Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 02:04 AM EDT

PDB ID	:	3LQ2
Title	:	E. coli pyruvate dehydrogenase complex E1 E235A mutant with low TDP concentration
Authors	:	Furey, W.
Deposited on	:	2010-02-08
Resolution	:	1.96 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 (i) 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 (i)) were used in the production of this report:

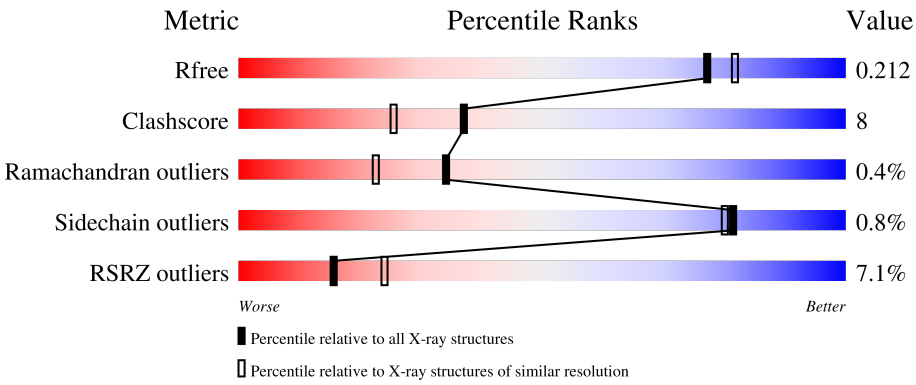
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	6%, 74%, 16%, •, 10%
1	B	886	7%, 77%, 13%, 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	888	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13395 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.

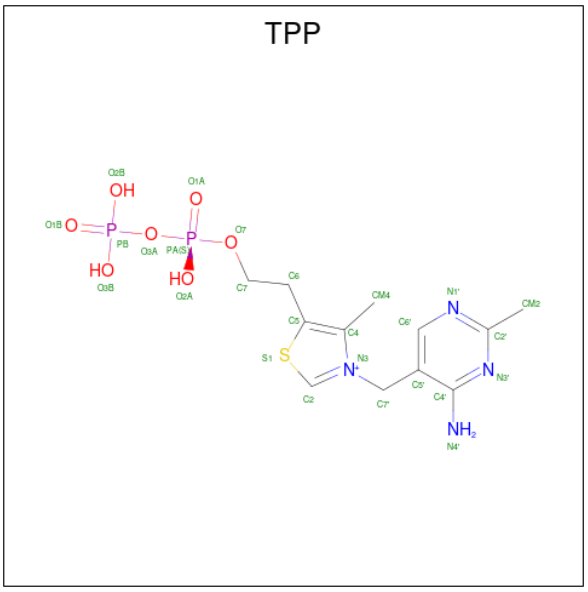
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

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

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
			Total	C	N	O	P	S		
2	A	1	26	12	4	7	2	1	0	0

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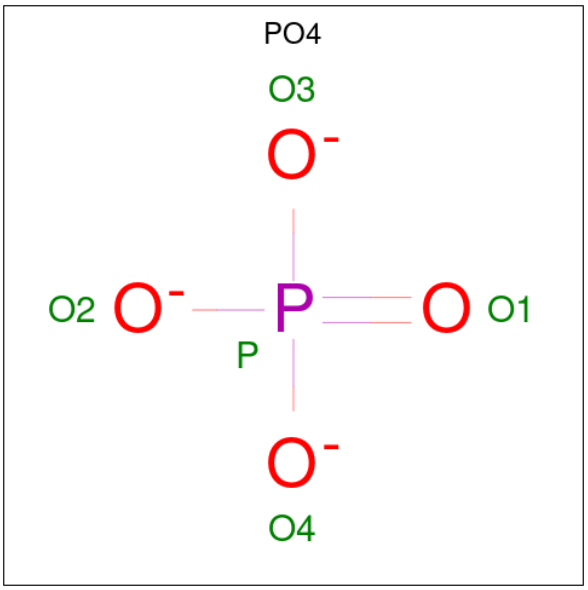
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	B	1	26	12	4	7	2	1	0	0

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

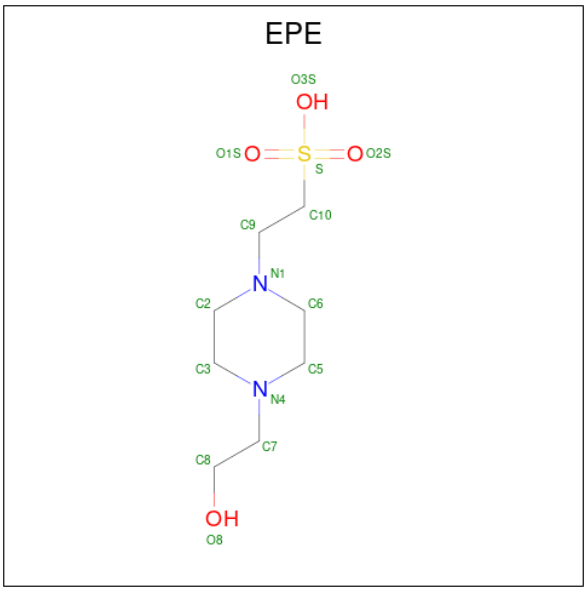
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

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



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

- Molecule 6 is water.

