Full wwPDB X-ray Structure Validation Report (i)

Jul 28, 2021 – 04:49 PM EDT

PDB ID	:	2IEA
Title	:	E. coli pyruvate dehydrogenase
Authors	:	Furey, W.; Arjunan, P.
Deposited on	:	2006-09-18
Resolution	:	1.85 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 following versions of software and data (see references (i)) were used in the production of this report:

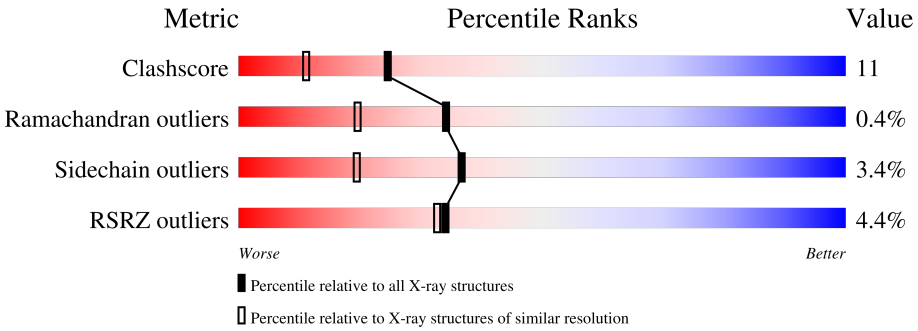
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.22

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	3% 73% 16% • 10%
1	B	886	5% 71% 17% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13418 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.

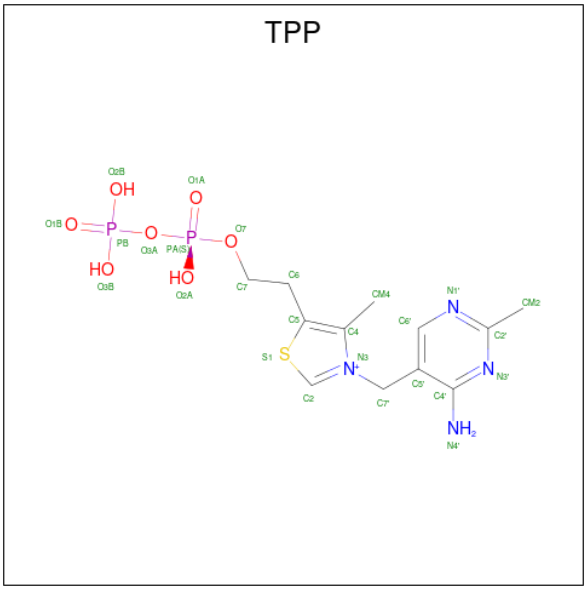
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

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

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

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

- Molecule 4 is water.

