Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 02:54 AM EDT

PDB ID	:	3LQ4
Title	:	E. coli pyruvate dehydrogenase complex E1 E235A mutant with high TDP concentration
Authors	:	Furey, W.
Deposited on	:	2010-02-08
Resolution	:	1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

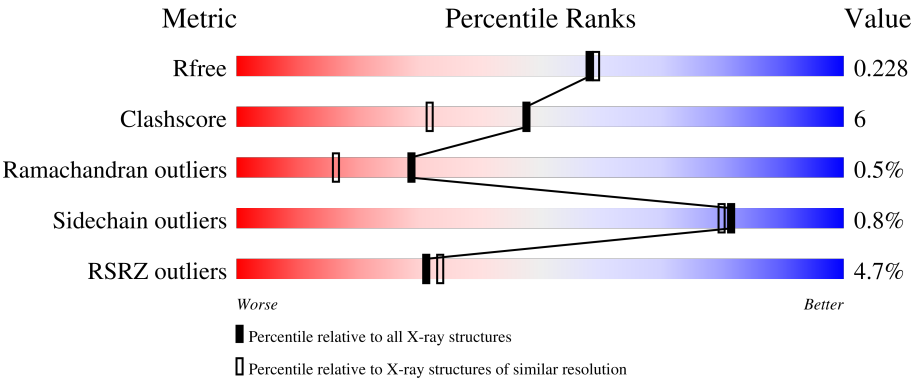
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	5% 77% 13% 10%
1	B	886	3% 81% 9% · 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13440 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.

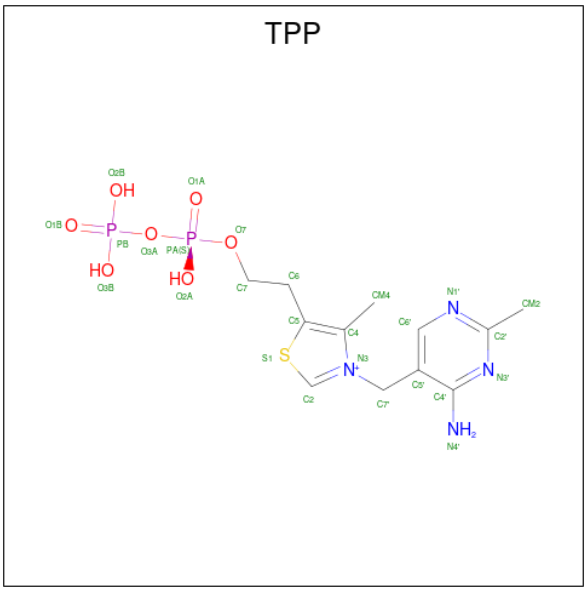
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	1	0
			6347	4022	1096	1203	26			
1	B	801	Total	C	N	O	S	0	0	0
			6337	4016	1093	1202	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	ALA	GLU	engineered mutation	UNP P0AFG9
B	235	ALA	GLU	engineered mutation	UNP P0AFG9

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



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

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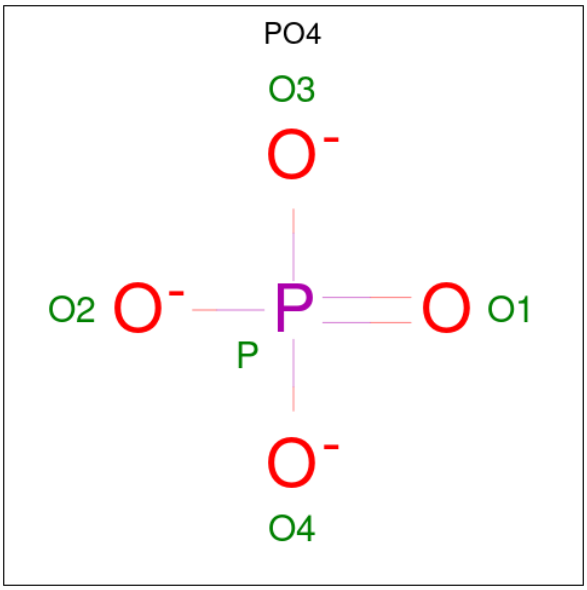
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

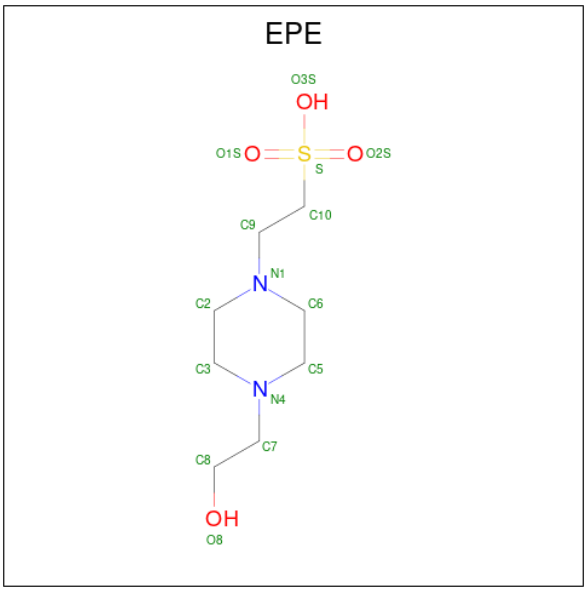
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 6 is water.

