



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2021 – 05:01 PM EDT

PDB ID : 3M49
Title : Crystal Structure of Transketolase Complexed with Thiamine Diphosphate from *Bacillus anthracis*
Authors : Maltseva, N.; Kim, Y.; Kwon, K.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2010-03-10
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.22
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) : 2.22

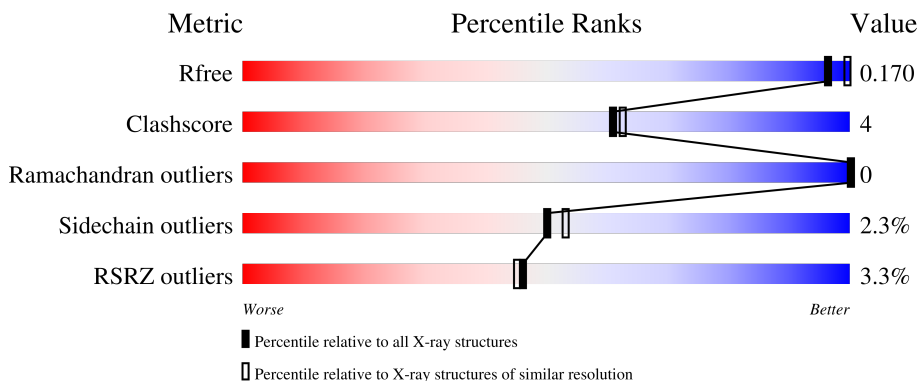
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	690	 89% 7%
1	B	690	 87% 9%

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
3	SO4	A	702	-	-	X	-
4	FMT	A	721	-	-	X	-
5	GOL	A	720	-	-	X	-
5	GOL	B	705	-	-	X	-
9	TRS	A	714[B]	-	X	-	-

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 11757 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
			Total	C	N	O	S	Se			
1	A	665	5167	3246	878	1019	1	23	0	10	0
1	B	664	5218	3271	890	1034	1	22	0	15	0

There are 48 discrepancies between the modelled and reference sequences:

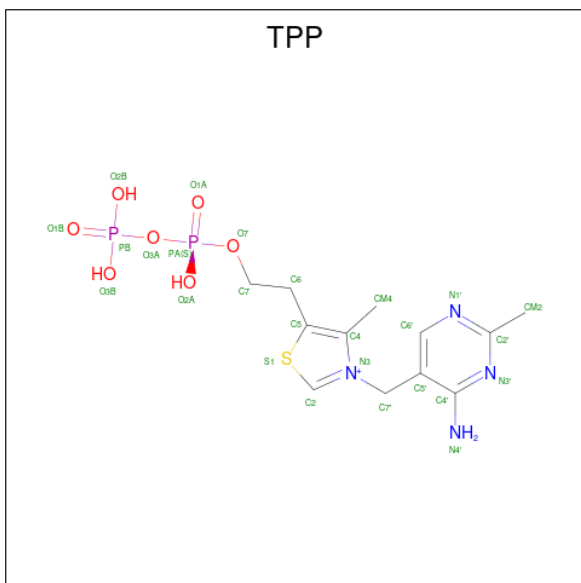
Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MSE	-	expression tag	UNP Q81Y15
A	-22	HIS	-	expression tag	UNP Q81Y15
A	-21	HIS	-	expression tag	UNP Q81Y15
A	-20	HIS	-	expression tag	UNP Q81Y15
A	-19	HIS	-	expression tag	UNP Q81Y15
A	-18	HIS	-	expression tag	UNP Q81Y15
A	-17	HIS	-	expression tag	UNP Q81Y15
A	-16	SER	-	expression tag	UNP Q81Y15
A	-15	SER	-	expression tag	UNP Q81Y15
A	-14	GLY	-	expression tag	UNP Q81Y15
A	-13	VAL	-	expression tag	UNP Q81Y15
A	-12	ASP	-	expression tag	UNP Q81Y15
A	-11	LEU	-	expression tag	UNP Q81Y15
A	-10	GLY	-	expression tag	UNP Q81Y15
A	-9	THR	-	expression tag	UNP Q81Y15
A	-8	GLU	-	expression tag	UNP Q81Y15
A	-7	ASN	-	expression tag	UNP Q81Y15
A	-6	LEU	-	expression tag	UNP Q81Y15
A	-5	TYR	-	expression tag	UNP Q81Y15
A	-4	PHE	-	expression tag	UNP Q81Y15
A	-3	GLN	-	expression tag	UNP Q81Y15
A	-2	SER	-	expression tag	UNP Q81Y15
A	-1	ASN	-	expression tag	UNP Q81Y15
A	0	ALA	-	expression tag	UNP Q81Y15
B	-23	MSE	-	expression tag	UNP Q81Y15

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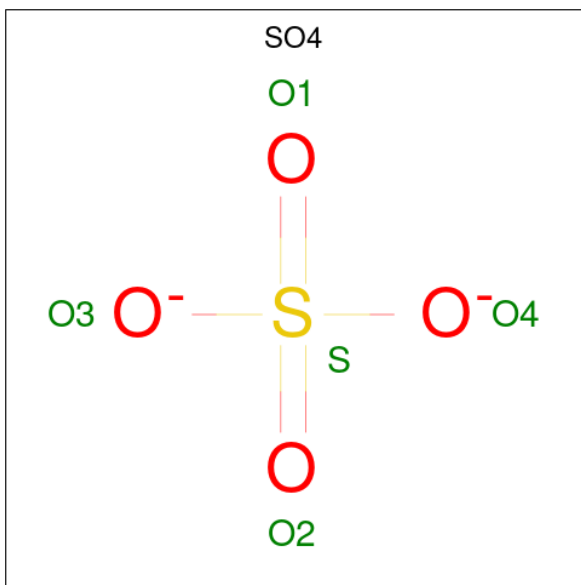
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	HIS	-	expression tag	UNP Q81Y15
B	-21	HIS	-	expression tag	UNP Q81Y15
B	-20	HIS	-	expression tag	UNP Q81Y15
B	-19	HIS	-	expression tag	UNP Q81Y15
B	-18	HIS	-	expression tag	UNP Q81Y15
B	-17	HIS	-	expression tag	UNP Q81Y15
B	-16	SER	-	expression tag	UNP Q81Y15
B	-15	SER	-	expression tag	UNP Q81Y15
B	-14	GLY	-	expression tag	UNP Q81Y15
B	-13	VAL	-	expression tag	UNP Q81Y15
B	-12	ASP	-	expression tag	UNP Q81Y15
B	-11	LEU	-	expression tag	UNP Q81Y15
B	-10	GLY	-	expression tag	UNP Q81Y15
B	-9	THR	-	expression tag	UNP Q81Y15
B	-8	GLU	-	expression tag	UNP Q81Y15
B	-7	ASN	-	expression tag	UNP Q81Y15
B	-6	LEU	-	expression tag	UNP Q81Y15
B	-5	TYR	-	expression tag	UNP Q81Y15
B	-4	PHE	-	expression tag	UNP Q81Y15
B	-3	GLN	-	expression tag	UNP Q81Y15
B	-2	SER	-	expression tag	UNP Q81Y15
B	-1	ASN	-	expression tag	UNP Q81Y15
B	0	ALA	-	expression tag	UNP Q81Y15

