



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 4, 2024 – 03:08 AM EST

PDB ID : 1NGS  
Title : COMPLEX OF TRANSKETOLASE WITH THIAMIN DIPHOSPHATE,  
CA<sup>2+</sup> AND ACCEPTOR SUBSTRATE ERYTHROSE-4-PHOSPHATE  
Authors : Nilsson, U.; Lindqvist, Y.; Schneider, G.  
Deposited on : 1996-09-25  
Resolution : 2.40 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](mailto: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>.

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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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

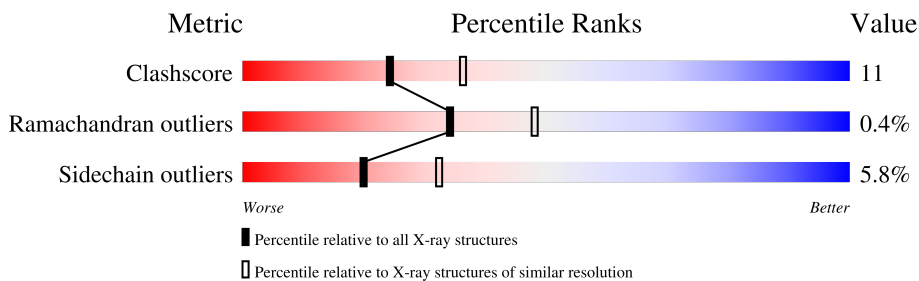
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	680	
1	B	680	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10928 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.

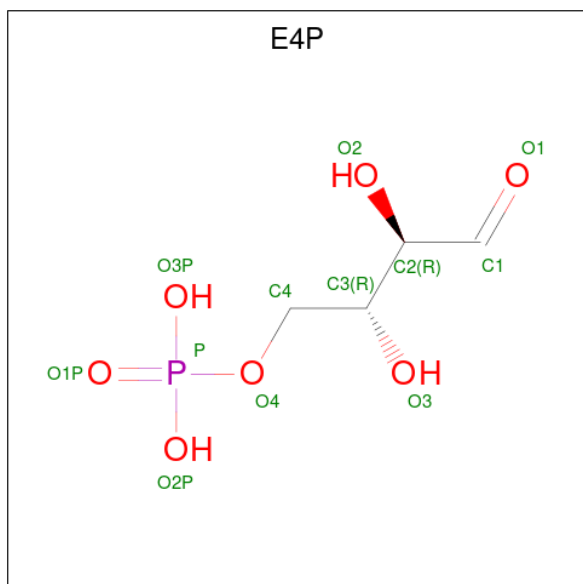
- Molecule 1 is a protein called TRANSKETOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	678	5198	3312	884	990	12	0	0	0
1	B	678	5198	3312	884	990	12	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

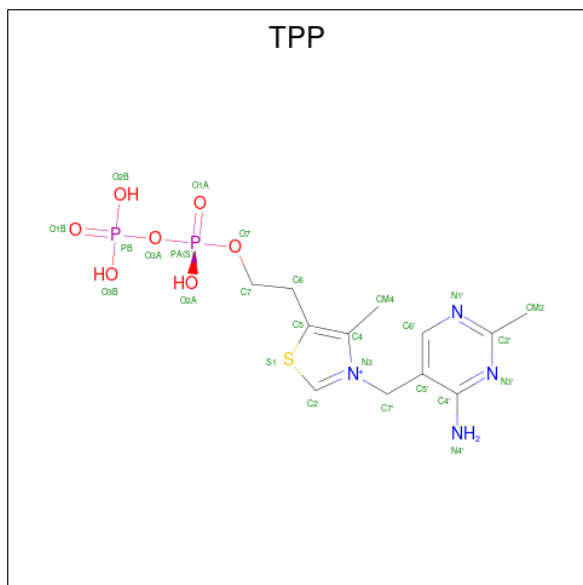
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ERYTHROSE-4-PHOSPHATE (three-letter code: E4P) (formula: C<sub>4</sub>H<sub>9</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			12	4	7	1		
3	B	1	Total	C	O	P	0	0
			12	4	7	1		

- Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



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.