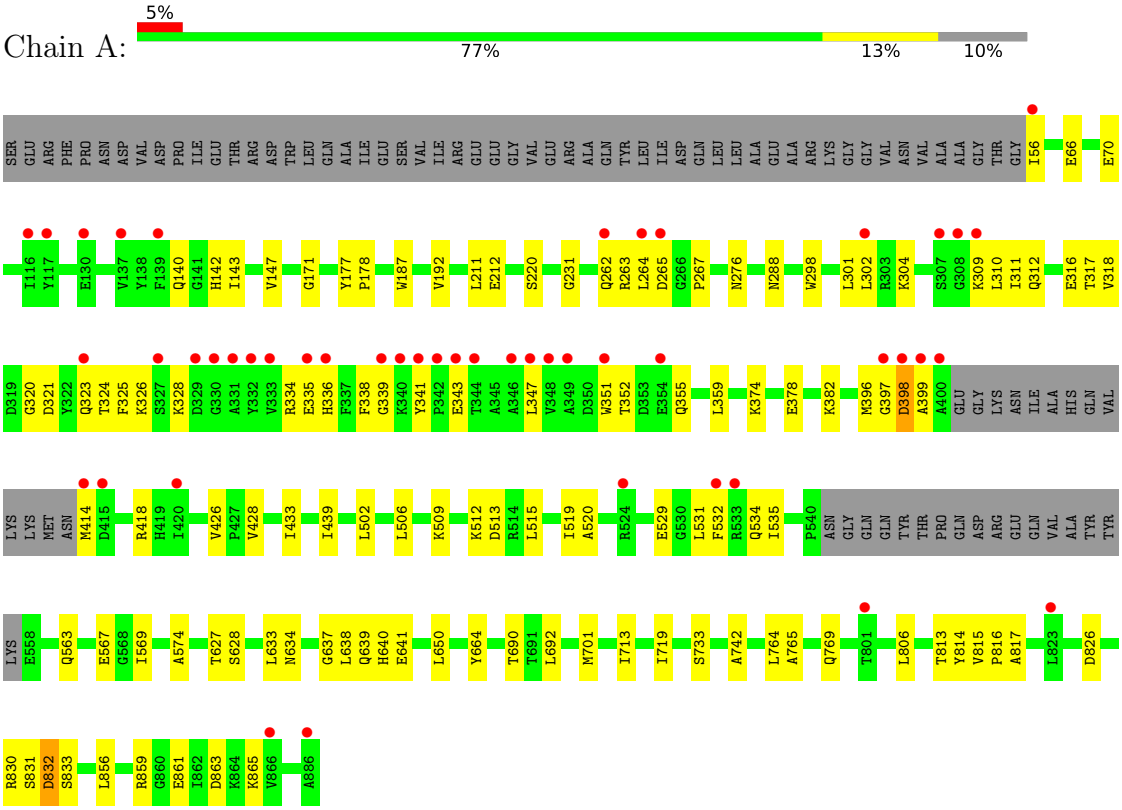
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	340	Total	O	0	0
			340	340		
6	B	337	Total	O	0	0
			337	337		

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.

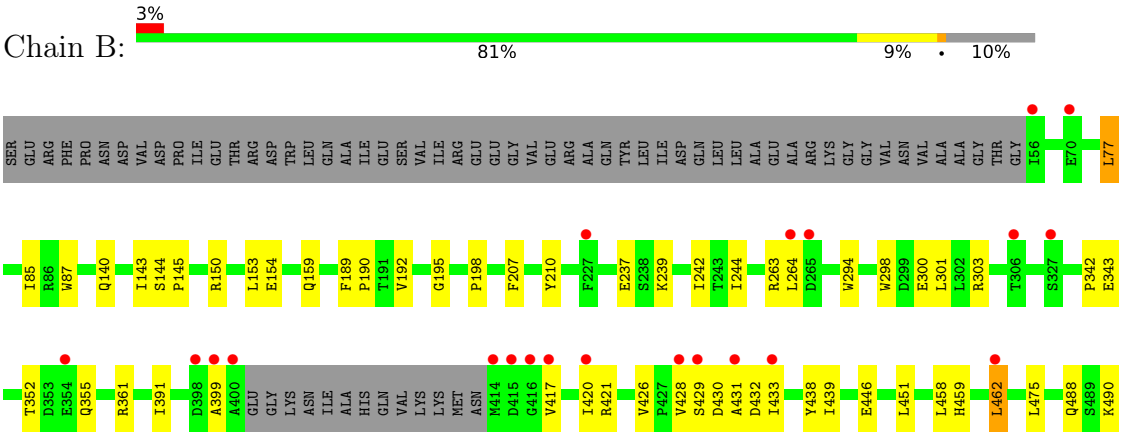
• Molecule 1: Pyruvate dehydrogenase E1 component

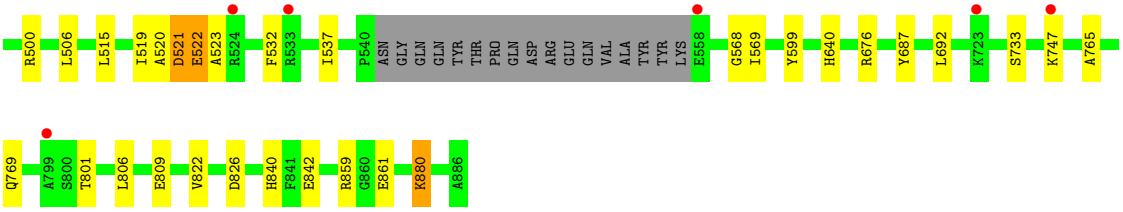
Chain A:



• Molecule 1: Pyruvate dehydrogenase E1 component

Chain B:




R500
L506
L515
I519
A520
D521
E522
A523
R524
F532
R533
I537
P540
ASN
GLY
GLN
GLN
TYR
THR
PRO
GLN
ASP
ARG
GLU
GLN
VAL
ALA
TYR
TYR
LYS
E558
G568
I569
Y599
H640
R676
Y687
L692
K723
S733
K747
A765
Q769
A799
S800
T801
L806
E809
V822
D826
H840
F841
E842
R859
G860
E861
K880
A886

