



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:37 PM UTC

PDB ID : 5HHT / pdb_00005hht
Title : Crystal structure of E. coli transketolase triple variant Ser385Tyr/Asp469Thr /Arg520Gln
Authors : Dai, S.; Tittmann, K.
Deposited on : 2016-01-11
Resolution : 1.50 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

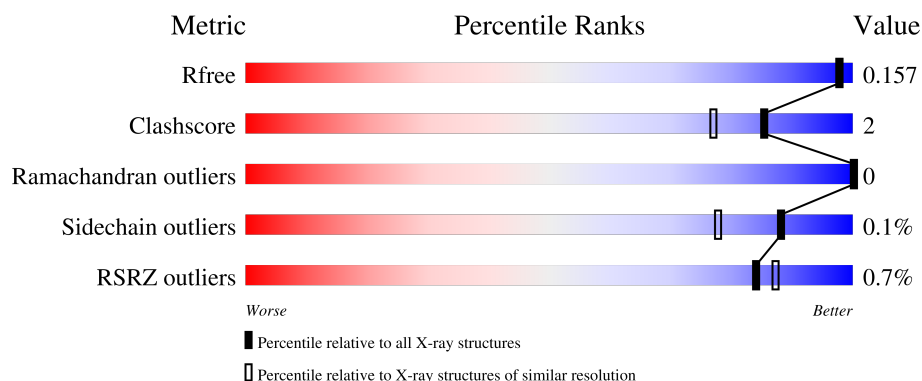
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

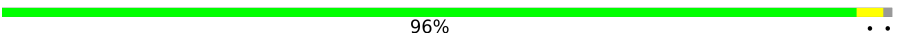
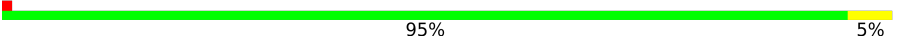
The reported resolution of this entry is 1.50 Å.

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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	669	 96%
1	B	669	 95% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12313 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	17	0
			5161	3275	878	980	28			
1	B	667	Total	C	N	O	S	0	16	0
			5204	3303	888	981	32			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	TYR	SER	engineered mutation	UNP P27302
A	469	THR	ASP	engineered mutation	UNP P27302
A	520	GLN	ARG	engineered mutation	UNP P27302
A	664	HIS	-	expression tag	UNP P27302
A	665	HIS	-	expression tag	UNP P27302
A	666	HIS	-	expression tag	UNP P27302
A	667	HIS	-	expression tag	UNP P27302
A	668	HIS	-	expression tag	UNP P27302
A	669	HIS	-	expression tag	UNP P27302
B	385	TYR	SER	engineered mutation	UNP P27302
B	469	THR	ASP	engineered mutation	UNP P27302
B	520	GLN	ARG	engineered mutation	UNP P27302
B	664	HIS	-	expression tag	UNP P27302
B	665	HIS	-	expression tag	UNP P27302
B	666	HIS	-	expression tag	UNP P27302
B	667	HIS	-	expression tag	UNP P27302
B	668	HIS	-	expression tag	UNP P27302
B	669	HIS	-	expression tag	UNP P27302

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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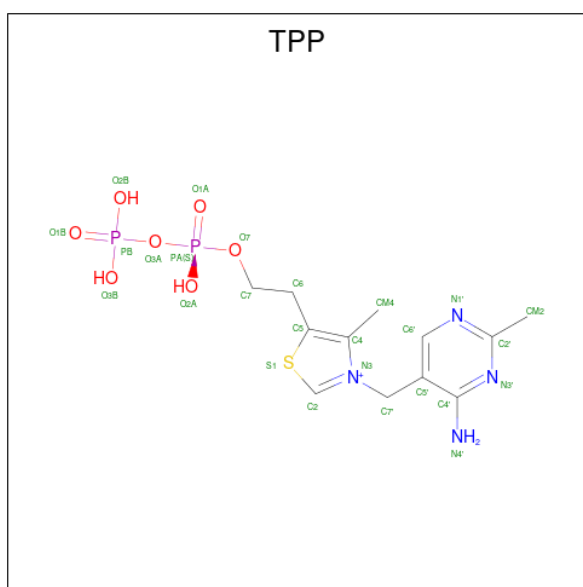
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (CCD ID: 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		

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



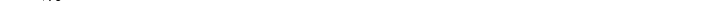
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

