



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:43 AM UTC

PDB ID : 8R3Q / pdb_00008r3q
Title : Transketolase from Plasmodium falciparum 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 : 1.88 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

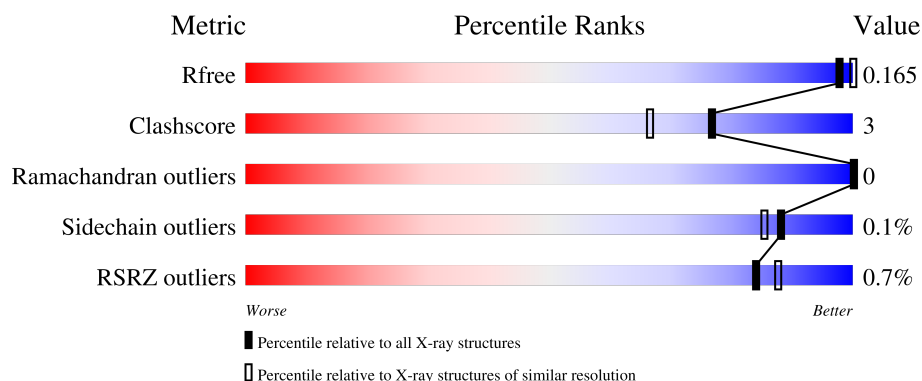
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

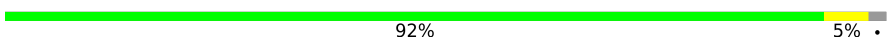
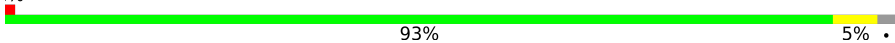
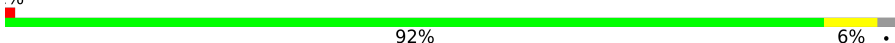
The reported resolution of this entry is 1.88 Å.

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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	687	
1	B	687	
1	C	687	
1	D	687	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24764 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	B	670	Total	C	N	O	S	0	6	0
			5376	3418	921	1014	23			
1	A	671	Total	C	N	O	S	0	4	0
			5372	3421	916	1012	23			
1	C	674	Total	C	N	O	S	0	11	0
			5456	3470	932	1029	25			
1	D	676	Total	C	N	O	S	0	9	0
			5451	3466	931	1028	26			

There are 60 discrepancies between the modelled and reference sequences:

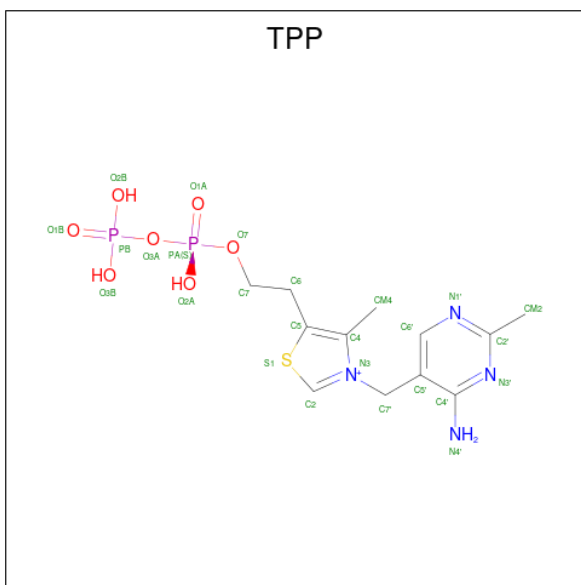
Chain	Residue	Modelled	Actual	Comment	Reference
B	673	GLU	-	expression tag	UNP C6KSV3
B	674	ASN	-	expression tag	UNP C6KSV3
B	675	LEU	-	expression tag	UNP C6KSV3
B	676	TYR	-	expression tag	UNP C6KSV3
B	677	PHE	-	expression tag	UNP C6KSV3
B	678	GLN	-	expression tag	UNP C6KSV3
B	679	GLY	-	expression tag	UNP C6KSV3
B	680	LEU	-	expression tag	UNP C6KSV3
B	681	GLU	-	expression tag	UNP C6KSV3
B	682	HIS	-	expression tag	UNP C6KSV3
B	683	HIS	-	expression tag	UNP C6KSV3
B	684	HIS	-	expression tag	UNP C6KSV3
B	685	HIS	-	expression tag	UNP C6KSV3
B	686	HIS	-	expression tag	UNP C6KSV3
B	687	HIS	-	expression tag	UNP C6KSV3
A	673	GLU	-	expression tag	UNP C6KSV3
A	674	ASN	-	expression tag	UNP C6KSV3
A	675	LEU	-	expression tag	UNP C6KSV3
A	676	TYR	-	expression tag	UNP C6KSV3
A	677	PHE	-	expression tag	UNP C6KSV3
A	678	GLN	-	expression tag	UNP C6KSV3

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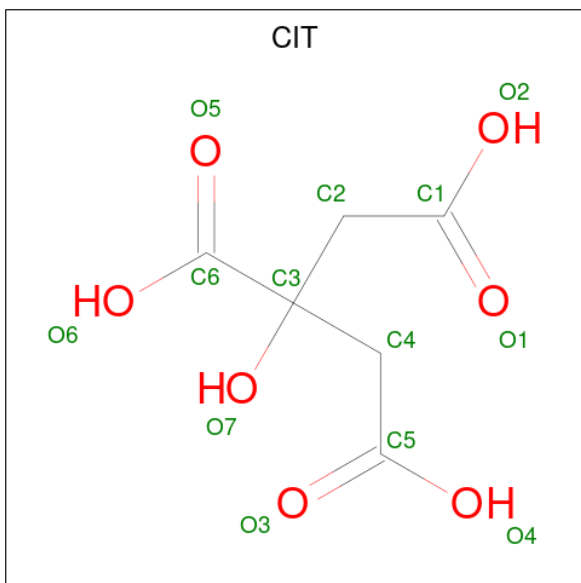
Chain	Residue	Modelled	Actual	Comment	Reference
A	679	GLY	-	expression tag	UNP C6KSV3
A	680	LEU	-	expression tag	UNP C6KSV3
A	681	GLU	-	expression tag	UNP C6KSV3
A	682	HIS	-	expression tag	UNP C6KSV3
A	683	HIS	-	expression tag	UNP C6KSV3
A	684	HIS	-	expression tag	UNP C6KSV3
A	685	HIS	-	expression tag	UNP C6KSV3
A	686	HIS	-	expression tag	UNP C6KSV3
A	687	HIS	-	expression tag	UNP C6KSV3
C	673	GLU	-	expression tag	UNP C6KSV3
C	674	ASN	-	expression tag	UNP C6KSV3
C	675	LEU	-	expression tag	UNP C6KSV3
C	676	TYR	-	expression tag	UNP C6KSV3
C	677	PHE	-	expression tag	UNP C6KSV3
C	678	GLN	-	expression tag	UNP C6KSV3
C	679	GLY	-	expression tag	UNP C6KSV3
C	680	LEU	-	expression tag	UNP C6KSV3
C	681	GLU	-	expression tag	UNP C6KSV3
C	682	HIS	-	expression tag	UNP C6KSV3
C	683	HIS	-	expression tag	UNP C6KSV3
C	684	HIS	-	expression tag	UNP C6KSV3
C	685	HIS	-	expression tag	UNP C6KSV3
C	686	HIS	-	expression tag	UNP C6KSV3
C	687	HIS	-	expression tag	UNP C6KSV3
D	673	GLU	-	expression tag	UNP C6KSV3
D	674	ASN	-	expression tag	UNP C6KSV3
D	675	LEU	-	expression tag	UNP C6KSV3
D	676	TYR	-	expression tag	UNP C6KSV3
D	677	PHE	-	expression tag	UNP C6KSV3
D	678	GLN	-	expression tag	UNP C6KSV3
D	679	GLY	-	expression tag	UNP C6KSV3
D	680	LEU	-	expression tag	UNP C6KSV3
D	681	GLU	-	expression tag	UNP C6KSV3
D	682	HIS	-	expression tag	UNP C6KSV3
D	683	HIS	-	expression tag	UNP C6KSV3
D	684	HIS	-	expression tag	UNP C6KSV3
D	685	HIS	-	expression tag	UNP C6KSV3
D	686	HIS	-	expression tag	UNP C6KSV3
D	687	HIS	-	expression tag	UNP C6KSV3