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.21Å 142.22Å 82.85Å 90.00° 101.87° 90.00°	Depositor
Resolution (Å)	32.52 – 1.98 32.52 – 1.96	Depositor EDS
% Data completeness (in resolution range)	83.7 (32.52-1.98) 82.6 (32.52-1.96)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.06 (at 1.97Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.199 , 0.236 0.193 , 0.228	Depositor DCC
R_{free} test set	5434 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13440	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, MG, EPE, TPP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/6491	0.57	1/8776 (0.0%)
1	B	0.33	0/6480	0.58	0/8761
All	All	0.32	0/12971	0.57	1/17537 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	GLY	N-CA-C	5.22	126.15	113.10

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	6347	0	6184	92	0
1	B	6337	0	6178	72	0
2	A	26	0	16	6	0
2	B	26	0	16	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	17	3	0
6	A	340	0	0	2	0
6	B	337	0	0	4	0
All	All	13440	0	12411	153	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 6.

All (153) 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:302:LEU:HD11	1:A:311:ILE:HD11	1.51	0.93
1:B:421:ARG:HD3	1:B:433:ILE:HD11	1.53	0.90
1:A:192:VAL:HG21	1:B:640:HIS:HE1	1.35	0.89
1:B:421:ARG:CD	1:B:433:ILE:HD11	2.13	0.78
1:B:421:ARG:HD3	1:B:433:ILE:CD1	2.13	0.78
1:A:323:GLN:HA	1:A:326:LYS:HE3	1.65	0.76
1:B:264:LEU:HB2	2:B:887:TPP:H62	1.72	0.72
1:A:192:VAL:CG2	1:B:640:HIS:HE1	2.02	0.72
1:A:320:GLY:O	1:A:323:GLN:HG2	1.89	0.72
1:A:192:VAL:HG21	1:B:640:HIS:CE1	2.22	0.70
2:A:887:TPP:H61	1:B:569:ILE:HD11	1.76	0.67
1:A:264:LEU:HB2	2:A:887:TPP:H62	1.78	0.65
2:A:887:TPP:HM41	1:B:569:ILE:HG12	1.80	0.63
1:B:154:GLU:HG2	1:B:451:LEU:HD21	1.81	0.63
1:A:640:HIS:HE1	1:B:192:VAL:HG21	1.63	0.63
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.29	0.62
1:A:832:ASP:OD2	1:A:833:SER:N	2.25	0.61
1:A:302:LEU:CD1	1:A:311:ILE:HD11	2.29	0.60
1:A:426:VAL:HG12	1:A:428:VAL:HG23	1.84	0.59
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.84	0.59
1:A:765:ALA:O	1:A:769:GLN:HG3	2.02	0.59
1:B:522:GLU:HG2	1:B:599:TYR:HE1	1.69	0.58
1:B:429:SER:HB3	1:B:432:ASP:OD2	2.04	0.58
1:A:640:HIS:HE1	1:B:192:VAL:CG2	2.16	0.57
1:A:192:VAL:CG2	1:B:640:HIS:CE1	2.86	0.57
1:B:809:GLU:HG2	1:B:822:VAL:HG21	1.86	0.57
1:A:863:ASP:OD2	1:A:865:LYS:HB2	2.04	0.57
1:A:352:THR:OG1	1:A:355:GLN:HG3	2.04	0.56
1:A:856:LEU:HD22	1:A:861:GLU:OE1	2.04	0.56
1:A:70:GLU:OE2	5:A:890:EPE:H21	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLU:HG2	1:B:599:TYR:CE1	2.41	0.56
1:A:140:GLN:O	1:A:143:ILE:HG13	2.06	0.56
1:B:417:VAL:O	1:B:420:ILE:HG12	2.06	0.55
1:A:304:LYS:HE3	1:A:347:LEU:HD23	1.88	0.55
1:B:801:THR:HB	6:B:1199:HOH:O	2.05	0.55
1:B:842:GLU:OE2	1:B:880:LYS:HE3	2.07	0.54
1:A:567:GLU:HG3	1:A:574:ALA:HA	1.89	0.54
1:A:813:THR:HG23	1:A:814:TYR:CE1	2.42	0.54
2:A:887:TPP:H2	6:B:1137:HOH:O	2.08	0.54
1:A:56:ILE:HD13	1:A:276:ASN:HB3	1.90	0.53
1:A:304:LYS:HE3	1:A:347:LEU:CD2	2.39	0.53
1:B:429:SER:C	1:B:431:ALA:H	2.11	0.53
1:B:77:LEU:HD11	1:B:446:GLU:HG2	1.89	0.53
1:A:813:THR:CG2	1:A:814:TYR:CZ	2.91	0.53
1:A:529:GLU:OE1	1:A:529:GLU:N	2.41	0.52
1:B:421:ARG:HD2	1:B:428:VAL:HG13	1.91	0.52
1:A:212:GLU:OE2	1:A:220:SER:HB3	2.08	0.52
1:A:263:ARG:HG3	1:A:264:LEU:H	1.75	0.52
1:A:529:GLU:HA	1:A:532:PHE:CD2	2.45	0.52
1:B:747:LYS:HG2	6:B:989:HOH:O	2.10	0.52
1:A:264:LEU:HD13	1:B:522:GLU:OE1	2.09	0.51
1:A:265:ASP:OD2	1:B:522:GLU:HA	2.10	0.51
1:B:150:ARG:O	1:B:154:GLU:HG3	2.10	0.51
1:B:140:GLN:O	1:B:143:ILE:HG13	2.11	0.51
1:A:414:MET:HE1	1:A:433:ILE:HG23	1.94	0.50
1:B:519:ILE:HD12	1:B:523:ALA:HB2	1.93	0.50
1:B:237:GLU:H	1:B:237:GLU:CD	2.15	0.50
1:B:506:LEU:HD23	1:B:515:LEU:HD12	1.93	0.50
1:A:831:SER:O	1:A:832:ASP:HB2	2.10	0.50
2:A:887:TPP:CM4	1:B:569:ILE:HG12	2.42	0.50
1:B:85:ILE:HG12	1:B:153:LEU:HD12	1.93	0.50
1:B:859:ARG:NH1	1:B:861:GLU:CD	2.65	0.49
1:B:488:GLN:OE1	1:B:500:ARG:NH1	2.45	0.49
1:A:531:LEU:HD23	1:A:534:GLN:HE21	1.77	0.49
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.93	0.49
1:A:813:THR:HG23	1:A:814:TYR:CD1	2.47	0.49
1:A:312:GLN:O	1:A:316:GLU:HG2	2.12	0.49
1:A:414:MET:O	1:A:418:ARG:HG3	2.13	0.49
1:B:244:ILE:N	1:B:244:ILE:HD12	2.28	0.48
1:A:142[O]:HIS:ND1	1:A:142[O]:HIS:N	2.58	0.48