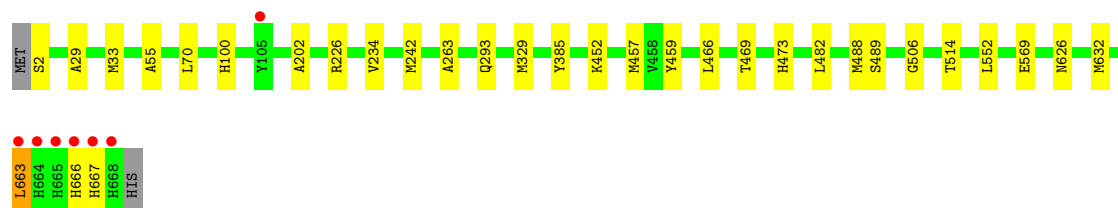
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	885	Total	O	0	0
			885	885		
5	B	865	Total	O	0	0
			865	865		

- Molecule 1: Transketolase 1



- Chain B:  95% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.94Å 102.04Å 133.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.38 – 1.50 44.38 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.38-1.50) 97.7 (44.38-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.31 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.126 , 0.157 0.127 , 0.157	Depositor DCC
R_{free} test set	9625 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	7.8	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12313	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: TPP, CA, 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	0.74	1/5329 (0.0%)	0.85	0/7221
1	B	0.75	0/5377	0.86	1/7287 (0.0%)
All	All	0.74	1/10706 (0.0%)	0.86	1/14508 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	MET	SD-CE	-6.31	1.63	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	663	LEU	N-CA-C	-7.89	102.56	112.90

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	5161	0	5069	21	0
1	B	5204	0	5100	32	0
2	A	60	0	89	4	0
2	B	84	0	125	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	26	0	16	0	0
4	B	26	0	16	0	0
5	A	885	0	0	4	3
5	B	865	0	0	6	2
All	All	12313	0	10415	45	3

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 (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ALA:HB3	2:B:721:EDO:H11	1.55	0.88
1:B:2:SER:N	5:B:801:HOH:O	2.09	0.85
1:A:100[B]:HIS:HE1	1:B:473:HIS:CE1	2.03	0.75
1:A:336:ASP:OD2	1:A:340:LYS:NZ	2.20	0.74
1:B:55:ALA:HB2	2:B:720:EDO:H22	1.69	0.73
1:A:29:ALA:HB1	1:A:33[B]:MET:HE2	1.75	0.69
1:A:100[B]:HIS:CE1	1:B:473:HIS:CE1	2.83	0.66
1:A:100[A]:HIS:HE1	1:B:469:THR:HG23	1.62	0.64
1:B:506:GLY:HA2	1:B:514[B]:THR:HG21	1.79	0.64
1:B:569[B]:GLU:OE1	5:B:803:HOH:O	2.15	0.63
1:A:473:HIS:CE1	1:B:100[B]:HIS:HE1	2.17	0.62
1:B:663:LEU:O	1:B:667:HIS:ND1	2.33	0.61
1:A:100[A]:HIS:CE1	1:B:469:THR:HG23	2.38	0.58
1:B:329:MET:HB3	2:B:720:EDO:H12	1.86	0.57
1:B:226:ARG:NH2	5:B:820:HOH:O	2.38	0.57
1:B:234:VAL:O	5:B:804:HOH:O	2.19	0.54
1:A:473:HIS:CE1	1:B:100[B]:HIS:CE1	2.96	0.53
1:A:89:ASN:OD1	2:A:710:EDO:H12	2.10	0.52
1:A:326:THR:HG22	1:A:330:LYS:HE2	1.91	0.52
1:B:202:ALA:HB2	1:B:242[B]:MET:SD	2.51	0.51
1:B:385:TYR:CD1	2:B:719:EDO:H21	2.46	0.51
1:A:510:GLN:O	5:A:801:HOH:O	2.19	0.51
1:B:489:SER:HB3	1:B:514[B]:THR:HG22	1.94	0.50
1:A:85:GLU:OE1	2:A:710:EDO:H11	2.12	0.49
1:A:534:ALA:HA	2:A:716:EDO:H12	1.95	0.49
1:B:626:ASN:O	1:B:666:HIS:NE2	2.45	0.49
1:A:2:SER:HB2	5:A:1385:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HE2	2:A:710:EDO:H21	1.95	0.47
1:B:33[B]:MET:HE3	1:B:70:LEU:HD22	1.97	0.47
1:A:469:THR:HG23	1:B:100[A]:HIS:HE1	1.79	0.47
1:B:242[B]:MET:HE2	1:B:242[B]:MET:HB3	1.87	0.47
1:A:488:MET:HB2	1:A:488:MET:HE2	1.72	0.45
1:B:452:LYS:HE3	5:B:1453:HOH:O	2.16	0.45
1:B:482:LEU:HD22	1:B:488[A]:MET:CE	2.48	0.43
1:B:552:LEU:HG	1:B:663:LEU:HD21	2.00	0.43
1:A:442:ARG:NH1	5:A:831:HOH:O	2.52	0.43
1:A:593:ASP:OD2	5:A:803:HOH:O	2.21	0.43
1:A:469:THR:HG23	1:B:100[A]:HIS:CE1	2.53	0.42
1:B:466:LEU:C	1:B:466:LEU:HD12	2.44	0.42
1:B:632[B]:MET:HE2	1:B:632[B]:MET:HB3	1.91	0.42
1:B:482:LEU:HD22	1:B:488[A]:MET:HE3	2.02	0.41
1:A:466:LEU:HD12	1:A:466:LEU:C	2.46	0.41
1:B:29:ALA:HB1	1:B:33[B]:MET:HE2	2.02	0.41
1:B:293:GLN:NE2	5:B:806:HOH:O	2.21	0.40
1:B:457[B]:MET:HB3	1:B:459:TYR:CZ	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1458:HOH:O	5:A:1563:HOH:O[3_655]	2.08	0.12
5:A:1446:HOH:O	5:B:1483:HOH:O[4_545]	2.09	0.11
5:A:1435:HOH:O	5:B:1154:HOH:O[3_545]	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	676/669 (101%)	663 (98%)	13 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	681/669 (102%)	671 (98%)	10 (2%)	0	100	100
All	All	1357/1338 (101%)	1334 (98%)	23 (2%)	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	531/522 (102%)	530 (100%)	1 (0%)	87	77
1	B	536/522 (103%)	536 (100%)	0	100	100
All	All	1067/1044 (102%)	1066 (100%)	1 (0%)	88	78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER