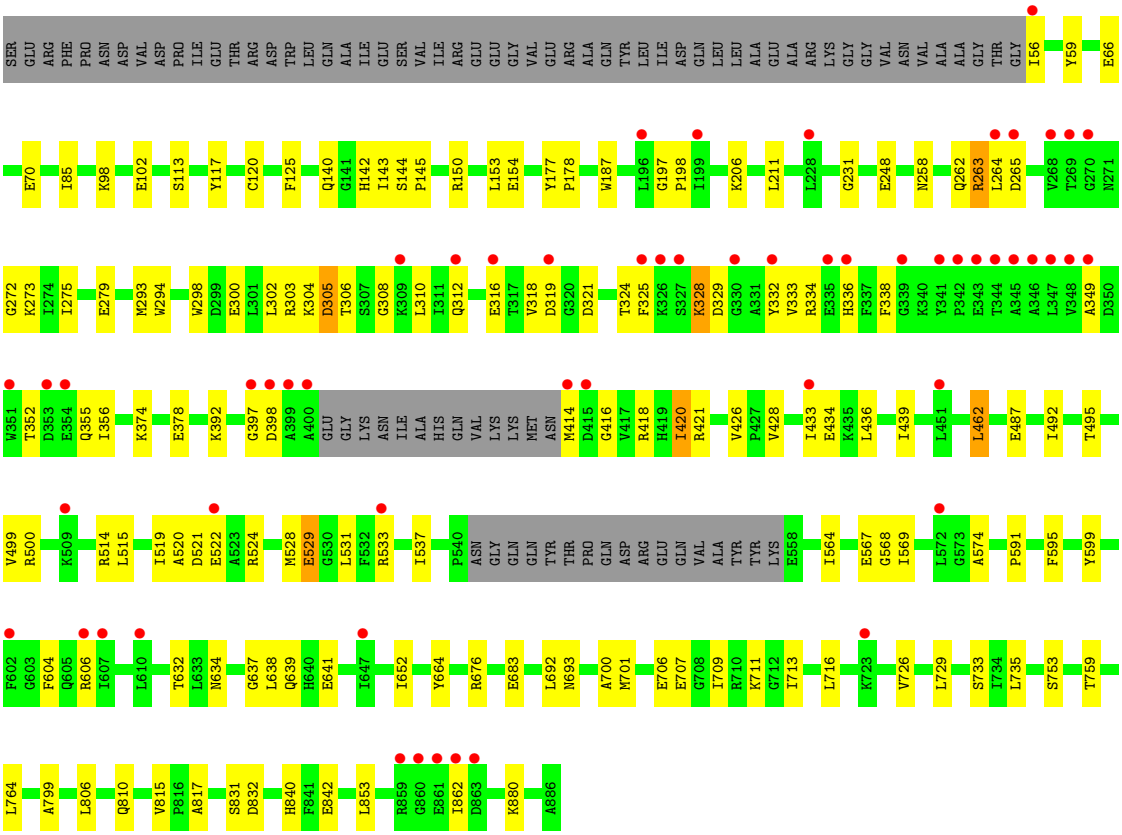
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	305	305	305	0	0
			Total	O		
6	B	327	327	327	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

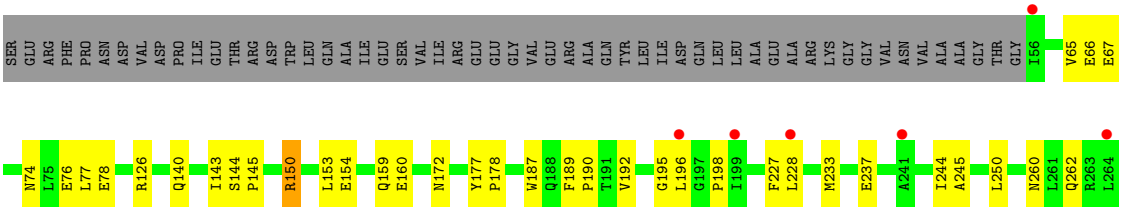
• Molecule 1: Pyruvate dehydrogenase E1 component

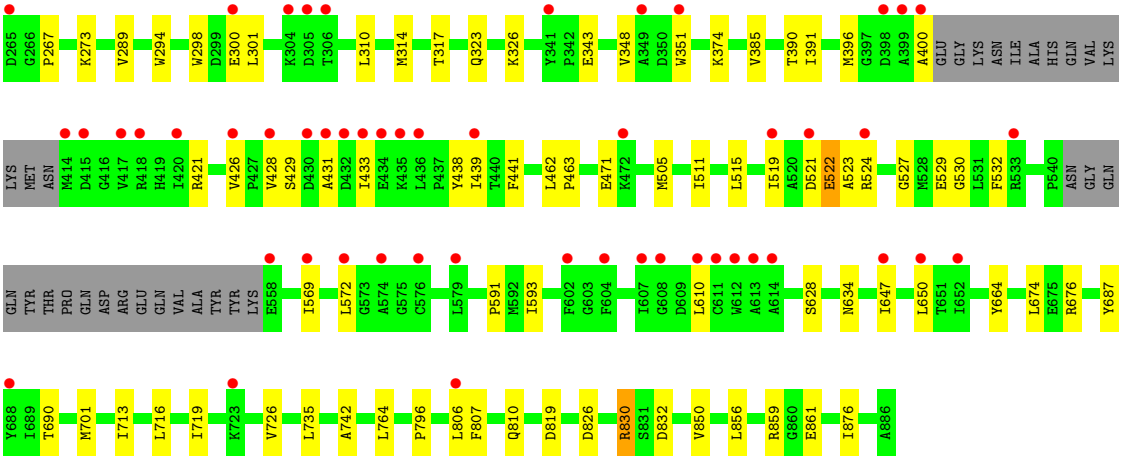
Chain A: 6% 74% 16% • 10%



• Molecule 1: Pyruvate dehydrogenase E1 component

Chain B: 7% 77% 13% 10%




D265 G266 P267 K273 V289 W294 W298 D299 E300 L301 K304 D305 T306 L310 M314 T317 Q323 K326 Y341 P342 E343 V348 A349 D350 W351 K374 V385 T390 I391 M396 G397 D398 A399 A400 GLU GLY LYS ASN ILE ALA HIS GLN VAL LYS
LYS MET ASN M414 D415 G416 V417 R418 H419 I420 R421 V426 P427 V428 S429 D430 A431 D432 I433 E434 K435 L436 P437 Y438 I439 T440 F441 L462 P463 E471 K472 M505 I511 L515 I519 A520 D521 E522 A523 R524 G527 M528 E529 G530 L531 F532 R533 P540 ASN GLY GLN
GLN TYR THR PRO GLN ASP ARG GLU GLN VAL ALA TYR TYR LYS E558 I569 L572 G573 A574 G575 C576 L579 P591 M592 I593 F602 G603 F604 I607 G608 D609 L610 G611 W612 A613 A614 S628 N634 I647 L650 T651 I652 Y664 L674 E675 R676 Y687
Y688 I689 T690 M701 I713 L716 I719 K723 V726 L735 A742 L764 P796 L806 F807 Q810 D819 D826 R830 S831 D832 V850 L856 R859 G860 E861 I876 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	80.65Å 141.77Å 83.42Å 90.00° 103.36° 90.00°	Depositor
Resolution (Å)	41.32 – 1.96 41.32 – 1.96	Depositor EDS
% Data completeness (in resolution range)	89.4 (41.32-1.96) 89.6 (41.32-1.96)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 1.97Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.223 0.187 , 0.212	Depositor DCC
R_{free} test set	5861 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13395	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, PO4, 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	0.33	0/6491	0.57	0/8776
1	B	0.34	0/6480	0.58	0/8761
All	All	0.33	0/12971	0.58	0/17537