1:A:262:GLN:HA	1:A:267:PRO:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:LYS:O	1:A:378:GLU:HG3	2.13	0.48
1:A:288:ASN:HB2	1:A:382:LYS:HE3	1.96	0.48
1:B:532:PHE:CE2	1:B:537:ILE:HD11	2.48	0.48
1:A:262:GLN:HB2	6:A:912:HOH:O	2.13	0.48
1:A:806:LEU:HD11	1:B:806:LEU:HD11	1.96	0.48
1:B:144:SER:OG	1:B:145:PRO:HD3	2.14	0.48
1:A:309:LYS:HE3	1:A:341:TYR:CD2	2.49	0.47
1:A:512:LYS:HG3	1:A:513:ASP:N	2.29	0.47
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.96	0.47
1:B:765:ALA:O	1:B:769:GLN:HG3	2.14	0.47
1:A:318:VAL:HG22	1:A:321:ASP:OD2	2.14	0.47
1:B:361:ARG:HD2	1:B:391:ILE:HG13	1.97	0.46
1:B:429:SER:C	1:B:431:ALA:N	2.68	0.46
1:A:634:ASN:HB2	1:A:832:ASP:O	2.15	0.46
1:B:87:TRP:CD1	1:B:439:ILE:HG12	2.50	0.46
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.50	0.46
1:A:426:VAL:HG13	1:A:439:ILE:CD1	2.46	0.46
1:B:521:ASP:HB2	1:B:568:GLY:HA2	1.97	0.46
1:B:352:THR:OG1	1:B:355:GLN:HG3	2.16	0.46
1:A:325:PHE:HE1	1:A:336:HIS:HB2	1.81	0.46
1:B:207:PHE:O	1:B:210:TYR:HB3	2.16	0.46
1:B:426:VAL:HG12	1:B:428:VAL:HG12	1.98	0.46
1:A:231:GLY:C	1:B:569:ILE:HD12	2.37	0.45
1:A:692:LEU:HD13	1:A:733:SER:HB3	1.97	0.45
1:B:430:ASP:OD1	1:B:430:ASP:O	2.33	0.45
1:B:300:GLU:HG3	6:B:1140:HOH:O	2.17	0.45
1:A:650:LEU:C	1:A:650:LEU:HD12	2.37	0.45
1:B:859:ARG:HH12	1:B:861:GLU:CD	2.20	0.45
1:A:142[A]:HIS:NE2	2:A:887:TPP:S1	2.89	0.45
1:A:301:LEU:HD22	1:A:310:LEU:HD22	1.97	0.45
1:A:66:GLU:O	5:A:890:EPE:H81	2.17	0.45
1:A:502:LEU:HD23	1:A:531:LEU:HD11	1.99	0.45
1:A:519:ILE:HG22	1:A:520:ALA:N	2.32	0.45
1:B:189:PHE:HA	1:B:190:PRO:HD3	1.78	0.45
1:A:396:MET:O	1:A:398:ASP:N	2.50	0.44
1:B:264:LEU:HD23	1:B:264:LEU:O	2.17	0.44
1:A:192:VAL:O	1:A:192:VAL:HG22	2.17	0.44
1:A:506:LEU:HD23	1:A:515:LEU:HD12	2.00	0.44
1:A:531:LEU:HD23	1:A:534:GLN:NE2	2.33	0.44
1:A:639:GLN:OE1	1:B:192:VAL:HG12	2.18	0.43
1:B:303:ARG:HH11	1:B:303:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:ARG:HD3	1:B:687:TYR:OH	2.18	0.43
1:A:343:GLU:HA	6:A:956:HOH:O	2.17	0.43
1:A:664:TYR:CG	1:A:701:MET:HB2	2.53	0.43
1:A:815:VAL:HG12	1:A:817:ALA:H	1.83	0.43
1:A:637:GLY:O	1:A:641:GLU:HG3	2.18	0.43
1:A:351:TRP:HA	1:A:355:GLN:OE1	2.19	0.43
1:B:520:ALA:O	1:B:522:GLU:N	2.52	0.43
1:A:264:LEU:HB3	1:B:521:ASP:OD2	2.19	0.43
1:B:421:ARG:CD	1:B:428:VAL:HG13	2.49	0.43
1:B:342:PRO:HG2	1:B:343:GLU:OE1	2.19	0.43
1:A:628:SER:OG	1:A:690:THR:HB	2.19	0.42
1:B:840:HIS:O	1:B:880:LYS:NZ	2.48	0.42
1:A:320:GLY:O	1:A:323:GLN:CG	2.64	0.42
1:B:462:LEU:HD23	1:B:462:LEU:C	2.40	0.42
1:B:458:LEU:O	1:B:459:HIS:HB2	2.19	0.42
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.50	0.42
1:A:569:ILE:HD11	2:B:887:TPP:H61	2.02	0.42
1:A:815:VAL:HA	1:A:816:PRO:HD3	1.86	0.42
1:A:535:ILE:HB	1:A:563:GLN:HB3	2.02	0.41
1:B:692:LEU:HD13	1:B:733:SER:HB3	2.01	0.41
1:A:178:PRO:HA	1:A:187:TRP:CG	2.55	0.41
1:A:317:THR:CG2	1:A:321:ASP:HB2	2.51	0.41
1:A:321:ASP:O	1:A:324:THR:HB	2.20	0.41
1:A:335:GLU:O	1:A:339:GLY:HA3	2.20	0.41
1:B:87:TRP:CD2	1:B:426:VAL:HG11	2.56	0.41
1:B:490:LYS:HE3	1:B:490:LYS:HB2	1.93	0.41
1:A:638:LEU:HD23	1:A:638:LEU:C	2.40	0.41
1:A:509:LYS:HA	1:A:512:LYS:HE3	2.03	0.41
1:B:195:GLY:O	1:B:198:PRO:HG2	2.21	0.41
1:A:298:TRP:CE2	1:A:359:LEU:HB3	2.56	0.41
1:A:326:LYS:HG2	1:A:326:LYS:O	2.20	0.41
1:A:70:GLU:HG2	5:A:890:EPE:H21	2.02	0.41
1:A:813:THR:CG2	1:A:814:TYR:CE2	3.04	0.41
1:B:264:LEU:HD23	1:B:264:LEU:C	2.40	0.41
1:A:627:THR:HB	1:A:633:LEU:HD13	2.03	0.40
1:A:859:ARG:HH11	1:A:859:ARG:CB	2.34	0.40
1:B:294:TRP:HB3	1:B:298:TRP:CD1	2.57	0.40
1:B:421:ARG:HD3	1:B:433:ILE:HD12	2.00	0.40
1:A:143:ILE:HD12	1:A:147:VAL:HG23	2.04	0.40
1:A:334:ARG:HA	1:A:338:PHE:HB2	2.02	0.40
1:B:239:LYS:O	1:B:242:ILE:HG12	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	796/886 (90%)	756 (95%)	35 (4%)	5 (1%)	25	14
1	B	795/886 (90%)	759 (96%)	33 (4%)	3 (0%)	34	22
All	All	1591/1772 (90%)	1515 (95%)	68 (4%)	8 (0%)	29	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	397	GLY
1	A	328	LYS
1	A	399	ALA
1	B	399	ALA
1	A	398	ASP
1	B	263	ARG
1	B	521	ASP
1	A	832	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	665/734 (91%)	662 (100%)	3 (0%)	88	87
1	B	664/734 (90%)	657 (99%)	7 (1%)	73	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1329/1468 (90%)	1319 (99%)	10 (1%)	81 80

