



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:52 pm BST

PDB ID : 1RP7  
Title : E. COLI PYRUVATE DEHYDROGENASE INHIBITOR COMPLEX  
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Deposited on : 2003-12-03  
Resolution : 2.09 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.

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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)  
Xtriage (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) : 2.11

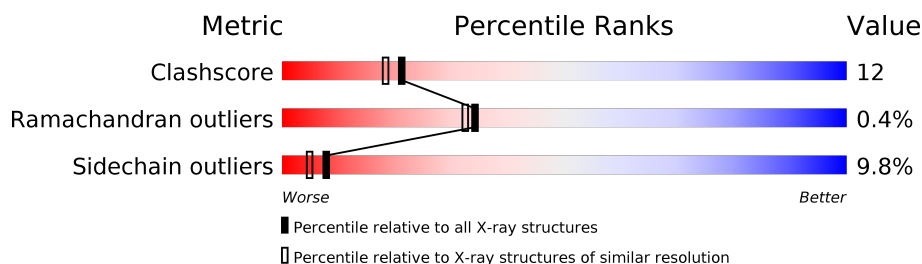
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.09 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 on 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	886	
1	B	886	

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13237 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.

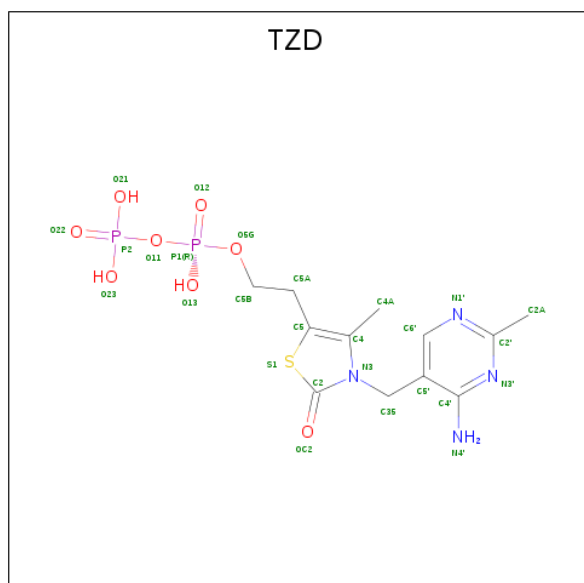
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total 6341	C 4018	N 1093	O 1204	S 26	0	0	0
1	B	801	Total 6341	C 4018	N 1093	O 1204	S 26	0	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is 2-{3-[4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-4-METHYL-2-OXO-2,3-DIHYDRO-1,3-THIAZOL-5-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TZD) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>8</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	223	Total	O	0	0
			223	223		
4	B	276	Total	O	0	0
			276	276		





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.55Å 141.84Å 82.17Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	8.00 – 2.09	Depositor
% Data completeness (in resolution range)	84.5 (8.00-2.09)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.192 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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: MG, TZD

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	0.36	0/6484	0.60	1/8766 (0.0%)
1	B	0.37	0/6484	0.61	1/8766 (0.0%)
All	All	0.36	0/12968	0.61	2/17532 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	171	GLY	N-CA-C	5.40	126.61	113.10
1	B	638	LEU	CA-CB-CG	5.35	127.61	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	803	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	6341	0	6179	162	0
1	B	6341	0	6179	154	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	15	0	0
3	B	27	0	15	1	0
4	A	223	0	0	2	0
4	B	276	0	0	10	0
All	All	13237	0	12388	304	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 12.