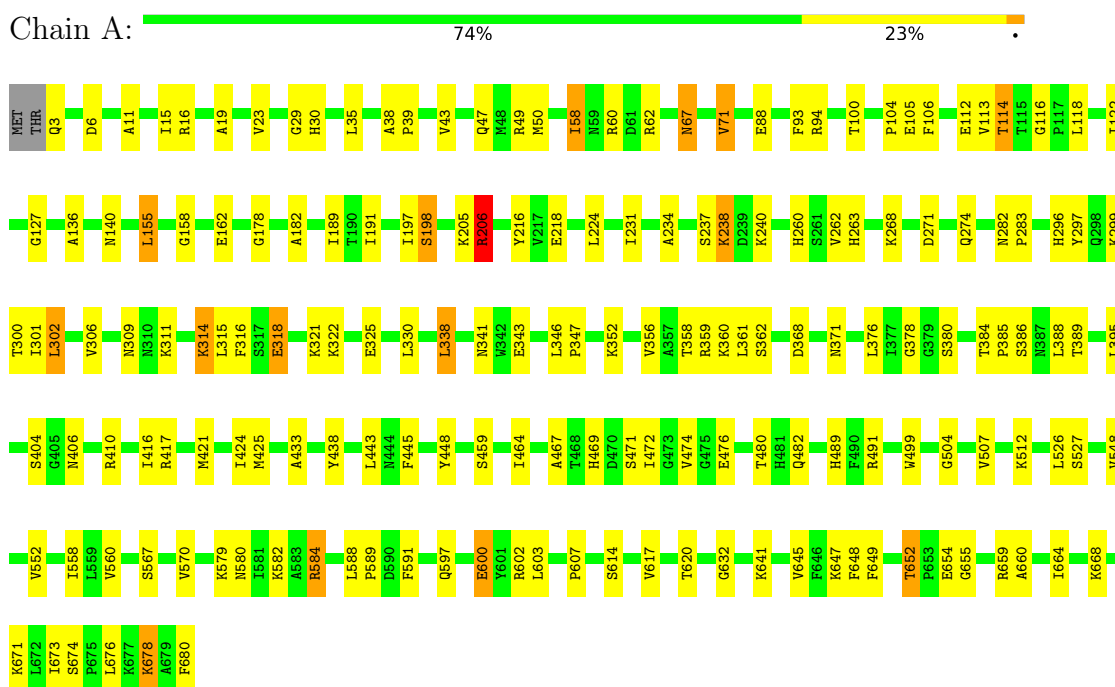
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	237	Total	O	0	0
			237	237		
5	B	217	Total	O	0	0
			217	217		

### 3 Residue-property plots

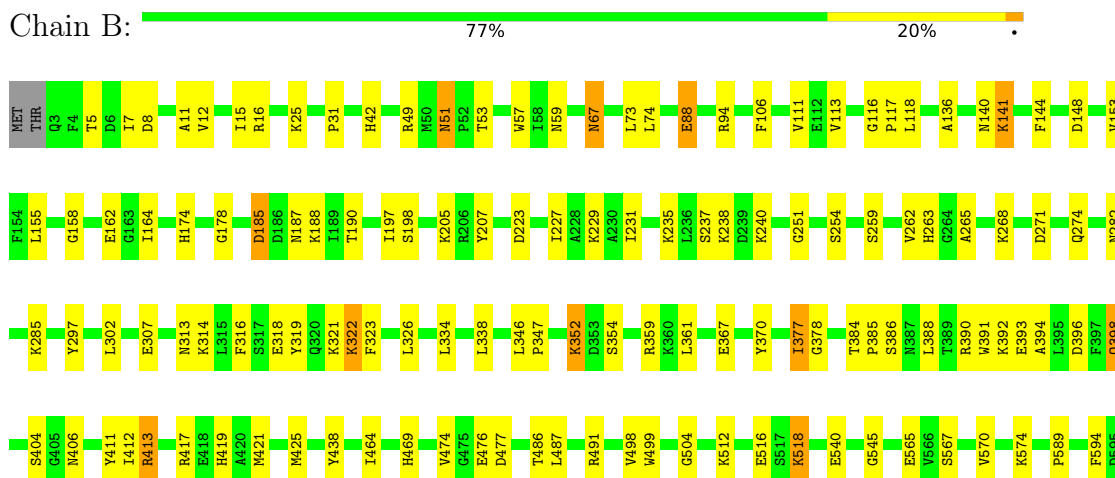
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

- Molecule 1: TRANSKETOLASE



- Molecule 1: TRANSKETOLASE





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.50Å 113.30Å 160.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.206 , 0.239	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	10928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 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, E4P

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	0.50	1/5324 (0.0%)	0.82	6/7230 (0.1%)
1	B	0.59	4/5324 (0.1%)	0.81	7/7230 (0.1%)
All	All	0.55	5/10648 (0.0%)	0.81	13/14460 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	GLU	CG-CD	14.33	1.73	1.51
1	B	88	GLU	CB-CG	13.39	1.77	1.52
1	B	88	GLU	CD-OE1	-10.22	1.14	1.25
1	A	600	GLU	CD-OE1	-6.28	1.18	1.25
1	B	600	GLU	CD-OE1	-5.45	1.19	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	GLU	OE1-CD-OE2	-9.87	111.45	123.30
1	A	206	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	A	58	ILE	CA-CB-CG1	-9.17	93.58	111.00
1	A	206	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	88	GLU	CG-CD-OE2	6.40	131.11	118.30
1	B	88	GLU	CG-CD-OE1	-6.19	105.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	600	GLU	OE1-CD-OE2	-6.17	115.90	123.30
1	A	116	GLY	N-CA-C	-5.94	98.25	113.10
1	B	88	GLU	CB-CG-CD	5.81	129.90	114.20
1	B	185	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	116	GLY	N-CA-C	-5.71	98.83	113.10
1	A	600	GLU	CG-CD-OE2	5.30	128.90	118.30
1	B	155	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	TYR	Sidechain

## 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	5198	0	5139	133	1
1	B	5198	0	5139	104	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	7	1	0
3	B	12	0	7	1	0
4	A	26	0	16	3	0
4	B	26	0	16	4	0
5	A	237	0	0	13	2
5	B	217	0	0	13	0
All	All	10928	0	10324	229	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 11.

