:B:292:PHE:O	1:B:296:VAL:HG13	2.18	0.43
1:A:480:ARG:NH1	1:A:613:ASN:HD21	2.11	0.43
1:B:293:LYS:HE3	1:B:293:LYS:HB2	1.77	0.42
1:B:549:LEU:HG	1:B:573:ILE:HD11	2.02	0.42
1:A:606:VAL:HG13	1:A:625:LEU:HD23	2.02	0.41
1:A:535:ALA:HB2	1:A:578:MET:HG3	2.02	0.41
1:B:309:LYS:NZ	5:B:815:HOH:O	2.52	0.41
1:C:150:VAL:HG22	1:C:179:VAL:HG13	2.02	0.41
1:A:404:PHE:CD2	1:A:411:MET:HG3	2.56	0.41
1:B:555:GLU:CD	1:B:608:MET:HG3	2.46	0.41
1:B:135:LYS:HG2	1:B:136:TYR:CE2	2.56	0.41
1:C:555:GLU:CD	1:C:608:MET:HG3	2.46	0.41
1:A:418:MET:HE3	1:A:426:VAL:HG11	2.03	0.41
1:B:480:ARG:HH11	1:B:613:ASN:HD21	1.67	0.41
1:A:372:LEU:O	1:A:426:VAL:HA	2.21	0.40
1:C:164:GLU:HB3	1:C:407:ARG:HD3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	657/673 (98%)	636 (97%)	21 (3%)	0	100	100
1	B	656/673 (98%)	633 (96%)	23 (4%)	0	100	100
1	C	655/673 (97%)	636 (97%)	19 (3%)	0	100	100
1	D	657/673 (98%)	643 (98%)	14 (2%)	0	100	100
All	All	2625/2692 (98%)	2548 (97%)	77 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	518/532 (97%)	510 (98%)	8 (2%)	57	72
1	B	516/532 (97%)	510 (99%)	6 (1%)	63	77
1	C	516/532 (97%)	503 (98%)	13 (2%)	42	55
1	D	517/532 (97%)	508 (98%)	9 (2%)	53	68
All	All	2067/2128 (97%)	2031 (98%)	36 (2%)	53	68

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LEU
1	A	121	THR
1	A	150	VAL
1	A	479	LEU
1	A	504	VAL
1	A	515	LEU
1	A	606	VAL
1	A	624	VAL

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Mol	Chain	Res	Type
1	B	121	THR
1	B	150	VAL
1	B	296	VAL
1	B	420	LEU
1	B	566	LEU
1	B	624	VAL
1	C	60	LEU
1	C	121	THR
1	C	150	VAL
1	C	361	LEU
1	C	372	LEU
1	C	387	LYS
1	C	398	LEU
1	C	444	LEU
1	C	447	LEU
1	C	479	LEU
1	C	504	VAL
1	C	515	LEU
1	C	624	VAL
1	D	43	LEU
1	D	86	ILE
1	D	121	THR
1	D	150	VAL
1	D	296	VAL
1	D	370	THR
1	D	504	VAL
1	D	620	LEU
1	D	624	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	GLN
1	A	358	GLN
1	A	382	ASN
1	A	612	GLN
1	A	613	ASN
1	B	44	HIS
1	B	355	ASN
1	B	382	ASN
1	B	396	ASN
1	B	475	HIS

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Mol	Chain	Res	Type
1	B	569	GLN
1	B	612	GLN
1	B	613	ASN
1	C	187	ASN
1	C	470	HIS
1	C	497	GLN
1	C	519	ASN
1	C	613	ASN
1	D	216	ASN
1	D	305	GLN
1	D	358	GLN
1	D	382	ASN
1	D	587	GLN
1	D	613	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	D	701	4	26,27,27	0.75	1 (3%)	38,40,40	0.38	0
3	EDO	B	701	-	3,3,3	0.46	0	2,2,2	0.34	0
2	TPP	C	701	4	26,27,27	0.48	0	38,40,40	0.36	0
3	EDO	A	702	-	3,3,3	0.38	0	2,2,2	0.38	0
2	TPP	B	702	4	26,27,27	0.53	0	38,40,40	0.38	0
2	TPP	A	701	4	26,27,27	0.46	0	38,40,40	0.35	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	D	701	4	-	7/17/17/17	0/2/2/2
3	EDO	B	701	-	-	1/1/1/1	-
2	TPP	C	701	4	-	5/17/17/17	0/2/2/2
3	EDO	A	702	-	-	1/1/1/1	-
2	TPP	B	702	4	-	4/17/17/17	0/2/2/2
2	TPP	A	701	4	-	7/17/17/17	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	TPP	PA-O3A	-3.37	1.55	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TPP	C7-O7-PA-O1A
2	A	701	TPP	C7-O7-PA-O3A
2	B	702	TPP	C5-C6-C7-O7
2	B	702	TPP	C7-O7-PA-O1A
2	B	702	TPP	C7-O7-PA-O2A
2	B	702	TPP	C7-O7-PA-O3A
2	C	701	TPP	C5-C6-C7-O7
2	C	701	TPP	C7-O7-PA-O1A
2	C	701	TPP	C7-O7-PA-O3A
2	D	701	TPP	C5-C6-C7-O7