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



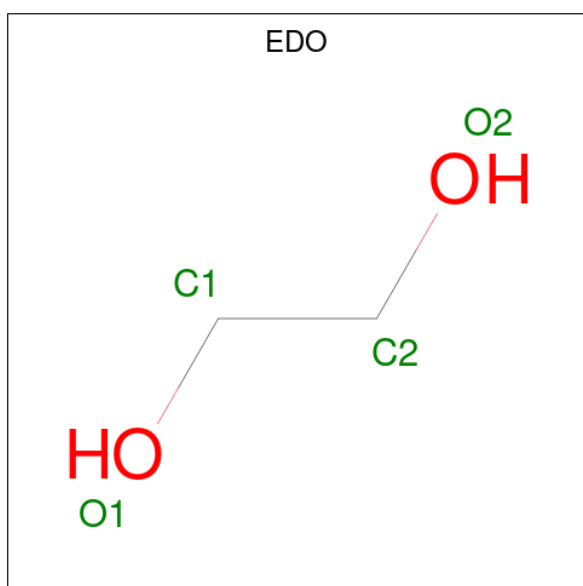
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: $\text{C}_6\text{H}_8\text{O}_7$).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

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

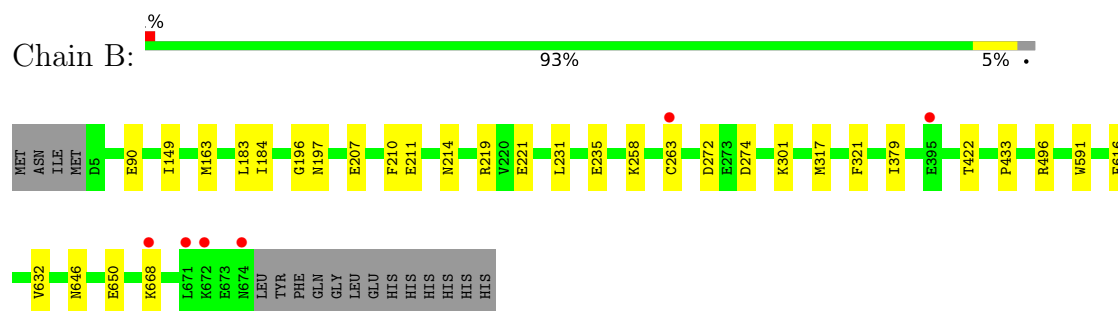
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	697	Total 697	O 697	0	0
6	A	746	Total 746	O 746	0	0
6	C	723	Total 723	O 723	0	0
6	D	763	Total 763	O 763	0	0

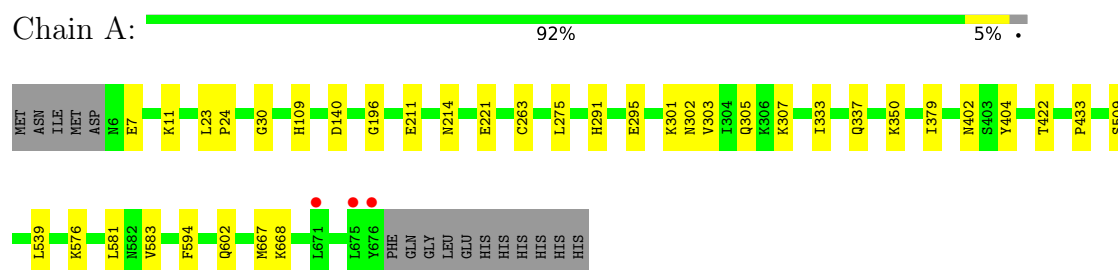
3 Residue-property plots [i](#)

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.