All (229) 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:88:GLU:CG	1:B:88:GLU:CB	1.77	1.61
1:A:58:ILE:CD1	1:A:58:ILE:CG1	1.84	1.51
1:A:58:ILE:HG12	5:A:981:HOH:O	1.47	1.09
1:B:307:GLU:HG3	5:B:1094:HOH:O	1.58	0.99
1:A:652:THR:HG22	1:A:655:GLY:H	1.35	0.91
1:A:58:ILE:HD12	1:A:58:ILE:HA	1.53	0.90
1:A:358:THR:HG22	1:A:526:LEU:HD22	1.53	0.88
1:B:67:ASN:HD22	1:B:67:ASN:H	1.19	0.88
1:B:51:ASN:HD21	1:B:53:THR:HB	1.38	0.87
1:A:67:ASN:H	1:A:67:ASN:HD22	1.19	0.87
1:A:58:ILE:CD1	1:A:58:ILE:HA	2.07	0.83
1:A:71:VAL:HG13	1:A:104:PRO:HD3	1.59	0.83
1:A:680:PHE:CG	1:B:659:ARG:HG2	2.13	0.82
1:A:322:LYS:HD2	5:A:1047:HOH:O	1.78	0.82
1:A:311:LYS:O	1:A:314:LYS:HG3	1.80	0.81
1:B:237:SER:HB2	5:B:974:HOH:O	1.80	0.81
1:B:487:LEU:O	1:B:491:ARG:HG3	1.79	0.80
4:B:682:TPP:H2	4:B:682:TPP:HN42	1.50	0.77
1:A:603:LEU:HD23	1:A:676:LEU:HD12	1.67	0.76
1:A:548:VAL:HG13	1:A:584:ARG:HD2	1.68	0.76
1:A:58:ILE:HG13	1:A:58:ILE:O	1.86	0.76
1:A:652:THR:HG22	1:A:655:GLY:N	2.00	0.75
1:A:106:PHE:H	1:A:114:THR:HG22	1.52	0.75
1:A:67:ASN:H	1:A:67:ASN:ND2	1.85	0.74
1:A:491:ARG:HD2	1:A:591:PHE:CD2	2.22	0.74
1:B:359:ARG:HD2	1:B:386:SER:O	1.87	0.74
4:B:682:TPP:HN42	4:B:682:TPP:C2	2.01	0.73
1:A:67:ASN:HD22	1:A:67:ASN:N	1.82	0.72
1:A:476:GLU:HB3	1:B:94:ARG:HD3	1.70	0.72
1:B:51:ASN:ND2	1:B:53:THR:HB	2.04	0.72
1:A:58:ILE:CD1	1:A:58:ILE:CB	2.68	0.72
1:A:105:GLU:HA	1:A:114:THR:HB	1.72	0.71
1:A:88:GLU:HG2	5:A:1099:HOH:O	1.91	0.70
1:A:296:HIS:CE1	5:A:908:HOH:O	2.45	0.69
1:B:67:ASN:HD22	1:B:67:ASN:N	1.88	0.68
1:B:67:ASN:H	1:B:67:ASN:ND2	1.91	0.68
1:A:58:ILE:CD1	1:A:58:ILE:CA	2.73	0.67
1:B:223:ASP:O	1:B:227:ILE:HG13	1.94	0.67
1:A:114:THR:HG23	1:A:459:SER:OG	1.96	0.66
1:A:680:PHE:CD1	1:B:659:ARG:HG2	2.30	0.65
1:A:433:ALA:HB2	5:A:981:HOH:O	1.97	0.65
1:A:358:THR:HG22	1:A:526:LEU:CD2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:LYS:HE2	5:B:1061:HOH:O	1.98	0.63
1:A:206:ARG:NH2	5:A:935:HOH:O	2.31	0.63
1:B:49:ARG:NH1	5:B:939:HOH:O	2.31	0.63
1:B:469:HIS:HB3	1:B:474:VAL:CG2	2.28	0.62
1:B:617:VAL:HG11	1:B:646:PHE:CE1	2.34	0.62
1:A:162:GLU:OE2	4:A:682:TPP:HM23	2.00	0.61
1:B:377:ILE:HD11	1:B:412:ILE:HD11	1.83	0.60
1:A:359:ARG:HD2	1:A:386:SER:O	2.01	0.60
1:A:6:ASP:HB3	5:A:1090:HOH:O	2.01	0.60
1:B:469:HIS:HB3	1:B:474:VAL:HG22	1.84	0.60
1:B:491:ARG:HD3	5:B:1029:HOH:O	2.02	0.59
1:A:314:LYS:HE2	1:A:315:LEU:HB2	1.84	0.59
1:A:395:LEU:HD21	1:A:406:ASN:ND2	2.17	0.59
1:A:30:HIS:NE2	3:A:900:E4P:C1	2.66	0.59
1:A:659:ARG:HD3	1:B:680:PHE:CD2	2.37	0.59
1:A:205:LYS:HG3	1:B:205:LYS:HE3	1.85	0.59
1:A:472:ILE:HG23	5:A:990:HOH:O	2.02	0.58
1:A:347:PRO:HG3	1:A:368:ASP:OD2	2.03	0.58
1:A:118:LEU:HD13	1:A:158:GLY:HA3	1.86	0.58
1:B:391:TRP:CD1	1:B:394:ALA:HB2	2.39	0.57
1:A:678:LYS:HB3	1:A:678:LYS:NZ	2.19	0.57
1:B:164:ILE:HD12	1:B:419:HIS:CD2	2.39	0.57
1:B:282:ASN:ND2	1:B:285:LYS:HD3	2.20	0.57
1:A:416:ILE:HD13	1:B:158:GLY:HA2	1.87	0.57
1:B:11:ALA:O	1:B:15:ILE:HG13	2.04	0.57
1:B:565:GLU:OE1	1:B:617:VAL:HG22	2.05	0.56
1:A:358:THR:HG23	1:A:507:VAL:CG2	2.35	0.56
1:A:376:LEU:O	1:A:410:ARG:HD2	2.06	0.56
1:B:271:ASP:O	1:B:274:GLN:HG3	2.06	0.56
1:A:361:LEU:HD13	1:A:504:GLY:HA2	1.86	0.55
1:B:74:LEU:HD21	1:B:111:VAL:HG22	1.88	0.55
1:A:198:SER:O	1:B:417:ARG:NH2	2.39	0.55
1:B:391:TRP:NE1	1:B:394:ALA:HB2	2.21	0.55
1:B:5:THR:OG1	1:B:7:ILE:HG22	2.06	0.55
1:A:647:LYS:NZ	1:A:647:LYS:HB3	2.22	0.55