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Mol	Chain	Res	Type	Atoms
2	D	701	TPP	C7-O7-PA-O1A
2	D	701	TPP	C7-O7-PA-O3A
3	A	702	EDO	O1-C1-C2-O2
2	A	701	TPP	PB-O3A-PA-O1A
2	D	701	TPP	PB-O3A-PA-O1A
3	B	701	EDO	O1-C1-C2-O2
2	A	701	TPP	C5-C6-C7-O7
2	A	701	TPP	C7-O7-PA-O2A
2	C	701	TPP	C7-O7-PA-O2A
2	D	701	TPP	C7-O7-PA-O2A
2	D	701	TPP	PB-O3A-PA-O2A
2	A	701	TPP	PB-O3A-PA-O2A
2	D	701	TPP	PA-O3A-PB-O2B
2	A	701	TPP	C5'-C7'-N3-C2
2	C	701	TPP	C5'-C7'-N3-C2

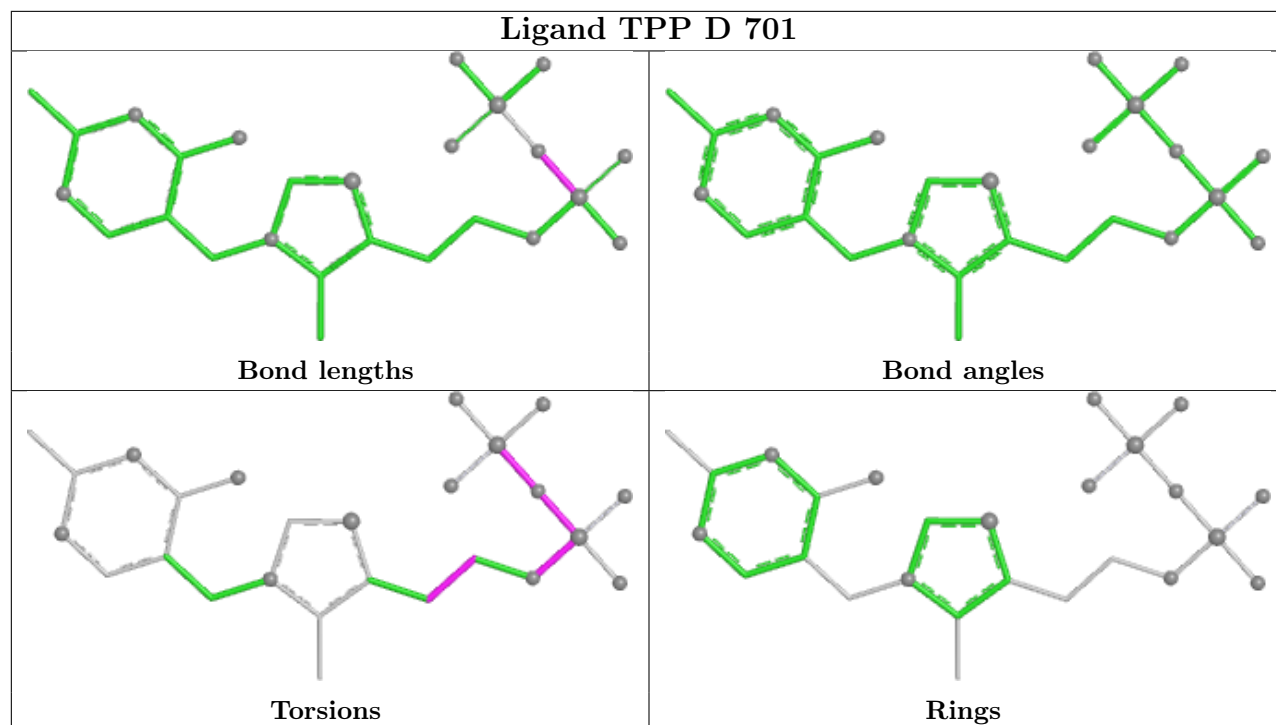
There are no ring outliers.

