



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2021 – 04:06 PM EDT

PDB ID : 3LPL  
Title : E. coli pyruvate dehydrogenase complex E1 component E571A mutant  
Authors : Furey, W.  
Deposited on : 2010-02-05  
Resolution : 2.10 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) : 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

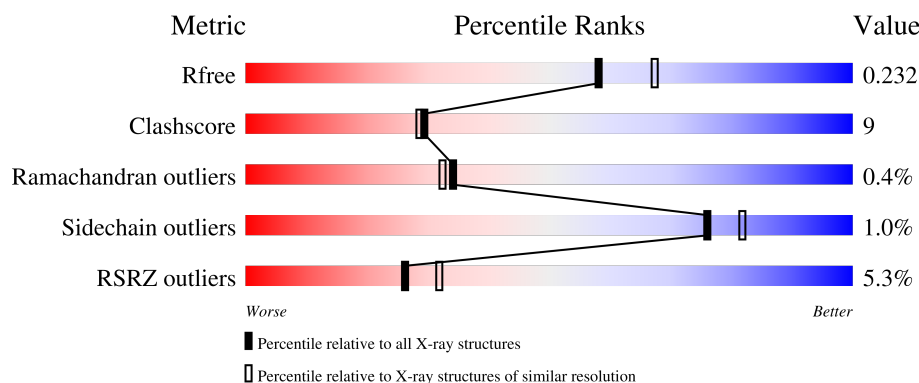
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 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  $\leq 5\%$ . 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	886	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 10%</div> </div> </div>
1	B	886	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>• 10%</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13497 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.

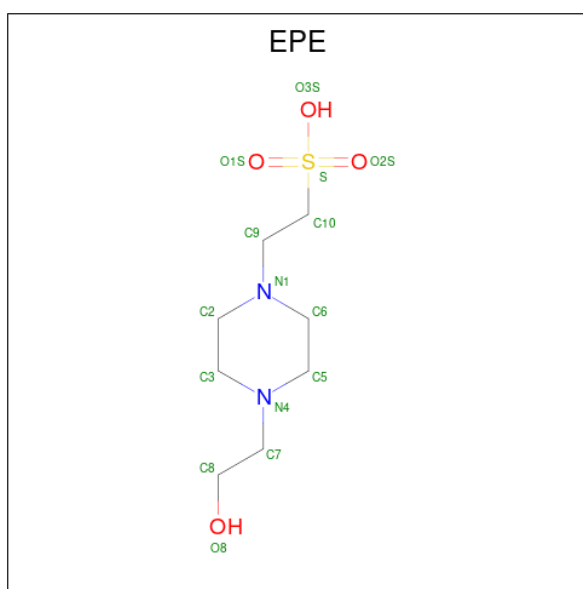
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	2	0
			6359	4031	1097	1205	26			
1	B	801	Total	C	N	O	S	0	1	0
			6349	4025	1094	1204	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	ALA	GLU	engineered mutation	UNP P0AFG9
B	571	ALA	GLU	engineered mutation	UNP P0AFG9

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



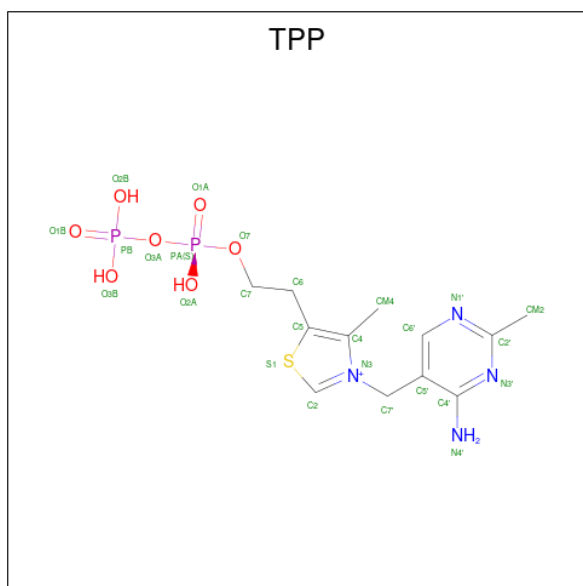
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			11	2	7	2		
3	B	1	Total	C	O	P	0	0
			11	2	7	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).

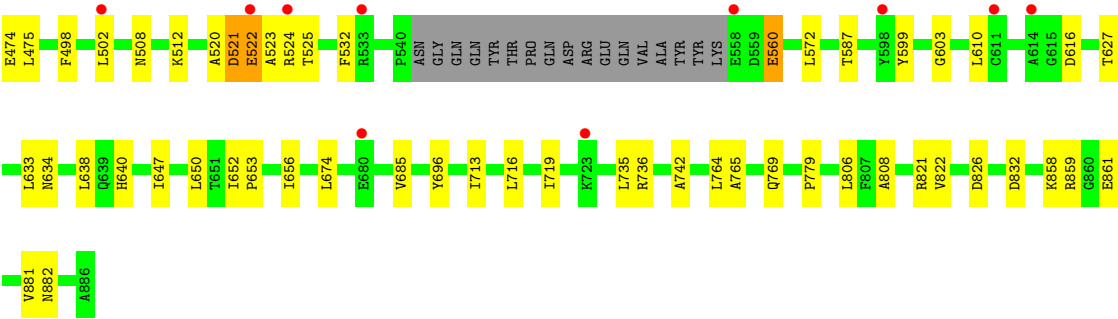


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	348	Total	O	0	0
			348	348		
6	B	377	Total	O	0	0
			377	377		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.82Å 142.22Å 82.52Å 90.00° 102.36° 90.00°	Depositor
Resolution (Å)	41.72 – 2.10 40.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (41.72-2.10) 94.5 (40.86-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.72 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197 , 0.238 0.195 , 0.232	Depositor DCC
$R_{free}$ test set	5122 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.0	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13497	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, TPP, MG, EPE

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	0/6504	0.71	1/8794 (0.0%)
1	B	0.56	0/6493	0.71	2/8779 (0.0%)
All	All	0.55	0/12997	0.71	3/17573 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	LEU	CA-CB-CG	5.47	127.88	115.30
1	B	126	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	126	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6359	0	6192	131	0
1	B	6349	0	6186	124	0
2	A	15	0	17	0	0
2	B	15	0	18	0	0
3	A	11	0	2	0	0
3	B	11	0	2	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	348	0	0	3	0
6	B	377	0	0	13	0
All	All	13497	0	12417	239	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 9.