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LEU
1	A	826	ASP
1	A	830	ARG
1	B	77	LEU
1	B	301	LEU
1	B	462	LEU
1	B	475	LEU
1	B	522	GLU
1	B	826	ASP
1	B	880	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	640	HIS

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	PO4	A	889	-	4,4,4	0.71	0	6,6,6	0.63	0
5	EPE	A	890	-	15,15,15	1.51	2 (13%)	18,20,20	2.16	5 (27%)
2	TPP	B	887	3	22,27,27	1.64	6 (27%)	29,40,40	1.06	1 (3%)
4	PO4	B	889	-	4,4,4	0.77	0	6,6,6	0.69	0
2	TPP	A	887	3	22,27,27	1.62	6 (27%)	29,40,40	1.08	1 (3%)

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	TPP	A	887	3	-	3/16/17/17	0/2/2/2
2	TPP	B	887	3	-	2/16/17/17	0/2/2/2
5	EPE	A	890	-	-	2/9/19/19	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	890	EPE	C10-S	4.13	1.83	1.77
2	A	887	TPP	C4'-N3'	3.82	1.40	1.35
2	B	887	TPP	C5'-C4'	3.53	1.49	1.42
2	B	887	TPP	C4'-N3'	3.42	1.39	1.35
2	A	887	TPP	C5'-C4'	3.33	1.48	1.42
5	A	890	EPE	O2S-S	2.93	1.53	1.45
2	A	887	TPP	C2'-N1'	2.64	1.38	1.34
2	B	887	TPP	C4-N3	2.59	1.42	1.39
2	B	887	TPP	C2'-N1'	2.55	1.38	1.34
2	A	887	TPP	C4-N3	2.55	1.41	1.39
2	A	887	TPP	C6'-N1'	2.07	1.38	1.34
2	B	887	TPP	C6'-N1'	2.03	1.38	1.34
2	A	887	TPP	C7'-N3	2.02	1.52	1.48
2	B	887	TPP	C7'-N3	2.00	1.52	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	890	EPE	O3S-S-O1S	4.34	121.89	111.27
5	A	890	EPE	O1S-S-C10	3.80	111.49	106.92
5	A	890	EPE	O3S-S-O2S	-3.51	102.70	111.27
5	A	890	EPE	O3S-S-C10	3.46	111.37	105.77
5	A	890	EPE	O2S-S-O1S	-3.32	102.46	113.95
2	A	887	TPP	C6'-N1'-C2'	2.52	120.25	115.96
2	B	887	TPP	C6'-N1'-C2'	2.44	120.12	115.96