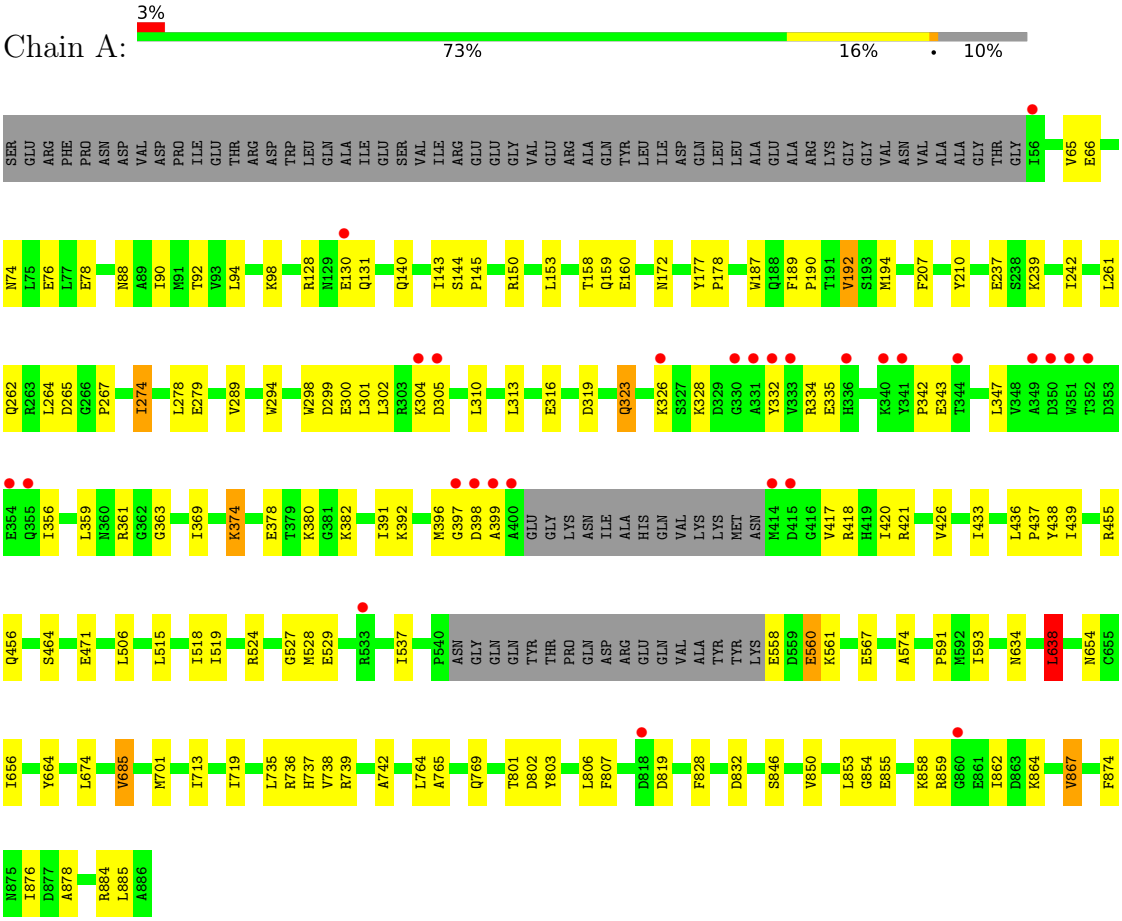
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	329	Total	O	0	0
			329	329		
4	B	353	Total	O	0	0
			353	353		

3 Residue-property plots

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

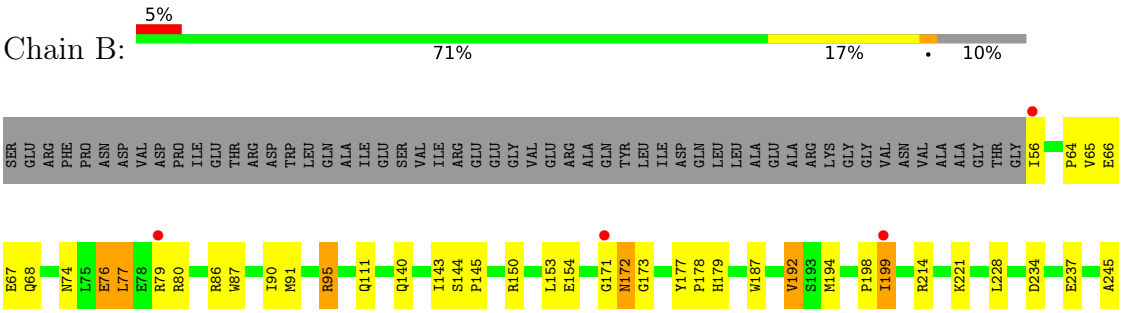
• Molecule 1: Pyruvate dehydrogenase E1 component