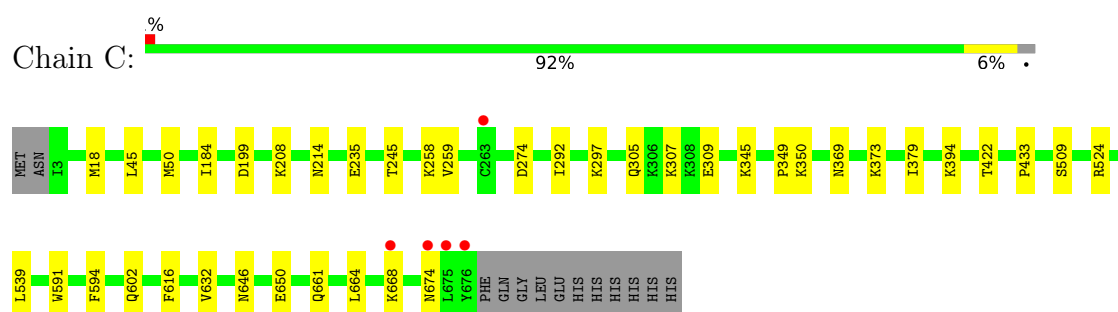
- Molecule 1: transketolase



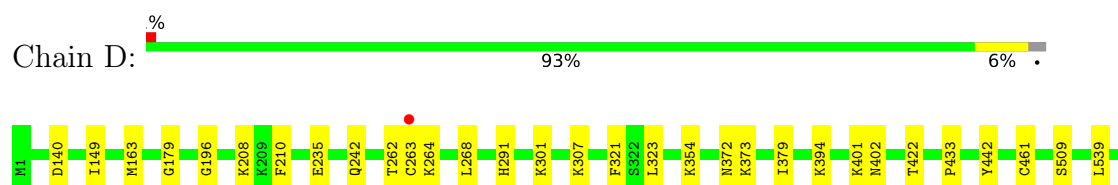
- Molecule 1: transketolase

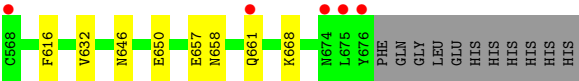


- Molecule 1: transketolase



- Molecule 1: transketolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.04Å 114.34Å 149.90Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	46.81 – 1.88 46.81 – 1.88	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.81-1.88) 100.0 (46.81-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.144 , 0.168 (Not available) , 0.165	Depositor DCC
R_{free} test set	13264 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24764	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: CIT, EDO, MG, TPP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/5503	0.53	0/7451
1	B	0.31	0/5506	0.52	0/7455
1	C	0.32	0/5587	0.52	0/7562
1	D	0.32	0/5582	0.53	0/7556
All	All	0.32	0/22178	0.53	0/30024

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 [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	5372	0	5254	29	0
1	B	5376	0	5252	24	0
1	C	5456	0	5330	34	0
1	D	5451	0	5328	37	0
2	A	26	0	16	0	0
2	B	26	0	16	0	0
2	C	26	0	16	2	0
2	D	26	0	16	1	0
3	A	13	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	5	0	0
3	C	13	0	5	2	0
3	D	13	0	5	0	0
4	A	8	0	12	2	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	746	0	0	12	1
6	B	697	0	0	11	1
6	C	723	0	0	12	1
6	D	763	0	0	9	1
All	All	24764	0	21278	126	2

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 3.