All (239) 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:415:ASP:O	1:B:418:ARG:HG2	1.46	1.14
1:B:430:ASP:HA	1:B:433:ILE:HD12	1.47	0.96
1:B:421:ARG:HG3	1:B:421:ARG:HH11	1.32	0.94
1:A:863:ASP:O	1:A:866:VAL:HG12	1.68	0.93
1:B:415:ASP:CG	1:B:418:ARG:HD3	1.93	0.89
1:B:430:ASP:HA	1:B:433:ILE:CD1	2.05	0.86
1:A:262:GLN:NE2	1:A:392:LYS:HD3	1.92	0.83
1:A:853:LEU:HB3	1:A:867:VAL:HG22	1.62	0.81
1:B:198:PRO:HG3	1:B:228:LEU:HD22	1.61	0.81
1:A:707:GLU:O	1:A:711:LYS:HG2	1.82	0.78
1:B:415:ASP:O	1:B:418:ARG:CG	2.32	0.77
1:A:863:ASP:OD2	1:A:865:LYS:HB2	1.85	0.76
1:B:194:MET:HE1	3:B:887:TPP:H72	1.66	0.75
1:A:414:MET:O	1:A:418:ARG:HG3	1.86	0.75
1:A:272:GLY:O	1:A:318:VAL:HG13	1.86	0.75
1:B:587:THR:HG22	6:B:911:HOH:O	1.86	0.74
1:A:806:LEU:HD11	1:B:806:LEU:HD11	1.70	0.74
1:A:140:GLN:O	1:A:143:ILE:HG13	1.87	0.73
1:A:263:ARG:O	1:A:392:LYS:NZ	2.22	0.72
1:A:736:ARG:NH2	1:A:737:HIS:NE2	2.36	0.72
1:A:301:LEU:HD21	1:A:351:TRP:CZ2	2.24	0.72
1:B:498:PHE:CZ	1:B:502:LEU:HD11	2.24	0.72
1:A:192:VAL:HG21	1:B:640:HIS:HE1	1.55	0.71
1:A:522:GLU:OE1	1:B:264:LEU:HD13	1.89	0.71
1:B:377:GLN:HG3	6:B:1085:HOH:O	1.91	0.71
1:A:334:ARG:HB3	1:A:356:ILE:CD1	2.20	0.70
1:A:863:ASP:OD2	1:A:865:LYS:HE3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:NH1	1:A:267:PRO:O	2.26	0.68
1:A:304:LYS:HE2	1:A:347:LEU:HD23	1.76	0.68
1:A:273:LYS:HE2	6:A:1156:HOH:O	1.94	0.67
1:A:277:GLU:OE2	1:B:243:THR:HG21	1.93	0.67
1:A:142[O]:HIS:ND1	1:A:142[O]:HIS:N	2.42	0.66
1:A:344:THR:HA	1:A:347:LEU:HD12	1.77	0.66
1:A:303:ARG:O	1:A:303:ARG:HG3	1.94	0.66
1:A:290:ILE:HD11	1:A:375:LYS:HD2	1.77	0.66
1:B:76:GLU:CD	1:B:76:GLU:H	1.98	0.66
1:B:719:ILE:HD12	1:B:742:ALA:HB1	1.76	0.66
1:A:312:GLN:O	1:A:316:GLU:HG2	1.96	0.65
1:A:286:GLY:O	1:A:382:LYS:HE3	1.95	0.65
1:B:415:ASP:OD2	1:B:418:ARG:HD3	1.95	0.65
1:A:518:ILE:C	1:A:519:ILE:HD12	2.17	0.65
1:A:263:ARG:HG3	1:A:264:LEU:N	2.13	0.63
1:A:199:ILE:HD13	1:A:572:LEU:HG	1.80	0.63
1:A:853:LEU:CB	1:A:867:VAL:HG22	2.28	0.63
1:A:298:TRP:HA	1:A:301:LEU:HD12	1.80	0.63
1:B:421:ARG:HH11	1:B:421:ARG:CG	2.08	0.63
1:B:656:ILE:HD11	1:B:685:VAL:HG21	1.81	0.62
1:A:634:ASN:HB2	1:A:832:ASP:O	1.98	0.62
1:A:352:THR:OG1	1:A:355:GLN:HG3	2.00	0.62
1:B:300:GLU:HG3	1:B:301:LEU:N	2.16	0.61
1:A:345:ALA:O	1:A:349:ALA:HB2	2.02	0.60
1:A:352:THR:HG23	1:A:355:GLN:OE1	2.01	0.60
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.31	0.60
1:B:192:VAL:HG22	1:B:192:VAL:O	2.01	0.60
1:B:522:GLU:HG3	1:B:599:TYR:HE1	1.66	0.60
1:A:302:LEU:HD23	1:A:310:LEU:HD23	1.83	0.59
1:A:433:ILE:HG22	1:A:434:GLU:OE2	2.01	0.59
1:A:192:VAL:HG22	1:A:192:VAL:O	2.03	0.59
1:A:840:HIS:HA	1:A:880:LYS:NZ	2.17	0.59
1:A:199:ILE:HD13	1:A:572:LEU:CD2	2.33	0.59
1:A:329:ASP:HA	1:A:357:TRP:CZ3	2.38	0.58
1:A:304:LYS:NZ	1:A:347:LEU:HA	2.17	0.58
1:B:696:TYR:HB3	1:B:736:ARG:HH11	1.67	0.58
1:B:421:ARG:HG3	1:B:421:ARG:NH1	2.09	0.58
1:A:524:ARG:HA	1:A:529:GLU:OE1	2.03	0.57
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.34	0.57
1:A:98:LYS:HD2	1:A:436:LEU:CD1	2.34	0.57
1:A:130:GLU:HB3	1:A:131:GLN:HE22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:VAL:HG12	1:A:319:ASP:N	2.19	0.57
1:B:274:ILE:HG13	1:B:278:LEU:HG	1.87	0.57
1:B:421:ARG:HD2	1:B:421:ARG:O	2.04	0.57
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.40	0.56
1:B:194:MET:CE	1:B:232:GLU:HB2	2.35	0.56
1:B:194:MET:HE3	6:B:1096:HOH:O	2.05	0.56
1:A:522:GLU:OE1	1:B:264:LEU:CD1	2.54	0.56
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.88	0.56
1:B:318:VAL:HG22	6:B:1234:HOH:O	2.06	0.55
1:A:294:TRP:HB3	1:A:298:TRP:CD1	2.42	0.55
1:A:519:ILE:HD11	1:A:528:MET:HE2	1.89	0.55
1:B:421:ARG:HD2	1:B:421:ARG:C	2.27	0.55