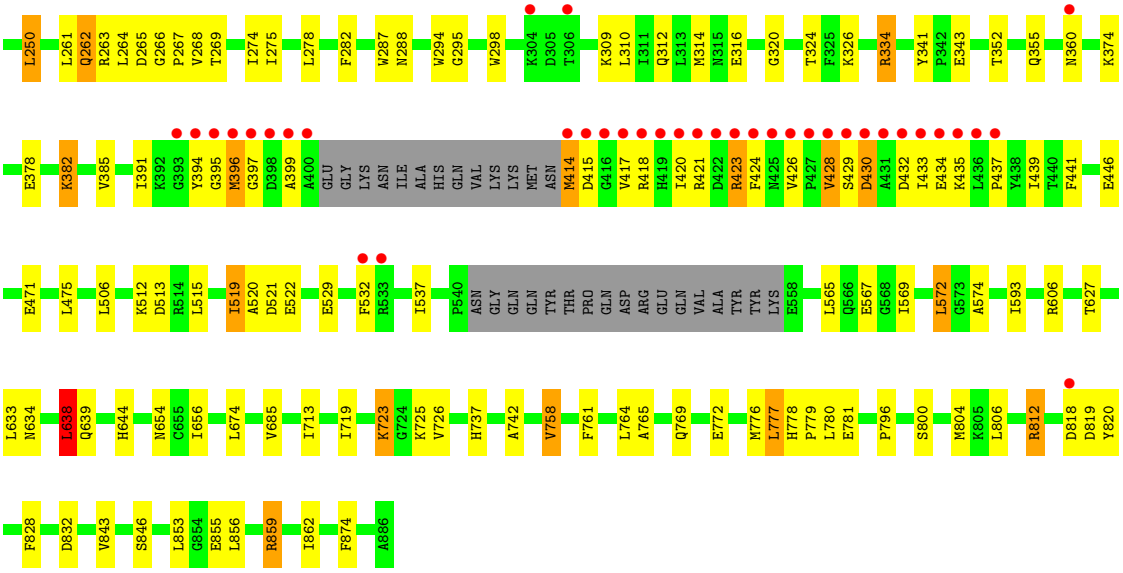
Chain A:



• Molecule 1: Pyruvate dehydrogenase E1 component

Chain B:




L250 L261 Q262 R263 L264 D265 G266 P267 V268 T269 I274 I275 L278 F282 W287 N288 W294 G295 W298 K304 D305 T306 K309 L310 I311 Q312 L313 M314 N315 E316 G320 T324 F325 K326 R334 Y341 P342 E343 T352 Q355 N360 K374
E378 K382 V385 I391 K392 G393 Y394 G395 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 D422 R423 F424 N425 V426 P427 V428 S429 D430 A431 D432 I433 E434 K435 L436 P437 Y438 I439 T440 F441 E446
E471 L475 L506 K512 D513 R514 L515 I519 A520 D521 E522 E529 F532 R533 I537 P540 ASN GLY GLN GLN TYR THR PRO GLN ASP ARG GLU GLN VAL ALA TYR TYR LYS E558 L565 Q566 E567 G568 I569 L572 G573 A574 I593 R606 T627
L633 N634 L638 Q639 H644 N654 C655 I656 L674 V685 I713 I719 K723 G724 K725 V726 H737 A742 V758 F761 L764 A765 Q769 E772 M776 L777 H778 P779 L780 E781 P796 S800 M804 K805 L806 R812 D818 D819 Y820
F828 D832 V843 S846 L853 G854 E855 L856 R859 I862 F874 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	81.69Å 141.60Å 82.46Å 90.00° 102.40° 90.00°	Depositor
Resolution (Å)	8.00 – 1.85 40.72 – 1.80	Depositor EDS
% Data completeness (in resolution range)	87.0 (8.00-1.85) 87.9 (40.72-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.73 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.177 , 0.203 0.180 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13418	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.30	0/6484	0.59	1/8766 (0.0%)
1	B	0.31	0/6484	0.59	1/8766 (0.0%)
All	All	0.31	0/12968	0.59	2/17532 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	638	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	638	LEU	CA-CB-CG	5.19	127.24	115.30

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	6341	0	6179	132	0
1	B	6341	0	6179	148	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	2	0
3	B	26	0	16	2	0
4	A	329	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	353	0	0	6	0
All	All	13418	0	12390	273	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 11.