All (126) 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:D:401:LYS:NZ	6:D:801:HOH:O	1.88	1.05
1:A:11:LYS:NZ	1:A:295:GLU:OE1	2.00	0.93
1:B:90:GLU:OE1	6:B:801:HOH:O	1.87	0.92
1:C:235:GLU:OE2	6:C:801:HOH:O	1.91	0.89
1:D:179:GLY:HA3	1:D:401:LYS:HE3	1.58	0.86
1:D:661:GLN:NE2	6:D:803:HOH:O	2.12	0.83
1:A:214:ASN:ND2	6:A:801:HOH:O	2.09	0.83
1:C:661:GLN:NE2	6:C:804:HOH:O	2.13	0.81
1:C:650:GLU:OE2	6:C:802:HOH:O	1.99	0.81
1:B:668:LYS:NZ	6:B:804:HOH:O	2.14	0.77
1:A:30:GLY:H	4:A:704:EDO:H22	1.50	0.76
1:C:524:ARG:HH21	3:C:702:CIT:H41	1.51	0.74
1:D:354:LYS:HA	1:D:354:LYS:HE2	1.69	0.73
1:B:272:ASP:OD2	6:B:802:HOH:O	2.06	0.73
1:A:221:GLU:HG2	6:A:1096:HOH:O	1.88	0.73
1:C:258:LYS:NZ	1:C:274:ASP:OD2	2.20	0.73
1:D:140:ASP:OD1	6:D:802:HOH:O	2.07	0.73
1:D:242:GLN:HE22	1:D:402:ASN:HD21	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199[B]:ASP:OD1	6:C:803:HOH:O	2.07	0.71
1:A:301:LYS:NZ	6:A:804:HOH:O	2.22	0.71
1:A:302:ASN:ND2	6:A:805:HOH:O	2.26	0.69
1:B:221:GLU:OE1	6:B:803:HOH:O	2.09	0.69
1:C:214:ASN:ND2	6:C:805:HOH:O	2.26	0.69
1:D:235:GLU:HG2	6:D:1387:HOH:O	1.97	0.64
1:B:646:ASN:O	1:B:650:GLU:HG3	1.98	0.62
1:C:235:GLU:HG3	6:C:1431:HOH:O	1.98	0.62
1:D:372:ASN:HD22	1:D:373:LYS:NZ	1.98	0.61
1:D:658:ASN:HA	1:D:661:GLN:HG2	1.83	0.60
1:D:242:GLN:NE2	1:D:402:ASN:HD21	2.00	0.59
1:A:333:ILE:O	1:A:337:GLN:HG3	2.03	0.58
1:D:372:ASN:HD22	1:D:373:LYS:HZ2	1.50	0.58
1:B:163:MET:HE1	1:B:210:PHE:CE1	2.39	0.58
1:C:45:LEU:O	1:C:50:MET:HG3	2.04	0.58
1:A:305:GLN:NE2	6:A:809:HOH:O	2.31	0.58
1:B:196:GLY:HA2	1:B:263:CYS:HB3	1.85	0.57
1:D:242:GLN:HE22	1:D:402:ASN:ND2	2.02	0.57
1:B:214:ASN:ND2	6:B:808:HOH:O	2.37	0.57
1:C:305[A]:GLN:O	1:C:309:GLU:HG3	2.05	0.56
1:A:295:GLU:H	1:A:295:GLU:CD	2.13	0.56
1:D:264:LYS:N	1:D:264:LYS:HD3	2.22	0.55
1:C:646:ASN:O	1:C:650:GLU:HG3	2.06	0.54
1:A:291:HIS:HD2	6:A:1431:HOH:O	1.90	0.54
1:C:394:LYS:HG3	6:C:818:HOH:O	2.08	0.54
1:B:207:GLU:O	1:B:211:GLU:HG3	2.09	0.53
1:C:208:LYS:HG3	1:D:208:LYS:HE3	1.89	0.53
1:C:664:LEU:O	1:C:668:LYS:HE2	2.08	0.53
1:B:163:MET:HE1	1:B:210:PHE:CZ	2.44	0.53
1:C:349:PRO:O	1:C:350:LYS:HE2	2.09	0.52
1:A:211:GLU:OE1	6:A:802:HOH:O	2.19	0.52
1:A:576:LYS:HE3	1:A:583:VAL:H	1.75	0.52
1:C:345:LYS:NZ	6:C:814:HOH:O	2.43	0.52
1:C:668:LYS:N	1:C:668:LYS:HD3	2.25	0.51
1:D:268:LEU:HD12	6:D:877:HOH:O	2.09	0.51
1:B:219:ARG:NH2	6:B:807:HOH:O	2.36	0.51
1:B:650:GLU:OE2	6:B:805:HOH:O	2.18	0.50
1:A:422:THR:HG23	1:A:433:PRO:HB2	1.92	0.50
1:C:305[B]:GLN:O	1:C:309:GLU:HG3	2.11	0.50
1:D:149:ILE:HD11	1:D:321:PHE:CE1	2.47	0.49
1:C:509[A]:SER:OG	1:C:539:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:LYS:HE3	1:D:208:LYS:HG3	1.93	0.49
1:D:394:LYS:N	1:D:394:LYS:HD3	2.27	0.49
1:B:183:LEU:C	1:B:184:ILE:HD12	2.38	0.49
1:B:301:LYS:HD3	1:B:301:LYS:C	2.38	0.49
1:D:323:LEU:HB3	6:D:1002:HOH:O	2.12	0.48
1:B:149:ILE:HD11	1:B:321:PHE:CE1	2.49	0.48
1:D:262:THR:HB	1:D:264:LYS:HE2	1.96	0.48
1:C:184:ILE:HD13	1:C:245:THR:HB	1.96	0.48
1:C:524:ARG:HH21	3:C:702:CIT:C4	2.25	0.48
1:D:646[A]:ASN:O	1:D:650:GLU:HG3	2.13	0.48
1:A:509[A]:SER:OG	1:A:539:LEU:HD12	2.14	0.47
1:D:509[A]:SER:OG	1:D:539:LEU:HD12	2.14	0.47
1:A:196:GLY:HA2	1:A:263:CYS:HB3	1.97	0.47
1:C:422:THR:HG23	1:C:433:PRO:HB2	1.97	0.47
1:B:149:ILE:HA	1:B:317:MET:HE1	1.97	0.47
1:C:674:ASN:ND2	6:C:820:HOH:O	2.48	0.47
1:A:109:HIS:HD2	6:A:1455:HOH:O	1.98	0.46
1:A:350:LYS:HE3	6:A:1268:HOH:O	2.15	0.46
1:C:18:MET:HA	1:C:18:MET:HE2	1.96	0.46
1:B:496:ARG:HD3	6:B:817:HOH:O	2.16	0.46
6:B:1196:HOH:O	4:A:704:EDO:H21	2.14	0.46
1:B:258:LYS:HE3	1:B:274:ASP:OD1	2.15	0.46
1:A:140[B]:ASP:OD2	1:A:404:TYR:HB2	2.16	0.46
1:D:616:PHE:HA	1:D:632:VAL:O	2.16	0.45
1:A:576:LYS:CE	1:A:583:VAL:H	2.30	0.45
1:B:231:LEU:O	1:B:235:GLU:HG3	2.15	0.45
1:D:668:LYS:HB3	1:D:668:LYS:HE3	1.67	0.45
1:A:402:ASN:OD1	6:A:803:HOH:O	2.21	0.45
1:A:7:GLU:HB2	6:A:1051:HOH:O	2.16	0.45
2:C:701:TPP:H2	6:D:996:HOH:O	2.15	0.45
2:D:701:TPP:H2	6:D:1047:HOH:O	2.17	0.45
1:D:379:ILE:O	1:D:433:PRO:HA	2.17	0.44
1:C:292:ILE:HG22	1:C:297:LYS:HG3	2.00	0.44
1:A:576:LYS:HE2	1:A:581:LEU:O	2.18	0.43
1:D:264:LYS:HD3	1:D:264:LYS:H	1.83	0.43
1:D:301:LYS:HD2	1:D:301:LYS:HA	1.77	0.43
1:B:379:ILE:O	1:B:433:PRO:HA	2.18	0.43
1:D:422:THR:HG23	1:D:433:PRO:HB2	2.00	0.43
1:C:369:ASN:OD1	1:C:394:LYS:HG2	2.19	0.43
1:C:258:LYS:HG3	1:C:259:VAL:HG13	2.01	0.43
2:C:701:TPP:H2	6:C:1086:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:658:ASN:HA	1:D:661:GLN:CG	2.48	0.43
1:D:163:MET:HE1	1:D:210:PHE:CE1	2.54	0.42
1:B:591:TRP:CD1	6:B:960:HOH:O	2.71	0.42
1:D:179:GLY:CA	1:D:401:LYS:HE3	2.39	0.42
1:D:264:LYS:H	1:D:264:LYS:CD	2.32	0.42
1:A:594:PHE:CZ	1:A:602:GLN:HA	2.54	0.42
1:A:23:LEU:HB2	1:A:24:PRO:HD3	2.01	0.42
1:A:668:LYS:HD2	6:A:834:HOH:O	2.20	0.42
1:D:196:GLY:HA2	1:D:263:CYS:HB3	2.01	0.42
1:C:349:PRO:C	1:C:350:LYS:HE2	2.45	0.42
1:A:581:LEU:HD22	1:A:667:MET:HE1	2.01	0.42
1:B:616:PHE:HA	1:B:632:VAL:O	2.20	0.42
1:D:646[B]:ASN:O	1:D:650:GLU:HG3	2.18	0.41
1:B:197:ASN:ND2	6:B:833:HOH:O	2.53	0.41
1:C:594:PHE:CZ	1:C:602:GLN:HA	2.55	0.41
1:D:657:GLU:CD	1:D:657:GLU:H	2.28	0.41
1:D:291:HIS:HE1	6:D:1439:HOH:O	2.03	0.41
1:A:379:ILE:O	1:A:433:PRO:HA	2.21	0.41
1:C:591:TRP:CD1	6:C:851:HOH:O	2.73	0.41
1:B:422:THR:HG23	1:B:433:PRO:HB2	2.01	0.41
1:C:373:LYS:NZ	6:C:836:HOH:O	2.54	0.41
1:C:616:PHE:HA	1:C:632:VAL:O	2.21	0.40
1:A:303:VAL:O	1:A:307:LYS:HG2	2.21	0.40
1:C:379:ILE:O	1:C:433:PRO:HA	2.20	0.40
1:A:275:LEU:HD23	1:A:275:LEU:HA	1.90	0.40
1:D:442:TYR:CZ	1:D:461:CYS:HB3	2.56	0.40

All (2) 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:B:1324:HOH:O	6:A:1423:HOH:O[2_655]	2.02	0.18
6:C:1469:HOH:O	6:D:1341:HOH:O[2_556]	2.10	0.10

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	673/687 (98%)	661 (98%)	12 (2%)	0	100	100
1	B	674/687 (98%)	661 (98%)	13 (2%)	0	100	100
1	C	683/687 (99%)	672 (98%)	11 (2%)	0	100	100
1	D	683/687 (99%)	671 (98%)	12 (2%)	0	100	100
All	All	2713/2748 (99%)	2665 (98%)	48 (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	586/597 (98%)	586 (100%)	0	100	100
1	B	587/597 (98%)	587 (100%)	0	100	100
1	C	596/597 (100%)	595 (100%)	1 (0%)	87	84
1	D	596/597 (100%)	595 (100%)	1 (0%)	87	84
All	All	2365/2388 (99%)	2363 (100%)	2 (0%)	88	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	307	LYS
1	D	307	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	97	GLN