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



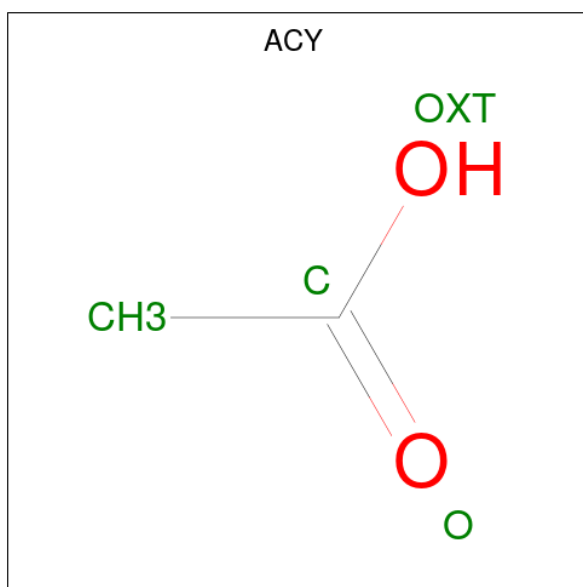
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



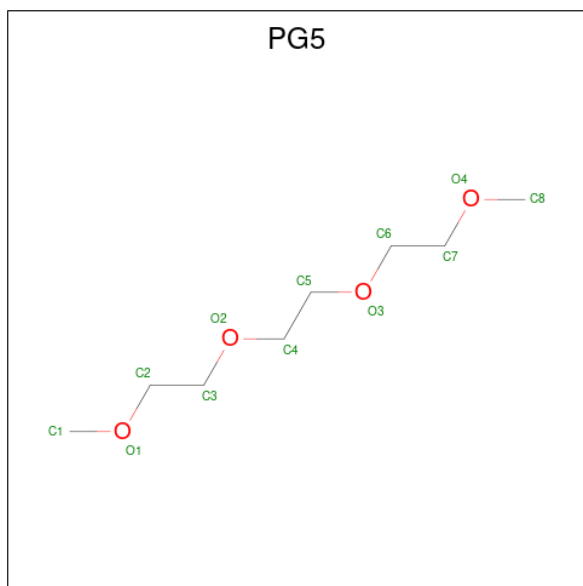
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 7 is 1-METHOXY-2-[2-(2-METHOXY-ETHOXY)]-ETHANE (three-letter code: PG5) (formula: $C_8H_{18}O_4$).



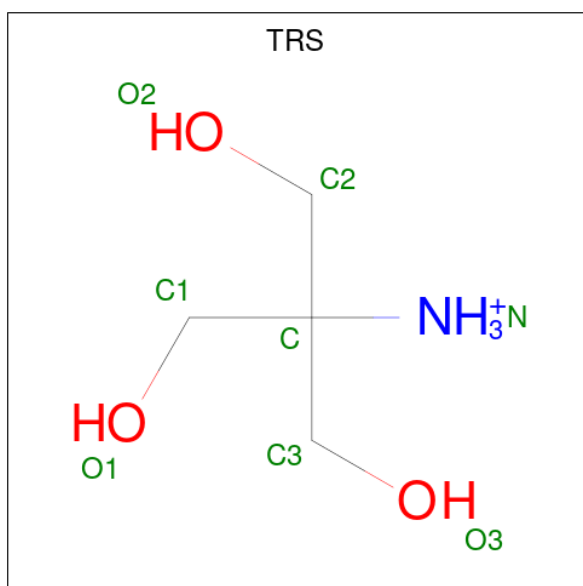
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).

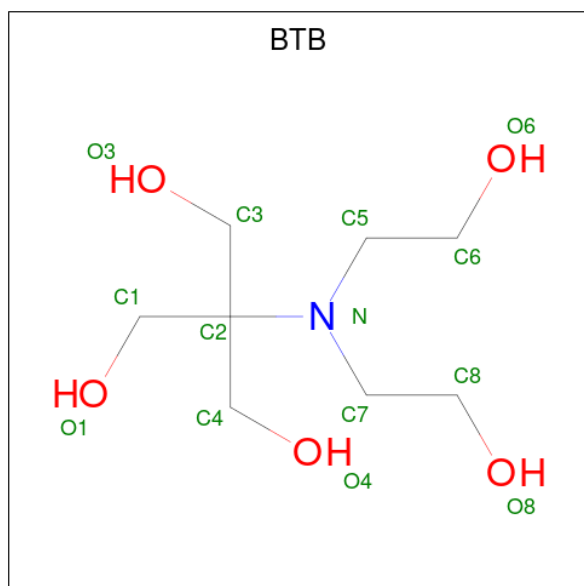


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	1
			16	8	2	6		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Mg 1 1	0	0

- Molecule 11 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C N O 14 8 1 5	0	0