All (304) 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:309:LYS:HG3	1:B:343:GLU:HG3	1.34	1.09
1:B:90:ILE:HG12	1:B:107:MET:HE3	1.37	1.01
1:A:64:PRO:HG2	1:A:67:GLU:HG3	1.47	0.96
1:B:509:LYS:HD2	1:B:509:LYS:H	1.30	0.95
1:B:198:PRO:HG3	1:B:228:LEU:HD22	1.52	0.91
1:B:490:LYS:HE2	1:B:500:ARG:HH22	1.35	0.90
1:B:194:MET:HB3	1:B:232:GLU:HG3	1.55	0.86
1:B:309:LYS:CG	1:B:343:GLU:HG3	2.11	0.80
1:B:432:ASP:HA	1:B:435:LYS:HD2	1.63	0.80
1:B:587:THR:HG21	4:B:923:HOH:O	1.83	0.79
1:A:326:LYS:HD2	1:A:391:ILE:HG23	1.62	0.78
1:B:309:LYS:HG3	1:B:343:GLU:CG	2.13	0.77
1:A:297:ARG:HB3	1:A:359:LEU:HD23	1.65	0.77
1:A:334:ARG:HB3	1:A:356:ILE:HD13	1.65	0.77
1:B:352:THR:OG1	1:B:355:GLN:HG3	1.86	0.75
1:A:638:LEU:HD22	1:A:828:PHE:HB3	1.69	0.74
1:B:300:GLU:HG3	1:B:301:LEU:N	2.02	0.74
1:A:867:VAL:HG22	1:B:779:PRO:HG3	1.70	0.72
1:B:326:LYS:HE2	1:B:391:ILE:HG23	1.71	0.72
1:A:277:GLU:OE2	1:B:243:THR:HG21	1.90	0.72
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.74	0.70
1:A:160:GLU:HG2	1:A:161:GLN:N	2.07	0.70
1:B:301:LEU:HD12	1:B:304:LYS:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:LYS:H	1:B:509:LYS:CD	2.05	0.69
4:A:1079:HOH:O	1:B:522:GLU:HG3	1.92	0.69
1:A:627:THR:HB	1:A:633:LEU:HD13	1.74	0.69
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.22	0.69
1:A:262:GLN:HA	1:A:267:PRO:HA	1.75	0.68
1:B:638:LEU:HD22	1:B:828:PHE:HB3	1.74	0.68
1:A:393:GLY:HA3	1:A:400:ALA:HB3	1.74	0.68
1:B:414:MET:O	1:B:433:ILE:HG23	1.94	0.67
1:B:490:LYS:HE2	1:B:500:ARG:NH2	2.08	0.66
1:B:361:ARG:HD2	1:B:391:ILE:HG13	1.77	0.66
1:A:348:VAL:O	1:A:351:TRP:HB2	1.96	0.66
1:A:140:GLN:O	1:A:143:ILE:HG13	1.95	0.65
1:B:323:GLN:HA	1:B:326:LYS:HD3	1.78	0.65
1:B:374:LYS:HE3	1:B:377:GLN:OE1	1.96	0.65
1:B:87:TRP:CD1	1:B:439:ILE:HG13	2.32	0.64
1:A:237:GLU:HG2	1:A:572:LEU:HD11	1.79	0.64
1:B:287:TRP:CE3	1:B:385:VAL:HG22	2.33	0.64
1:A:508:ASN:O	1:A:512:LYS:HB3	1.99	0.63
1:B:656:ILE:HD11	1:B:685:VAL:HG21	1.79	0.63
1:A:328:LYS:HG3	1:A:332:TYR:CD1	2.35	0.62
1:A:334:ARG:HG3	1:A:335:GLU:N	2.14	0.62
1:B:800:SER:OG	1:B:843:VAL:HG22	1.99	0.62
1:A:796:PRO:HG3	1:A:859:ARG:NE	2.15	0.61
1:B:415:ASP:OD1	1:B:433:ILE:HG21	1.99	0.61
1:A:334:ARG:HA	1:A:338:PHE:HB2	1.83	0.61
1:B:846:SER:OG	1:B:874:PHE:HB3	2.01	0.60
1:A:324:THR:HG23	1:A:328:LYS:HE3	1.82	0.60
1:A:298:TRP:CE2	1:A:359:LEU:HB3	2.37	0.60
1:A:98:LYS:HE2	1:A:436:LEU:HD12	1.82	0.60
1:A:313:LEU:HD21	1:A:337:PHE:O	2.02	0.59
1:B:112:SER:HB3	1:B:392:LYS:HA	1.85	0.59
1:A:418:ARG:HG2	1:A:433:ILE:HD13	1.84	0.59
1:A:561:LYS:NZ	1:A:561:LYS:HB2	2.17	0.59
1:A:867:VAL:CG2	1:B:779:PRO:HG3	2.32	0.59
1:A:344:THR:HA	1:A:347:LEU:HD12	1.85	0.59
1:A:192:VAL:HG22	4:A:1062:HOH:O	2.01	0.58
1:A:857:ALA:HA	1:A:862:ILE:HG13	1.84	0.58
1:B:522:GLU:HG2	1:B:599:TYR:OH	2.02	0.58
1:A:854:GLY:O	1:A:858:LYS:HG3	2.04	0.58
1:A:91:MET:O	1:A:95:ARG:HG3	2.03	0.58
1:B:420:ILE:HG13	1:B:421:ARG:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:LEU:HD11	1:B:446:GLU:HG2	1.85	0.57
1:A:821:ARG:HH11	1:A:851:ALA:HA	1.69	0.57
1:A:832:ASP:OD2	1:B:169:VAL:HB	2.04	0.57
1:A:335:GLU:O	1:A:339:GLY:HA3	2.04	0.57
1:A:853:LEU:O	1:A:862:ILE:HD11	2.05	0.56
1:B:681:LYS:HB2	4:B:1075:HOH:O	2.05	0.56
1:B:177:TYR:HB3	1:B:178:PRO:CD	2.35	0.56
1:B:509:LYS:HD2	1:B:509:LYS:N	2.12	0.56
1:A:859:ARG:NH1	1:A:861:GLU:OE1	2.39	0.56
1:A:294:TRP:HB3	1:A:298:TRP:CD1	2.41	0.56