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	6347	0	6184	114	0
1	B	6337	0	6178	89	0
2	A	26	0	16	5	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
5	A	15	0	17	2	0
6	A	305	0	0	2	0
6	B	327	0	0	3	0
All	All	13395	0	12411	197	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 8.

All (197) 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:117:TYR:CE2	1:A:143:ILE:HD13	2.03	0.93
1:A:117:TYR:CZ	1:A:143:ILE:CD1	2.51	0.92
1:A:117:TYR:CE2	1:A:143:ILE:CD1	2.56	0.88
1:A:264:LEU:HB2	2:A:887:TPP:H62	1.60	0.84
1:B:421:ARG:HD3	1:B:433:ILE:HD11	1.64	0.80
1:A:117:TYR:CZ	1:A:143:ILE:HD11	2.21	0.74
1:A:537:ILE:HD13	1:A:564:ILE:HB	1.70	0.73
1:A:117:TYR:CZ	1:A:143:ILE:HD13	2.19	0.72
2:A:887:TPP:H61	1:B:569:ILE:HD11	1.71	0.72
1:A:334:ARG:HB3	1:A:356:ILE:HD13	1.75	0.69
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.27	0.65
1:A:522:GLU:HG2	1:A:522:GLU:O	1.97	0.65
1:A:840:HIS:HA	1:A:880:LYS:HZ1	1.63	0.64
1:A:264:LEU:HD23	1:A:264:LEU:O	2.00	0.62
1:A:522:GLU:HG3	1:A:599:TYR:HE1	1.66	0.61
1:A:499:VAL:HG22	1:A:528:MET:HE3	1.82	0.61
1:B:140:GLN:O	1:B:143:ILE:HG13	2.01	0.60
1:A:140:GLN:O	1:A:143:ILE:HG12	2.01	0.60
1:A:692:LEU:HD13	1:A:733:SER:HB3	1.84	0.60
1:A:487:GLU:HG2	1:A:700:ALA:N	2.17	0.59
1:A:706:GLU:H	1:A:706:GLU:CD	2.06	0.59
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.84	0.59
1:A:522:GLU:HG3	1:A:599:TYR:CE1	2.37	0.59
1:B:74:ASN:O	1:B:78:GLU:HG3	2.02	0.59
1:A:840:HIS:HA	1:A:880:LYS:NZ	2.19	0.58
1:A:639:GLN:OE1	1:B:192:VAL:HG12	2.05	0.57
1:A:524:ARG:HA	1:A:529:GLU:OE1	2.05	0.57
1:B:859:ARG:HB2	1:B:861:GLU:HG2	1.87	0.56
1:B:195:GLY:O	1:B:198:PRO:HD2	2.05	0.56
1:B:326:LYS:HD2	1:B:391:ILE:HG23	1.87	0.56
1:B:150:ARG:O	1:B:154:GLU:HG3	2.07	0.55
1:B:67:GLU:HG2	1:B:67:GLU:O	2.05	0.55
1:B:647:ILE:O	1:B:650:LEU:HG	2.06	0.55
1:A:374:LYS:O	1:A:378:GLU:HG3	2.06	0.55
2:A:887:TPP:H61	1:B:569:ILE:CD1	2.38	0.55
1:A:352:THR:OG1	1:A:355:GLN:HG3	2.06	0.54
1:B:228:LEU:HD12	1:B:228:LEU:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HG12	1:A:153:LEU:HD12	1.90	0.54
1:A:304:LYS:O	1:A:306:THR:HG23	2.08	0.54
1:A:462:LEU:C	1:A:462:LEU:HD12	2.28	0.54
1:A:853:LEU:O	1:A:862:ILE:HD11	2.08	0.54
1:A:144:SER:OG	1:A:145:PRO:HD3	2.08	0.53
1:A:264:LEU:HD13	1:B:522:GLU:OE2	2.08	0.53
1:A:125:PHE:HB3	1:A:462:LEU:HD21	1.89	0.53
1:B:529:GLU:HG2	1:B:530:GLY:H	1.73	0.53
1:A:434:GLU:HB2	6:A:1045:HOH:O	2.09	0.53
1:A:318:VAL:HG12	1:A:319:ASP:N	2.24	0.53
1:B:198:PRO:HG3	1:B:228:LEU:CD2	2.39	0.53
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.91	0.52
1:A:113:SER:HB3	1:A:258:ASN:ND2	2.25	0.52
1:B:830:ARG:HH11	1:B:830:ARG:HG3	1.75	0.52
1:A:806:LEU:HD11	1:B:806:LEU:HD11	1.92	0.52
1:A:294:TRP:HB3	1:A:298:TRP:CD1	2.44	0.52
1:A:492:ILE:HD13	1:A:500:ARG:NH1	2.26	0.51
1:A:637:GLY:O	1:A:641:GLU:HG3	2.10	0.51
1:B:126:ARG:HH11	1:B:126:ARG:HB3	1.75	0.51
1:B:126:ARG:NH1	6:B:955:HOH:O	2.44	0.51
1:B:462:LEU:C	1:B:462:LEU:HD12	2.31	0.51
1:A:499:VAL:HG22	1:A:528:MET:CE	2.41	0.51
1:B:650:LEU:HD12	1:B:650:LEU:C	2.32	0.50
1:B:807:PHE:O	1:B:810:GLN:HG2	2.10	0.50
1:A:632:THR:HG22	1:A:693:ASN:OD1	2.11	0.50
1:B:421:ARG:HD2	1:B:428:VAL:O	2.11	0.50
1:B:593:ILE:HD13	1:B:674:LEU:HD11	1.93	0.50