1:B:572:LEU:HD12	1:B:610:LEU:HD22	1.88	0.54
1:B:656:ILE:CG1	1:B:685:VAL:HG21	2.37	0.54
1:B:498:PHE:CE1	1:B:502:LEU:HD21	2.43	0.54
1:B:210:TYR:CZ	1:B:214:ARG:HD2	2.43	0.54
1:B:508:ASN:O	1:B:512:LYS:HB3	2.08	0.53
1:B:112:SER:HB3	1:B:392:LYS:HA	1.90	0.53
1:B:421:ARG:NH2	1:B:430:ASP:HB2	2.23	0.53
1:A:842:GLU:OE2	1:A:880:LYS:HE2	2.08	0.53
1:B:472:LYS:HE3	1:B:474:GLU:OE2	2.09	0.53
1:B:140:GLN:O	1:B:143:ILE:HG13	2.09	0.53
1:A:98:LYS:HD2	1:A:436:LEU:HD12	1.90	0.52
1:A:819:ASP:OD2	1:A:855:GLU:HG2	2.09	0.52
1:B:498:PHE:CE2	1:B:502:LEU:HD11	2.44	0.52
1:B:421:ARG:CG	1:B:421:ARG:NH1	2.70	0.52
1:A:212:GLU:OE2	1:A:220:SER:HB3	2.10	0.52
1:A:507:LYS:HA	1:A:507:LYS:HE2	1.91	0.52
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.92	0.52
1:B:265:ASP:OD1	1:B:265:ASP:O	2.28	0.52
1:B:194:MET:HE3	1:B:232:GLU:HB2	1.92	0.52
1:B:304:LYS:NZ	6:B:1242:HOH:O	2.40	0.52
1:A:393:GLY:HA3	1:A:400:ALA:HB1	1.92	0.52
1:A:144:SER:OG	1:A:145:PRO:HD3	2.10	0.51
1:B:634:ASN:HB2	1:B:832:ASP:O	2.10	0.51
1:A:397:GLY:O	1:A:398:ASP:C	2.48	0.51
1:A:716:LEU:HD13	1:A:739:ARG:NH1	2.25	0.51
1:B:736:ARG:NH1	6:B:1233:HOH:O	2.33	0.51
1:A:206:LYS:HD2	1:A:248:GLU:HG3	1.92	0.51
1:A:262:GLN:HA	1:A:267:PRO:HA	1.92	0.51
1:B:587:THR:HG21	6:B:970:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASP:C	1:B:417:VAL:H	2.13	0.51
1:A:318:VAL:CG1	1:A:319:ASP:N	2.74	0.51
1:A:396:MET:O	1:A:397:GLY:O	2.27	0.51
1:B:859:ARG:NH1	1:B:861:GLU:OE1	2.44	0.51
1:B:475:LEU:HD22	1:B:674:LEU:HG	1.93	0.51
1:B:198:PRO:HG3	1:B:228:LEU:CD2	2.35	0.51
1:B:656:ILE:CD1	1:B:685:VAL:HG21	2.40	0.51
1:A:508:ASN:O	1:A:512:LYS:HB3	2.11	0.50
1:A:192:VAL:CG2	1:B:640:HIS:HE1	2.23	0.50
1:A:519:ILE:HD11	1:A:528:MET:CE	2.40	0.50
1:B:523:ALA:CB	1:B:532:PHE:HZ	2.25	0.50
1:B:206:LYS:HD2	6:B:1056:HOH:O	2.12	0.50
1:B:159:GLN:NE2	1:B:438:TYR:HD2	2.10	0.50
1:B:420:ILE:C	1:B:420:ILE:HD12	2.33	0.50
1:A:528:MET:HE1	1:A:531:LEU:HD12	1.94	0.49
1:A:334:ARG:HB3	1:A:356:ILE:HD13	1.94	0.49
1:B:126:ARG:HD3	6:B:1184:HOH:O	2.12	0.49
1:B:415:ASP:OD1	1:B:418:ARG:HD3	2.10	0.49
1:A:301:LEU:CD2	1:A:351:TRP:CZ2	2.96	0.49
1:A:304:LYS:HZ1	1:A:347:LEU:HA	1.76	0.49
1:A:519:ILE:CG2	1:A:520:ALA:N	2.76	0.49
1:A:370:TYR:OH	1:A:374:LYS:HE3	2.12	0.49
1:B:808:ALA:HB3	1:B:822:VAL:CG1	2.42	0.49
1:A:716:LEU:HD13	1:A:739:ARG:CZ	2.42	0.49
1:A:199:ILE:HD13	1:A:572:LEU:CG	2.43	0.49
1:A:331:ALA:O	1:A:334:ARG:HG2	2.12	0.49
1:A:263:ARG:NE	1:B:521:ASP:OD1	2.45	0.49
1:A:616:ASP:OD2	1:B:638:LEU:HD22	2.13	0.48
1:A:638:LEU:HD22	1:B:616:ASP:CG	2.33	0.48
1:B:656:ILE:HG12	1:B:685:VAL:HG21	1.95	0.48
1:A:326:LYS:HD2	1:A:391:ILE:HG23	1.95	0.48
1:B:398:ASP:OD1	1:B:398:ASP:N	2.46	0.48
1:B:429:SER:C	1:B:431:ALA:N	2.67	0.48
1:A:192:VAL:HG21	1:B:640:HIS:CE1	2.43	0.48
1:B:178:PRO:HA	1:B:187:TRP:CG	2.49	0.48
1:B:262:GLN:NE2	1:B:392:LYS:HD3	2.29	0.48
1:A:353:ASP:O	1:A:356:ILE:N	2.47	0.47
1:B:466:GLN:CD	6:B:952:HOH:O	2.52	0.47
1:B:524:ARG:HB3	1:B:524:ARG:CZ	2.44	0.47
1:B:627:THR:HB	1:B:633:LEU:HD22	1.95	0.47
1:A:736:ARG:NH2	1:A:737:HIS:CE1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:HIS:HE1	1:B:192:VAL:HG21	1.79	0.47
1:B:107:MET:CE	1:B:396:MET:HE1	2.45	0.47
1:B:309:LYS:HG3	1:B:343:GLU:CG	2.44	0.47
1:B:429:SER:C	1:B:431:ALA:H	2.16	0.47
1:B:524:ARG:HB3	1:B:524:ARG:NH1	2.29	0.47
1:A:332:TYR:O	1:A:332:TYR:CD1	2.68	0.46
1:A:664:TYR:CG	1:A:701:MET:HB2	2.49	0.46
1:B:417:VAL:CG2	1:B:433:ILE:CG2	2.93	0.46
1:B:656:ILE:HG12	1:B:685:VAL:HG22	1.97	0.46
1:A:178:PRO:HA	1:A:187:TRP:CG	2.50	0.46
1:A:304:LYS:CE	1:A:347:LEU:HD23	2.43	0.46
1:A:862:ILE:HD12	1:A:866:VAL:CG1	2.45	0.46
1:A:334:ARG:NE	1:A:353:ASP:OD1	2.47	0.46