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	887	TPP	C4-C5-C6-C7
2	A	887	TPP	PB-O3A-PA-O7
2	B	887	TPP	C4-C5-C6-C7
2	B	887	TPP	PA-O3A-PB-O2B
5	A	890	EPE	C9-C10-S-O1S
5	A	890	EPE	C9-C10-S-O2S
2	A	887	TPP	PA-O3A-PB-O2B

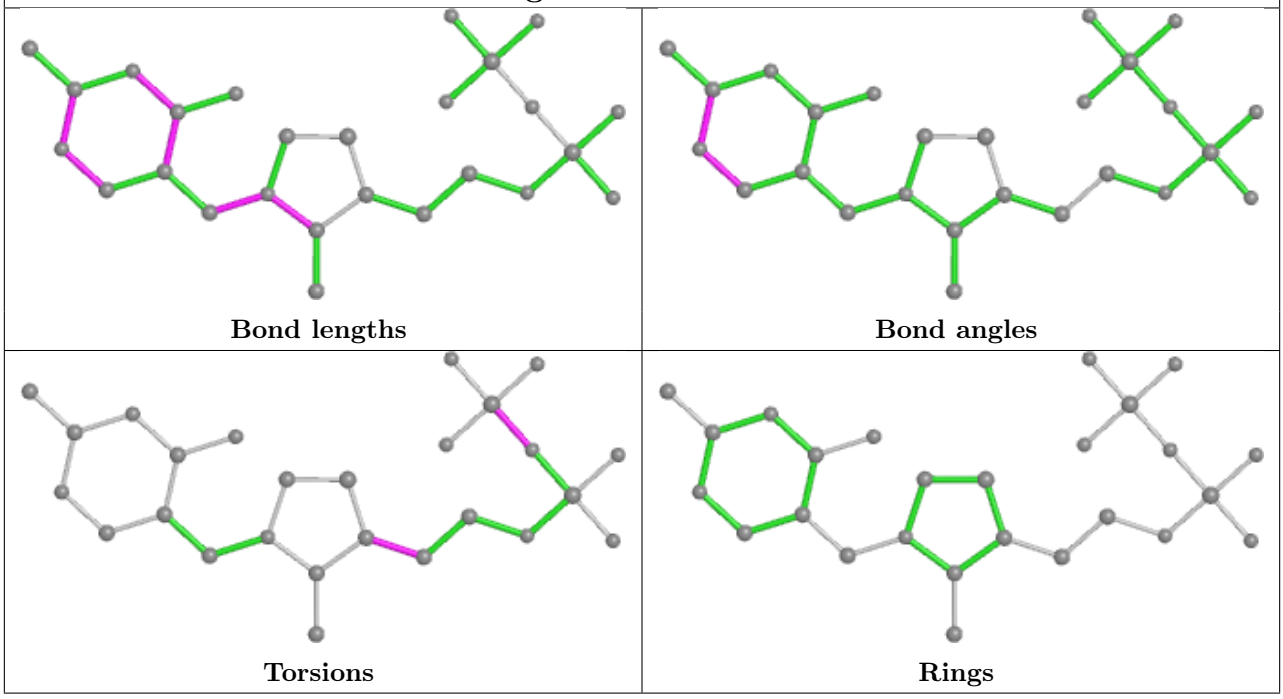
There are no ring outliers.

3 monomers are involved in 11 short contacts:

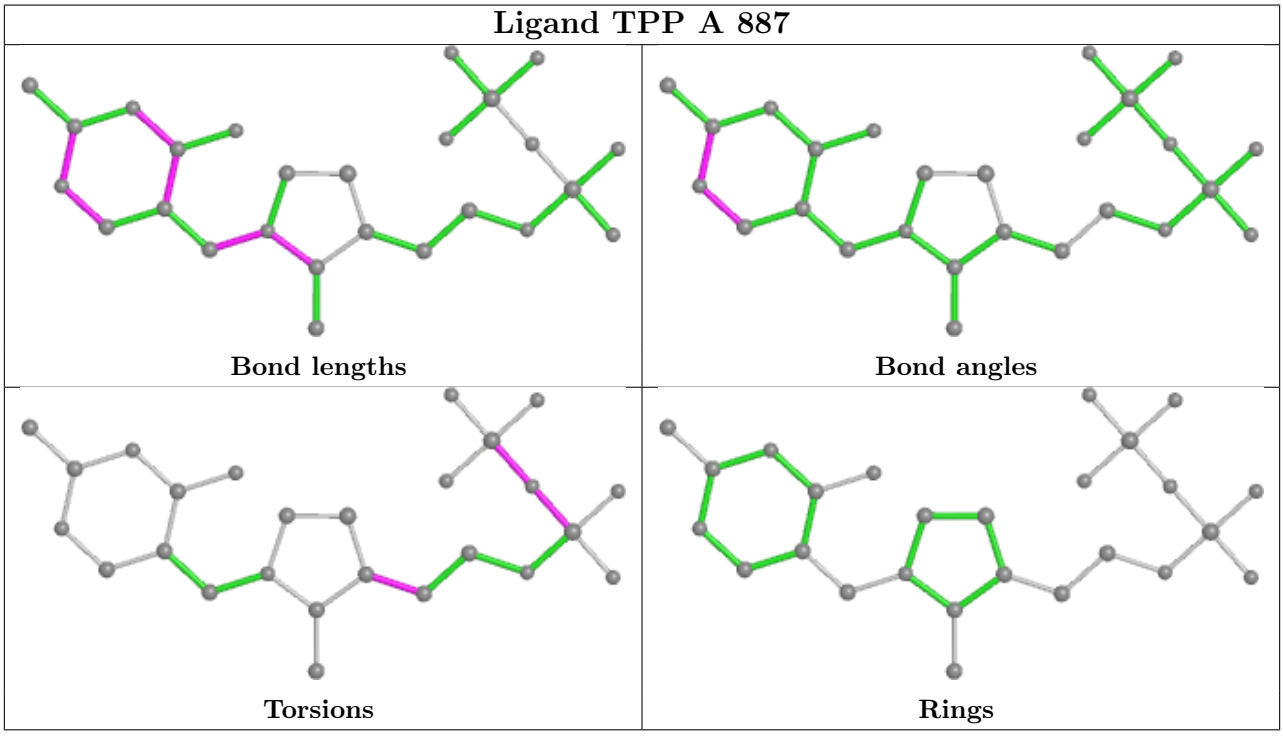
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	890	EPE	3	0
2	B	887	TPP	2	0
2	A	887	TPP	6	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TPP B 887