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	276	GLN
1	A	455	GLN
1	B	258	HIS
1	B	276	GLN
1	B	522	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 2 are monoatomic - leaving 38 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	EDO	A	710	-	3,3,3	0.45	0	2,2,2	0.33	0
2	EDO	A	713	-	3,3,3	0.50	0	2,2,2	0.53	0
2	EDO	B	706	-	3,3,3	0.61	0	2,2,2	0.36	0
2	EDO	B	709	-	3,3,3	0.31	0	2,2,2	1.40	0
2	EDO	B	720	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	A	705	-	3,3,3	0.57	0	2,2,2	0.61	0
2	EDO	B	714	-	3,3,3	0.62	0	2,2,2	0.23	0
2	EDO	B	716	-	3,3,3	0.43	0	2,2,2	0.72	0
2	EDO	A	711	-	3,3,3	0.99	0	2,2,2	0.56	0
2	EDO	B	701	-	3,3,3	0.40	0	2,2,2	0.76	0
2	EDO	B	704	-	3,3,3	0.65	0	2,2,2	0.07	0
2	EDO	B	719	-	3,3,3	0.34	0	2,2,2	0.33	0
2	EDO	A	714	-	3,3,3	0.51	0	2,2,2	0.26	0
2	EDO	A	701	-	3,3,3	0.49	0	2,2,2	0.60	0
2	EDO	B	703	-	3,3,3	0.54	0	2,2,2	0.68	0
2	EDO	A	712	-	3,3,3	0.33	0	2,2,2	0.32	0
2	EDO	B	708	-	3,3,3	0.57	0	2,2,2	0.70	0
2	EDO	A	715	-	3,3,3	0.51	0	2,2,2	0.42	0
2	EDO	B	722	-	3,3,3	0.39	0	2,2,2	0.77	0
4	TPP	B	711	3	26,27,27	1.51	3 (11%)	38,40,40	1.48	7 (18%)
2	EDO	B	713	-	3,3,3	0.49	0	2,2,2	0.51	0
2	EDO	B	718	-	3,3,3	0.54	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TPP	A	703	3	26,27,27	1.42	3 (11%)	38,40,40	1.61	8 (21%)
2	EDO	B	721	-	3,3,3	0.51	0	2,2,2	0.48	0
2	EDO	A	708	-	3,3,3	0.45	0	2,2,2	0.28	0
2	EDO	B	715	-	3,3,3	0.46	0	2,2,2	0.40	0
2	EDO	B	707	-	3,3,3	0.46	0	2,2,2	0.53	0
2	EDO	B	710	-	3,3,3	0.47	0	2,2,2	0.47	0
2	EDO	B	702	-	3,3,3	0.45	0	2,2,2	0.52	0
2	EDO	B	705	-	3,3,3	0.77	0	2,2,2	0.91	0
2	EDO	A	706	-	3,3,3	0.54	0	2,2,2	0.31	0
2	EDO	A	709	-	3,3,3	0.44	0	2,2,2	0.64	0
2	EDO	A	717	-	3,3,3	0.56	0	2,2,2	0.37	0
2	EDO	B	723	-	3,3,3	0.35	0	2,2,2	0.66	0
2	EDO	A	716	-	3,3,3	0.36	0	2,2,2	0.86	0
2	EDO	A	704	-	3,3,3	0.59	0	2,2,2	0.04	0
2	EDO	B	717	-	3,3,3	0.61	0	2,2,2	0.15	0
2	EDO	A	707	-	3,3,3	0.39	0	2,2,2	0.44	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	EDO	A	710	-	-	1/1/1/1	-
2	EDO	A	713	-	-	0/1/1/1	-
2	EDO	B	706	-	-	1/1/1/1	-