1:B:177:TYR:CD2	1:B:192:VAL:HG21	2.46	0.50
1:A:262:GLN:OE1	1:A:392:LYS:HB3	2.13	0.49
1:B:227:PHE:C	1:B:228:LEU:HD12	2.33	0.49
1:B:505:MET:HB3	1:B:515:LEU:HD11	1.95	0.49
1:A:56:ILE:HG23	1:A:279:GLU:OE1	2.12	0.48
1:A:272:GLY:O	1:A:318:VAL:HG13	2.13	0.48
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.94	0.48
1:A:98:LYS:HD2	1:A:436:LEU:CD1	2.44	0.48
1:B:396:MET:HB2	1:B:400:ALA:CB	2.44	0.48
1:A:329:ASP:O	1:A:333:VAL:HG23	2.12	0.48
1:A:664:TYR:CG	1:A:701:MET:HB2	2.49	0.48
1:A:334:ARG:HH22	1:A:349:ALA:HA	1.78	0.48
1:A:606:ARG:HH12	1:B:196:LEU:HD13	1.79	0.48
1:A:334:ARG:HA	1:A:338:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ARG:HB3	1:B:126:ARG:NH1	2.29	0.48
1:A:302:LEU:HD23	1:A:310:LEU:HD23	1.95	0.48
1:B:65:VAL:HG23	1:B:66:GLU:OE2	2.13	0.48
1:B:426:VAL:HG13	1:B:439:ILE:CD1	2.44	0.48
1:A:273:LYS:HA	1:A:319:ASP:OD2	2.14	0.47
1:A:416:GLY:O	1:A:420:ILE:HG23	2.14	0.47
1:B:426:VAL:HG13	1:B:439:ILE:HD11	1.95	0.47
1:B:426:VAL:CG1	1:B:439:ILE:HD11	2.44	0.47
1:A:70:GLU:OE2	5:A:890:EPE:H21	2.14	0.47
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.49	0.47
1:A:634:ASN:HB2	1:A:832:ASP:O	2.14	0.47
1:A:676:ARG:HH21	1:A:683:GLU:CD	2.17	0.47
1:B:178:PRO:HA	1:B:187:TRP:CG	2.49	0.47
1:A:102:GLU:HG3	6:B:1213:HOH:O	2.14	0.47
1:A:178:PRO:HA	1:A:187:TRP:CG	2.49	0.47
1:B:76:GLU:H	1:B:76:GLU:CD	2.18	0.47
1:A:420:ILE:HG13	1:A:421:ARG:N	2.28	0.47
1:A:300:GLU:HA	1:A:300:GLU:OE1	2.15	0.47
1:A:150:ARG:O	1:A:154:GLU:HG3	2.15	0.46
1:A:426:VAL:HG12	1:A:428:VAL:HG23	1.97	0.46
1:A:729:LEU:HD12	1:A:729:LEU:N	2.30	0.46
1:B:471:GLU:OE2	1:B:591:PRO:HD2	2.16	0.46
1:A:263:ARG:O	1:A:392:LYS:NZ	2.49	0.46
1:A:305:ASP:OD2	1:A:308:GLY:HA2	2.16	0.46
1:B:429:SER:C	1:B:431:ALA:H	2.19	0.46
1:B:153:LEU:HD21	1:B:441:PHE:CE2	2.51	0.46
1:A:831:SER:O	1:A:832:ASP:HB2	2.15	0.45
1:B:719:ILE:HD12	1:B:742:ALA:HB1	1.96	0.45
1:B:153:LEU:HD21	1:B:441:PHE:HE2	1.80	0.45
1:A:258:ASN:ND2	6:A:1010:HOH:O	2.49	0.45
2:A:887:TPP:H2	6:B:1201:HOH:O	2.17	0.45
1:A:521:ASP:HB2	1:A:568:GLY:HA2	1.98	0.45
1:B:126:ARG:HH11	1:B:126:ARG:CB	2.29	0.45
1:B:189:PHE:HA	1:B:190:PRO:HD3	1.86	0.45
1:B:198:PRO:HG3	1:B:228:LEU:HD21	1.97	0.45
1:B:245:ALA:HA	1:B:250:LEU:HD12	1.98	0.45
1:B:716:LEU:HD11	1:B:735:LEU:HD21	1.98	0.45
1:A:414:MET:O	1:A:418:ARG:HG3	2.17	0.45
1:A:709:ILE:HG23	1:A:759:THR:HG21	1.98	0.45
1:A:98:LYS:HD2	1:A:436:LEU:HD12	1.99	0.45
1:A:325:PHE:HE1	1:A:336:HIS:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LYS:CD	1:B:391:ILE:HG23	2.47	0.44
1:A:414:MET:HE1	1:A:433:ILE:O	2.17	0.44
1:B:310:LEU:O	1:B:314:MET:HG3	2.17	0.44
1:A:638:LEU:C	1:A:638:LEU:HD23	2.38	0.44
1:B:343:GLU:H	1:B:343:GLU:CD	2.21	0.44
1:B:348:VAL:O	1:B:351:TRP:HB2	2.17	0.44
1:A:414:MET:HE2	1:A:434:GLU:HA	2.00	0.44
1:A:842:GLU:OE2	1:A:880:LYS:HE2	2.17	0.44
1:A:206:LYS:HD2	1:A:248:GLU:HG3	2.00	0.44
1:A:142[O]:HIS:ND1	1:A:142[O]:HIS:N	2.61	0.44
1:A:569:ILE:HD11	2:B:887:TPP:H61	1.99	0.44
1:B:519:ILE:HD12	1:B:523:ALA:HB2	1.99	0.44
1:A:312:GLN:O	1:A:316:GLU:HG2	2.18	0.44
1:B:262:GLN:HA	1:B:267:PRO:HA	1.99	0.44
1:B:300:GLU:HG3	1:B:301:LEU:N	2.33	0.44
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.48	0.44