Ligand TPP A 887



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^{th} 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	801/886 (90%)	0.29	48 (5%)	21	23	22, 34, 72, 87	0
1	B	801/886 (90%)	0.10	27 (3%)	45	48	19, 33, 57, 87	0
All	All	1602/1772 (90%)	0.20	75 (4%)	31	33	19, 34, 64, 87	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	ALA	12.6
1	B	399	ALA	10.8
1	B	400	ALA	9.6
1	A	398	ASP	7.4
1	B	414	MET	6.7
1	A	399	ALA	6.6
1	A	397	GLY	6.4
1	A	331	ALA	5.2
1	A	335	GLU	5.1
1	A	342	PRO	4.9
1	A	302	LEU	4.6
1	A	348	VAL	4.5
1	A	329	ASP	4.3
1	B	306	THR	4.2
1	B	415	ASP	4.1
1	A	344	THR	4.0
1	B	416	GLY	3.9
1	A	349	ALA	3.9
1	A	264	LEU	3.7
1	A	323	GLN	3.7
1	A	341	TYR	3.4
1	B	398	ASP	3.4
1	B	420	ILE	3.4
1	A	330	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	332	TYR	3.4
1	B	354	GLU	3.3
1	B	428	VAL	3.3
1	A	117	TYR	3.3
1	A	347	LEU	3.1
1	A	265	ASP	3.1
1	A	354	GLU	3.0
1	A	351	TRP	3.0
1	B	417	VAL	3.0
1	A	886	ALA	3.0
1	A	533	ARG	2.9
1	B	524	ARG	2.9
1	B	56	ILE	2.9
1	B	265	ASP	2.8
1	A	339	GLY	2.8
1	A	420	ILE	2.8
1	A	415	ASP	2.7
1	B	264	LEU	2.7
1	B	533	ARG	2.7
1	B	462	LEU	2.6
1	A	309	LYS	2.6
1	A	56	ILE	2.6
1	A	137	VAL	2.5
1	A	866	VAL	2.5
1	B	431	ALA	2.5
1	A	336	HIS	2.5
1	A	343	GLU	2.4
1	A	307	SER	2.3
1	B	327	SER	2.3
1	A	532	PHE	2.3
1	A	262	GLN	2.3
1	A	327	SER	2.3
1	A	308	GLY	2.3
1	A	524	ARG	2.3
1	A	333	VAL	2.3
1	A	346	ALA	2.3
1	B	558	GLU	2.2
1	B	433	ILE	2.2
1	A	414	MET	2.2
1	A	801	THR	2.2
1	A	130	GLU	2.2
1	B	227	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	70	GLU	2.2
1	B	747	LYS	2.2
1	A	116	ILE	2.1
1	B	429	SER	2.1
1	B	799	ALA	2.1
1	B	723	LYS	2.1
1	A	823	LEU	2.1
1	A	139	PHE	2.0
1	A	340	LYS	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)