1:B:627:THR:HB	1:B:633:LEU:HD22	1.88	0.55
1:A:153:LEU:HD21	1:A:441:PHE:CE2	2.41	0.55
1:A:863:ASP:O	1:A:866:VAL:HG22	2.07	0.55
1:B:489:SER:HB2	1:B:490:LYS:NZ	2.22	0.55
1:A:352:THR:OG1	1:A:354:GLU:HG2	2.07	0.55
1:B:664:TYR:O	1:B:668:VAL:HG23	2.07	0.54
1:A:663:ALA:O	1:A:666:VAL:HG13	2.07	0.54
1:A:806:LEU:HD11	1:B:806:LEU:HD11	1.88	0.54
1:A:656:ILE:HG12	1:A:685:VAL:HG13	1.89	0.54
1:B:294:TRP:HB3	1:B:298:TRP:CD1	2.43	0.54
1:A:177:TYR:CG	1:A:192:VAL:HG11	2.43	0.54
1:B:426:VAL:HG12	1:B:428:VAL:HG12	1.89	0.54
1:A:524:ARG:HA	1:A:529:GLU:OE1	2.08	0.53
1:B:106:HIS:HD2	4:B:1161:HOH:O	1.90	0.53
1:B:537:ILE:HG22	1:B:558:GLU:HA	1.91	0.53
1:B:297:ARG:HB2	1:B:359:LEU:HD23	1.90	0.53
1:A:561:LYS:HB2	1:A:561:LYS:HZ2	1.73	0.53
1:A:585:TYR:O	1:A:589:ASN:HA	2.08	0.53
1:B:213:HIS:HB3	1:B:560:GLU:O	2.09	0.53
1:B:532:PHE:HD1	1:B:564:ILE:HD12	1.73	0.53
1:B:694:GLU:CD	1:B:736:ARG:HH12	2.12	0.53
1:A:177:TYR:CD2	1:A:192:VAL:HG11	2.44	0.52
1:B:323:GLN:O	1:B:326:LYS:HG2	2.08	0.52
1:B:490:LYS:CE	1:B:500:ARG:HH22	2.17	0.52
1:B:64:PRO:HB2	1:B:66:GLU:OE2	2.09	0.52
1:A:507:LYS:HA	1:A:507:LYS:HE3	1.90	0.52
1:B:164:ASN:HB3	1:B:173:GLY:HA2	1.91	0.52
1:B:442:PRO:HG2	1:B:445:SER:HB3	1.90	0.52
1:A:396:MET:HB3	1:A:399:ALA:HB3	1.93	0.51
1:A:130:GLU:HG3	1:A:131:GLN:NE2	2.25	0.51
1:A:537:ILE:O	1:A:558:GLU:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:SER:OG	1:B:145:PRO:HD3	2.10	0.51
1:A:827:GLY:CA	1:A:884:ARG:HA	2.40	0.51
1:B:140:GLN:O	1:B:143:ILE:HG13	2.10	0.51
1:A:314:MET:HA	1:A:322:TYR:OH	2.11	0.51
1:B:195:GLY:C	1:B:198:PRO:HD2	2.32	0.51
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.91	0.51
1:B:91:MET:O	1:B:95:ARG:HG3	2.10	0.51
1:B:506:LEU:HD23	1:B:515:LEU:HD12	1.92	0.50
1:B:537:ILE:HD11	1:B:566:GLN:HB3	1.92	0.50
1:B:76:GLU:CD	1:B:76:GLU:H	2.15	0.50
1:B:721:GLY:HA3	1:B:752:GLY:N	2.27	0.50
1:B:178:PRO:HA	1:B:187:TRP:CG	2.47	0.50
1:B:177:TYR:CD2	1:B:192:VAL:HG11	2.46	0.50
1:B:309:LYS:HD2	1:B:341:TYR:CD2	2.46	0.50
1:A:304:LYS:HE2	1:A:347:LEU:HD23	1.93	0.50
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.93	0.50
1:B:509:LYS:HD3	4:B:1145:HOH:O	2.12	0.50
1:B:736:ARG:NH1	4:B:1081:HOH:O	2.44	0.50
1:A:317:THR:HB	1:A:322:TYR:CE2	2.47	0.50
1:B:273:LYS:HG2	4:B:1042:HOH:O	2.11	0.50
1:A:324:THR:O	1:A:328:LYS:HG2	2.11	0.49
1:A:420:ILE:HG13	1:A:421:ARG:N	2.26	0.49
1:B:195:GLY:O	1:B:198:PRO:HD2	2.12	0.49
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.42	0.49
1:A:352:THR:OG1	1:A:355:GLN:HG3	2.12	0.49
1:B:164:ASN:CB	1:B:173:GLY:HA2	2.42	0.49
1:B:415:ASP:OD1	1:B:418:ARG:HB3	2.13	0.49
1:A:638:LEU:CD2	1:A:828:PHE:HB3	2.42	0.49
1:A:304:LYS:NZ	1:A:347:LEU:O	2.45	0.49
1:A:418:ARG:HG2	1:A:433:ILE:CD1	2.42	0.49
1:A:304:LYS:HE2	1:A:347:LEU:CD2	2.43	0.49
1:A:197:GLY:N	1:A:198:PRO:HD2	2.28	0.49
1:B:317:THR:HB	1:B:322:TYR:CE2	2.47	0.49
1:B:881:VAL:HG12	4:B:1147:HOH:O	2.11	0.49
1:A:153:LEU:HD21	1:A:441:PHE:HE2	1.78	0.49
1:A:120:CYS:HB3	1:A:125:PHE:CE1	2.48	0.49
1:A:298:TRP:CZ2	1:A:359:LEU:HB3	2.48	0.49
1:B:508:ASN:O	1:B:512:LYS:HB3	2.13	0.48
1:B:856:LEU:HB3	1:B:861:GLU:HB3	1.93	0.48
1:A:578:TRP:CD1	1:A:594:PRO:HB2	2.48	0.48
1:A:130:GLU:HG3	1:A:131:GLN:HE22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLY:HA3	1:A:353:ASP:O	2.14	0.48
1:A:821:ARG:NH1	1:A:851:ALA:HA	2.28	0.48
1:B:87:TRP:CZ2	1:B:428:VAL:HG11	2.48	0.48