All (273) 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:801:THR:HG22	1:A:803:TYR:H	1.26	1.00
1:B:396:MET:HB2	1:B:399:ALA:HB3	1.47	0.94
1:A:854:GLY:O	1:A:858:LYS:HD3	1.69	0.91
1:B:421:ARG:HE	1:B:433:ILE:HD11	1.34	0.90
1:B:421:ARG:HB2	1:B:426:VAL:HB	1.55	0.89
1:B:800:SER:OG	1:B:843:VAL:HG23	1.76	0.86
1:B:192:VAL:HG23	4:B:920:HOH:O	1.74	0.86
1:B:268:VAL:HB	1:B:274:ILE:HG21	1.59	0.83
1:A:396:MET:HB3	1:A:399:ALA:HB3	1.59	0.83
1:A:192:VAL:HG22	4:A:891:HOH:O	1.76	0.82
1:B:638:LEU:HD22	1:B:828:PHE:HB3	1.60	0.82
1:B:414:MET:HE2	1:B:415:ASP:HB2	1.59	0.82
1:A:261:LEU:HB2	1:A:323:GLN:HE22	1.43	0.81
1:A:735:LEU:O	1:A:738:VAL:HG22	1.81	0.79
1:B:287:TRP:CE3	1:B:385:VAL:HG23	2.18	0.78
1:A:177:TYR:CG	1:A:192:VAL:HG11	2.21	0.76
1:B:282:PHE:CD2	1:B:385:VAL:HG21	2.21	0.75
1:A:326:LYS:HE2	1:A:391:ILE:HG23	1.68	0.75
1:A:801:THR:HG22	1:A:803:TYR:N	2.01	0.73
1:B:77:LEU:HD11	1:B:446:GLU:HG2	1.71	0.72
1:A:638:LEU:HD22	1:A:828:PHE:HB3	1.71	0.72
1:A:801:THR:HG21	1:A:807:PHE:HD2	1.54	0.72
1:B:199:ILE:HD13	1:B:572:LEU:HD13	1.71	0.71
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.21	0.71
1:B:421:ARG:NE	1:B:433:ILE:HD11	2.05	0.71
1:B:418:ARG:HA	1:B:421:ARG:HG2	1.75	0.69
1:A:88:ASN:O	1:A:92:THR:HG23	1.92	0.69
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.23	0.68
1:B:656:ILE:HG12	1:B:685:VAL:HG21	1.76	0.68
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.76	0.67
1:B:288:ASN:HB2	1:B:382:LYS:HE3	1.76	0.67
1:A:140:GLN:O	1:A:143:ILE:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:HG2	1:A:433:ILE:HD13	1.77	0.66
1:A:518:ILE:C	1:A:519:ILE:HD12	2.15	0.66
1:A:342:PRO:HG2	1:A:343:GLU:OE2	1.95	0.66
1:B:274:ILE:HD12	1:B:275:ILE:N	2.11	0.66
1:B:429:SER:O	1:B:433:ILE:HG13	1.96	0.66
1:B:430:ASP:OD2	1:B:430:ASP:N	2.28	0.65
1:B:76:GLU:CD	1:B:76:GLU:H	1.97	0.65
1:A:158:THR:OG1	1:A:160:GLU:HG2	1.98	0.64
1:A:884:ARG:NH1	4:A:1047:HOH:O	2.30	0.64
1:A:328:LYS:HG3	1:A:332:TYR:CD2	2.33	0.64
1:A:524:ARG:HG2	1:A:529:GLU:HG2	1.81	0.63
1:A:261:LEU:HB2	1:A:323:GLN:NE2	2.12	0.63
1:A:90:ILE:O	1:A:94:LEU:HD23	1.99	0.62
1:B:199:ILE:HD11	1:B:237:GLU:HB3	1.81	0.62
1:A:519:ILE:HD11	1:A:528:MET:HE3	1.82	0.62
1:B:221:LYS:HE3	4:B:1072:HOH:O	2.00	0.62
1:A:177:TYR:CD1	1:A:192:VAL:HG11	2.34	0.61
1:A:519:ILE:HD11	1:A:528:MET:CE	2.29	0.61