2	EDO	B	709	-	-	1/1/1/1	-
2	EDO	B	720	-	-	0/1/1/1	-
2	EDO	A	705	-	-	0/1/1/1	-
2	EDO	B	714	-	-	0/1/1/1	-
2	EDO	B	716	-	-	0/1/1/1	-
2	EDO	A	711	-	-	0/1/1/1	-
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	B	704	-	-	1/1/1/1	-
2	EDO	B	719	-	-	0/1/1/1	-
2	EDO	A	714	-	-	0/1/1/1	-
2	EDO	A	701	-	-	0/1/1/1	-
2	EDO	B	703	-	-	0/1/1/1	-
2	EDO	A	712	-	-	0/1/1/1	-
2	EDO	B	708	-	-	0/1/1/1	-
2	EDO	A	715	-	-	0/1/1/1	-
2	EDO	B	722	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TPP	B	711	3	-	4/17/17/17	0/2/2/2
2	EDO	B	713	-	-	1/1/1/1	-
2	EDO	B	718	-	-	0/1/1/1	-
4	TPP	A	703	3	-	3/17/17/17	0/2/2/2
2	EDO	B	721	-	-	0/1/1/1	-
2	EDO	A	708	-	-	0/1/1/1	-
2	EDO	B	715	-	-	0/1/1/1	-
2	EDO	B	707	-	-	0/1/1/1	-
2	EDO	B	710	-	-	0/1/1/1	-
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	B	705	-	-	0/1/1/1	-
2	EDO	A	706	-	-	0/1/1/1	-
2	EDO	A	709	-	-	0/1/1/1	-
2	EDO	A	717	-	-	1/1/1/1	-
2	EDO	B	723	-	-	0/1/1/1	-
2	EDO	A	716	-	-	1/1/1/1	-
2	EDO	A	704	-	-	0/1/1/1	-
2	EDO	B	717	-	-	1/1/1/1	-
2	EDO	A	707	-	-	0/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	711	TPP	C5-C4	4.25	1.44	1.35
4	A	703	TPP	C5-C4	3.82	1.43	1.35
4	B	711	TPP	C5'-C4'	3.20	1.48	1.42
4	A	703	TPP	C5'-C4'	3.08	1.47	1.42
4	B	711	TPP	C2-N3	2.87	1.39	1.32
4	A	703	TPP	C4-N3	-2.12	1.35	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	TPP	CM4-C4-C5	-3.40	119.03	127.75
4	B	711	TPP	C6'-N1'-C2'	3.14	121.22	116.07
4	B	711	TPP	C5'-C6'-N1'	-3.00	118.95	123.83
4	A	703	TPP	CM4-C4-N3	2.94	127.35	120.57
4	B	711	TPP	O7-C7-C6	-2.76	97.55	108.63
4	A	703	TPP	C6'-N1'-C2'	2.75	120.59	116.07
4	A	703	TPP	C2-S1-C5	2.69	93.00	91.22
4	B	711	TPP	CM4-C4-C5	-2.68	120.88	127.75
4	A	703	TPP	O3B-PB-O1B	2.62	121.06	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	711	TPP	O2A-PA-O3A	2.55	114.17	107.27
4	B	711	TPP	CM4-C4-N3	2.42	126.16	120.57
4	A	703	TPP	O7-C7-C6	-2.13	100.08	108.63
4	A	703	TPP	C5'-C7'-N3	-2.10	108.44	112.97
4	A	703	TPP	O7-PA-O1A	-2.08	100.67	108.94
4	B	711	TPP	C7-C6-C5	-2.04	106.32	112.73