1:A:821:ARG:HH11	1:A:851:ALA:HA	1.81	0.46
1:A:396:MET:O	1:A:397:GLY:C	2.53	0.46
1:B:462:LEU:HB2	1:B:463:PRO:HA	1.98	0.45
1:B:206:LYS:NZ	6:B:1204:HOH:O	2.41	0.45
1:B:808:ALA:HB3	1:B:822:VAL:HG11	1.98	0.45
1:B:821:ARG:NH2	1:B:858:LYS:HE2	2.31	0.45
1:A:263:ARG:CG	1:A:264:LEU:N	2.78	0.45
1:B:265:ASP:O	1:B:265:ASP:CG	2.54	0.45
1:A:846:SER:HB2	1:A:874:PHE:CG	2.52	0.45
1:B:765:ALA:O	1:B:769:GLN:HG3	2.16	0.45
1:A:131:GLN:NE2	1:A:131:GLN:N	2.64	0.45
1:B:143:ILE:HD12	1:B:143:ILE:C	2.37	0.44
1:B:192:VAL:O	1:B:192:VAL:CG2	2.65	0.44
1:A:290:ILE:CD1	1:A:375:LYS:HD2	2.46	0.44
1:A:466:GLN:NE2	6:A:1162:HOH:O	2.50	0.44
1:B:87:TRP:CZ3	1:B:421:ARG:HB3	2.52	0.44
1:A:326:LYS:O	1:A:357:TRP:HH2	2.00	0.44
1:B:194:MET:HE2	1:B:232:GLU:HB2	1.99	0.44
1:B:233:MET:HB2	6:B:1150:HOH:O	2.17	0.44
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.99	0.44
1:B:195:GLY:C	1:B:198:PRO:HD2	2.38	0.44
1:B:415:ASP:C	1:B:417:VAL:N	2.71	0.44
1:A:640:HIS:HE1	1:B:192:VAL:CG2	2.31	0.43
1:A:263:ARG:HG2	1:A:266:GLY:O	2.18	0.43
1:A:426:VAL:HG13	1:A:439:ILE:HD11	2.00	0.43
1:A:323:GLN:O	1:A:326:LYS:HB3	2.18	0.43
1:A:765:ALA:O	1:A:769:GLN:HG3	2.18	0.43
1:A:462:LEU:HB2	1:A:463:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:SER:O	1:B:433:ILE:HG13	2.18	0.43
1:A:647:ILE:O	1:A:650:LEU:HG	2.19	0.43
1:B:523:ALA:CB	1:B:532:PHE:CZ	3.01	0.43
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.87	0.43
1:A:262:GLN:CD	1:A:392:LYS:HD3	2.38	0.42
1:B:301:LEU:HD13	1:B:351:TRP:CZ2	2.54	0.42
1:A:434:GLU:H	1:A:434:GLU:CD	2.22	0.42
1:A:569:ILE:HD13	1:B:194:MET:CE	2.49	0.42
1:B:107:MET:HE3	1:B:396:MET:CE	2.48	0.42
1:A:300:GLU:OE1	1:A:303:ARG:NH1	2.52	0.42
1:B:87:TRP:CE3	1:B:420:ILE:HD11	2.54	0.42
1:B:361:ARG:HD2	1:B:391:ILE:HG13	2.01	0.42
1:A:426:VAL:HG12	1:A:428:VAL:HG23	2.02	0.42
1:A:862:ILE:HD12	1:A:866:VAL:HG11	2.01	0.42
1:B:525:THR:O	1:B:525:THR:CG2	2.67	0.42
1:A:567:GLU:HG3	1:A:574:ALA:HA	2.01	0.42
1:A:597:ILE:HD13	1:A:624:ILE:CG2	2.50	0.42
1:B:309:LYS:HB2	1:B:343:GLU:HG3	2.02	0.42
1:A:265:ASP:OD2	1:B:523:ALA:N	2.43	0.42
1:A:638:LEU:HD21	1:B:616:ASP:HB2	2.02	0.42
1:B:560:GLU:O	1:B:560:GLU:HG2	2.20	0.42
1:B:309:LYS:HG3	1:B:343:GLU:HG3	2.02	0.42
1:B:716:LEU:HD11	1:B:735:LEU:HD21	2.02	0.41
1:B:397:GLY:O	1:B:398:ASP:C	2.57	0.41
1:A:300:GLU:CD	1:A:303:ARG:NH1	2.73	0.41
1:A:326:LYS:O	1:A:357:TRP:CH2	2.74	0.41
1:A:839:HIS:HB3	6:A:1212:HOH:O	2.20	0.41
1:A:327:SER:O	1:A:328:LYS:O	2.38	0.41
1:A:488:GLN:OE1	1:A:500:ARG:NH2	2.53	0.41
1:B:647:ILE:O	1:B:650:LEU:HG	2.20	0.41
1:B:195:GLY:O	1:B:198:PRO:HD2	2.20	0.41
1:A:300:GLU:OE2	1:A:303:ARG:NH1	2.54	0.41
1:B:498:PHE:CZ	1:B:502:LEU:HD21	2.55	0.41
1:A:326:LYS:HB3	1:A:326:LYS:NZ	2.36	0.41
1:B:523:ALA:HB1	1:B:532:PHE:CZ	2.56	0.41
1:B:652:ILE:HA	1:B:653:PRO:HD3	1.89	0.41
1:B:881:VAL:HG22	1:B:882:ASN:N	2.36	0.41
1:A:197:GLY:N	1:A:198:PRO:HD2	2.36	0.41
1:B:274:ILE:O	1:B:278:LEU:HG	2.20	0.41
1:B:520:ALA:O	1:B:522:GLU:N	2.54	0.40
1:B:603:GLY:HA3	6:B:1060:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:O	1:A:192:VAL:CG2	2.68	0.40
1:A:194:MET:HE2	1:A:194:MET:HA	2.04	0.40
1:A:864:LYS:HD3	1:B:779:PRO:O	2.20	0.40
1:A:329:ASP:HA	1:A:357:TRP:CE3	2.57	0.40
1:A:397:GLY:O	1:A:399:ALA:N	2.54	0.40
1:A:806:LEU:HA	1:A:809:GLU:HB2	2.04	0.40
1:B:428:VAL:O	1:B:428:VAL:HG13	2.21	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	797/886 (90%)	761 (96%)	31 (4%)	5 (1%)	25	21
1	B	796/886 (90%)	755 (95%)	39 (5%)	2 (0%)	41	41
All	All	1593/1772 (90%)	1516 (95%)	70 (4%)	7 (0%)	34	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	LYS
1	A	398	ASP
1	A	399	ALA
1	A	397	GLY
1	B	521	ASP
1	B	522	GLU
1	A	638	LEU