1:A:514:ARG:NH1	1:A:591:PRO:HG2	2.33	0.43
1:A:264:LEU:HD13	1:B:522:GLU:CD	2.38	0.43
1:A:321:ASP:O	1:A:324:THR:HB	2.19	0.43
1:B:527:GLY:HA2	1:B:529:GLU:OE1	2.18	0.43
1:A:426:VAL:HG13	1:A:439:ILE:CD1	2.47	0.43
1:A:716:LEU:HD11	1:A:735:LEU:HD21	2.01	0.43
1:B:726:VAL:HG12	1:B:796:PRO:HG2	1.99	0.43
1:B:237:GLU:H	1:B:237:GLU:CD	2.20	0.43
1:B:529:GLU:HG2	1:B:530:GLY:N	2.33	0.43
1:B:628:SER:OG	1:B:690:THR:HB	2.19	0.43
1:B:572:LEU:HD12	1:B:610:LEU:HD22	2.00	0.43
1:B:273:LYS:NZ	1:B:317:THR:O	2.43	0.43
1:A:59:TYR:CE1	1:A:273:LYS:HE3	2.54	0.42
1:B:289:VAL:HG12	1:B:385:VAL:CG1	2.48	0.42
2:A:887:TPP:HM41	1:B:569:ILE:HG12	2.00	0.42
1:B:428:VAL:HG23	1:B:439:ILE:HD11	2.01	0.42
1:A:66:GLU:O	5:A:890:EPE:H81	2.20	0.42
1:A:707:GLU:OE2	1:A:711:LYS:HE2	2.20	0.42
1:A:729:LEU:O	1:A:799:ALA:HA	2.18	0.42
1:A:178:PRO:HA	1:A:187:TRP:CD2	2.54	0.42
1:A:318:VAL:CG1	1:A:319:ASP:N	2.81	0.42
1:A:604:PHE:HE2	1:A:652:ILE:HD12	1.83	0.42
1:A:519:ILE:HG22	1:A:520:ALA:N	2.34	0.42
1:B:244:ILE:N	1:B:244:ILE:HD12	2.35	0.42
1:B:664:TYR:CG	1:B:701:MET:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:GLU:HG3	1:A:574:ALA:HA	2.01	0.42
1:B:462:LEU:HB2	1:B:463:PRO:HA	2.02	0.42
1:A:520:ALA:O	1:A:521:ASP:HB3	2.20	0.42
1:B:326:LYS:HD2	1:B:391:ILE:CG2	2.49	0.42
1:A:197:GLY:N	1:A:198:PRO:HD2	2.34	0.42
1:A:231:GLY:C	1:B:569:ILE:HD12	2.40	0.42
1:A:328:LYS:HG3	1:A:332:TYR:CE1	2.55	0.42
1:A:117:TYR:CE2	1:A:143:ILE:HD12	2.50	0.42
1:B:676:ARG:HD3	1:B:687:TYR:OH	2.20	0.42
1:B:856:LEU:HB3	1:B:861:GLU:HB2	2.01	0.41
1:A:515:LEU:HD22	1:A:595:PHE:HE1	1.86	0.41
1:A:265:ASP:OD2	1:B:524:ARG:HG3	2.20	0.41
1:B:144:SER:OG	1:B:145:PRO:HD3	2.20	0.41
1:B:160:GLU:OE2	1:B:172:ASN:ND2	2.52	0.41
1:B:260:ASN:HA	1:B:390:THR:O	2.20	0.41
1:B:301:LEU:HD21	1:B:351:TRP:CZ2	2.55	0.41
1:A:529:GLU:O	1:A:533:ARG:NH1	2.54	0.41
1:A:495:THR:O	1:A:499:VAL:HG23	2.20	0.41
1:A:300:GLU:OE1	1:A:303:ARG:NH2	2.53	0.41
1:A:120:CYS:HB3	1:A:125:PHE:CE1	2.56	0.41
1:A:713:ILE:HG22	1:A:764:LEU:HD21	2.01	0.41
1:A:815:VAL:HG12	1:A:817:ALA:H	1.86	0.41
1:B:228:LEU:HD23	1:B:233:MET:SD	2.61	0.41
1:B:374:LYS:HD2	1:B:374:LYS:HA	1.94	0.41
1:B:850:VAL:HG21	1:B:876:ILE:HD12	2.03	0.41
1:A:275:ILE:HD12	1:A:293:MET:HE1	2.02	0.41
1:A:726:VAL:O	1:A:753:SER:HA	2.21	0.41
1:B:323:GLN:NE2	1:B:323:GLN:HA	2.36	0.40
1:B:634:ASN:HB2	1:B:832:ASP:O	2.22	0.40
1:A:328:LYS:HG3	1:A:332:TYR:CD1	2.57	0.40
1:A:528:MET:HE2	1:A:531:LEU:HD12	2.02	0.40
1:B:65:VAL:HG23	1:B:66:GLU:CD	2.41	0.40
1:B:195:GLY:C	1:B:198:PRO:HD2	2.40	0.40
1:B:294:TRP:HB3	1:B:298:TRP:CD1	2.57	0.40
1:B:529:GLU:HA	1:B:532:PHE:CD2	2.56	0.40
1:A:569:ILE:HG12	2:B:887:TPP:HM41	2.03	0.40
1:B:511:ILE:HD12	1:B:515:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	796/886 (90%)	759 (95%)	32 (4%)	5 (1%)	25	14
1	B	795/886 (90%)	761 (96%)	33 (4%)	1 (0%)	51	43
All	All	1591/1772 (90%)	1520 (96%)	65 (4%)	6 (0%)	34	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ARG
1	A	328	LYS
1	A	305	ASP
1	A	397	GLY
1	A	398	ASP
1	B	521	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%)	660 (99%)	5 (1%)	81	80
1	B	664/734 (90%)	658 (99%)	6 (1%)	78	77
All	All	1329/1468 (90%)	1318 (99%)	11 (1%)	81	80