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	711	TPP	C5-C6-C7-O7
4	B	711	TPP	C7-O7-PA-O2A
4	B	711	TPP	C7-O7-PA-O3A
2	B	706	EDO	O1-C1-C2-O2
2	A	717	EDO	O1-C1-C2-O2
2	A	716	EDO	O1-C1-C2-O2
4	A	703	TPP	S1-C5-C6-C7
4	A	703	TPP	C5-C6-C7-O7
4	A	703	TPP	C4-C5-C6-C7
2	A	710	EDO	O1-C1-C2-O2
2	B	709	EDO	O1-C1-C2-O2
2	B	717	EDO	O1-C1-C2-O2
2	B	713	EDO	O1-C1-C2-O2
2	B	722	EDO	O1-C1-C2-O2
2	B	704	EDO	O1-C1-C2-O2
4	B	711	TPP	S1-C5-C6-C7

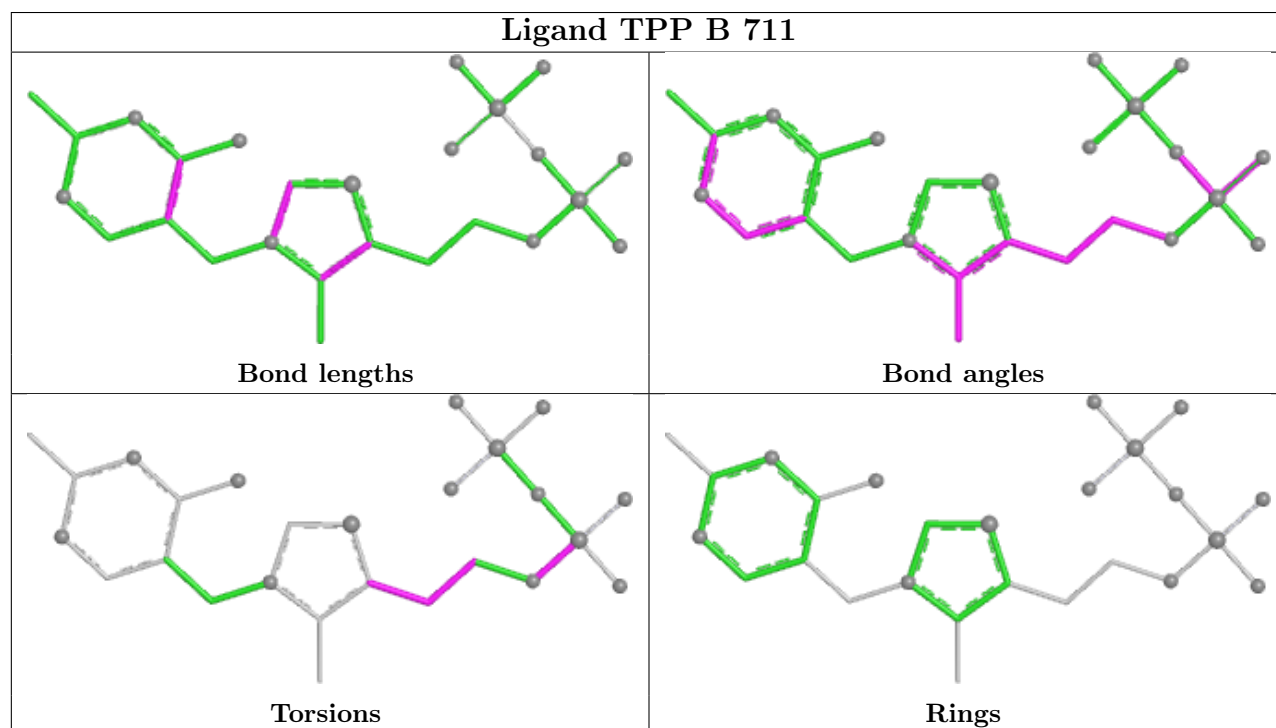
There are no ring outliers.