### 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	666/734 (91%)	661 (99%)	5 (1%)	81	86
1	B	665/734 (91%)	657 (99%)	8 (1%)	71	77
All	All	1331/1468 (91%)	1318 (99%)	13 (1%)	76	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	LEU
1	A	309	LYS
1	A	502	LEU
1	A	638	LEU
1	A	826	ASP
1	B	77	LEU
1	B	79	ARG
1	B	243	THR
1	B	301	LEU
1	B	382	LYS
1	B	421	ARG
1	B	560	GLU
1	B	826	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	172	ASN
1	A	466	GLN
1	A	534	GLN

### 5.3.3 RNA

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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	TPP	A	887	4	8,10,27	1.61	1 (12%)	12,15,40	1.16	1 (8%)
2	EPE	A	889	-	15,15,15	1.34	3 (20%)	18,20,20	2.29	7 (38%)
5	PO4	A	890	-	4,4,4	0.43	0	6,6,6	0.63	0
3	TPP	B	887	4	8,10,27	1.62	1 (12%)	12,15,40	1.16	1 (8%)
2	EPE	B	889	-	15,15,15	1.66	2 (13%)	18,20,20	2.35	6 (33%)
5	PO4	B	890	-	4,4,4	0.56	0	6,6,6	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	A	889	-	-	3/9/19/19	0/1/1/1
2	EPE	B	889	-	-	0/9/19/19	0/1/1/1
3	TPP	A	887	4	-	3/10/10/17	-
3	TPP	B	887	4	-	4/10/10/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	889	EPE	O1S-S	4.02	1.56	1.45
3	B	887	TPP	PB-O1B	3.42	1.61	1.50
3	A	887	TPP	PB-O1B	3.37	1.61	1.50
2	B	889	EPE	C10-S	3.26	1.82	1.77
2	A	889	EPE	C10-S	3.03	1.81	1.77
2	A	889	EPE	O1S-S	2.73	1.53	1.45
2	A	889	EPE	C5-N4	2.24	1.53	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	889	EPE	O3S-S-O2S	4.60	122.51	111.27
2	B	889	EPE	O3S-S-O2S	4.53	122.35	111.27
2	B	889	EPE	O3S-S-C10	4.19	112.54	105.77
2	B	889	EPE	O2S-S-C10	4.07	111.82	106.92
2	A	889	EPE	O2S-S-C10	4.06	111.80	106.92
2	A	889	EPE	O3S-S-O1S	-3.91	101.72	111.27
2	B	889	EPE	O3S-S-O1S	-3.79	102.02	111.27
2	B	889	EPE	O2S-S-O1S	-3.68	101.20	113.95
2	A	889	EPE	O2S-S-O1S	-3.38	102.26	113.95
2	A	889	EPE	C9-N1-C2	-3.22	103.01	111.23
3	A	887	TPP	PA-O3A-PB	-2.62	123.83	132.83
2	B	889	EPE	O1S-S-C10	-2.60	103.78	106.92
3	B	887	TPP	PA-O3A-PB	-2.59	123.93	132.83
2	A	889	EPE	C6-C5-N4	-2.24	106.05	110.64
2	A	889	EPE	O3S-S-C10	2.05	109.08	105.77

There are no chirality outliers.