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Mol	Chain	Res	Type
1	B	152	ASN
1	B	232	HIS
1	B	302	ASN
1	B	338	ASN
1	B	406	ASN
1	B	440	ASN
1	B	661	GLN
1	B	669	ASN
1	A	51	ASN
1	A	97	GLN
1	A	152	ASN
1	A	214	ASN
1	A	302	ASN
1	A	402	ASN
1	A	406	ASN
1	A	493	ASN
1	A	525	ASN
1	A	537	GLN
1	A	612	ASN
1	A	638	GLN
1	C	97	GLN
1	C	232	HIS
1	C	287	GLN
1	C	302	ASN
1	C	316	ASN
1	C	440	ASN
1	C	493	ASN
1	C	646	ASN
1	D	6	ASN
1	D	51	ASN
1	D	109	HIS
1	D	214	ASN
1	D	232	HIS
1	D	240	ASN
1	D	242	GLN
1	D	243	GLN
1	D	316	ASN
1	D	342	ASN
1	D	343	ASN
1	D	372	ASN
1	D	440	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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\# Z > 2$
3	CIT	A	703	-	12,12,12	1.13	0	17,17,17	1.56	2 (11%)
3	CIT	B	702	-	12,12,12	1.00	0	17,17,17	1.71	3 (17%)
3	CIT	C	702	-	12,12,12	1.12	0	17,17,17	1.53	3 (17%)
2	TPP	D	701	5	26,27,27	0.83	1 (3%)	38,40,40	0.50	0
3	CIT	D	702	-	12,12,12	1.12	0	17,17,17	1.44	2 (11%)
4	EDO	C	703	-	3,3,3	0.41	0	2,2,2	0.64	0
4	EDO	D	703	-	3,3,3	0.37	0	2,2,2	0.58	0
4	EDO	A	704	-	3,3,3	0.39	0	2,2,2	0.41	0
2	TPP	B	701	5	26,27,27	0.82	1 (3%)	38,40,40	0.52	0
4	EDO	B	703	-	3,3,3	0.41	0	2,2,2	0.15	0
4	EDO	A	701	-	3,3,3	0.42	0	2,2,2	0.67	0
2	TPP	C	701	5	26,27,27	1.02	1 (3%)	38,40,40	0.46	0
2	TPP	A	702	5	26,27,27	1.03	1 (3%)	38,40,40	0.48	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
3	CIT	A	703	-	-	3/16/16/16	-
3	CIT	B	702	-	-	4/16/16/16	-
3	CIT	C	702	-	-	9/16/16/16	-
2	TPP	D	701	5	-	2/17/17/17	0/2/2/2
3	CIT	D	702	-	-	9/16/16/16	-
4	EDO	C	703	-	-	0/1/1/1	-
4	EDO	D	703	-	-	0/1/1/1	-
4	EDO	A	704	-	-	0/1/1/1	-
2	TPP	B	701	5	-	2/17/17/17	0/2/2/2
4	EDO	B	703	-	-	1/1/1/1	-
4	EDO	A	701	-	-	0/1/1/1	-
2	TPP	C	701	5	-	2/17/17/17	0/2/2/2
2	TPP	A	702	5	-	3/17/17/17	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	TPP	PA-O3A	-4.91	1.54	1.59
2	A	702	TPP	PA-O3A	-4.76	1.54	1.59
2	B	701	TPP	PA-O3A	-3.74	1.55	1.59
2	D	701	TPP	PA-O3A	-3.31	1.55	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	CIT	O6-C6-C3	4.37	121.53	113.14
3	A	703	CIT	O6-C6-C3	3.71	120.26	113.14
3	C	702	CIT	O6-C6-C3	3.70	120.25	113.14
3	D	702	CIT	O6-C6-C3	3.46	119.78	113.14
3	B	702	CIT	O2-C1-C2	2.61	122.61	114.35
3	C	702	CIT	O2-C1-C2	2.54	122.39	114.35
3	A	703	CIT	C3-C2-C1	-2.51	107.07	113.92
3	C	702	CIT	O2-C1-O1	-2.15	117.81	123.33
3	D	702	CIT	O2-C1-C2	2.13	121.10	114.35
3	B	702	CIT	O2-C1-O1	-2.02	118.14	123.33

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	TPP	C7-O7-PA-O1A
2	D	701	TPP	C7-O7-PA-O1A
3	B	702	CIT	O7-C3-C4-C5
3	B	702	CIT	C6-C3-C4-C5
3	C	702	CIT	O7-C3-C6-O5
3	C	702	CIT	O7-C3-C6-O6
3	C	702	CIT	C4-C3-C6-O5
3	C	702	CIT	C4-C3-C6-O6
3	D	702	CIT	O7-C3-C4-C5
3	D	702	CIT	C6-C3-C4-C5
3	B	702	CIT	C2-C3-C4-C5
3	D	702	CIT	C2-C3-C4-C5
3	A	703	CIT	C1-C2-C3-O7
3	A	703	CIT	C1-C2-C3-C6
3	A	703	CIT	C1-C2-C3-C4
3	C	702	CIT	C1-C2-C3-O7
2	B	701	TPP	C5-C6-C7-O7
2	A	702	TPP	C5-C6-C7-O7
2	C	701	TPP	C5-C6-C7-O7
2	D	701	TPP	C5-C6-C7-O7
3	C	702	CIT	C2-C3-C6-O5
3	D	702	CIT	C2-C3-C6-O5
2	B	701	TPP	C7-O7-PA-O1A
2	C	701	TPP	C7-O7-PA-O1A
3	C	702	CIT	C2-C3-C6-O6
3	D	702	CIT	C2-C3-C6-O6
3	D	702	CIT	C4-C3-C6-O5
3	D	702	CIT	C4-C3-C6-O6
4	B	703	EDO	O1-C1-C2-O2
3	C	702	CIT	O1-C1-C2-C3
3	B	702	CIT	O1-C1-C2-C3
3	C	702	CIT	O2-C1-C2-C3
3	D	702	CIT	O1-C1-C2-C3
3	D	702	CIT	O2-C1-C2-C3
2	A	702	TPP	S1-C5-C6-C7

There are no ring outliers.