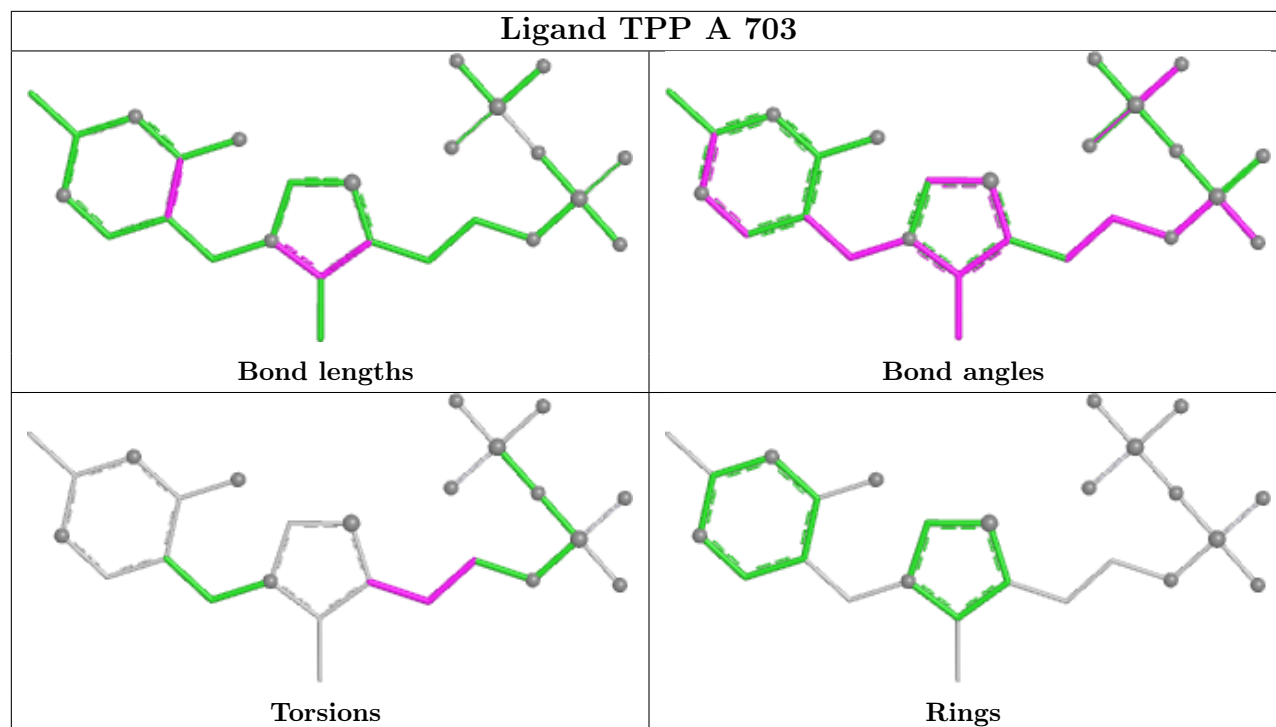
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	710	EDO	3	0
2	B	720	EDO	2	0
2	B	719	EDO	1	0
2	B	721	EDO	1	0
2	A	716	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 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.





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 [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	662/669 (98%)	-0.77	2 (0%)	90 91	3, 7, 17, 32	16 (2%)
1	B	667/669 (99%)	-0.72	7 (1%)	79 82	3, 7, 17, 86	16 (2%)
All	All	1329/1338 (99%)	-0.75	9 (0%)	84 87	3, 7, 17, 86	32 (2%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	TYR	7.0
1	B	666	HIS	6.0
1	B	664	HIS	5.1
1	B	667	HIS	5.1
1	B	665	HIS	4.6
1	B	668	HIS	4.1
1	A	105	TYR	3.1
1	A	2	SER	2.8
1	B	663	LEU	2.4

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.