1:B:567:GLU:HG3	1:B:574:ALA:HA	1.96	0.48
1:A:780:LEU:HD12	1:B:864:LYS:HB3	1.95	0.48
1:A:434:GLU:CD	1:A:434:GLU:H	2.16	0.48
1:B:585:TYR:O	1:B:589:ASN:HA	2.14	0.48
1:B:811:VAL:O	1:B:815:VAL:HG23	2.14	0.48
1:A:567:GLU:HG3	1:A:574:ALA:HA	1.95	0.48
1:B:638:LEU:CD2	1:B:828:PHE:HB3	2.43	0.48
1:A:635:GLY:HA3	1:B:103:LEU:O	2.14	0.47
1:A:95:ARG:HD2	1:A:438:TYR:OH	2.14	0.47
1:B:134:GLY:O	1:B:222:GLN:HG2	2.14	0.47
1:B:807:PHE:O	1:B:810:GLN:HG2	2.14	0.47
1:A:206:LYS:HD2	1:A:248:GLU:HG3	1.95	0.47
1:A:535:ILE:HB	1:A:563:GLN:HB3	1.97	0.47
1:A:821:ARG:HD2	1:A:855:GLU:CG	2.45	0.47
1:B:489:SER:HB2	1:B:490:LYS:HZ1	1.79	0.47
1:B:877:ASP:O	1:B:880:LYS:HG2	2.13	0.47
1:A:300:GLU:O	1:A:304:LYS:HB2	2.14	0.47
1:B:262:GLN:HA	1:B:267:PRO:HA	1.96	0.47
1:B:421:ARG:HA	1:B:426:VAL:CG2	2.44	0.47
1:A:664:TYR:CG	1:A:701:MET:HB2	2.49	0.47
1:B:106:HIS:CD2	4:B:1161:HOH:O	2.68	0.47
1:B:421:ARG:HG2	1:B:433:ILE:HD11	1.97	0.47
1:B:230:ASP:OD1	1:B:230:ASP:N	2.47	0.46
1:B:87:TRP:CD2	1:B:426:VAL:HG11	2.50	0.46
1:A:144:SER:N	1:A:145:PRO:CD	2.79	0.46
1:B:194:MET:H	1:B:194:MET:HG2	1.52	0.46
1:B:207:PHE:O	1:B:210:TYR:HB3	2.16	0.46
1:B:720:GLU:HA	1:B:720:GLU:OE1	2.15	0.46
1:B:855:GLU:O	1:B:859:ARG:HG3	2.15	0.46
1:A:729:LEU:HD12	1:A:729:LEU:N	2.30	0.46
1:A:272:GLY:O	1:A:318:VAL:HG22	2.16	0.46
1:B:341:TYR:HB2	1:B:344:THR:OG1	2.16	0.46
1:A:138:TYR:HB2	1:A:226:ALA:HA	1.97	0.46
1:A:286:GLY:O	1:A:382:LYS:HE3	2.15	0.46
1:A:634:ASN:HB2	1:A:832:ASP:O	2.15	0.46
1:A:726:VAL:O	1:A:753:SER:HA	2.16	0.46
1:B:239:LYS:HA	1:B:242:ILE:HG23	1.97	0.46
1:A:505:MET:HB3	1:A:515:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:CD2	1:A:446:GLU:HG2	2.46	0.45
1:A:806:LEU:HA	1:A:809:GLU:HB2	1.98	0.45
1:B:421:ARG:HG3	1:B:422:ASP:N	2.31	0.45
1:A:479:GLN:HG2	1:A:480:ASP:N	2.31	0.45
1:B:274:ILE:O	1:B:278:LEU:HB2	2.15	0.45
1:B:418:ARG:O	1:B:421:ARG:HG3	2.16	0.45
1:A:762:THR:O	1:A:766:ARG:HG3	2.16	0.45
1:A:864:LYS:O	1:A:867:VAL:HG13	2.17	0.45
1:B:808:ALA:O	1:B:811:VAL:HG22	2.16	0.45
1:A:144:SER:OG	1:A:145:PRO:HD3	2.17	0.45
1:A:647:ILE:O	1:A:650:LEU:HG	2.17	0.45
1:B:125:PHE:O	1:B:458:LEU:HB3	2.17	0.44
1:B:716:LEU:HD13	1:B:739:ARG:CZ	2.47	0.44
1:A:426:VAL:HG13	1:A:439:ILE:CD1	2.46	0.44
1:A:827:GLY:HA2	1:A:884:ARG:HA	1.99	0.44
1:B:194:MET:CB	1:B:232:GLU:HG3	2.38	0.44
1:B:330:GLY:HA3	1:B:353:ASP:O	2.17	0.44
1:A:198:PRO:O	1:A:202:ILE:HG13	2.17	0.44
1:A:236:PRO:HD3	1:B:570:ASN:OD1	2.17	0.44
1:A:59:TYR:N	1:A:315:ASN:OD1	2.40	0.44
1:A:334:ARG:NH2	1:A:351:TRP:O	2.51	0.44
1:B:421:ARG:HG3	1:B:421:ARG:HH11	1.82	0.44
1:A:328:LYS:HD2	1:A:332:TYR:CD2	2.53	0.44
1:B:397:GLY:O	1:B:398:ASP:C	2.56	0.44
1:B:488:GLN:HB2	1:B:698:MET:HB2	2.00	0.44
1:A:519:ILE:HD11	1:A:528:MET:HG3	1.99	0.44
1:A:521:ASP:N	1:A:566:GLN:OE1	2.44	0.44
1:B:144:SER:N	1:B:145:PRO:CD	2.81	0.44
1:B:309:LYS:HD2	1:B:341:TYR:CG	2.53	0.44
1:A:859:ARG:HD3	1:A:861:GLU:OE1	2.17	0.43
1:B:540:PRO:HA	1:B:560:GLU:HB2	2.00	0.43
1:A:723:LYS:HG2	1:A:750:GLY:HA3	2.00	0.43
1:B:529:GLU:OE1	1:B:529:GLU:N	2.51	0.43
1:A:862:ILE:HD12	1:A:866:VAL:HG22	1.98	0.43
1:B:309:LYS:CB	1:B:343:GLU:HG3	2.48	0.43
1:B:532:PHE:CD1	1:B:564:ILE:HD12	2.53	0.43
1:A:328:LYS:HD2	1:A:332:TYR:CE2	2.53	0.43
1:B:274:ILE:H	1:B:274:ILE:HG13	1.54	0.43
1:A:309:LYS:HB3	1:A:344:THR:HG23	2.01	0.43
1:A:416:GLY:O	1:A:420:ILE:HG23	2.18	0.43