4 monomers are involved in 7 short contacts:

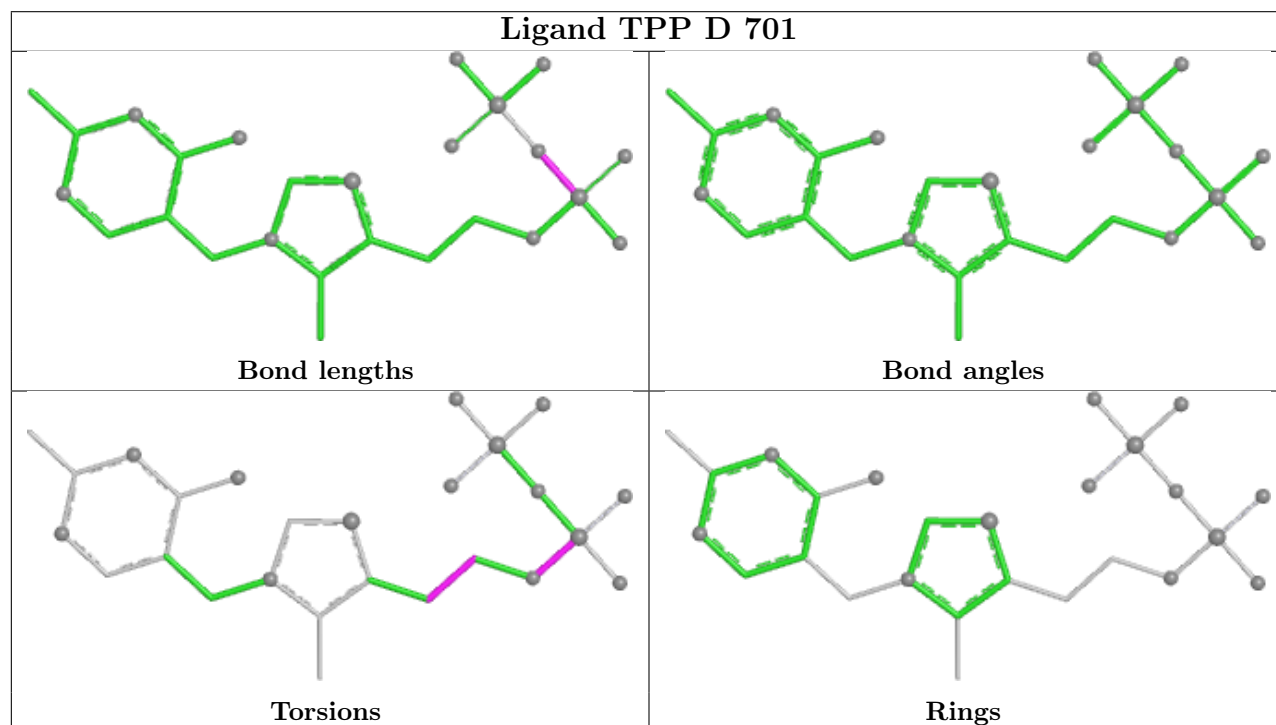
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	CIT	2	0
2	D	701	TPP	1	0
4	A	704	EDO	2	0

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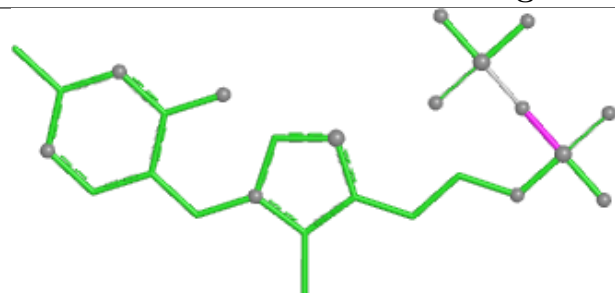
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	TPP	2	0

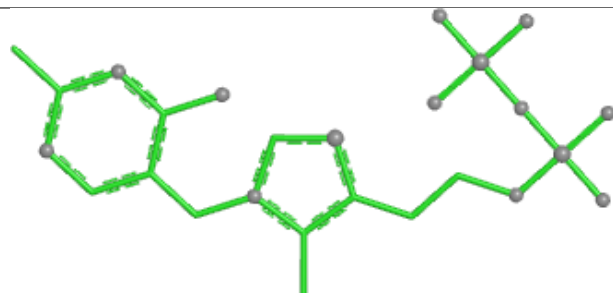
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