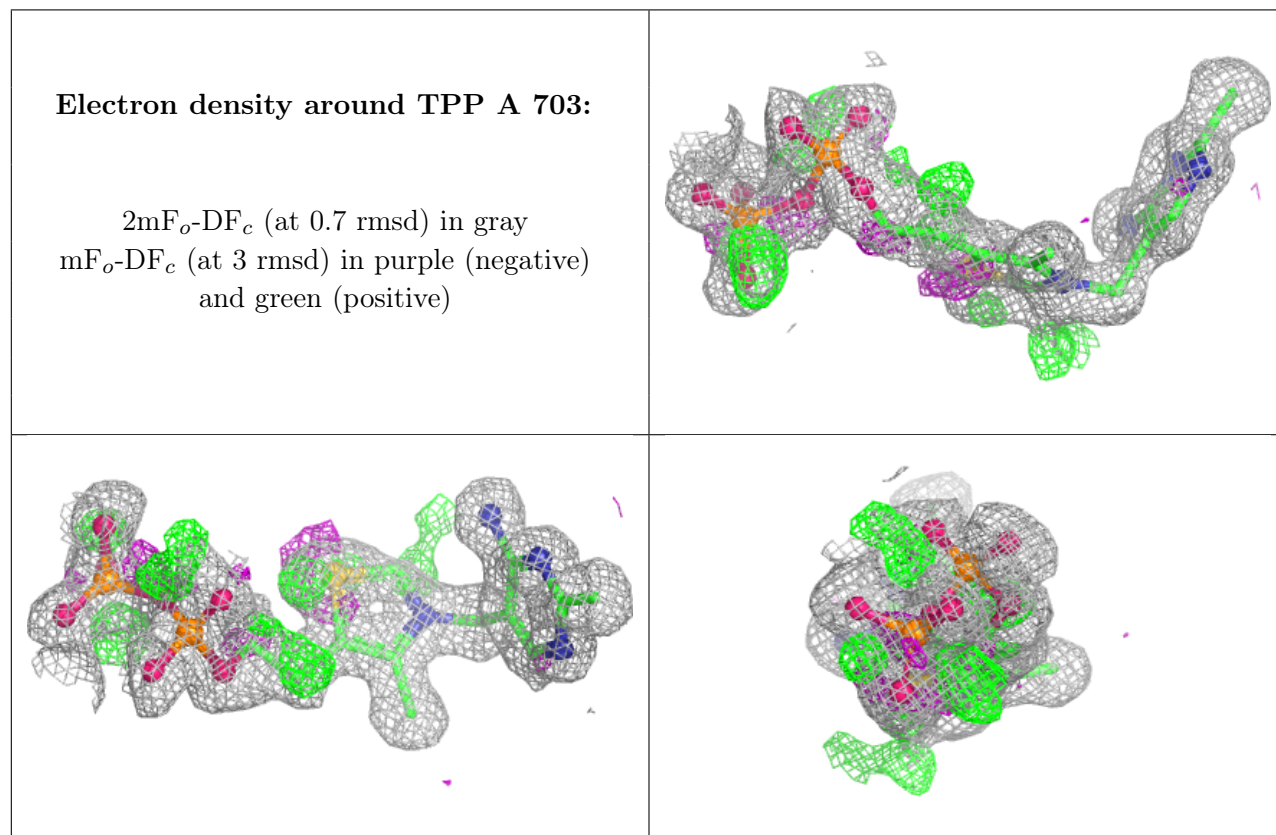
6.4 Ligands [i](#)