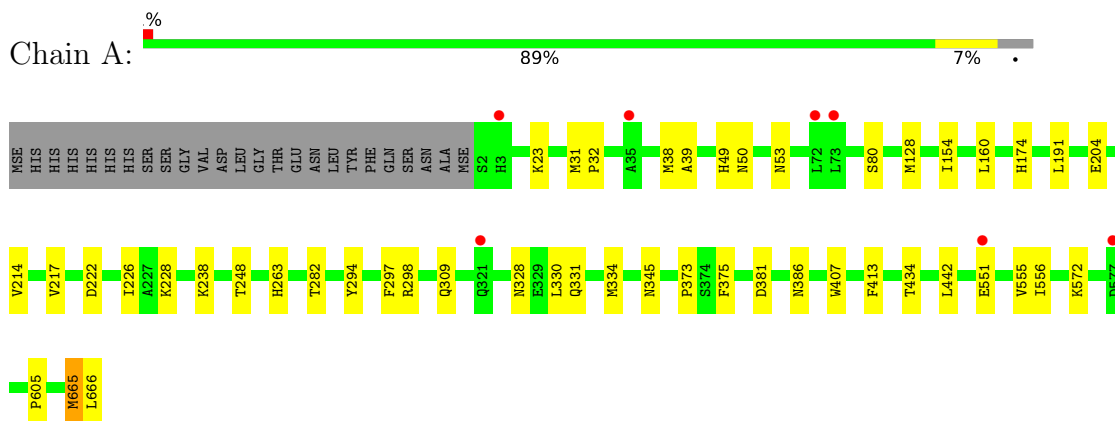
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	567	Total O 567 567	0	0
12	B	563	Total O 563 563	0	0

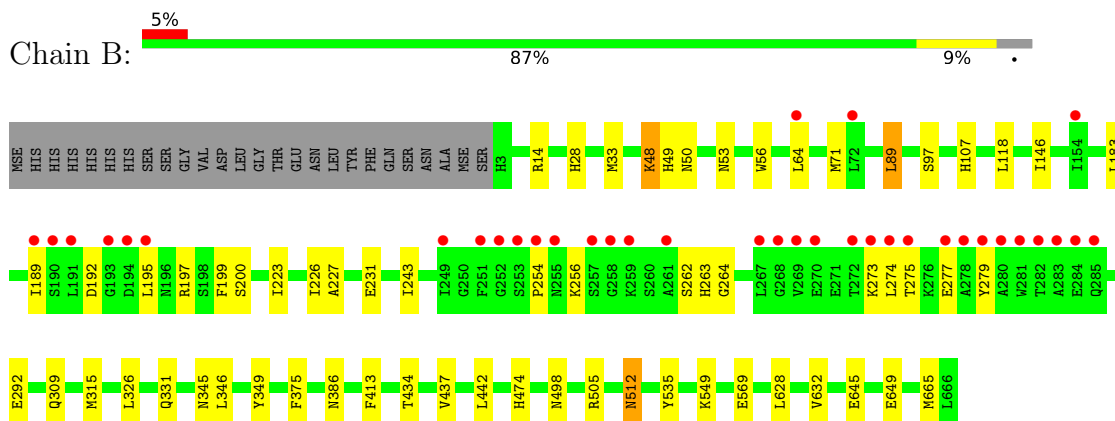
3 Residue-property plots [i](#)

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



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.33Å 132.09Å 137.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.73 – 2.00 31.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (31.73-2.00) 99.2 (31.73-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.23 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.137 , 0.172 0.133 , 0.170	Depositor DCC
R_{free} test set	5109 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.374	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for -h,l,k	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11757	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, PEG, GOL, FMT, TRS, MG, BTB, PG5, TPP, SO4

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	0.55	0/5256	0.61	0/7098
1	B	0.53	0/5307	0.60	0/7166
All	All	0.54	0/10563	0.60	0/14264

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	5167	0	4992	41	0
1	B	5218	0	5020	42	0
2	A	26	0	16	6	0
2	B	26	0	16	6	0
3	A	30	0	0	4	0
3	B	15	0	0	0	0
4	A	18	0	6	2	0
4	B	18	0	6	2	0
5	A	30	0	40	11	0
5	B	18	0	24	4	0
6	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	12	0	18	0	0
8	A	14	0	20	1	0
9	A	16	0	24	2	0
10	A	1	0	0	0	0
11	B	14	0	19	2	0
12	A	567	0	0	6	0
12	B	563	0	0	7	0
All	All	11757	0	10204	94	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 4.