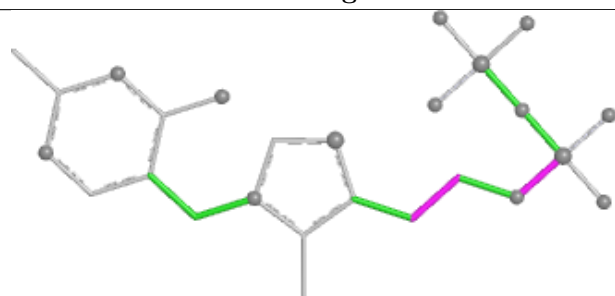
Ligand TPP B 701



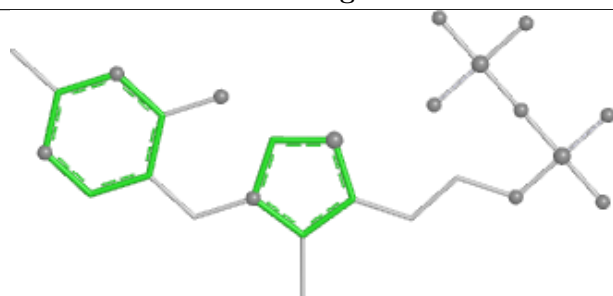
Bond lengths



Bond angles

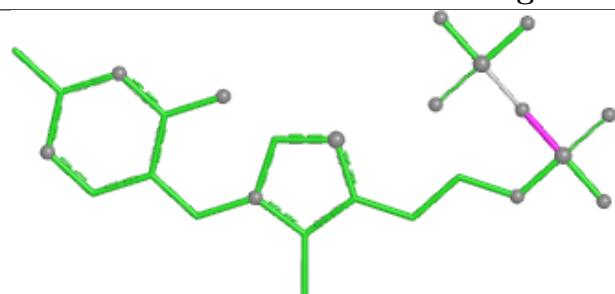


Torsions

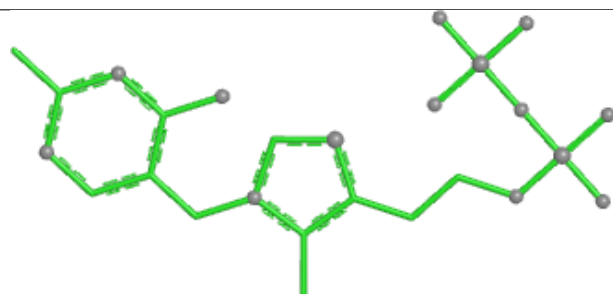


Rings

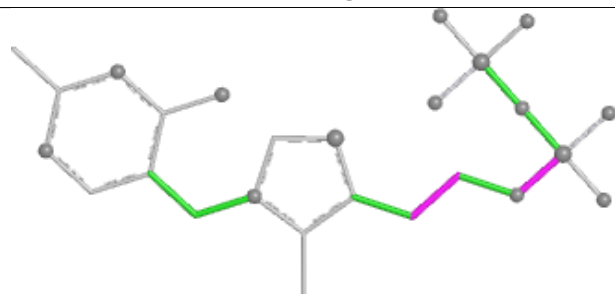
Ligand TPP C 701



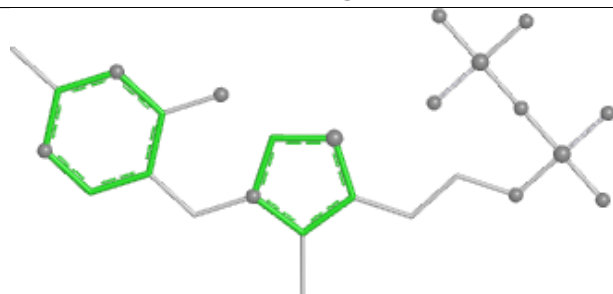
Bond lengths



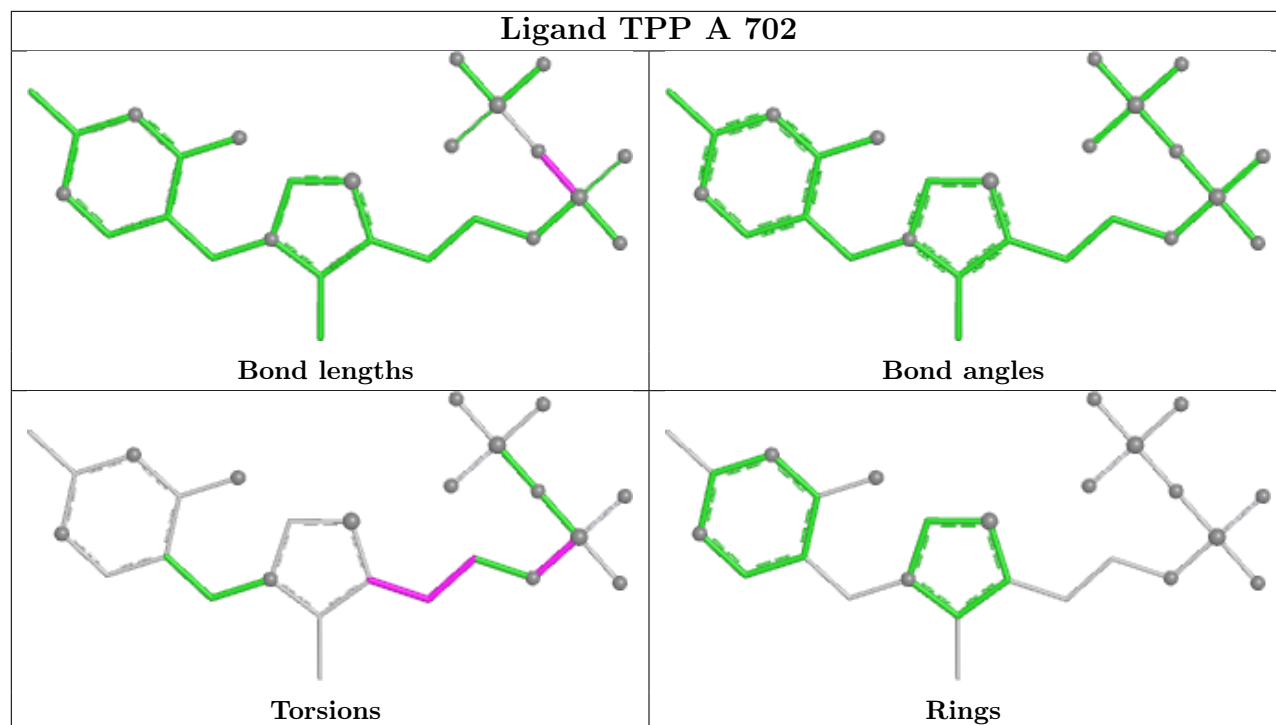
Bond angles



Torsions



Rings



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	671/687 (97%)	-0.63	3 (0%) 88 92	6, 15, 30, 57	4 (0%)
1	B	670/687 (97%)	-0.53	6 (0%) 81 85	6, 17, 34, 59	6 (0%)
1	C	674/687 (98%)	-0.54	5 (0%) 84 88	7, 16, 32, 56	11 (1%)
1	D	676/687 (98%)	-0.61	6 (0%) 81 85	6, 16, 31, 54	9 (1%)
All	All	2691/2748 (97%)	-0.58	20 (0%) 84 88	6, 16, 32, 59	30 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	676	TYR	4.3
1	D	568	CYS	4.1
1	A	676	TYR	4.0
1	C	676	TYR	3.5
1	C	675	LEU	3.4
1	D	675	LEU	3.3
1	B	263	CYS	3.2
1	D	674	ASN	3.1
1	B	671	LEU	3.1
1	A	675	LEU	2.9
1	B	674	ASN	2.9
1	A	671	LEU	2.6
1	B	672	LYS	2.6
1	B	395	GLU	2.5
1	D	263	CYS	2.4
1	C	263	CYS	2.4
1	B	668	LYS	2.2
1	C	668	LYS	2.1
1	D	661	GLN	2.1
1	C	674	ASN	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 [i](#)