1:B:49:ARG:HE	1:B:57:TRP:HH2	1.53	0.54
1:A:384:THR:HB	1:A:385:PRO:HD3	1.89	0.54
1:B:359:ARG:HG2	1:B:388:LEU:HD12	1.89	0.54
1:B:259:SER:O	1:B:262:VAL:HG22	2.07	0.54
1:A:6:ASP:CG	5:A:1088:HOH:O	2.46	0.54
1:A:380:SER:HB2	1:A:389:THR:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:GLU:O	1:B:662:LYS:HG2	2.08	0.53
1:B:487:LEU:HD22	1:B:498:VAL:CG1	2.39	0.53
1:A:671:LYS:HG3	1:A:671:LYS:O	2.08	0.53
1:B:594:PHE:O	1:B:602:ARG:HD2	2.07	0.53
1:B:231:ILE:O	1:B:235:LYS:HG3	2.10	0.52
1:A:416:ILE:HG22	1:B:162:GLU:OE2	2.10	0.52
1:A:71:VAL:HG13	1:A:104:PRO:CD	2.37	0.52
1:B:42:HIS:ND1	1:B:297:TYR:OH	2.38	0.52
1:A:112:GLU:O	1:A:113:VAL:HG13	2.10	0.52
1:B:251:GLY:O	1:B:254:SER:HB3	2.10	0.52
1:A:58:ILE:CD1	1:A:62:ARG:NH2	2.73	0.51
1:A:417:ARG:HD3	5:A:943:HOH:O	2.10	0.51
1:A:155:LEU:HD21	1:A:182:ALA:HB1	1.92	0.51
1:A:136:ALA:O	1:A:140:ASN:HB2	2.11	0.50
1:B:141:LYS:HG2	1:B:323:PHE:CE2	2.46	0.50
1:A:552:VAL:HG21	1:A:582:LYS:HB3	1.94	0.49
1:B:396:ASP:OD2	1:B:413:ARG:HD2	2.12	0.49
1:A:23:VAL:HG13	1:A:29:GLY:HA3	1.94	0.49
1:B:144:PHE:CD1	1:B:144:PHE:N	2.81	0.49
1:B:499:TRP:HA	1:B:589:PRO:O	2.13	0.49
1:B:438:TYR:HA	1:B:464:ILE:O	2.13	0.49
1:B:635:ARG:HD3	1:B:636:PHE:O	2.13	0.49
1:A:178:GLY:HA2	1:A:240:LYS:O	2.13	0.48
1:A:302:LEU:O	1:A:306:VAL:HG23	2.13	0.48
1:B:178:GLY:HA2	1:B:240:LYS:O	2.12	0.48
1:A:659:ARG:HG3	1:A:659:ARG:HH11	1.77	0.48
1:B:393:GLU:O	1:B:393:GLU:HG2	2.13	0.48
1:A:356:VAL:CG1	1:A:360:LYS:HD3	2.44	0.48
1:A:421:MET:O	1:A:425:MET:HG3	2.14	0.48
1:A:271:ASP:O	1:A:274:GLN:HG3	2.13	0.48
1:A:469:HIS:HB3	1:A:474:VAL:HG22	1.96	0.48
1:B:378:GLY:HA3	1:B:438:TYR:CZ	2.49	0.48
1:A:58:ILE:HD12	1:A:60:ARG:HH21	1.79	0.47
1:A:268:LYS:O	1:A:271:ASP:HB3	2.13	0.47
1:A:43:VAL:CG2	1:A:224:LEU:HD22	2.45	0.47
1:A:238:LYS:HD3	1:A:238:LYS:H	1.80	0.47
1:A:438:TYR:HA	1:A:464:ILE:O	2.14	0.47
1:B:390:ARG:HD3	1:B:411:TYR:CG	2.49	0.47
1:A:11:ALA:O	1:A:15:ILE:HG13	2.15	0.47
1:A:19:ALA:O	1:A:23:VAL:HG23	2.15	0.47
1:A:191:ILE:HD12	4:A:682:TPP:HM43	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:LYS:HB3	1:A:678:LYS:HZ3	1.80	0.47
5:A:1057:HOH:O	3:B:900:E4P:H3	2.15	0.47
1:B:540:GLU:CD	5:B:1102:HOH:O	2.53	0.47
1:B:322:LYS:HB3	1:B:323:PHE:CE1	2.51	0.46
1:A:16:ARG:NH2	5:A:1077:HOH:O	2.49	0.46
1:A:262:VAL:HG12	1:A:262:VAL:O	2.15	0.46
1:B:635:ARG:HD2	1:B:649:PHE:HE1	1.81	0.46
1:B:384:THR:N	1:B:385:PRO:HD2	2.31	0.46
1:A:389:THR:OG1	1:A:438:TYR:HE2	1.99	0.46
1:B:136:ALA:O	1:B:140:ASN:HB2	2.15	0.46
1:B:512:LYS:O	1:B:516:GLU:HG3	2.16	0.46
1:A:127:GLY:HA2	1:A:424:ILE:HG23	1.98	0.46
1:B:118:LEU:HG	4:B:682:TPP:N4'	2.31	0.45
1:B:316:PHE:O	1:B:319:TYR:HB3	2.16	0.45
1:A:361:LEU:HD13	1:A:504:GLY:CA	2.47	0.45
1:A:378:GLY:HA3	1:A:438:TYR:CZ	2.51	0.45
1:A:443:LEU:HA	1:A:467:ALA:HB1	1.99	0.45
1:A:338:LEU:HD12	1:A:338:LEU:HA	1.88	0.45
1:B:390:ARG:HG2	1:B:411:TYR:CZ	2.52	0.45
1:B:185:ASP:OD2	5:B:923:HOH:O	2.21	0.45
1:B:318:GLU:O	1:B:321:LYS:HB2	2.16	0.45
1:B:111:VAL:O	5:B:1081:HOH:O	2.21	0.45
1:A:316:PHE:CE1	1:A:330:LEU:HD23	2.51	0.45
1:B:25:LYS:HB3	5:B:929:HOH:O	2.16	0.45
1:B:282:ASN:HD22	1:B:285:LYS:HD3	1.81	0.45
1:B:398:GLN:HE21	1:B:398:GLN:HA	1.82	0.45
1:A:191:ILE:HG12	1:A:263:HIS:CD2	2.52	0.45
1:A:471:SER:O	1:A:474:VAL:HG23	2.17	0.45
1:A:346:LEU:HA	1:A:347:PRO:HD3	1.82	0.44
1:A:597:GLN:O	1:A:602:ARG:NH1	2.50	0.44
1:B:647:LYS:HE2	1:B:647:LYS:HB3	1.80	0.44