1:A:656:ILE:HG12	1:A:685:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ILE:O	1:B:500:ARG:HG3	2.19	0.43
1:B:558:GLU:O	1:B:558:GLU:HG2	2.18	0.43
1:A:681:LYS:HD3	1:A:683:GLU:HB2	1.99	0.43
1:B:326:LYS:HE3	4:B:1063:HOH:O	2.19	0.43
1:A:532:PHE:CD1	1:A:532:PHE:N	2.86	0.43
1:A:560:GLU:HG3	1:A:560:GLU:H	1.53	0.43
1:A:728:LEU:HD12	1:A:742:ALA:HB2	2.01	0.43
1:A:521:ASP:O	1:B:265:ASP:HB2	2.18	0.43
1:B:471:GLU:OE2	1:B:591:PRO:HD2	2.18	0.43
1:A:348:VAL:HA	1:A:351:TRP:CD1	2.53	0.42
1:A:458:LEU:O	1:A:459:HIS:HB2	2.18	0.42
1:A:692:LEU:HD13	1:A:733:SER:HB3	1.99	0.42
1:B:177:TYR:HB3	1:B:178:PRO:HD2	1.99	0.42
1:B:450:TYR:O	1:B:454:GLN:HG2	2.20	0.42
1:B:421:ARG:CG	1:B:421:ARG:HH11	2.32	0.42
1:A:301:LEU:HD23	1:A:351:TRP:CZ2	2.55	0.42
1:A:524:ARG:HD3	1:B:265:ASP:OD2	2.19	0.42
1:B:263:ARG:HE	1:B:263:ARG:HB2	1.44	0.42
1:B:263:ARG:HG3	1:B:268:VAL:HG22	2.01	0.42
1:A:716:LEU:HD13	1:A:739:ARG:CZ	2.50	0.42
1:A:815:VAL:HG12	1:A:817:ALA:H	1.84	0.42
1:A:867:VAL:HG22	1:B:779:PRO:CG	2.47	0.42
1:B:348:VAL:HB	1:B:356:ILE:HD11	2.02	0.42
1:B:528:MET:C	1:B:530:GLY:H	2.23	0.42
1:A:296:SER:O	1:A:299:ASP:HB2	2.18	0.42
1:B:79:ARG:HG2	1:B:82:ARG:NH2	2.35	0.42
1:A:312:GLN:NE2	1:A:316:GLU:OE1	2.52	0.42
1:B:350:ASP:OD1	1:B:350:ASP:N	2.48	0.42
1:A:194:MET:H	1:A:194:MET:HG2	1.56	0.42
1:A:60:ILE:HG21	1:A:311:ILE:HD12	2.01	0.42
1:A:442:PRO:HG2	1:A:445:SER:HB3	2.02	0.42
1:B:365:ASP:HB3	1:B:368:LYS:HB2	2.01	0.42
1:B:260:ASN:HA	1:B:390:THR:O	2.20	0.42
1:A:77:LEU:HD22	1:A:446:GLU:HG2	2.01	0.42
1:B:737:HIS:HE1	4:B:1081:HOH:O	2.02	0.42
1:A:262:GLN:HG2	1:A:323:GLN:NE2	2.34	0.42
1:A:87:TRP:HE3	1:A:420:ILE:HD11	1.85	0.42
1:B:203:TYR:HB2	1:B:576:CYS:HB3	2.02	0.42
1:A:352:THR:O	1:A:355:GLN:N	2.50	0.41
1:A:857:ALA:CA	1:A:862:ILE:HG13	2.50	0.41
1:A:328:LYS:HG3	1:A:332:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:MET:CB	1:A:515:LEU:HD11	2.50	0.41
1:B:206:LYS:HD3	1:B:248:GLU:OE1	2.20	0.41
1:A:106:HIS:CD2	1:A:106:HIS:N	2.88	0.41
1:A:164:ASN:CB	1:A:173:GLY:HA2	2.50	0.41
1:A:502:LEU:HA	1:A:502:LEU:HD23	1.92	0.41
1:A:846:SER:HB2	1:A:874:PHE:HB3	2.01	0.41
1:B:189:PHE:HA	1:B:190:PRO:HD3	1.80	0.41
1:B:79:ARG:HG2	1:B:82:ARG:HH21	1.85	0.41
1:A:178:PRO:HA	1:A:187:TRP:CG	2.54	0.41
1:A:356:ILE:HG22	1:A:357:TRP:N	2.35	0.41
1:A:862:ILE:HD12	1:A:866:VAL:CG2	2.50	0.41
1:B:558:GLU:O	1:B:558:GLU:CG	2.68	0.41
1:A:177:TYR:HB3	1:A:178:PRO:HD2	2.03	0.41
1:A:217:LYS:NZ	1:A:588:ASN:HB3	2.36	0.41
1:A:230:ASP:N	1:A:230:ASP:OD1	2.51	0.41
1:B:282:PHE:CD2	1:B:385:VAL:HG21	2.56	0.41
1:A:260:ASN:O	1:A:262:GLN:HG3	2.21	0.41
1:A:56:ILE:HG23	1:A:279:GLU:OE1	2.21	0.41
1:A:864:LYS:HD3	1:B:779:PRO:O	2.21	0.41
1:B:506:LEU:CD2	1:B:515:LEU:HD12	2.50	0.41
1:A:514:ARG:HG3	1:A:514:ARG:HH11	1.86	0.41
1:A:727:GLN:HG2	1:A:754:ASP:HB2	2.03	0.41
1:A:851:ALA:O	1:A:855:GLU:HG3	2.21	0.41
1:B:528:MET:C	1:B:530:GLY:N	2.74	0.41
1:A:352:THR:O	1:A:355:GLN:HB2	2.21	0.40
1:A:143:ILE:HD12	1:A:143:ILE:C	2.41	0.40
1:B:343:GLU:H	1:B:343:GLU:HG2	1.55	0.40
1:B:527:GLY:HA2	1:B:529:GLU:OE1	2.21	0.40
1:B:391:ILE:O	1:B:394:TYR:HB2	2.22	0.40
1:B:664:TYR:CG	1:B:701:MET:HB2	2.57	0.40
1:A:160:GLU:CD	1:A:172:ASN:OD1	2.60	0.40
1:A:488:GLN:OE1	1:A:500:ARG:NH2	2.55	0.40
1:A:674:LEU:HD23	1:A:674:LEU:HA	1.96	0.40
1:B:194:MET:HG2	3:B:887:TZD:N3'	2.36	0.40
1:B:626:GLY:O	1:B:627:THR:C	2.60	0.40