2 monomers are involved in 3 short contacts:

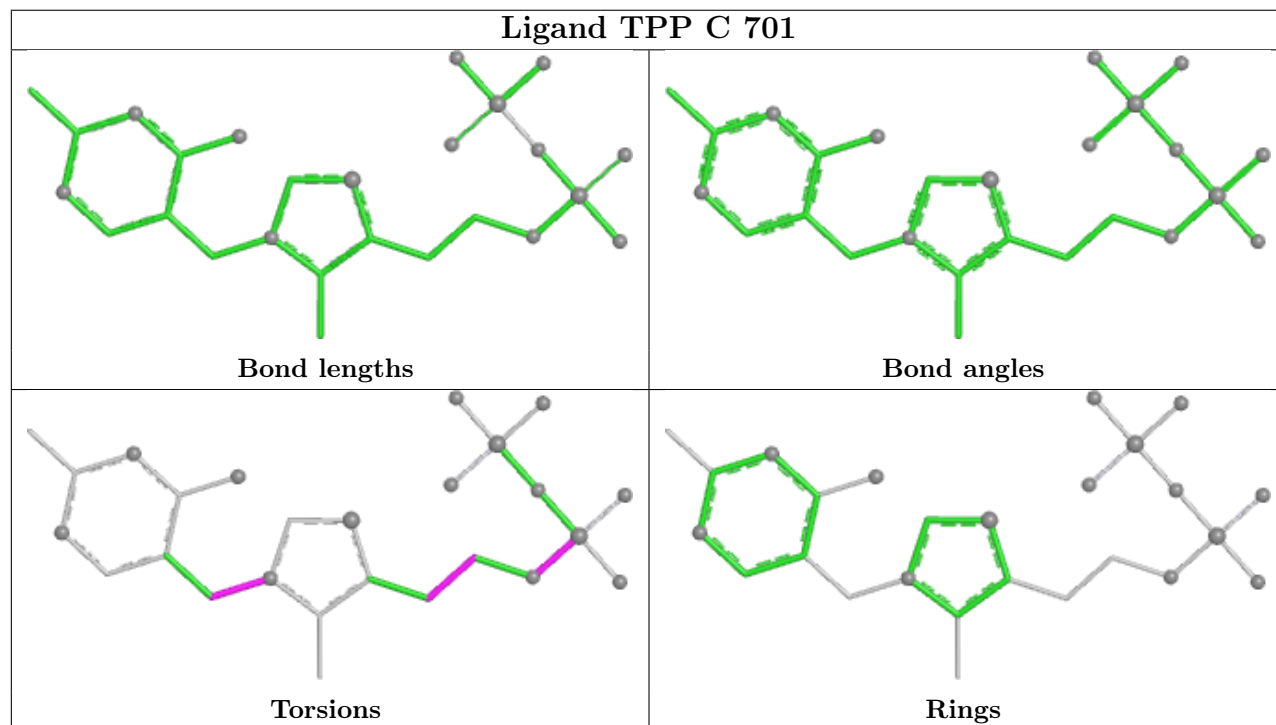
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	TPP	1	0
2	A	701	TPP	2	0