1:A:318:GLU:O	1:A:321:LYS:HB2	2.18	0.44
1:B:617:VAL:HG11	1:B:646:PHE:HE1	1.79	0.44
1:A:620:THR:HG22	1:A:632:GLY:HA3	2.00	0.44
1:B:596:LYS:CB	1:B:596:LYS:NZ	2.80	0.44
1:A:94:ARG:HB3	1:B:476:GLU:HG2	2.00	0.44
1:A:94:ARG:NH2	1:B:477:ASP:OD1	2.51	0.44
1:A:106:PHE:HB2	1:A:114:THR:HG22	2.00	0.44
1:A:489:HIS:CD2	1:A:489:HIS:C	2.92	0.44
1:B:88:GLU:HB2	5:B:1077:HOH:O	2.17	0.44
1:B:106:PHE:O	5:B:1081:HOH:O	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:GLY:HA3	1:B:238:LYS:O	2.18	0.44
1:A:378:GLY:HA3	1:A:438:TYR:CE1	2.53	0.44
1:A:58:ILE:HD12	1:A:62:ARG:NH2	2.33	0.43
1:A:673:ILE:HG22	1:A:674:SER:O	2.17	0.43
1:B:594:PHE:O	1:B:602:ARG:CD	2.66	0.43
1:A:316:PHE:HE1	1:A:330:LEU:HD23	1.83	0.43
1:A:445:PHE:O	1:A:448:TYR:HB2	2.19	0.43
1:B:518:LYS:HB2	1:B:518:LYS:HE3	1.70	0.43
1:B:421:MET:O	1:B:425:MET:HG3	2.19	0.43
1:B:390:ARG:HG2	1:B:411:TYR:CE2	2.53	0.43
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.85	0.43
1:A:189:ILE:HD12	1:A:260:HIS:HB3	2.00	0.43
1:A:300:THR:HG21	5:A:908:HOH:O	2.18	0.43
1:B:51:ASN:ND2	1:B:53:THR:H	2.16	0.43
1:A:216:TYR:CD1	1:A:216:TYR:N	2.85	0.43
1:B:12:VAL:O	1:B:16:ARG:HG3	2.19	0.43
1:A:297:TYR:CD1	1:A:301:ILE:HD12	2.54	0.43
1:B:567:SER:O	1:B:570:VAL:HB	2.19	0.43
1:B:545:GLY:O	1:B:589:PRO:HD2	2.19	0.43
1:B:346:LEU:HA	1:B:347:PRO:HD3	1.93	0.42
1:B:565:GLU:HB3	1:B:615:VAL:HG12	2.01	0.42
1:A:384:THR:HB	1:A:385:PRO:CD	2.49	0.42
1:B:49:ARG:NH2	1:B:59:ASN:HD22	2.16	0.42
1:A:71:VAL:CG1	1:A:104:PRO:HD3	2.39	0.42
1:B:361:LEU:HD13	1:B:504:GLY:HA2	2.01	0.42
1:A:16:ARG:HD3	1:A:35:LEU:O	2.20	0.42
1:B:187:ASN:O	1:B:188:LYS:HB2	2.20	0.42
1:A:114:THR:CG2	1:A:459:SER:OG	2.67	0.42
1:A:359:ARG:HG2	1:A:388:LEU:HD12	2.01	0.41
1:A:371:ASN:H	1:A:371:ASN:ND2	2.18	0.41
1:A:359:ARG:HB2	1:A:527:SER:O	2.20	0.41
1:A:480:THR:HB	1:B:117:PRO:HD3	2.02	0.41
1:A:491:ARG:HD2	1:A:591:PHE:CG	2.54	0.41
1:A:641:LYS:O	1:A:645:VAL:HG23	2.20	0.41
1:B:613:MET:HA	1:B:629:GLN:O	2.20	0.41
1:A:654:GLU:H	1:A:654:GLU:CD	2.24	0.41
1:A:499:TRP:HA	1:A:589:PRO:O	2.21	0.41
1:B:190:THR:HG22	4:B:682:TPP:O2A	2.20	0.41
1:A:567:SER:O	1:A:570:VAL:HB	2.20	0.41
1:A:647:LYS:HB3	1:A:647:LYS:HZ2	1.86	0.41
1:A:191:ILE:HD12	4:A:682:TPP:CM4	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ASN:HA	1:A:283:PRO:HD2	1.86	0.41
1:A:38:ALA:HB3	1:A:39:PRO:HD3	2.02	0.41
1:A:93:PHE:CZ	1:A:94:ARG:HD2	2.55	0.41
1:A:558:ILE:CD1	1:A:607:PRO:HD2	2.50	0.41
1:B:322:LYS:HB3	1:B:323:PHE:CD1	2.55	0.41
1:B:398:GLN:O	1:B:406:ASN:HA	2.21	0.41
1:A:362:SER:HB2	1:A:526:LEU:HD13	2.02	0.41
1:B:7:ILE:HG23	1:B:8:ASP:N	2.36	0.41
1:A:472:ILE:HA	1:A:482:GLN:HG2	2.03	0.40
1:B:31:PRO:HG3	1:B:265:ALA:O	2.21	0.40
1:B:352:LYS:HE3	1:B:352:LYS:HB2	1.91	0.40
1:A:58:ILE:CD1	1:A:62:ARG:HH22	2.34	0.40
1:A:231:ILE:O	1:A:234:ALA:HB3	2.21	0.40
1:A:660:ALA:O	1:A:664:ILE:HG13	2.22	0.40
1:B:88:GLU:CB	5:B:1077:HOH:O	2.69	0.40
1:B:263:HIS:CD2	1:B:263:HIS:C	2.94	0.40
1:A:178:GLY:HA3	1:A:238:LYS:O	2.21	0.40
1:A:560:VAL:O	1:A:614:SER:HA	2.20	0.40
1:B:174:HIS:CD2	5:B:903:HOH:O	2.74	0.40
1:B:406:ASN:C	1:B:406:ASN:OD1	2.60	0.40
1:A:380:SER:HB2	1:A:389:THR:CG2	2.51	0.40
1:A:648:PHE:HE2	1:A:649:PHE:CZ	2.39	0.40
1:B:390:ARG:NE	1:B:394:ALA:HB3	2.36	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)
1:B:313:ASN:OD1	5:A:1009:HOH:O[3_555]	2.12	0.08
1:A:579:LYS:NZ	5:A:954:HOH:O[3_555]	2.17	0.03