There are no symmetry-related clashes.



## 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	795/886 (90%)	752 (95%)	40 (5%)	3 (0%)	34	32
1	B	795/886 (90%)	755 (95%)	37 (5%)	3 (0%)	34	32
All	All	1590/1772 (90%)	1507 (95%)	77 (5%)	6 (0%)	34	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	GLY
1	A	305	ASP
1	B	627	THR
1	B	398	ASP
1	A	399	ALA
1	B	521	ASP

### 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	665/735 (90%)	605 (91%)	60 (9%)	9	6
1	B	665/735 (90%)	595 (90%)	70 (10%)	7	4
All	All	1330/1470 (90%)	1200 (90%)	130 (10%)	8	5

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	94	LEU
1	A	97	SER
1	A	130	GLU
1	A	159	GLN
1	A	160	GLU
1	A	168	GLU
1	A	172	ASN
1	A	182	LEU
1	A	192	VAL
1	A	194	MET
1	A	211	LEU
1	A	214	ARG
1	A	216	LEU
1	A	262	GLN
1	A	264	LEU
1	A	278	LEU
1	A	301	LEU
1	A	303	ARG
1	A	310	LEU
1	A	312	GLN
1	A	318	VAL
1	A	334	ARG
1	A	340	LYS
1	A	350	ASP
1	A	354	GLU
1	A	375	LYS
1	A	398	ASP
1	A	420	ILE
1	A	434	GLU
1	A	435	LYS
1	A	443	GLU
1	A	457	LYS
1	A	464	SER
1	A	479	GLN
1	A	486	GLU
1	A	507	LYS
1	A	509	LYS
1	A	519	ILE
1	A	533	ARG
1	A	558	GLU
1	A	560	GLU
1	A	561	LYS