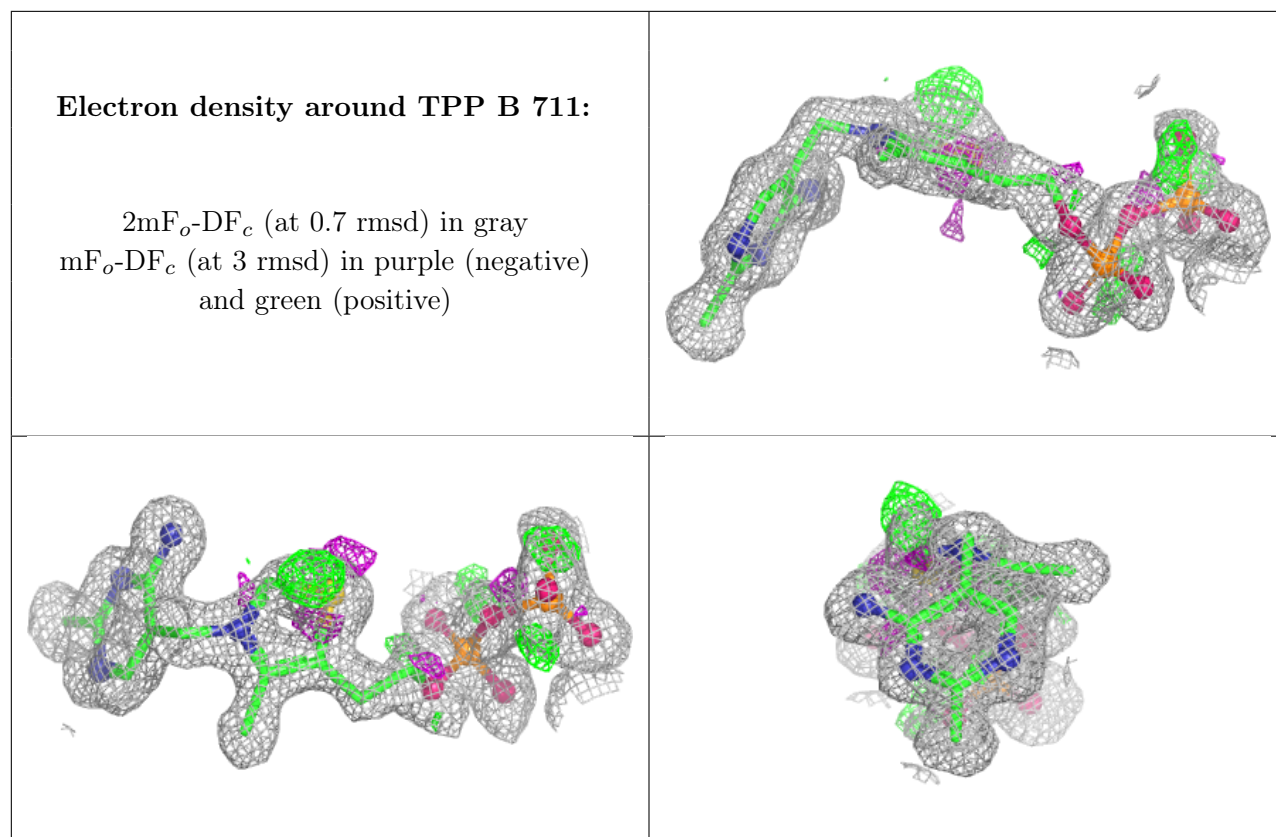
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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	EDO	B	721	4/4	0.74	0.19	34,35,36,36	0
2	EDO	A	708	4/4	0.79	0.14	30,32,33,36	0
2	EDO	B	709	4/4	0.82	0.15	25,30,30,31	0
2	EDO	A	716	4/4	0.84	0.17	14,23,28,30	0
2	EDO	A	717	4/4	0.87	0.14	18,25,29,33	0
2	EDO	B	720	4/4	0.87	0.12	27,28,30,32	0
2	EDO	B	706	4/4	0.87	0.12	20,24,27,32	0
2	EDO	A	705	4/4	0.88	0.15	19,20,22,24	0
2	EDO	A	701	4/4	0.88	0.11	22,23,25,26	0
2	EDO	A	712	4/4	0.89	0.12	26,27,30,32	0
2	EDO	A	710	4/4	0.89	0.12	25,26,26,29	0
2	EDO	B	708	4/4	0.89	0.11	17,18,19,20	0
2	EDO	B	719	4/4	0.90	0.11	27,31,32,33	0
2	EDO	A	715	4/4	0.90	0.15	21,22,24,24	0
2	EDO	B	707	4/4	0.90	0.11	19,19,22,26	0
2	EDO	B	722	4/4	0.90	0.12	28,29,31,32	0
2	EDO	A	711	4/4	0.91	0.17	8,15,16,17	0
2	EDO	B	715	4/4	0.91	0.12	21,25,27,31	0
2	EDO	A	714	4/4	0.92	0.09	16,22,24,25	0
2	EDO	B	714	4/4	0.93	0.12	11,19,22,27	0
2	EDO	A	704	4/4	0.93	0.10	17,21,24,24	0
2	EDO	B	718	4/4	0.94	0.13	9,14,15,17	0
2	EDO	A	706	4/4	0.94	0.10	13,14,19,23	0
2	EDO	A	707	4/4	0.94	0.09	20,20,21,22	0
2	EDO	B	705	4/4	0.94	0.10	8,10,12,13	0
2	EDO	B	717	4/4	0.94	0.10	17,20,20,20	0
2	EDO	B	710	4/4	0.95	0.08	19,19,21,23	0
2	EDO	B	713	4/4	0.95	0.10	19,20,21,24	0
2	EDO	B	723	4/4	0.95	0.12	12,19,24,27	0
2	EDO	A	713	4/4	0.96	0.10	13,16,16,23	0
2	EDO	B	701	4/4	0.97	0.06	13,14,18,20	0
2	EDO	B	704	4/4	0.97	0.06	12,14,16,16	0
4	TPP	A	703	26/26	0.97	0.06	5,9,19,21	0
4	TPP	B	711	26/26	0.97	0.06	4,10,19,21	0
2	EDO	B	703	4/4	0.98	0.04	10,10,11,15	0
2	EDO	A	709	4/4	0.98	0.09	10,16,16,17	0
2	EDO	B	716	4/4	0.98	0.05	10,11,12,13	0
2	EDO	B	702	4/4	0.98	0.05	6,8,13,15	0
3	CA	A	702	1/1	1.00	0.02	4,4,4,4	0
3	CA	B	712	1/1	1.00	0.01	5,5,5,5	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.