## 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	676/680 (99%)	645 (95%)	28 (4%)	3 (0%)	34	48
1	B	676/680 (99%)	644 (95%)	29 (4%)	3 (0%)	34	48
All	All	1352/1360 (99%)	1289 (95%)	57 (4%)	6 (0%)	34	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	SER
1	B	617	VAL
1	A	617	VAL
1	B	198	SER
1	A	198	SER
1	B	148	ASP

### 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	552/554 (100%)	519 (94%)	33 (6%)	19	31
1	B	552/554 (100%)	521 (94%)	31 (6%)	21	34
All	All	1104/1108 (100%)	1040 (94%)	64 (6%)	20	32

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	47	GLN
1	A	49	ARG
1	A	50	MET
1	A	67	ASN
1	A	71	VAL
1	A	100	THR
1	A	114	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	122	ILE
1	A	155	LEU
1	A	197	ILE
1	A	206	ARG
1	A	218	GLU
1	A	238	LYS
1	A	299	LYS
1	A	302	LEU
1	A	309	ASN
1	A	314	LYS
1	A	318	GLU
1	A	325	GLU
1	A	338	LEU
1	A	341	ASN
1	A	343	GLU
1	A	352	LYS
1	A	404	SER
1	A	512	LYS
1	A	580	ASN
1	A	584	ARG
1	A	588	LEU
1	A	600	GLU
1	A	652	THR
1	A	668	LYS
1	A	678	LYS
1	B	51	ASN
1	B	67	ASN
1	B	73	LEU
1	B	113	VAL
1	B	141	LYS
1	B	153	VAL
1	B	197	ILE
1	B	229	LYS
1	B	268	LYS
1	B	302	LEU
1	B	314	LYS
1	B	322	LYS
1	B	326	LEU
1	B	338	LEU
1	B	352	LYS
1	B	354	SER
1	B	367	GLU