All (10) torsion outliers are listed below:

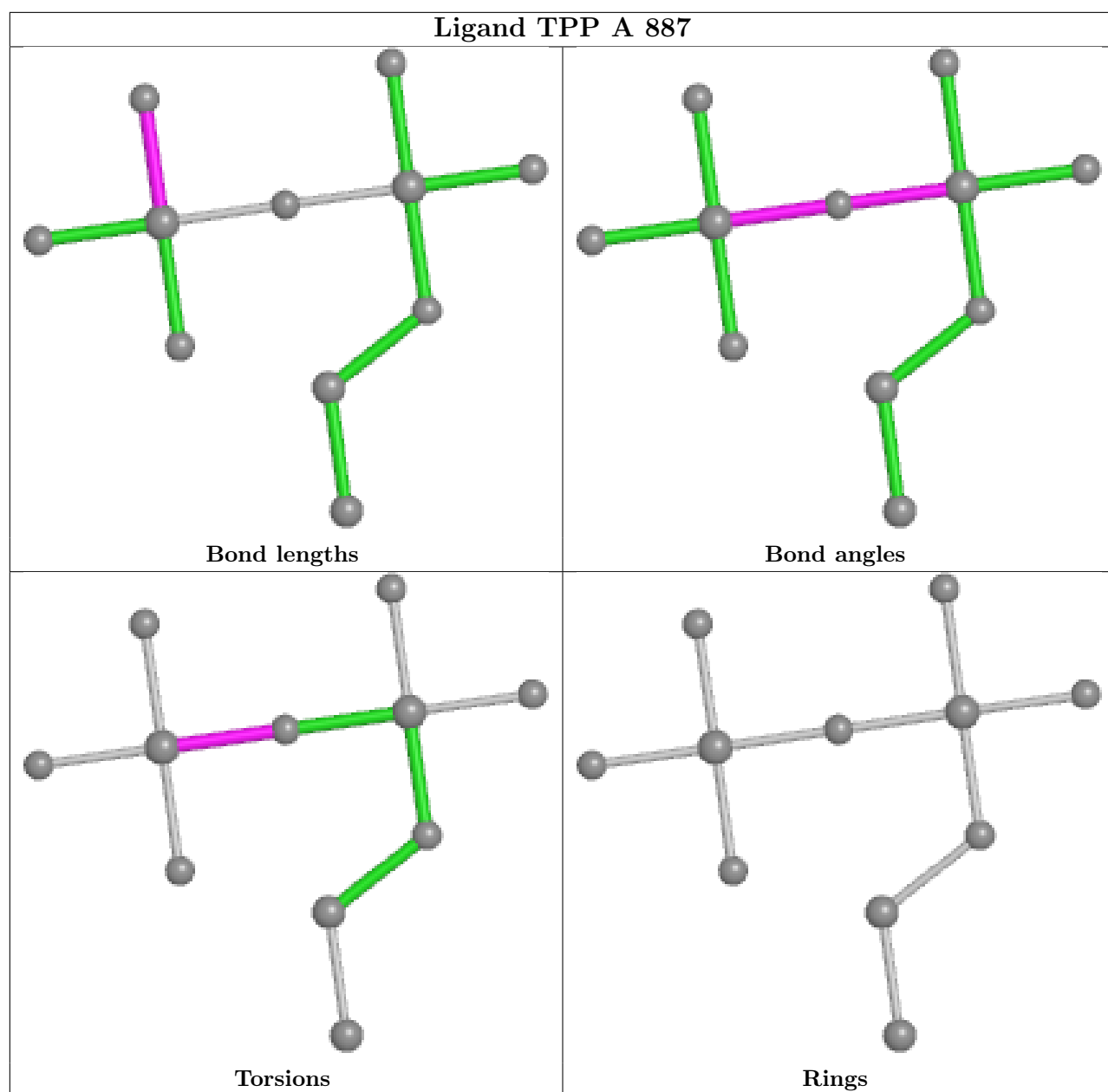
Mol	Chain	Res	Type	Atoms
2	A	889	EPE	C9-C10-S-O1S
2	A	889	EPE	C9-C10-S-O3S
3	A	887	TPP	PA-O3A-PB-O3B
3	A	887	TPP	PA-O3A-PB-O2B
2	A	889	EPE	C9-C10-S-O2S
3	B	887	TPP	PA-O3A-PB-O1B
3	A	887	TPP	PA-O3A-PB-O1B
3	B	887	TPP	PA-O3A-PB-O2B
3	B	887	TPP	PA-O3A-PB-O3B
3	B	887	TPP	C7-O7-PA-O1A