1:A:524:ARG:HA	1:A:529:GLU:OE2	2.01	0.61
1:B:245:ALA:HA	1:B:250:LEU:HD22	1.83	0.61
1:B:177:TYR:CB	1:B:192:VAL:HG21	2.31	0.61
1:B:506:LEU:HD23	1:B:515:LEU:HD12	1.82	0.60
1:B:654:ASN:O	1:B:685:VAL:HG23	2.01	0.60
1:B:430:ASP:HA	1:B:433:ILE:HD12	1.84	0.60
1:B:171:GLY:O	1:B:173:GLY:N	2.29	0.59
1:B:352:THR:OG1	1:B:355:GLN:HG3	2.03	0.59
1:B:656:ILE:CG1	1:B:685:VAL:HG21	2.32	0.59
1:B:64:PRO:HG2	1:B:67:GLU:HB2	1.85	0.59
1:A:261:LEU:HD23	1:A:274:ILE:HD11	1.85	0.58
1:B:417:VAL:HA	1:B:420:ILE:HG12	1.84	0.58
1:A:506:LEU:HD13	1:A:515:LEU:HD12	1.84	0.58
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.85	0.58
1:B:287:TRP:CE3	1:B:385:VAL:CG2	2.87	0.58
1:B:199:ILE:CD1	1:B:237:GLU:HB3	2.34	0.58
1:A:471:GLU:HG2	4:A:1006:HOH:O	2.03	0.57
1:B:853:LEU:O	1:B:862:ILE:HD11	2.04	0.57
1:A:65:VAL:HG11	1:A:299:ASP:OD1	2.05	0.57
1:A:560:GLU:CD	1:A:560:GLU:H	2.08	0.57
1:A:326:LYS:CE	1:A:391:ILE:HG23	2.33	0.56
1:A:801:THR:HG21	1:A:807:PHE:CD2	2.39	0.56
1:B:150:ARG:O	1:B:154:GLU:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ILE:HD12	1:B:56:ILE:O	2.06	0.56
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.71	0.56
1:A:304:LYS:HE2	1:A:347:LEU:HD12	1.88	0.55
1:B:140:GLN:O	1:B:143:ILE:HG13	2.06	0.55
1:B:261:LEU:HD23	1:B:274:ILE:HD11	1.88	0.55
1:B:519:ILE:HD13	1:B:519:ILE:H	1.71	0.55
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.88	0.55
1:A:426:VAL:HG13	1:A:439:ILE:CD1	2.37	0.55
1:A:527:GLY:HA2	1:A:529:GLU:OE2	2.07	0.55
1:B:262:GLN:HG3	1:B:266:GLY:O	2.06	0.55
1:B:269:THR:OG1	1:B:274:ILE:HG23	2.06	0.55
1:B:435:LYS:HD2	1:B:437:PRO:HB3	1.87	0.55
1:B:86:ARG:O	1:B:90:ILE:HD13	2.07	0.54
1:B:87:TRP:CZ3	1:B:421:ARG:HB3	2.42	0.54
1:B:434:GLU:CD	1:B:434:GLU:H	2.09	0.54
1:A:323:GLN:OE1	1:A:326:LYS:HD2	2.08	0.54
1:B:274:ILE:HD12	1:B:275:ILE:HG13	1.88	0.54
1:B:312:GLN:O	1:B:316:GLU:HG2	2.08	0.54
1:A:739:ARG:HD2	4:A:1089:HOH:O	2.08	0.54
1:A:323:GLN:O	1:A:326:LYS:HB3	2.07	0.53
1:A:471:GLU:OE2	1:A:591:PRO:HD2	2.08	0.53
1:B:778:HIS:HB3	1:B:781:GLU:OE1	2.09	0.53
1:A:853:LEU:O	1:A:862:ILE:HD11	2.08	0.53
1:A:374:LYS:O	1:A:378:GLU:HG3	2.08	0.53
1:B:421:ARG:CB	1:B:426:VAL:HB	2.35	0.53
1:A:159:GLN:HG3	1:A:438:TYR:CD1	2.43	0.53
1:B:532:PHE:CD1	1:B:537:ILE:HD11	2.44	0.53
1:A:262:GLN:NE2	1:A:392:LYS:HD3	2.24	0.53