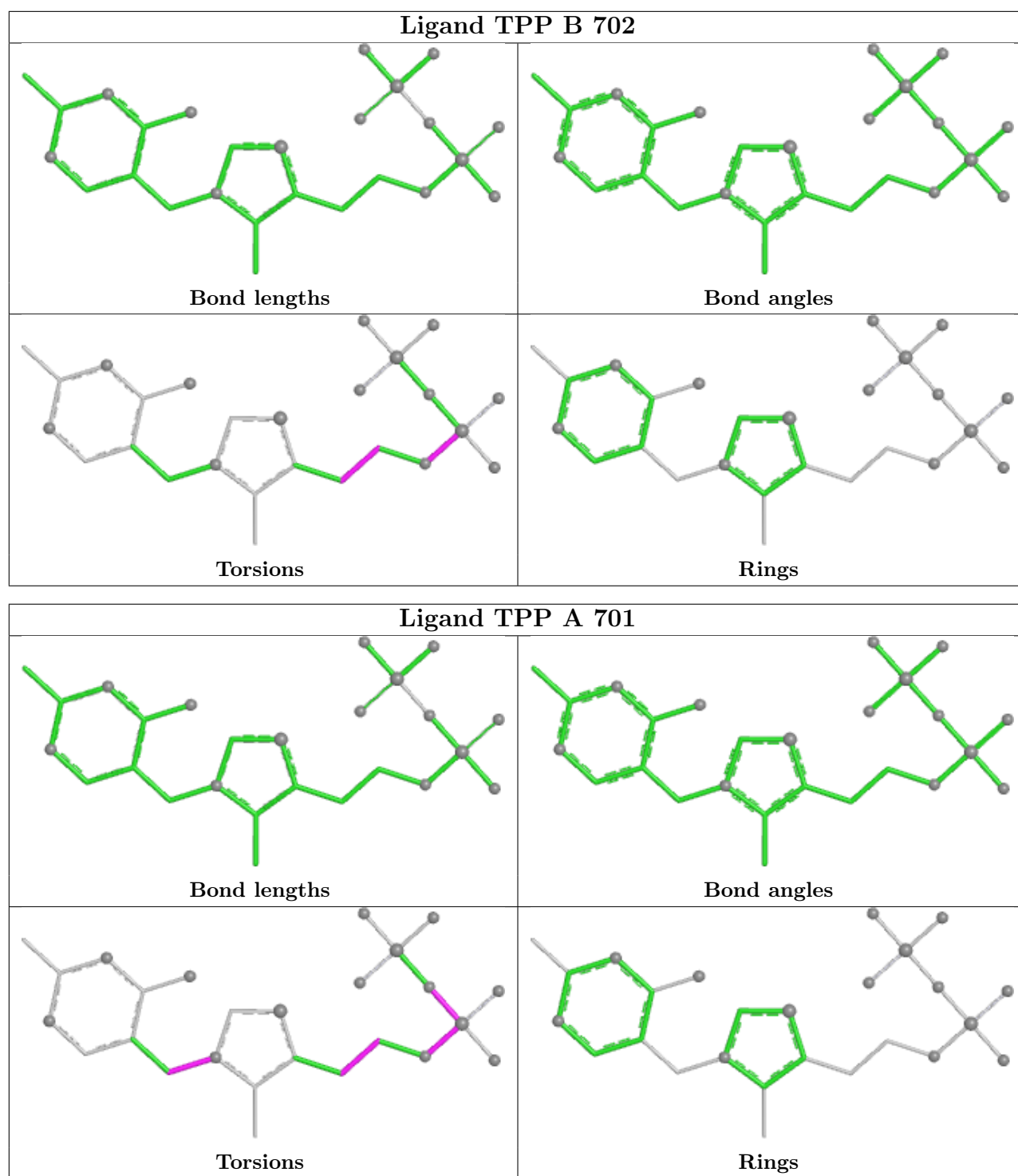
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand TPP D 701



Ligand TPP C 701





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	658/673 (97%)	-0.63	2 (0%) 90 92	8, 14, 24, 63	1 (0%)
1	B	658/673 (97%)	-0.59	3 (0%) 87 90	8, 14, 26, 58	0
1	C	657/673 (97%)	-0.59	1 (0%) 91 92	8, 15, 27, 59	0
1	D	658/673 (97%)	-0.60	2 (0%) 90 92	8, 14, 25, 66	1 (0%)
All	All	2631/2692 (97%)	-0.60	8 (0%) 90 92	8, 14, 26, 66	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	4.6
1	B	658	LYS	3.9
1	D	658	LYS	3.8
1	A	1	MET	3.6
1	A	658	LYS	2.7
1	D	1	MET	2.3
1	C	658	LYS	2.2
1	B	2	SER	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