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	LEU
1	A	420	ILE
1	A	462	LEU
1	A	529	GLU
1	A	810	GLN
1	B	77	LEU
1	B	150	ARG
1	B	522	GLU
1	B	819	ASP
1	B	826	ASP
1	B	830	ARG

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	534	GLN
1	B	106	HIS
1	B	172	ASN
1	B	466	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 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	$\#\|Z\| > 2$
2	TPP	B	887	3	22,27,27	1.64	6 (27%)	29,40,40	1.06	1 (3%)
5	EPE	A	890	-	15,15,15	1.48	2 (13%)	18,20,20	2.13	5 (27%)
4	PO4	A	889	-	4,4,4	0.71	0	6,6,6	0.64	0
2	TPP	A	887	3	22,27,27	1.55	4 (18%)	29,40,40	1.06	1 (3%)
4	PO4	B	889	-	4,4,4	0.70	0	6,6,6	0.70	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
5	EPE	A	890	-	-	3/9/19/19	0/1/1/1
2	TPP	B	887	3	-	1/16/17/17	0/2/2/2
2	TPP	A	887	3	-	6/16/17/17	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	890	EPE	C10-S	3.94	1.83	1.77
2	B	887	TPP	C4'-N3'	3.62	1.40	1.35
2	A	887	TPP	C4'-N3'	3.58	1.40	1.35
2	B	887	TPP	C5'-C4'	3.52	1.48	1.42
2	A	887	TPP	C5'-C4'	3.34	1.48	1.42
5	A	890	EPE	O2S-S	2.92	1.53	1.45
2	A	887	TPP	C2'-N1'	2.64	1.38	1.34
2	B	887	TPP	C2'-N1'	2.62	1.38	1.34
2	B	887	TPP	C4-N3	2.59	1.42	1.39
2	A	887	TPP	C4-N3	2.37	1.41	1.39
2	B	887	TPP	C6'-N1'	2.12	1.38	1.34
2	B	887	TPP	C7'-N3	2.09	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	4.40	122.02	111.27
5	A	890	EPE	O3S-S-O2S	-3.60	102.47	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	890	EPE	O3S-S-C10	3.55	111.50	105.77
5	A	890	EPE	O1S-S-C10	3.45	111.07	106.92
5	A	890	EPE	O2S-S-O1S	-3.27	102.63	113.95
2	A	887	TPP	C6'-N1'-C2'	2.48	120.18	115.96
2	B	887	TPP	C6'-N1'-C2'	2.44	120.12	115.96

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	887	TPP	C5-C6-C7-O7
2	A	887	TPP	PB-O3A-PA-O7
2	A	887	TPP	PA-O3A-PB-O2B
2	A	887	TPP	PA-O3A-PB-O3B
2	B	887	TPP	C4-C5-C6-C7
5	A	890	EPE	C9-C10-S-O3S
5	A	890	EPE	C9-C10-S-O1S
5	A	890	EPE	C9-C10-S-O2S
2	A	887	TPP	PA-O3A-PB-O1B
2	A	887	TPP	C4-C5-C6-C7

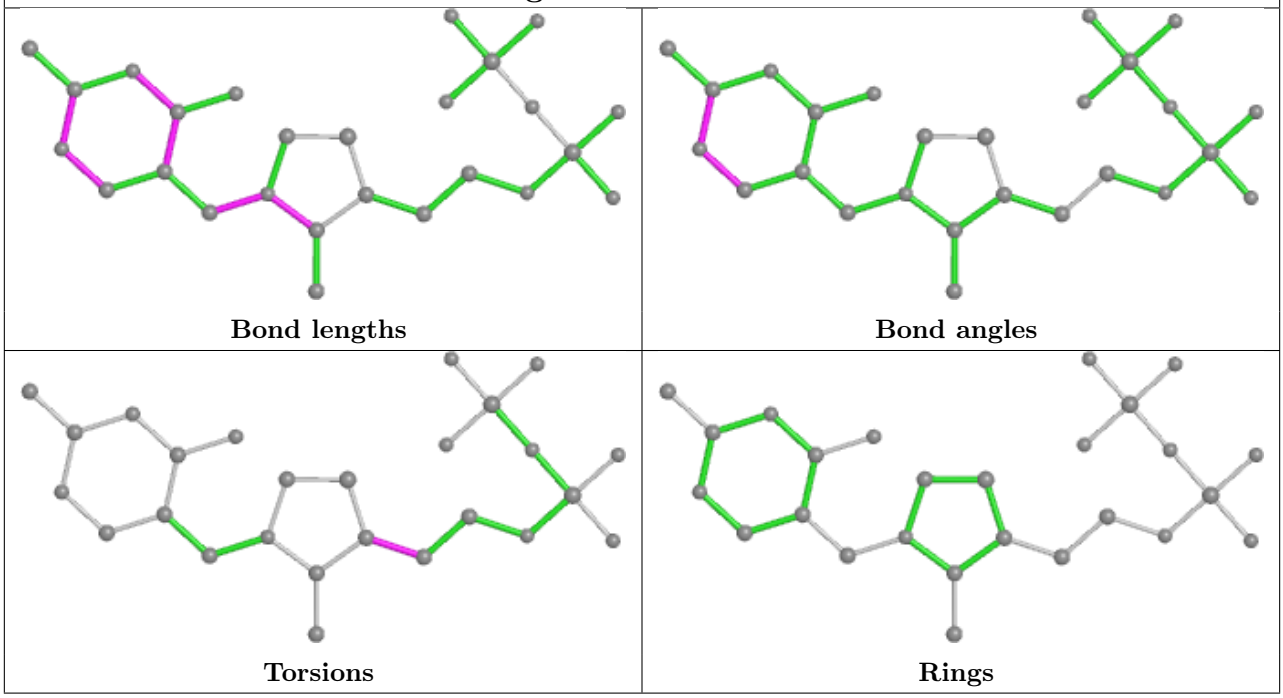
There are no ring outliers.