All (94) 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:282:THR:H	5:A:720:GOL:H12	1.17	1.10
5:B:705:GOL:H31	12:B:876:HOH:O	1.61	0.99
1:B:349:TYR:H	1:B:498:ASN:HD21	1.15	0.92
3:A:702:SO4:O2	2:B:701:TPP:H2	1.71	0.91
3:A:702:SO4:O2	2:B:701:TPP:C2	2.18	0.91
3:A:702:SO4:S	2:B:701:TPP:H2	2.20	0.81
1:B:50:ASN:HD22	1:B:309:GLN:HE21	1.30	0.77
1:B:50:ASN:HD22	1:B:309:GLN:NE2	1.83	0.75
5:B:705:GOL:C3	12:B:876:HOH:O	2.23	0.75
5:A:720:GOL:H32	12:A:1100:HOH:O	1.87	0.74
2:A:701:TPP:O3B	12:A:1039:HOH:O	2.06	0.73
1:A:282:THR:N	5:A:720:GOL:H12	1.99	0.72
1:B:535:TYR:HB3	5:B:705:GOL:H32	1.77	0.67
1:B:349:TYR:H	1:B:498:ASN:ND2	1.93	0.66
4:B:707:FMT:O1	12:B:1028:HOH:O	2.14	0.65
2:A:701:TPP:H2	2:A:701:TPP:HN42	1.62	0.63
1:A:38[B]:MSE:CG	1:A:39:ALA:N	2.61	0.63
1:A:174:HIS:HD2	1:B:200:SER:OG	1.82	0.62
1:A:248:THR:H	4:A:721:FMT:C	2.13	0.61
1:B:53[A]:ASN:HB2	1:B:309:GLN:HE22	1.65	0.60
1:B:53[B]:ASN:HB3	1:B:309:GLN:HE22	1.66	0.60
1:A:53:ASN:ND2	1:A:309:GLN:OE1	2.35	0.59
1:A:38[B]:MSE:HG3	1:A:39:ALA:N	2.14	0.58
1:B:505[B]:ARG:NH2	5:B:705:GOL:O1	2.37	0.58
1:B:146:ILE:HD13	1:B:315:MSE:HE3	1.86	0.57
1:A:53:ASN:HB3	1:A:309:GLN:HE22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ASN:HD22	1:B:512:ASN:C	2.07	0.56
1:B:254:PRO:HG2	1:B:274:LEU:HB3	1.87	0.56
1:B:97:SER:O	1:B:107[A]:HIS:HE1	1.89	0.56
1:B:118:LEU:HD11	2:B:701:TPP:S1	2.47	0.55
1:B:345:ASN:O	11:B:703:BTB:H11	2.07	0.54
1:A:282:THR:OG1	5:A:720:GOL:C1	2.56	0.54
1:B:48:LYS:HD3	1:B:56:TRP:CH2	2.42	0.54
1:A:555:VAL:CG2	1:A:666:LEU:HD21	2.38	0.53
1:A:204:GLU:HG3	1:A:214:VAL:HG11	1.90	0.53
1:B:53[B]:ASN:ND2	1:B:309:GLN:OE1	2.41	0.52
1:B:28:HIS:CD2	1:B:264:GLY:HA2	2.45	0.52
2:A:701:TPP:HN42	2:A:701:TPP:C2	2.24	0.51
1:B:197:ARG:HD2	12:B:1201:HOH:O	2.10	0.51
1:A:228:LYS:HE3	12:A:850:HOH:O	2.10	0.51
1:B:345:ASN:O	11:B:703:BTB:H52	2.10	0.50
1:A:555:VAL:HG22	1:A:666:LEU:HD21	1.94	0.50
1:A:23:LYS:O	5:A:724:GOL:H2	2.12	0.50
1:A:407:TRP:CZ3	1:B:192:ASP:HB3	2.47	0.50
1:A:191:LEU:HD11	5:A:719:GOL:C3	2.42	0.49
1:A:572:LYS:HB3	1:A:572:LYS:NZ	2.28	0.49
1:A:407:TRP:HZ3	1:B:192:ASP:HB3	1.77	0.49
3:A:702:SO4:O2	2:B:701:TPP:S1	2.70	0.49
1:A:282:THR:H	5:A:720:GOL:C1	2.06	0.49
1:A:128:MSE:SE	12:A:927:HOH:O	2.79	0.49
8:A:717:PEG:H42	4:A:721:FMT:O1	2.13	0.49
1:A:282:THR:OG1	5:A:720:GOL:H12	2.13	0.48
1:B:256:LYS:HB3	1:B:262:SER:HB3	1.94	0.48
1:A:263:HIS:CE1	2:A:701:TPP:H72	2.49	0.48
1:A:298:ARG:HH12	9:A:714[B]:TRS:HN1	1.61	0.48
1:B:189:ILE:O	12:B:954:HOH:O	2.20	0.48
1:A:381:ASP:OD2	2:B:701:TPP:H61	2.13	0.48
1:B:28:HIS:HB3	1:B:263:HIS:O	2.14	0.48
1:A:31[B]:MSE:HB3	1:A:32:PRO:HD3	1.96	0.47
1:A:222:ASP:O	1:A:226:ILE:HD12	2.15	0.47
1:A:572:LYS:HG3	12:A:1118:HOH:O	2.15	0.47
1:B:227:ALA:O	1:B:231[A]:GLU:HG3	2.15	0.47
1:A:217:VAL:HG11	1:A:226:ILE:HG13	1.96	0.47
1:B:183:LEU:CD2	1:B:243:ILE:HD12	2.45	0.46
1:A:38[A]:MSE:CE	1:A:154:ILE:HG23	2.45	0.46
1:A:345:ASN:O	5:A:705:GOL:H32	2.15	0.46
1:B:549:LYS:HD3	1:B:549:LYS:HA	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LEU:CD1	1:B:505[B]:ARG:HD2	2.47	0.45
1:A:556:ILE:HD11	1:A:605:PRO:HD2	1.99	0.45
1:B:273:LYS:O	1:B:277:GLU:HG3	2.17	0.45
1:B:346:LEU:HD12	1:B:505[B]:ARG:HD2	1.99	0.44
1:B:292:GLU:HG2	12:B:1004:HOH:O	2.16	0.44
1:B:223:ILE:HA	1:B:226:ILE:HD12	2.00	0.44
1:B:645:GLU:O	1:B:649[B]:GLU:HG3	2.18	0.44
1:A:191:LEU:HB2	2:A:701:TPP:H62	2.00	0.43
1:A:331:GLN:HA	1:A:334:MSE:CE	2.48	0.43
1:A:282:THR:OG1	5:A:720:GOL:H11	2.19	0.43
1:A:294:TYR:CE2	9:A:714[A]:TRS:H11	2.54	0.42
1:B:275:THR:HG22	1:B:279:TYR:CE1	2.54	0.42
1:B:14:ARG:HD3	1:B:33:MSE:O	2.19	0.42
1:B:71:MSE:HE1	1:B:89:LEU:HG	2.02	0.42
1:A:665:MSE:HB3	1:A:665:MSE:HE2	1.55	0.42
1:A:373:PRO:HD2	12:A:991:HOH:O	2.19	0.42
1:B:386:ASN:HD21	1:B:434:THR:HA	1.85	0.42
1:A:263:HIS:ND1	2:A:701:TPP:O1B	2.46	0.42
1:B:195:LEU:HG	1:B:199:PHE:HB3	2.03	0.41
1:A:330:LEU:O	1:A:334:MSE:HG3	2.20	0.41
5:A:704:GOL:H32	5:A:720:GOL:O1	2.20	0.41
1:A:386:ASN:HD21	1:A:434:THR:HA	1.86	0.41
1:B:50:ASN:ND2	1:B:309:GLN:NE2	2.62	0.41
1:B:437:VAL:HG11	1:B:474:HIS:HA	2.02	0.41
1:A:80[A]:SER:HA	1:A:297:PHE:HB3	2.03	0.40
4:B:711:FMT:H	12:B:1158:HOH:O	2.21	0.40
1:B:33:MSE:HE3	1:B:275:THR:HG21	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	673/690 (98%)	660 (98%)	13 (2%)	0	100	100
1	B	677/690 (98%)	663 (98%)	14 (2%)	0	100	100
All	All	1350/1380 (98%)	1323 (98%)	27 (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	538/527 (102%)	528 (98%)	10 (2%)	57	61
1	B	542/527 (103%)	528 (97%)	14 (3%)	46	48
All	All	1080/1054 (102%)	1056 (98%)	24 (2%)	50	55