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Mol	Chain	Res	Type
1	A	572	LEU
1	A	586	SER
1	A	638	LEU
1	A	666	VAL
1	A	685	VAL
1	A	690	THR
1	A	711	LYS
1	A	738	VAL
1	A	743	GLU
1	A	747	LYS
1	A	780	LEU
1	A	793	ASN
1	A	819	ASP
1	A	826	ASP
1	A	859	ARG
1	A	867	VAL
1	A	885	LEU
1	B	65	VAL
1	B	68	GLN
1	B	70	GLU
1	B	77	LEU
1	B	97	SER
1	B	172	ASN
1	B	175	SER
1	B	192	VAL
1	B	194	MET
1	B	196	LEU
1	B	206	LYS
1	B	209	LYS
1	B	211	LEU
1	B	221	LYS
1	B	228	LEU
1	B	234	ASP
1	B	243	THR
1	B	263	ARG
1	B	264	LEU
1	B	265	ASP
1	B	274	ILE
1	B	278	LEU
1	B	297	ARG
1	B	300	GLU
1	B	301	LEU

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Mol	Chain	Res	Type
1	B	303	ARG
1	B	309	LYS
1	B	326	LYS
1	B	340	LYS
1	B	343	GLU
1	B	368	LYS
1	B	374	LYS
1	B	375	LYS
1	B	377	GLN
1	B	380	LYS
1	B	382	LYS
1	B	385	VAL
1	B	398	ASP
1	B	420	ILE
1	B	421	ARG
1	B	429	SER
1	B	433	ILE
1	B	443	GLU
1	B	475	LEU
1	B	484	LEU
1	B	488	GLN
1	B	490	LYS
1	B	509	LYS
1	B	512	LYS
1	B	522	GLU
1	B	533	ARG
1	B	537	ILE
1	B	539	SER
1	B	560	GLU
1	B	587	THR
1	B	610	LEU
1	B	638	LEU
1	B	680	GLU
1	B	685	VAL
1	B	718	THR
1	B	723	LYS
1	B	725	LYS
1	B	747	LYS
1	B	780	LEU
1	B	784	ARG
1	B	818	ASP
1	B	843	VAL

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Mol	Chain	Res	Type
1	B	846	SER
1	B	861	GLU
1	B	880	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	466	GLN
1	A	737	HIS
1	B	106	HIS
1	B	466	GLN
1	B	737	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TZD	A	889	2	23,28,28	1.56	6 (26%)	28,42,42	1.09	2 (7%)
3	TZD	B	887	2	23,28,28	1.65	5 (21%)	28,42,42	1.10	2 (7%)

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	TZD	A	889	2	-	3/16/17/17	0/2/2/2
3	TZD	B	887	2	-	5/16/17/17	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TZD	C4'-N3'	3.86	1.40	1.35
3	A	889	TZD	C4'-N3'	3.69	1.40	1.35
3	B	887	TZD	C5'-C4'	3.61	1.49	1.42
3	A	889	TZD	C5'-C4'	3.31	1.48	1.42
3	B	887	TZD	C2'-N1'	2.65	1.38	1.34
3	B	887	TZD	OC2-C2	2.45	1.25	1.21
3	A	889	TZD	C2'-N1'	2.41	1.38	1.34
3	A	889	TZD	C5A-C5	-2.35	1.49	1.50
3	B	887	TZD	C5A-C5	-2.29	1.49	1.50
3	A	889	TZD	C6'-N1'	2.13	1.38	1.34
3	A	889	TZD	OC2-C2	2.07	1.24	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	887	TZD	C6'-N1'-C2'	2.59	120.37	115.96
3	A	889	TZD	C6'-N1'-C2'	2.54	120.28	115.96
3	B	887	TZD	C5-C4-N3	2.17	112.20	107.66
3	A	889	TZD	C5-C4-N3	2.01	111.87	107.66