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Mol	Chain	Res	Type
1	B	370	TYR
1	B	377	ILE
1	B	392	LYS
1	B	398	GLN
1	B	404	SER
1	B	413	ARG
1	B	486	THR
1	B	518	LYS
1	B	574	LYS
1	B	625	LYS
1	B	635	ARG
1	B	647	LYS
1	B	671	LYS
1	B	674	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	120	GLN
1	A	296	HIS
1	A	341	ASN
1	A	371	ASN
1	A	387	ASN
1	A	580	ASN
1	B	27	ASN
1	B	51	ASN
1	B	54	ASN
1	B	67	ASN
1	B	92	GLN
1	B	120	GLN
1	B	149	ASN
1	B	309	ASN
1	B	398	GLN

### 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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	E4P	B	900	-	9,11,11	1.67	2 (22%)	12,15,15	1.10	1 (8%)
4	TPP	A	682	2	22,27,27	2.57	3 (13%)	29,40,40	1.80	11 (37%)
4	TPP	B	682	2	22,27,27	2.30	5 (22%)	29,40,40	2.38	9 (31%)
3	E4P	A	900	-	9,11,11	1.84	2 (22%)	12,15,15	1.08	1 (8%)

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	E4P	B	900	-	-	5/10/12/12	-
4	TPP	A	682	2	-	5/16/17/17	0/2/2/2
4	TPP	B	682	2	-	3/16/17/17	0/2/2/2
3	E4P	A	900	-	-	4/10/12/12	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	682	TPP	C4-N3	-10.25	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	682	TPP	C4-N3	-8.77	1.32	1.39
3	A	900	E4P	P-O4	-3.80	1.48	1.60
3	B	900	E4P	P-O4	-3.65	1.48	1.60
3	A	900	E4P	P-O1P	3.12	1.60	1.50
4	A	682	TPP	C4'-N3'	2.94	1.39	1.35
4	B	682	TPP	PB-O2B	-2.75	1.44	1.54
4	A	682	TPP	C7'-N3	2.66	1.53	1.48
3	B	900	E4P	P-O1P	2.60	1.58	1.50
4	B	682	TPP	C2'-N3'	-2.17	1.30	1.34
4	B	682	TPP	PA-O2A	-2.10	1.45	1.55
4	B	682	TPP	PB-O3B	-2.02	1.47	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	682	TPP	O2A-PA-O7	-5.10	84.04	107.75
4	B	682	TPP	O2B-PB-O3A	-4.82	88.46	104.64
4	B	682	TPP	O3B-PB-O3A	4.62	120.12	104.64
4	B	682	TPP	C6-C5-C4	-4.43	123.88	127.43
4	B	682	TPP	PA-O3A-PB	4.14	147.05	132.83
4	A	682	TPP	PA-O3A-PB	3.58	145.12	132.83
4	A	682	TPP	C5-C4-N3	3.53	114.63	107.57
4	B	682	TPP	O7-PA-O1A	-3.34	96.03	109.07
4	B	682	TPP	C5'-C7'-N3	-3.06	108.19	113.28
4	A	682	TPP	O3A-PB-O1B	-2.96	94.77	111.19
4	B	682	TPP	C6'-N1'-C2'	2.82	120.76	115.96
3	A	900	E4P	P-O4-C4	-2.69	110.88	118.30
4	A	682	TPP	N1'-C2'-N3'	-2.59	121.08	125.54
4	B	682	TPP	C5-C4-N3	2.56	112.69	107.57
4	A	682	TPP	O2A-PA-O7	-2.54	95.96	107.75
3	B	900	E4P	P-O4-C4	-2.52	111.34	118.30
4	A	682	TPP	CM4-C4-N3	-2.51	119.33	122.53
4	A	682	TPP	O3B-PB-O1B	2.45	120.28	110.68
4	A	682	TPP	C6'-N1'-C2'	2.45	120.13	115.96
4	A	682	TPP	O7-PA-O1A	2.30	118.04	109.07
4	A	682	TPP	CM2-C2'-N3'	2.19	120.56	117.15
4	A	682	TPP	C5'-C7'-N3	-2.15	109.69	113.28

There are no chirality outliers.