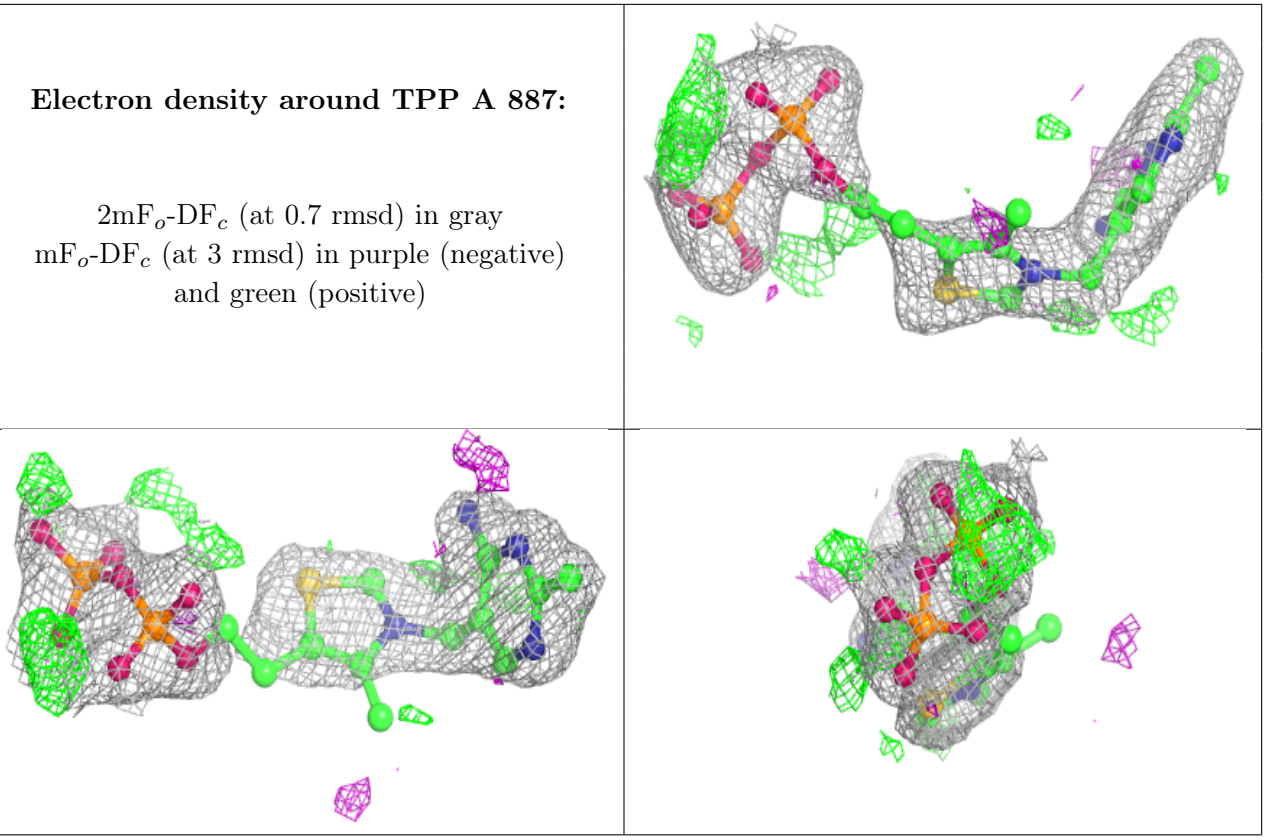
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MG	A	888	1/1	0.80	0.27	44,44,44,44	1
5	EPE	A	890	15/15	0.88	0.14	43,46,62,63	0
3	MG	B	888	1/1	0.89	0.17	36,36,36,36	0
2	TPP	A	887	26/26	0.94	0.14	37,42,44,45	17
2	TPP	B	887	26/26	0.97	0.11	34,40,41,43	7
4	PO4	B	889	5/5	0.98	0.07	57,58,58,59	0
4	PO4	A	889	5/5	0.98	0.07	46,48,49,49	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.

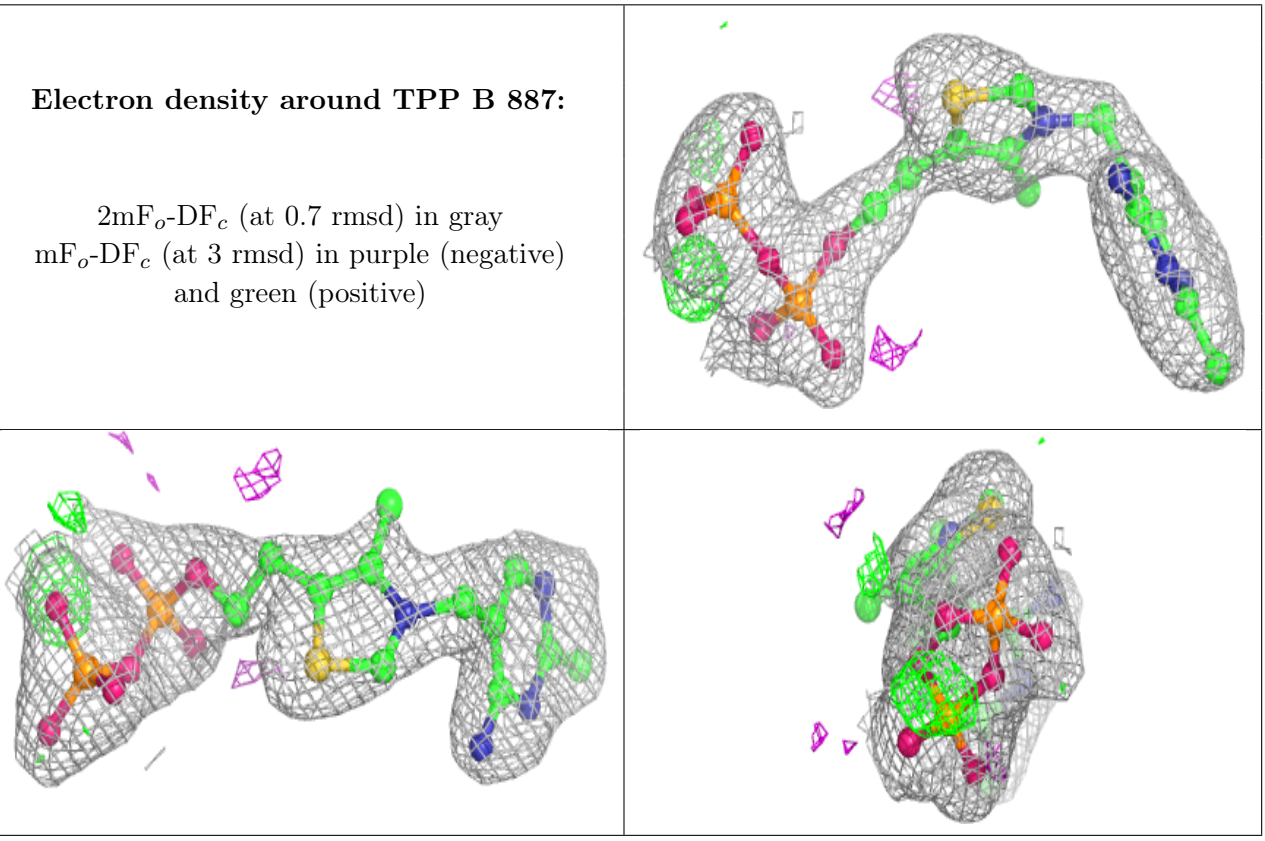
Electron density around TPP A 887:

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



Electron density around TPP B 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.