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	50	ASN
1	A	160	LEU
1	A	238	LYS
1	A	328	ASN
1	A	375	PHE
1	A	413	PHE
1	A	442	LEU
1	A	551	GLU
1	A	665	MSE
1	B	48	LYS
1	B	49	HIS
1	B	64	LEU
1	B	89	LEU
1	B	326	LEU
1	B	331	GLN
1	B	375	PHE
1	B	413	PHE

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Mol	Chain	Res	Type
1	B	442	LEU
1	B	512	ASN
1	B	569	GLU
1	B	628	LEU
1	B	632	VAL
1	B	665	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	53	ASN
1	A	174	HIS
1	A	309	GLN
1	A	386	ASN
1	B	263	HIS
1	B	309	GLN
1	B	386	ASN
1	B	498	ASN
1	B	512	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 1 is 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
5	GOL	A	704	-	5,5,5	0.35	0	5,5,5	0.16	0
3	SO4	B	714	-	4,4,4	0.57	0	6,6,6	0.35	0
3	SO4	A	708	-	4,4,4	0.14	0	6,6,6	0.18	0
5	GOL	A	720	-	5,5,5	0.24	0	5,5,5	1.05	0
4	FMT	A	721	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	A	702	-	4,4,4	0.58	0	6,6,6	0.24	0
5	GOL	A	705	-	5,5,5	0.32	0	5,5,5	0.72	0
5	GOL	A	724	-	5,5,5	0.66	0	5,5,5	0.92	0
4	FMT	B	711	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	707	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	A	722	-	4,4,4	0.15	0	6,6,6	0.22	0
5	GOL	A	719	-	5,5,5	0.30	0	5,5,5	0.46	0
4	FMT	A	718	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	713	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	A	706	-	4,4,4	0.17	0	6,6,6	0.31	0
4	FMT	A	723	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	A	709	-	4,4,4	0.14	0	6,6,6	0.18	0
4	FMT	B	709	-	0,2,2	0.00	-	0,1,1	0.00	-
3	SO4	B	702	-	4,4,4	0.13	0	6,6,6	0.23	0
7	PG5	A	712	-	11,11,11	0.48	0	10,10,10	1.02	0
9	TRS	A	714[A]	-	7,7,7	0.38	0	9,9,9	1.44	2 (22%)
3	SO4	A	707	-	4,4,4	0.15	0	6,6,6	0.10	0
4	FMT	A	715	-	0,2,2	0.00	-	0,1,1	0.00	-
2	TPP	B	701	-	22,27,27	1.33	3 (13%)	29,40,40	2.99	8 (27%)
8	PEG	A	717	-	6,6,6	0.58	0	5,5,5	1.54	1 (20%)
8	PEG	A	713	-	6,6,6	0.55	0	5,5,5	1.67	1 (20%)
9	TRS	A	714[B]	-	7,7,7	0.32	0	9,9,9	1.15	1 (11%)
4	FMT	A	710	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	A	703	-	0,2,2	0.00	-	0,1,1	0.00	-
6	ACY	A	711	-	1,3,3	1.73	0	0,3,3	0.00	-
11	BTB	B	703	-	13,13,13	1.10	1 (7%)	7,16,16	0.76	0
3	SO4	B	708	-	4,4,4	0.09	0	6,6,6	0.14	0
5	GOL	B	712	-	5,5,5	0.30	0	5,5,5	0.49	0
2	TPP	A	701	10	22,27,27	1.41	3 (13%)	29,40,40	1.83	11 (37%)
4	FMT	B	706	-	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	B	704	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	705	-	5,5,5	0.31	0	5,5,5	1.47	2 (40%)
5	GOL	B	710	-	5,5,5	0.38	0	5,5,5	0.22	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
8	PEG	A	713	-	-	1/4/4/4	-
5	GOL	A	704	-	-	2/4/4/4	-
5	GOL	A	719	-	-	0/4/4/4	-
9	TRS	A	714[B]	-	-	9/9/9/9	-
7	PG5	A	712	-	-	4/9/9/9	-
9	TRS	A	714[A]	-	-	6/9/9/9	-
11	BTB	B	703	-	-	4/21/21/21	-
5	GOL	A	720	-	-	0/4/4/4	-
5	GOL	A	724	-	-	2/4/4/4	-
2	TPP	A	701	10	-	5/16/17/17	0/2/2/2
5	GOL	A	705	-	-	0/4/4/4	-
5	GOL	B	712	-	-	2/4/4/4	-
2	TPP	B	701	-	-	5/16/17/17	0/2/2/2
8	PEG	A	717	-	-	2/4/4/4	-
5	GOL	B	705	-	-	2/4/4/4	-
5	GOL	B	710	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	TPP	C4-N3	-4.17	1.36	1.39
2	B	701	TPP	C5'-C4'	3.81	1.49	1.42
2	B	701	TPP	C4-N3	-3.40	1.36	1.39
2	A	701	TPP	C5'-C4'	2.71	1.47	1.42
2	A	701	TPP	C7'-N3	-2.63	1.43	1.48
11	B	703	BTB	C5-N	-2.36	1.44	1.48
2	B	701	TPP	C6-C5	2.20	1.51	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	TPP	C6-C5-C4	12.96	137.84	127.43
2	B	701	TPP	C6'-N1'-C2'	4.53	123.68	115.96
2	B	701	TPP	C5'-C7'-N3	-3.72	107.08	113.28
2	A	701	TPP	C6'-N1'-C2'	3.54	121.98	115.96
2	A	701	TPP	N4'-C4'-N3'	3.47	121.94	117.03
2	B	701	TPP	N1'-C2'-N3'	-3.22	120.00	125.54
2	A	701	TPP	PA-O3A-PB	-2.94	122.75	132.83
2	B	701	TPP	C7'-N3-C2	-2.88	120.15	125.35
2	B	701	TPP	CM2-C2'-N1'	2.86	120.28	117.14
2	A	701	TPP	N1'-C2'-N3'	-2.61	121.05	125.54
9	A	714[B]	TRS	O1-C1-C	2.60	119.23	111.00
2	A	701	TPP	CM4-C4-N3	2.56	125.79	122.53
2	B	701	TPP	C5'-C6'-N1'	-2.54	119.58	123.82
9	A	714[A]	TRS	O2-C2-C	-2.45	103.22	111.00
2	A	701	TPP	CM4-C4-C5	-2.33	122.50	127.60
2	A	701	TPP	C5'-C6'-N1'	-2.29	120.00	123.82
2	A	701	TPP	C5'-C7'-N3	-2.20	109.61	113.28
8	A	713	PEG	O2-C3-C4	2.17	119.59	110.07
2	A	701	TPP	O3B-PB-O2B	2.17	115.92	107.64
9	A	714[A]	TRS	C1-C-N	2.17	114.45	107.98
5	B	705	GOL	O2-C2-C3	-2.16	99.61	109.12
2	B	701	TPP	C5-C4-N3	2.15	111.88	107.57
2	A	701	TPP	CM2-C2'-N3'	2.08	120.39	117.15
2	A	701	TPP	C5-C4-N3	2.07	111.71	107.57
5	B	705	GOL	O1-C1-C2	-2.04	100.44	110.20
8	A	717	PEG	O2-C2-C1	2.00	118.87	110.07