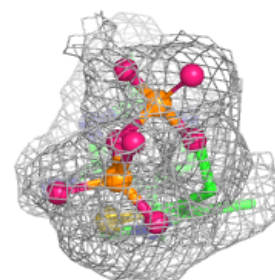
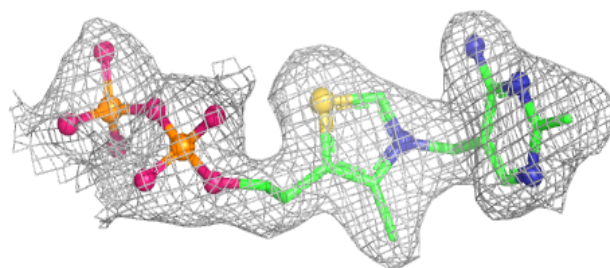
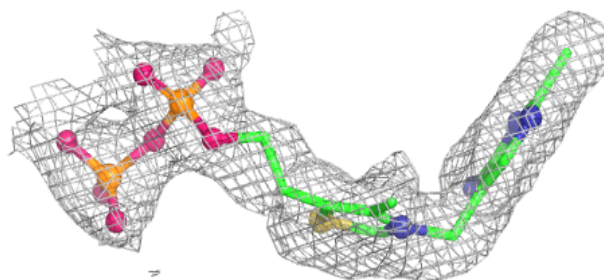
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	701	4/4	0.79	0.20	47,47,47,48	0
3	EDO	A	702	4/4	0.90	0.15	47,47,48,48	0
2	TPP	B	702	26/26	0.97	0.06	10,17,24,25	0
2	TPP	C	701	26/26	0.97	0.06	10,17,21,24	0
4	MG	A	703	1/1	0.97	0.03	11,11,11,11	0
2	TPP	D	701	26/26	0.98	0.06	10,16,22,26	0
2	TPP	A	701	26/26	0.98	0.06	5,15,20,24	0
4	MG	B	703	1/1	0.99	0.04	12,12,12,12	0
4	MG	C	702	1/1	0.99	0.04	11,11,11,11	0
4	MG	D	702	1/1	1.00	0.04	8,8,8,8	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.

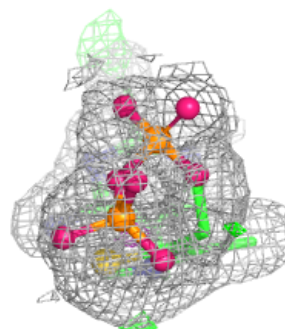
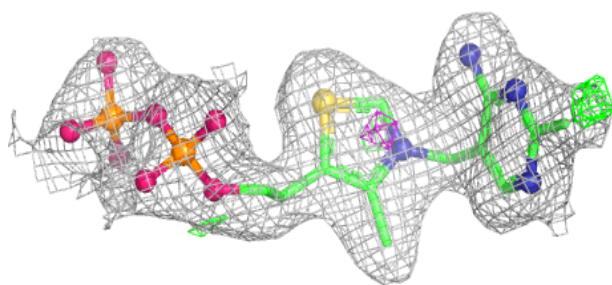
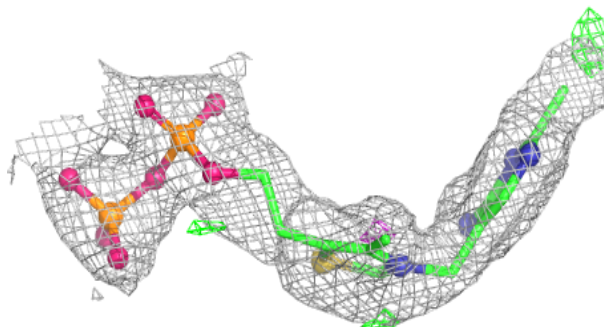
Electron density around TPP B 702:

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

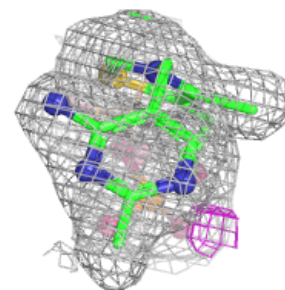
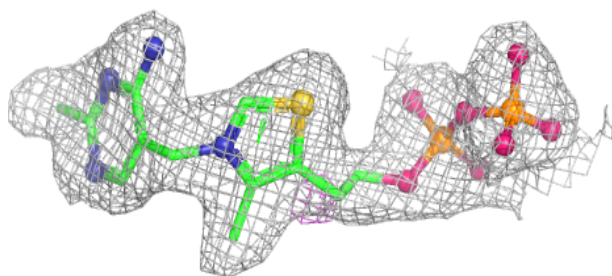
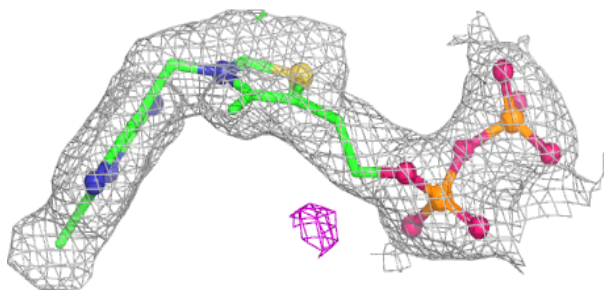


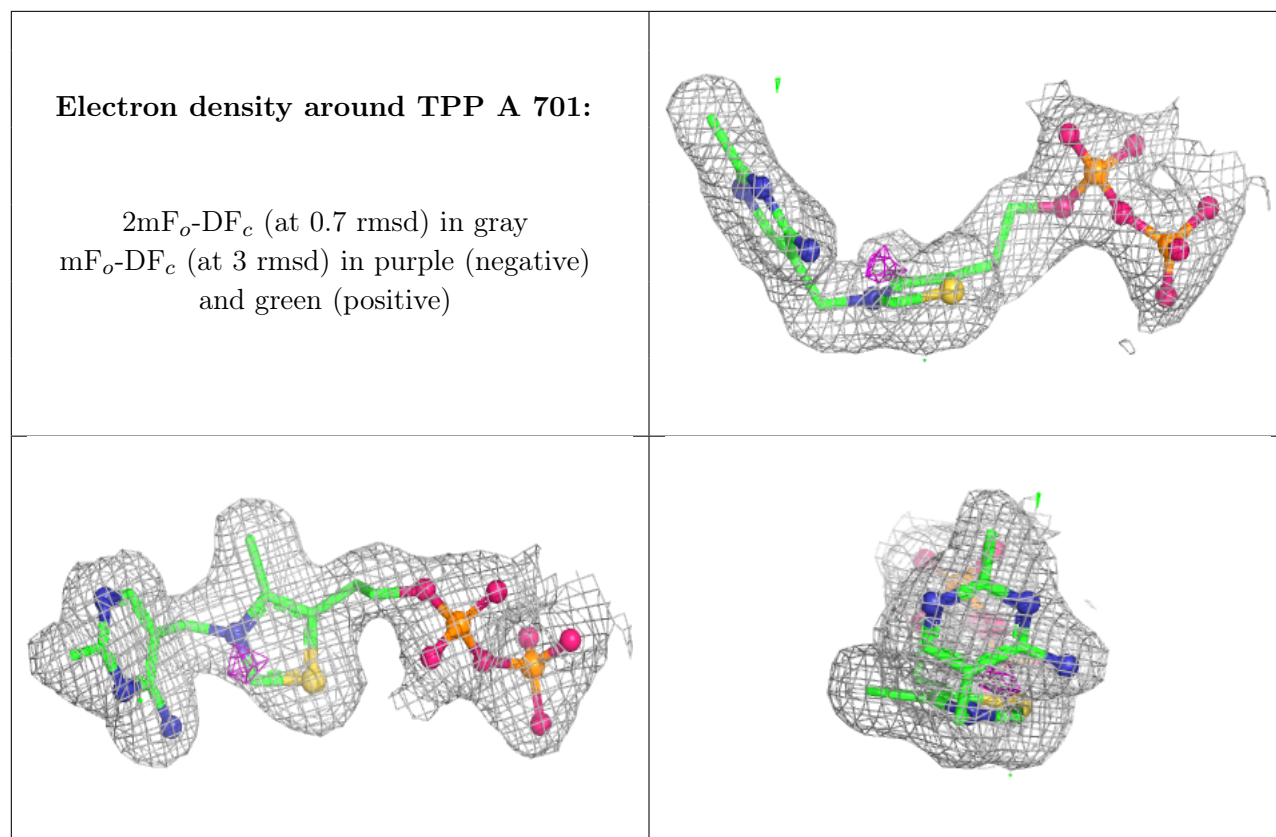
Electron density around TPP C 701:

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

**Electron density around TPP D 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.