1:A:654:ASN:O	1:A:685:VAL:HG22	2.10	0.52
1:B:295:GLY:HA3	1:B:360:ASN:ND2	2.24	0.52
1:B:644:HIS:HB3	1:B:804:MET:CE	2.38	0.52
1:A:261:LEU:CD2	1:A:274:ILE:HD11	2.40	0.52
1:A:864:LYS:HB3	1:B:780:LEU:HD23	1.90	0.52
1:B:843:VAL:HG22	1:B:843:VAL:O	2.09	0.52
1:A:301:LEU:HD23	1:A:304:LYS:HD3	1.91	0.52
1:B:177:TYR:HB3	1:B:192:VAL:HG22	1.92	0.51
1:B:194:MET:HE1	3:B:887:TPP:H72	1.91	0.51
1:A:801:THR:HG22	1:A:802:ASP:N	2.25	0.51
1:B:519:ILE:HD13	1:B:565:LEU:O	2.11	0.51
1:A:274:ILE:HG13	1:A:319:ASP:OD2	2.10	0.51
1:A:456:GLN:HA	1:A:456:GLN:NE2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:O	1:B:68:GLN:HG2	2.11	0.51
1:B:287:TRP:HE3	1:B:385:VAL:HG23	1.69	0.51
1:B:326:LYS:CD	1:B:391:ILE:HG23	2.41	0.51
1:A:736:ARG:NH1	1:A:737:HIS:HE1	2.10	0.50
1:B:177:TYR:CB	1:B:192:VAL:CG2	2.89	0.50
1:A:262:GLN:HA	1:A:267:PRO:HA	1.93	0.50
1:A:864:LYS:O	1:A:867:VAL:HG13	2.10	0.50
1:A:150:ARG:HH21	1:A:455:ARG:HD3	1.76	0.50
1:A:361:ARG:HD2	1:A:391:ILE:HD12	1.93	0.50
4:A:1042:HOH:O	3:B:887:TPP:H2	2.11	0.50
1:A:66:GLU:H	1:A:66:GLU:CD	2.15	0.50
1:A:801:THR:CG2	1:A:802:ASP:N	2.74	0.50
1:B:421:ARG:HG3	1:B:421:ARG:HH11	1.76	0.50
1:B:199:ILE:HD13	1:B:572:LEU:CD1	2.39	0.50
1:B:320:GLY:O	1:B:324:THR:HG23	2.12	0.50
1:A:855:GLU:O	1:A:859:ARG:HG3	2.12	0.49
1:B:326:LYS:HD3	1:B:391:ILE:HG23	1.92	0.49
1:A:656:ILE:HD11	1:A:685:VAL:HG21	1.94	0.49
1:B:719:ILE:HD12	1:B:742:ALA:HB1	1.94	0.49
1:B:737:HIS:HE1	4:B:906:HOH:O	1.95	0.49
1:A:735:LEU:HD12	1:A:738:VAL:CG2	2.42	0.49
1:B:309:LYS:HG2	1:B:343:GLU:HG2	1.95	0.49
1:B:627:THR:HB	1:B:633:LEU:HD22	1.93	0.49
1:B:56:ILE:HD12	1:B:56:ILE:C	2.33	0.49
1:A:567:GLU:HG3	1:A:574:ALA:HA	1.95	0.49
1:A:537:ILE:HB	1:A:558:GLU:HG2	1.95	0.48
1:B:74:ASN:OD1	1:B:76:GLU:HG2	2.13	0.48
1:B:519:ILE:HD13	1:B:519:ILE:N	2.27	0.48
1:B:177:TYR:HB2	1:B:192:VAL:HG21	1.94	0.48
1:A:301:LEU:HA	1:A:304:LYS:HD3	1.96	0.48
1:A:801:THR:HB	4:A:895:HOH:O	2.12	0.48
1:B:765:ALA:O	1:B:769:GLN:HG3	2.14	0.48
1:B:812:ARG:NE	1:B:820:TYR:HB3	2.28	0.48
1:A:130:GLU:HB3	1:A:131:GLN:NE2	2.28	0.48
1:B:812:ARG:HE	1:B:820:TYR:HB3	1.78	0.48
1:A:878:ALA:HA	1:B:777:LEU:HG	1.96	0.48
1:B:178:PRO:HA	1:B:187:TRP:CG	2.49	0.48
1:B:91:MET:O	1:B:95:ARG:CG	2.61	0.48
1:B:177:TYR:HB3	1:B:192:VAL:CG2	2.44	0.48