There are no chirality outliers.

All (46) 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	A	701	TPP	C7-O7-PA-O2A
2	A	701	TPP	C7-O7-PA-O3A
2	B	701	TPP	C4-C5-C6-C7
2	B	701	TPP	C5-C6-C7-O7
2	B	701	TPP	C7-O7-PA-O1A
2	B	701	TPP	C7-O7-PA-O2A
5	A	704	GOL	O1-C1-C2-C3
5	A	724	GOL	C1-C2-C3-O3
5	B	705	GOL	O1-C1-C2-C3
5	B	710	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	B	712	GOL	O1-C1-C2-C3
9	A	714[A]	TRS	C1-C-C2-O2
9	A	714[A]	TRS	C3-C-C2-O2
9	A	714[A]	TRS	N-C-C2-O2
9	A	714[A]	TRS	C1-C-C3-O3
9	A	714[B]	TRS	C3-C-C1-O1
9	A	714[B]	TRS	C1-C-C2-O2
9	A	714[B]	TRS	C3-C-C2-O2
9	A	714[B]	TRS	N-C-C2-O2
9	A	714[B]	TRS	C1-C-C3-O3
9	A	714[B]	TRS	C2-C-C3-O3
9	A	714[B]	TRS	N-C-C3-O3
11	B	703	BTB	C1-C2-C4-O4
11	B	703	BTB	C3-C2-C4-O4
11	B	703	BTB	N-C2-C4-O4
8	A	717	PEG	O2-C3-C4-O4
7	A	712	PG5	O3-C6-C7-O4
5	A	704	GOL	O1-C1-C2-O2
5	A	724	GOL	O2-C2-C3-O3
5	B	705	GOL	O1-C1-C2-O2
5	B	710	GOL	O1-C1-C2-O2
5	B	712	GOL	O1-C1-C2-O2
9	A	714[A]	TRS	C2-C-C3-O3
9	A	714[B]	TRS	C2-C-C1-O1
8	A	713	PEG	C1-C2-O2-C3
7	A	712	PG5	O1-C2-C3-O2
7	A	712	PG5	C2-C3-O2-C4
9	A	714[A]	TRS	N-C-C3-O3
9	A	714[B]	TRS	N-C-C1-O1
7	A	712	PG5	C3-C2-O1-C1
11	B	703	BTB	O1-C1-C2-N
8	A	717	PEG	C4-C3-O2-C2
2	B	701	TPP	C7-O7-PA-O3A
2	A	701	TPP	C4-C5-C6-C7

There are no ring outliers.

16 monomers are involved in 35 short contacts:

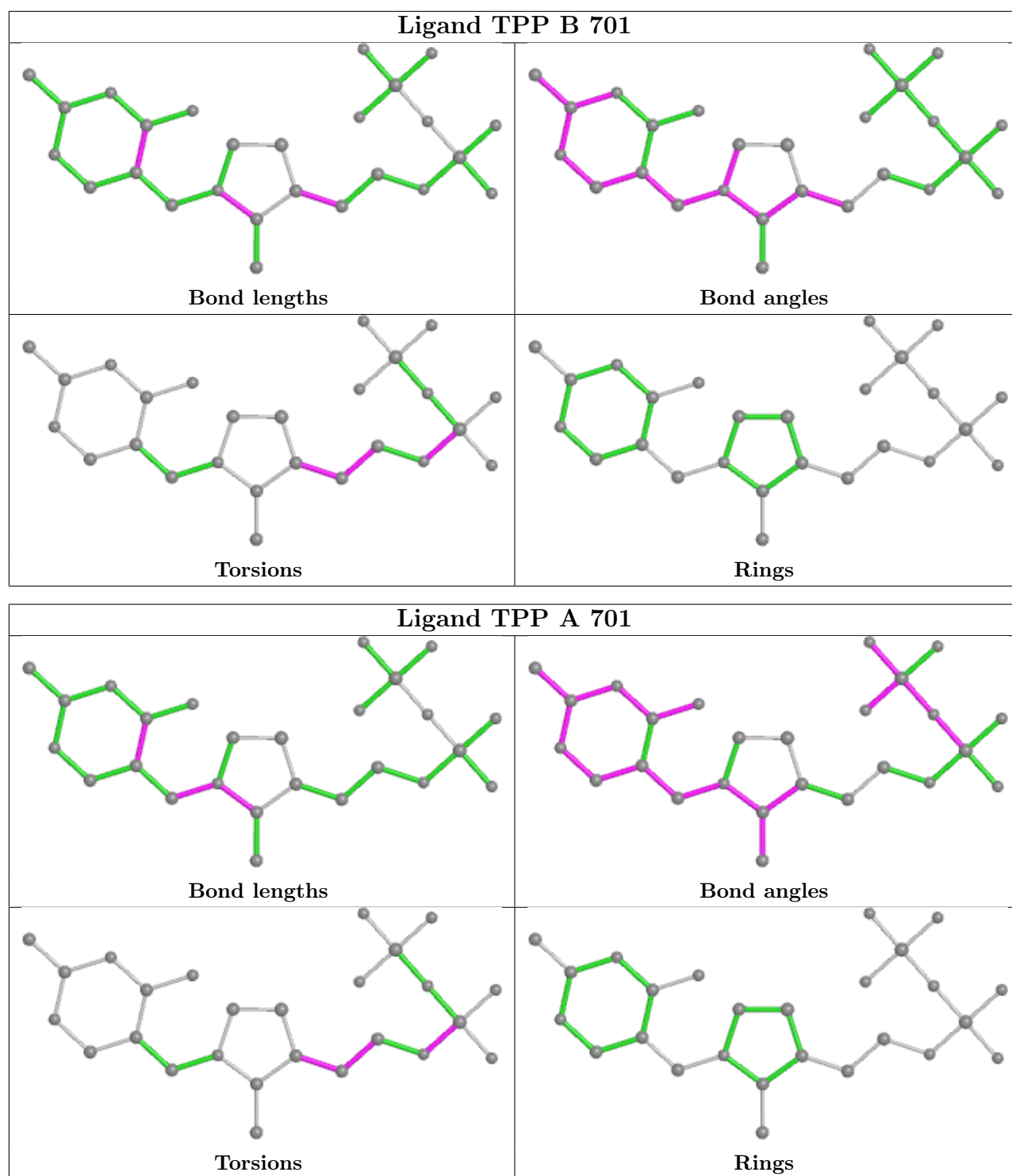
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	GOL	1	0
5	A	720	GOL	8	0
4	A	721	FMT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	SO4	4	0
5	A	705	GOL	1	0
5	A	724	GOL	1	0
4	B	711	FMT	1	0
4	B	707	FMT	1	0
5	A	719	GOL	1	0
9	A	714[A]	TRS	1	0
2	B	701	TPP	6	0
8	A	717	PEG	1	0
9	A	714[B]	TRS	1	0
11	B	703	BTB	2	0
2	A	701	TPP	6	0
5	B	705	GOL	4	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

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	644/690 (93%)	-0.45	7 (1%) 80 79	10, 17, 37, 69	0
1	B	643/690 (93%)	-0.33	36 (5%) 24 23	10, 19, 50, 105	0
All	All	1287/1380 (93%)	-0.39	43 (3%) 46 45	10, 18, 44, 105	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	274	LEU	5.8
1	B	284	GLU	5.0
1	B	282	THR	4.9
1	B	283	ALA	4.4
1	B	255	ASN	3.9
1	B	277	GLU	3.8
1	B	258	GLY	3.6
1	B	268	GLY	3.5
1	B	249	ILE	3.5
1	A	72	LEU	3.3
1	B	285	GLN	3.3
1	B	254	PRO	3.3
1	B	193	GLY	3.2
1	B	194	ASP	3.0
1	B	280	ALA	3.0
1	B	273	LYS	3.0
1	B	270	GLU	2.9
1	B	253	SER	2.9
1	B	281	TRP	2.9
1	B	191	LEU	2.8
1	B	257	SER	2.8
1	B	269	VAL	2.8
1	B	275	THR	2.7
1	B	190	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	189	ILE	2.6
1	B	252	GLY	2.6
1	B	267	LEU	2.4
1	B	259	LYS	2.4
1	A	73	LEU	2.4
1	B	261	ALA	2.4
1	A	551	GLU	2.4
1	B	278	ALA	2.4
1	B	279	TYR	2.3
1	B	272	THR	2.3
1	A	577	ASP	2.2
1	B	64	LEU	2.2
1	B	195	LEU	2.2
1	B	154	ILE	2.2
1	A	3	HIS	2.1
1	B	251	PHE	2.1
1	B	72	LEU	2.1
1	A	321	GLN	2.1
1	A	35	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FMT	B	706	3/3	0.55	0.20	57,57,58,60	0
9	TRS	A	714[A]	8/8	0.64	0.29	29,34,39,42	8
9	TRS	A	714[B]	8/8	0.64	0.29	27,32,36,38	8
4	FMT	B	713	3/3	0.70	0.29	54,54,59,60	0