All (17) torsion outliers are listed below:

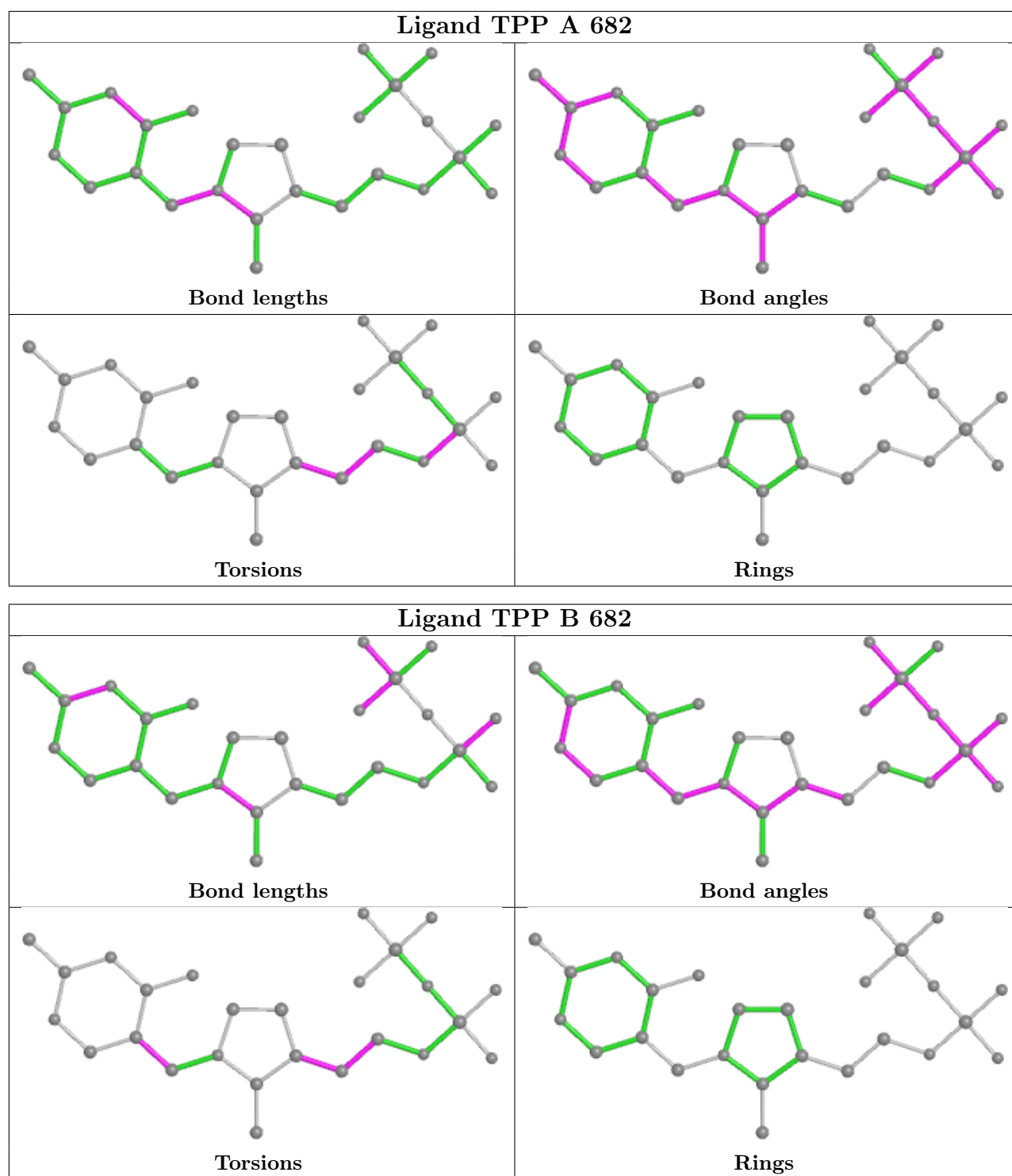
Mol	Chain	Res	Type	Atoms
3	A	900	E4P	C1-C2-C3-O3
3	A	900	E4P	C1-C2-C3-C4
3	A	900	E4P	O2-C2-C3-O3
3	A	900	E4P	O2-C2-C3-C4
3	B	900	E4P	C1-C2-C3-O3
3	B	900	E4P	C1-C2-C3-C4
3	B	900	E4P	O2-C2-C3-O3
3	B	900	E4P	O2-C2-C3-C4
4	A	682	TPP	C5-C6-C7-O7
4	A	682	TPP	C7-O7-PA-O3A
4	B	682	TPP	C4-C5-C6-C7
4	B	682	TPP	C5-C6-C7-O7
3	B	900	E4P	C4-O4-P-O1P
4	A	682	TPP	C7-O7-PA-O1A
4	A	682	TPP	C7-O7-PA-O2A
4	B	682	TPP	C6'-C5'-C7'-N3
4	A	682	TPP	C4-C5-C6-C7

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	900	E4P	1	0
4	A	682	TPP	3	0
4	B	682	TPP	4	0
3	A	900	E4P	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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.