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	889	TZD	P1-O11-P2-O21

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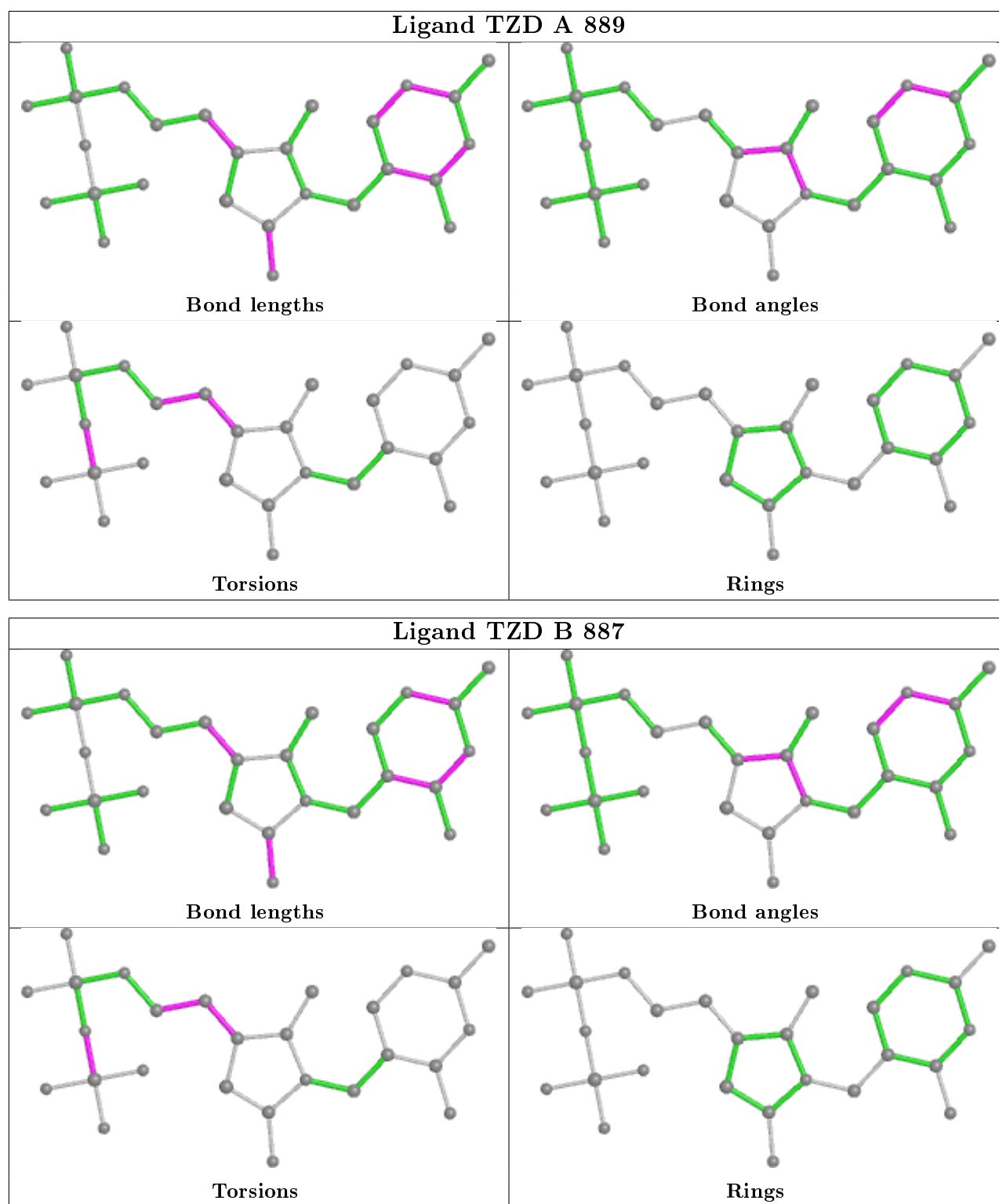
Mol	Chain	Res	Type	Atoms
3	B	887	TZD	C4-C5-C5A-C5B
3	B	887	TZD	P1-O11-P2-O21
3	B	887	TZD	P1-O11-P2-O23
3	A	889	TZD	C4-C5-C5A-C5B
3	B	887	TZD	P1-O11-P2-O22
3	A	889	TZD	C5-C5A-C5B-O5G
3	B	887	TZD	C5-C5A-C5B-O5G

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	887	TZD	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 ⓘ

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.