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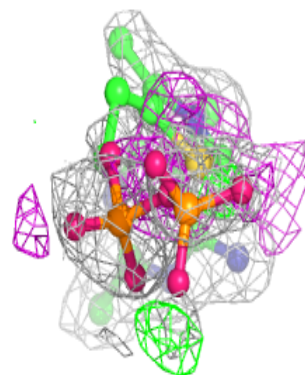
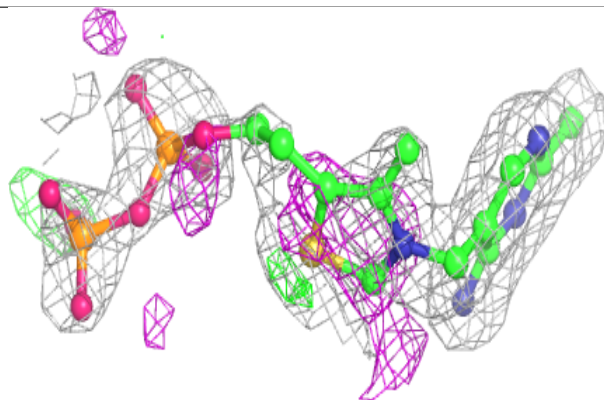
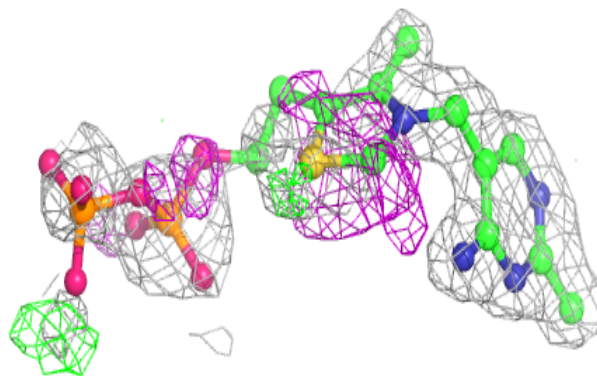
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PEG	A	717	7/7	0.73	0.26	62,66,68,71	0
7	PG5	A	712	12/12	0.75	0.21	52,57,59,60	0
5	GOL	B	710	6/6	0.78	0.18	68,69,70,71	0
5	GOL	B	712	6/6	0.78	0.21	62,63,66,70	0
6	ACY	A	711	4/4	0.80	0.22	72,74,75,76	0
3	SO4	A	707	5/5	0.81	0.30	118,119,120,121	0
5	GOL	A	705	6/6	0.83	0.24	32,45,48,48	0
4	FMT	A	703	3/3	0.83	0.18	41,41,45,45	0
4	FMT	B	704	3/3	0.84	0.24	47,47,52,52	0
3	SO4	B	702	5/5	0.85	0.23	71,75,78,82	0
4	FMT	B	707	3/3	0.86	0.18	51,51,55,58	0
4	FMT	A	715	3/3	0.86	0.15	33,33,43,48	0
4	FMT	A	710	3/3	0.87	0.12	58,58,58,59	0
3	SO4	B	714	5/5	0.87	0.36	71,77,78,79	0
4	FMT	A	723	3/3	0.87	0.12	59,59,59,60	0
4	FMT	A	718	3/3	0.88	0.13	49,49,51,54	0
4	FMT	A	721	3/3	0.88	0.23	39,39,45,45	0
3	SO4	A	702	5/5	0.88	0.27	60,72,75,77	0
8	PEG	A	713	7/7	0.89	0.28	48,49,55,56	0
3	SO4	A	722	5/5	0.89	0.30	75,77,80,85	0
3	SO4	A	709	5/5	0.89	0.38	79,83,89,90	5
4	FMT	B	711	3/3	0.89	0.18	40,40,47,50	0
5	GOL	B	705	6/6	0.90	0.33	51,58,63,63	0
2	TPP	B	701	26/26	0.90	0.18	11,41,123,137	0
5	GOL	A	720	6/6	0.90	0.39	41,51,53,58	0
11	BTB	B	703	14/14	0.90	0.23	27,43,50,51	0
4	FMT	B	709	3/3	0.91	0.18	47,47,53,60	0
5	GOL	A	719	6/6	0.92	0.12	38,42,43,44	0
3	SO4	A	706	5/5	0.93	0.11	59,65,69,73	0
5	GOL	A	724	6/6	0.93	0.38	19,35,46,46	0
2	TPP	A	701	26/26	0.95	0.12	11,30,67,82	0
5	GOL	A	704	6/6	0.96	0.21	19,36,48,54	0
3	SO4	A	708	5/5	0.97	0.17	65,67,69,71	0
3	SO4	B	708	5/5	0.97	0.11	39,48,54,57	0
10	MG	A	716	1/1	1.00	0.06	20,20,20,20	0

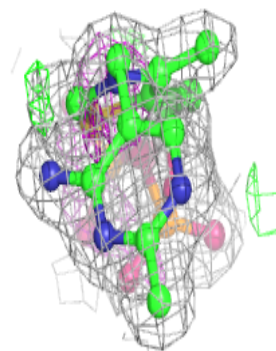
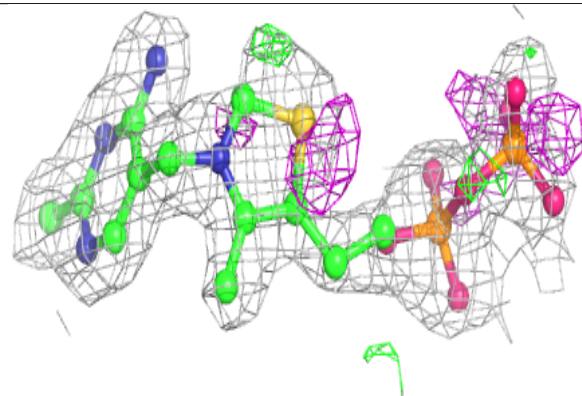
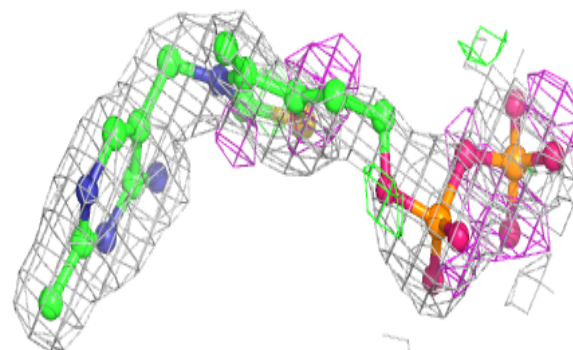
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP B 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 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.