3 monomers are involved in 9 short contacts:

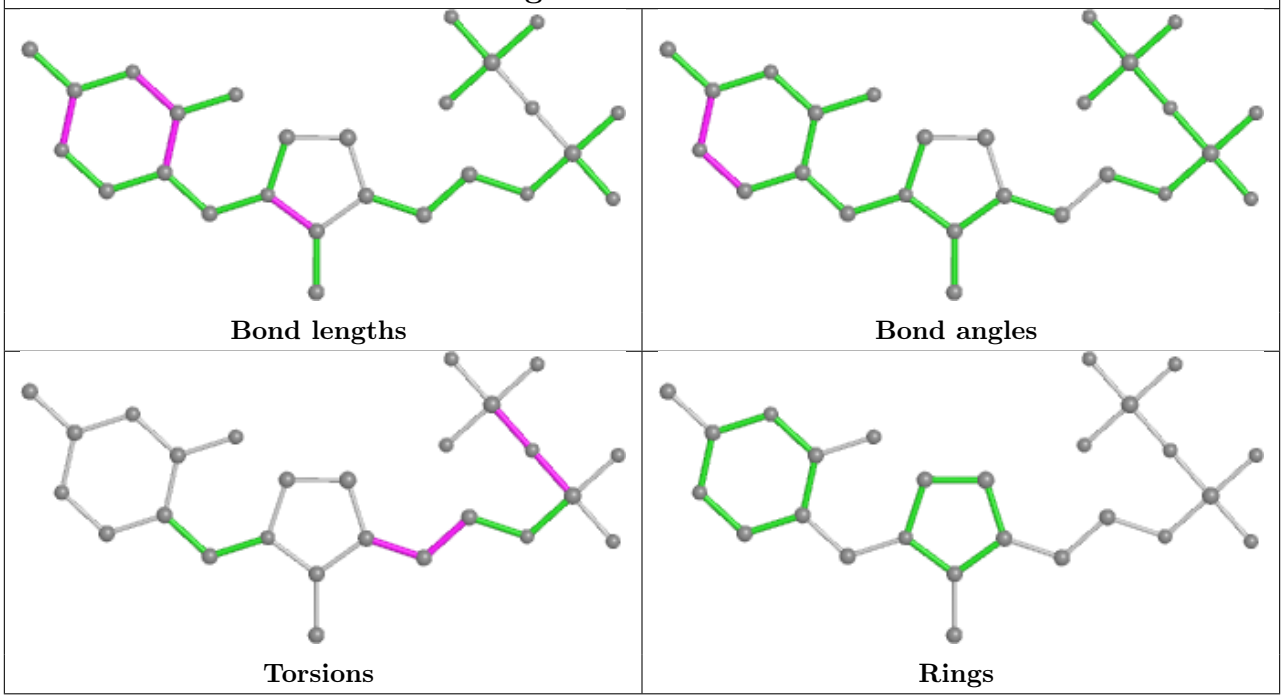
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	887	TPP	2	0
5	A	890	EPE	2	0
2	A	887	TPP	5	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	801/886 (90%)	0.44	56 (6%)	16	24	28, 41, 78, 92	0
1	B	801/886 (90%)	0.43	58 (7%)	15	23	26, 39, 63, 97	0
All	All	1602/1772 (90%)	0.43	114 (7%)	16	24	26, 40, 70, 97	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	ALA	13.0
1	A	400	ALA	10.5
1	B	414	MET	10.4
1	B	400	ALA	9.9
1	B	433	ILE	6.9
1	A	332	TYR	5.9
1	B	415	ASP	5.5
1	A	265	ASP	5.3
1	B	417	VAL	5.2
1	A	347	LEU	5.1
1	A	398	ASP	4.8
1	A	270	GLY	4.8
1	A	269	THR	4.6
1	A	341	TYR	4.4
1	A	522	GLU	4.4
1	B	56	ILE	4.3
1	B	398	ASP	4.1
1	A	330	GLY	4.0
1	A	264	LEU	4.0
1	A	268	VAL	3.8
1	A	339	GLY	3.8
1	A	344	THR	3.8
1	A	607	ILE	3.6
1	B	306	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	342	PRO	3.3
1	A	346	ALA	3.2
1	A	336	HIS	3.2
1	B	436	LEU	3.2
1	B	428	VAL	3.1
1	B	521	ASP	3.1
1	B	434	GLU	3.1
1	B	199	ILE	3.0
1	B	533	ARG	3.0
1	B	418	ARG	3.0
1	B	420	ILE	3.0
1	B	196	LEU	2.9
1	A	861	GLU	2.9
1	A	353	ASP	2.9
1	A	723	LYS	2.9
1	A	196	LEU	2.9
1	A	228	LEU	2.8
1	B	610	LEU	2.8
1	B	558	GLU	2.8
1	B	607	ILE	2.8
1	A	325	PHE	2.7
1	B	430	ASP	2.7
1	B	723	LYS	2.7
1	A	327	SER	2.7
1	A	319	ASP	2.6
1	A	399	ALA	2.6
1	B	569	ILE	2.6
1	A	414	MET	2.6
1	B	241	ALA	2.6
1	A	335	GLU	2.6
1	B	304	LYS	2.6
1	B	612	TRP	2.6
1	B	305	ASP	2.6
1	A	343	GLU	2.6
1	A	647	ILE	2.6
1	B	614	ALA	2.5
1	A	199	ILE	2.5
1	B	264	LEU	2.5
1	B	613	ALA	2.5
1	A	509	LYS	2.5
1	A	606	ARG	2.5
1	A	397	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	688	TYR	2.4
1	A	309	LYS	2.4
1	B	300	GLU	2.4
1	A	56	ILE	2.4
1	B	524	ARG	2.4
1	B	519	ILE	2.4
1	A	348	VAL	2.4
1	B	265	ASP	2.4
1	B	647	ILE	2.4
1	B	431	ALA	2.3
1	A	860	GLY	2.3
1	B	602	PHE	2.3
1	B	576	CYS	2.3
1	A	610	LEU	2.3
1	A	349	ALA	2.3
1	B	349	ALA	2.3
1	B	579	LEU	2.3
1	B	472	LYS	2.3
1	B	432	ASP	2.3
1	A	354	GLU	2.2
1	A	451	LEU	2.2
1	A	572	LEU	2.2
1	B	611	CYS	2.2
1	B	341	TYR	2.2
1	A	602	PHE	2.2
1	B	435	LYS	2.2
1	B	439	ILE	2.2
1	A	862	ILE	2.2
1	B	652	ILE	2.2
1	A	345	ALA	2.2
1	B	650	LEU	2.1
1	A	533	ARG	2.1
1	A	326	LYS	2.1
1	B	228	LEU	2.1
1	B	604	PHE	2.1
1	B	426	VAL	2.1
1	B	574	ALA	2.1
1	B	608	GLY	2.1
1	A	351	TRP	2.1
1	B	351	TRP	2.1
1	A	433	ILE	2.1
1	B	572	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	316	GLU	2.0
1	A	415	ASP	2.0
1	A	863	ASP	2.0
1	A	312	GLN	2.0
1	B	806	LEU	2.0
1	A	859	ARG	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)