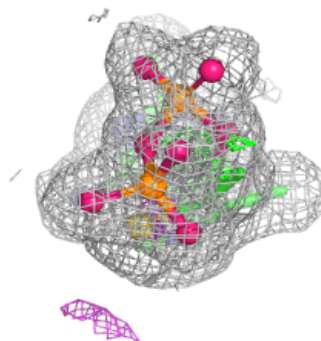
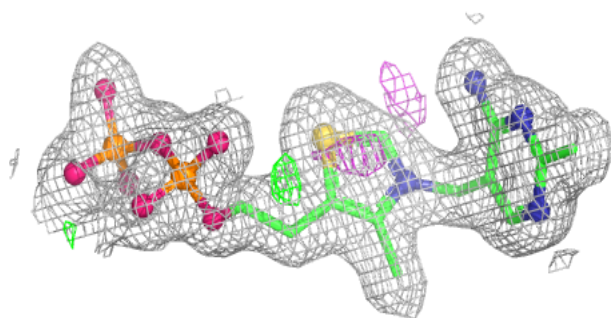
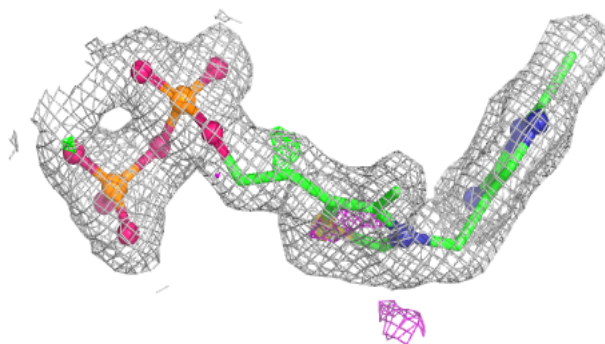
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	704	4/4	0.84	0.15	47,48,48,52	0
3	CIT	C	702	13/13	0.85	0.12	28,44,59,62	0
3	CIT	A	703	13/13	0.85	0.13	27,44,66,71	0
3	CIT	B	702	13/13	0.87	0.12	32,41,62,67	0
3	CIT	D	702	13/13	0.89	0.11	31,42,60,64	0
4	EDO	A	701	4/4	0.90	0.10	23,25,27,30	0
4	EDO	B	703	4/4	0.90	0.09	24,24,24,27	0
4	EDO	D	703	4/4	0.90	0.12	23,24,31,32	0
4	EDO	C	703	4/4	0.91	0.10	23,25,28,29	0
2	TPP	A	702	26/26	0.98	0.05	12,15,21,24	0
2	TPP	C	701	26/26	0.98	0.05	13,17,22,23	0
2	TPP	D	701	26/26	0.98	0.06	12,16,20,25	0
2	TPP	B	701	26/26	0.98	0.06	13,17,24,25	0
5	MG	B	704	1/1	0.98	0.03	16,16,16,16	0
5	MG	C	704	1/1	0.98	0.03	16,16,16,16	0
5	MG	D	704	1/1	0.98	0.02	15,15,15,15	0
5	MG	A	705	1/1	0.99	0.02	15,15,15,15	0

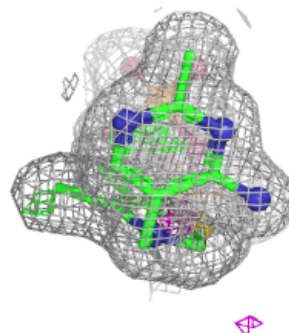
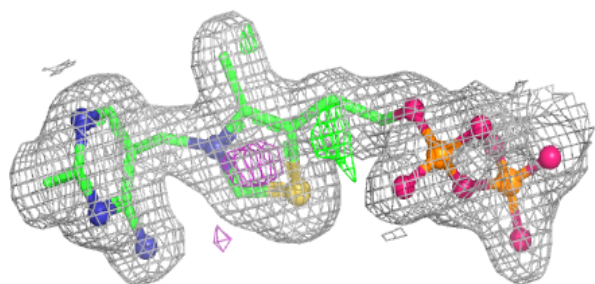
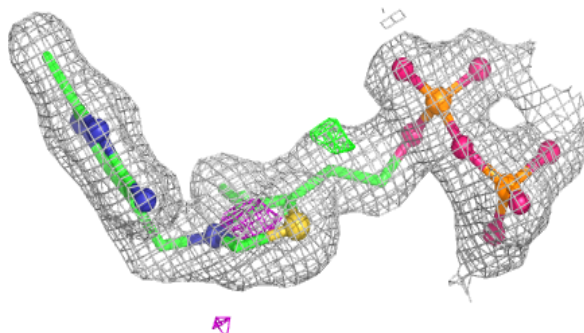
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 702:

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

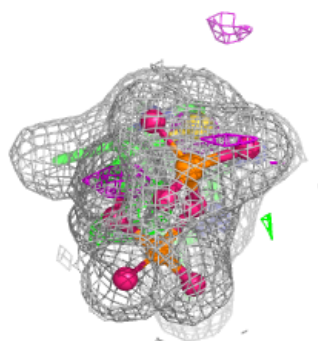
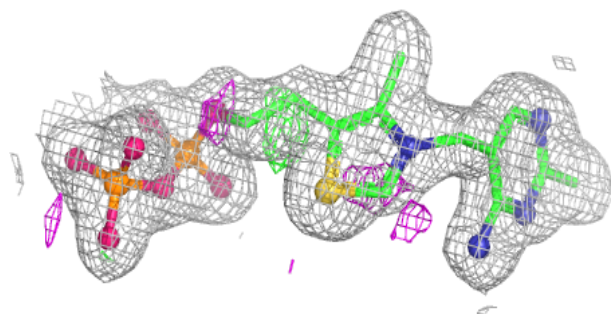
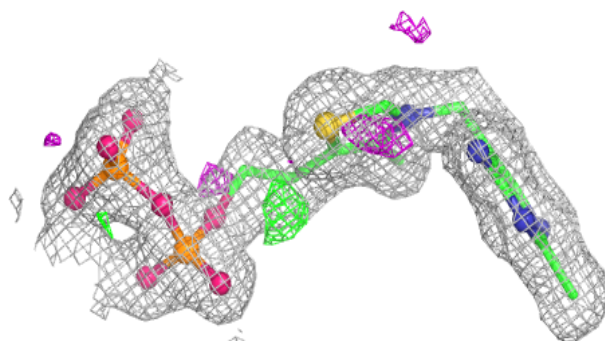
**Electron density around TPP C 701:**

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

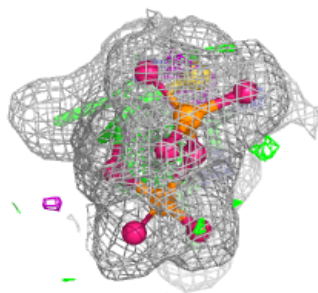
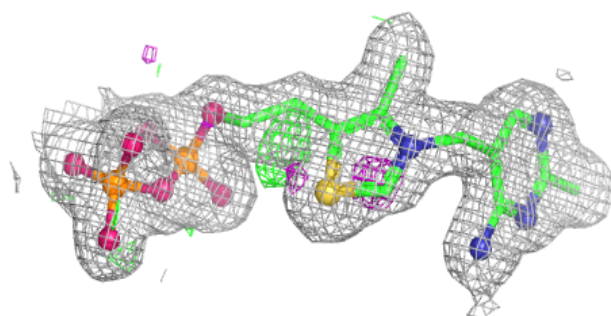
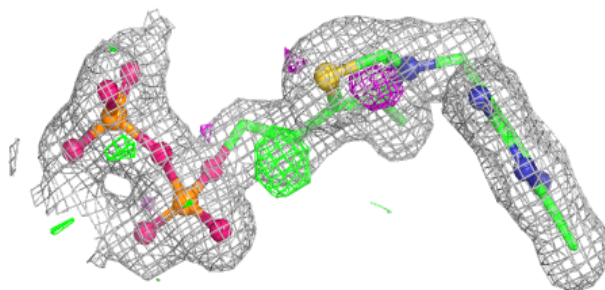


Electron density around TPP D 701:

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

**Electron density around TPP B 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.