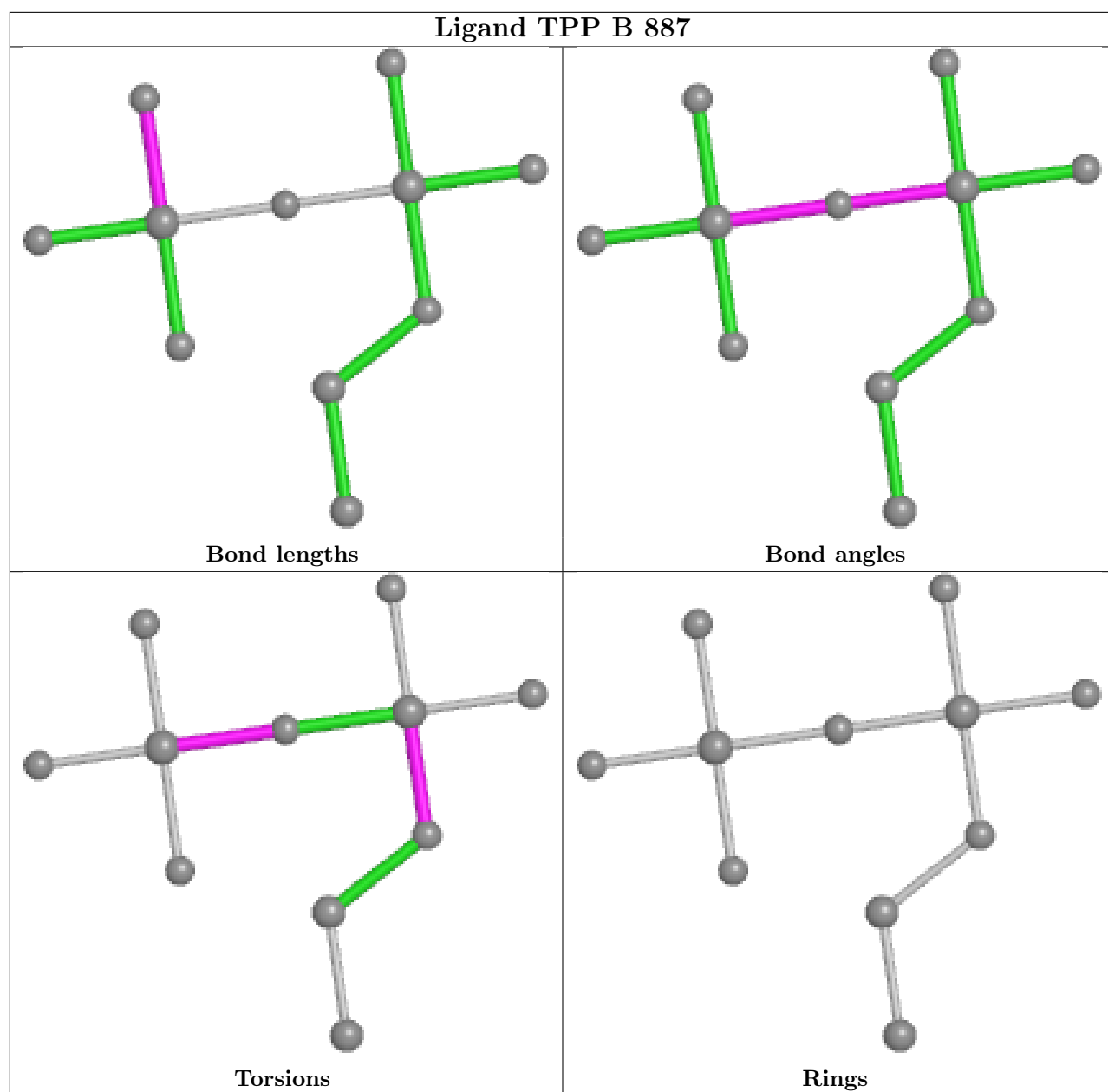
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	887	TPP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	801/886 (90%)	0.28	52 (6%) 18 23	17, 26, 40, 43	0
1	B	801/886 (90%)	0.17	33 (4%) 37 43	16, 25, 35, 45	0
All	All	1602/1772 (90%)	0.23	85 (5%) 26 32	16, 26, 38, 45	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	ALA	10.7
1	B	414	MET	8.7
1	B	400	ALA	8.6
1	A	400	ALA	8.2
1	A	398	ASP	7.3
1	A	349	ALA	7.0
1	A	354	GLU	5.0
1	B	415	ASP	5.0
1	B	398	ASP	5.0
1	A	341	TYR	4.8
1	B	416	GLY	4.7
1	B	533	ARG	4.4
1	B	598[A]	TYR	4.4
1	A	342	PRO	4.4
1	A	351	TRP	4.3
1	A	399	ALA	4.3
1	A	598[A]	TYR	4.2
1	B	428	VAL	4.1
1	A	263	ARG	4.1
1	B	418	ARG	4.0
1	A	325	PHE	3.9
1	A	350	ASP	3.7
1	A	264	LEU	3.7
1	A	524	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	305	ASP	3.6
1	B	433	ILE	3.5
1	B	417	VAL	3.5
1	A	333	VAL	3.5
1	A	330	GLY	3.4
1	A	326	LYS	3.3
1	B	431	ALA	3.3
1	A	418	ARG	3.2
1	B	56	ILE	3.2
1	B	436	LEU	3.1
1	A	130	GLU	3.1
1	B	434	GLU	3.1
1	A	533	ARG	3.0
1	A	336	HIS	3.0
1	A	348	VAL	3.0
1	A	56	ILE	3.0
1	A	397	GLY	3.0
1	A	344	THR	2.9
1	B	429	SER	2.9
1	A	866	VAL	2.7
1	A	268	VAL	2.7
1	B	397	GLY	2.7
1	A	335	GLU	2.7
1	A	327	SER	2.6
1	B	265	ASP	2.6
1	B	524	ARG	2.6
1	B	680	GLU	2.6
1	A	638	LEU	2.6
1	A	331	ALA	2.5
1	B	420	ILE	2.5
1	A	414	MET	2.5
1	A	338	PHE	2.5
1	B	558	GLU	2.5
1	A	340	LYS	2.4
1	B	723	LYS	2.4
1	A	332	TYR	2.4
1	A	265	ASP	2.4
1	A	352	THR	2.4
1	B	395	GLY	2.4
1	B	432	ASP	2.4
1	B	435	LYS	2.3
1	A	301	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	357	TRP	2.3
1	A	433	ILE	2.3
1	B	502	LEU	2.3
1	A	270	GLY	2.3
1	B	522	GLU	2.3
1	A	313	LEU	2.2
1	A	886	ALA	2.2
1	B	614	ALA	2.2
1	A	192	VAL	2.2
1	A	339	GLY	2.2
1	A	572	LEU	2.2
1	B	611	CYS	2.2
1	A	345	ALA	2.1
1	B	306	THR	2.1
1	B	430	ASP	2.1
1	A	160	GLU	2.0
1	A	337	PHE	2.0
1	A	353	ASP	2.0
1	A	356	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	888	1/1	0.88	0.30	56,56,56,56	0
2	EPE	B	889	15/15	0.89	0.30	38,38,39,39	0
3	TPP	A	887	11/26	0.90	0.16	41,42,42,42	0
2	EPE	A	889	15/15	0.93	0.13	31,32,33,33	0