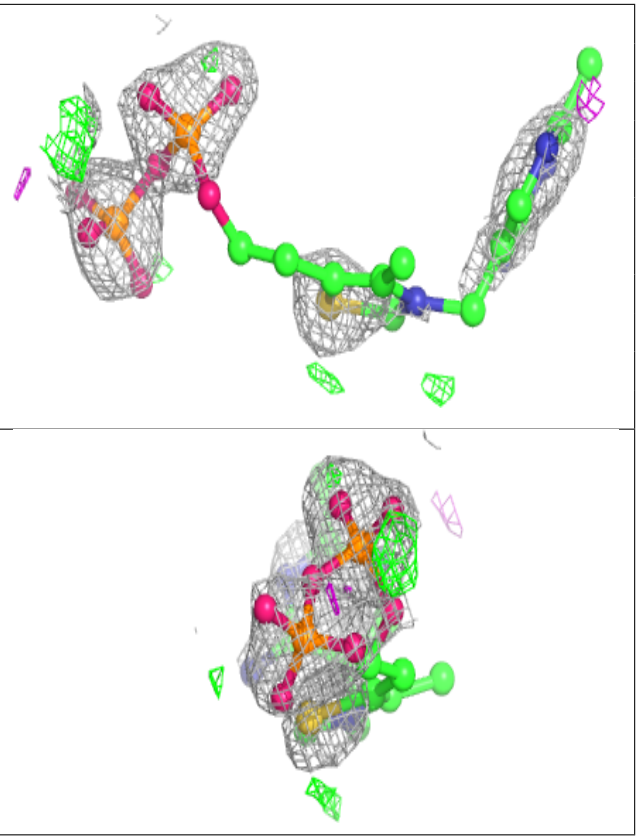
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

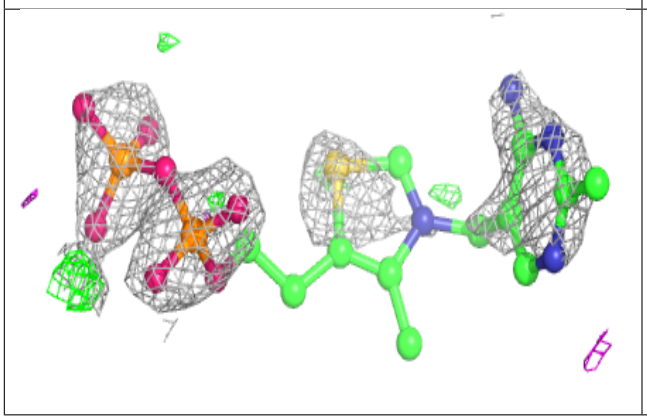
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	888	1/1	0.38	0.50	59,59,59,59	1
3	MG	B	888	1/1	0.70	0.22	48,48,48,48	1
2	TPP	A	887	26/26	0.88	0.34	46,51,52,52	26
5	EPE	A	890	15/15	0.92	0.12	49,52,67,68	0
2	TPP	B	887	26/26	0.94	0.20	40,44,46,47	26
4	PO4	B	889	5/5	0.97	0.07	59,59,61,61	0
4	PO4	A	889	5/5	0.97	0.07	52,53,53,54	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:

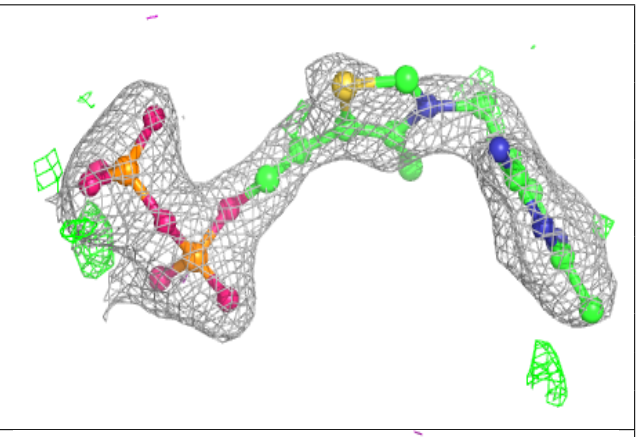
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

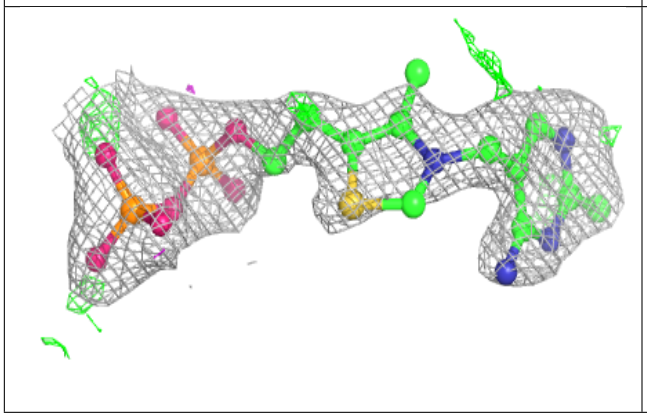


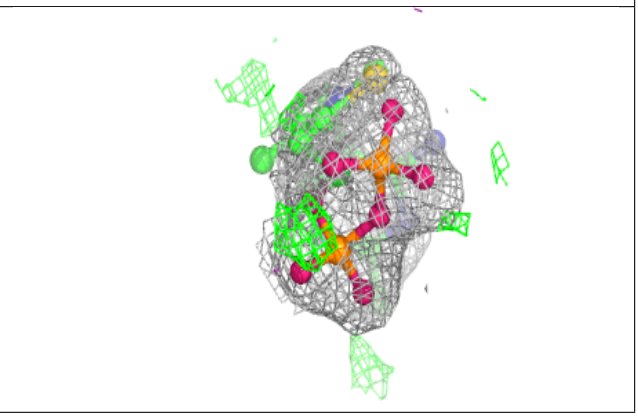


Electron density around TPP B 887:

$2mF_o$-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.