*Continued on next page...*

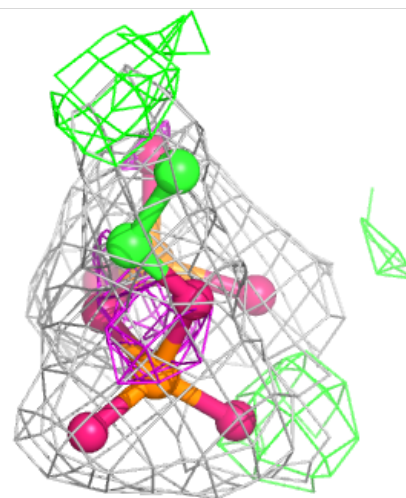
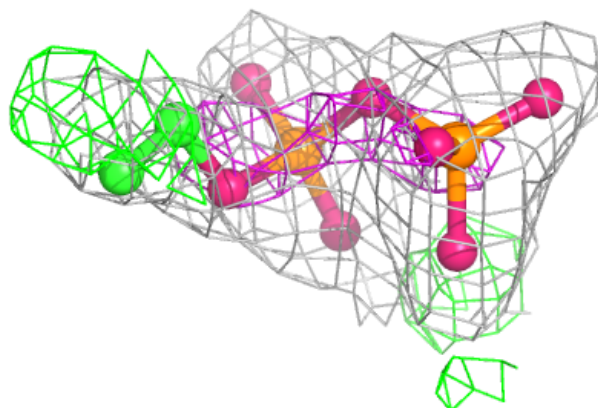
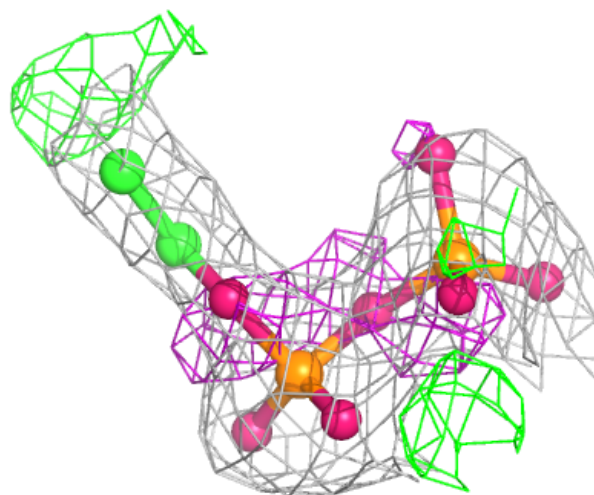
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	B	888	1/1	0.94	0.09	32,32,32,32	0
5	PO4	A	890	5/5	0.96	0.10	36,36,36,37	0
5	PO4	B	890	5/5	0.96	0.11	37,37,37,37	0
3	TPP	B	887	11/26	0.97	0.11	35,35,35,35	0

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

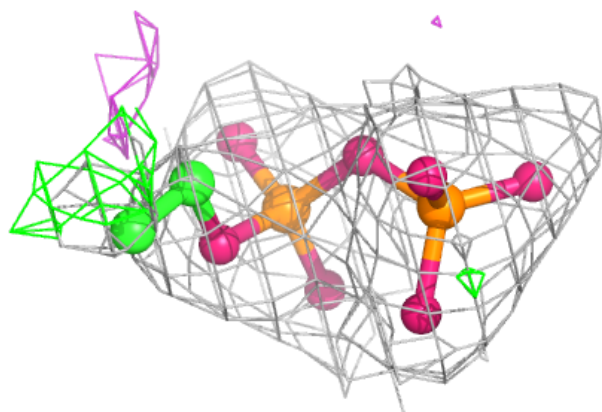
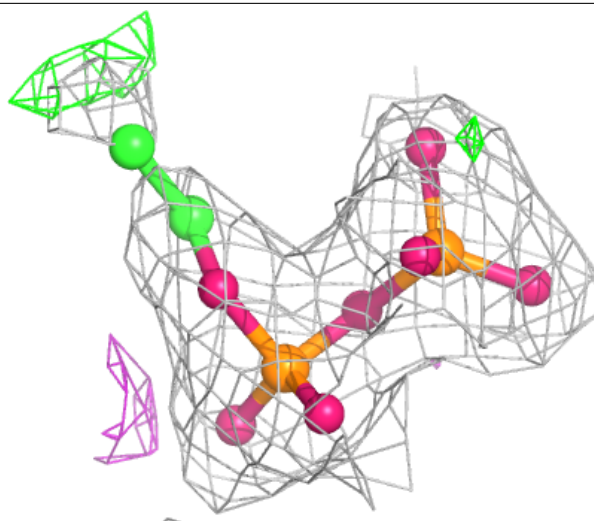
**Electron density around TPP A 887:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around TPP B 887:**

$2mF_o-DF_c$  (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.