1:B:91:MET:O	1:B:95:ARG:HG2	2.14	0.47
1:A:300:GLU:O	1:A:304:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:CD1	1:B:275:ILE:HG13	2.44	0.47
1:B:374:LYS:O	1:B:378:GLU:HG3	2.14	0.47
1:A:765:ALA:O	1:A:769:GLN:HG3	2.14	0.47
1:B:532:PHE:CG	1:B:537:ILE:HD11	2.50	0.47
1:A:864:LYS:HD3	1:B:779:PRO:O	2.15	0.47
1:B:198:PRO:HD3	1:B:228:LEU:HD22	1.96	0.47
1:B:396:MET:HA	1:B:420:ILE:CD1	2.44	0.47
1:A:279:GLU:HG3	1:A:289:VAL:HG11	1.97	0.47
1:A:846:SER:HB2	1:A:874:PHE:HB3	1.97	0.47
1:B:144:SER:OG	1:B:145:PRO:HD3	2.14	0.47
1:A:192:VAL:HG23	1:B:639:GLN:OE1	2.14	0.47
1:A:304:LYS:HE2	1:A:347:LEU:CD1	2.44	0.47
1:B:512:LYS:HG3	1:B:513:ASP:N	2.30	0.47
1:B:656:ILE:HG12	1:B:685:VAL:HG22	1.95	0.47
1:B:812:ARG:HD2	1:B:820:TYR:HD2	1.79	0.47
1:B:177:TYR:HB3	1:B:178:PRO:CD	2.45	0.46
1:B:294:TRP:HB3	1:B:298:TRP:CD1	2.50	0.46
1:A:300:GLU:HG3	1:A:301:LEU:N	2.29	0.46
1:B:79:ARG:HG3	1:B:80:ARG:N	2.30	0.46
1:B:421:ARG:HG3	1:B:421:ARG:NH1	2.30	0.46
1:A:560:GLU:HG2	1:A:561:LYS:HD2	1.98	0.46
1:B:638:LEU:CD2	1:B:828:PHE:HB3	2.38	0.46
1:A:819:ASP:OD2	1:A:855:GLU:HG2	2.15	0.46
1:A:638:LEU:HB3	1:B:179:HIS:CE1	2.51	0.46
3:A:887:TPP:H61	1:B:569:ILE:HD11	1.96	0.46
1:A:524:ARG:HG2	1:A:529:GLU:CG	2.42	0.46
1:B:153:LEU:HD21	1:B:441:PHE:HE1	1.81	0.46
1:A:305:ASP:OD1	1:A:310:LEU:HB3	2.16	0.45
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.99	0.45
1:B:506:LEU:CD2	1:B:515:LEU:HD12	2.46	0.45
1:B:395:GLY:HA3	1:B:424:PHE:CE1	2.51	0.45
1:B:334:ARG:HG2	4:B:1110:HOH:O	2.16	0.45
1:B:654:ASN:O	1:B:685:VAL:CG2	2.64	0.45
1:A:304:LYS:HG3	1:A:347:LEU:HD11	1.98	0.45
1:A:867:VAL:HG22	1:B:779:PRO:HG3	1.98	0.45
1:A:519:ILE:HD11	1:A:528:MET:HE2	1.99	0.45
1:A:65:VAL:HG11	1:A:299:ASP:CG	2.37	0.45
1:A:294:TRP:HB3	1:A:298:TRP:CD1	2.51	0.45
1:B:426:VAL:HG13	1:B:439:ILE:HD11	1.99	0.45
1:B:76:GLU:O	1:B:79:ARG:HG2	2.17	0.44
1:A:177:TYR:CG	1:A:192:VAL:CG1	2.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:TYR:CG	1:A:701:MET:HB2	2.52	0.44
1:B:263:ARG:NH1	1:B:267:PRO:O	2.50	0.44
1:A:98:LYS:HE2	1:A:436:LEU:HD12	1.98	0.44
1:B:143:ILE:HD12	1:B:143:ILE:C	2.38	0.44
1:A:380:LYS:HE2	4:A:1146:HOH:O	2.17	0.44
1:B:758:VAL:HG11	1:B:761:PHE:CZ	2.52	0.44
1:A:858:LYS:N	1:A:858:LYS:CD	2.80	0.44
1:A:143:ILE:C	1:A:143:ILE:HD12	2.38	0.44
1:A:237:GLU:H	1:A:237:GLU:CD	2.21	0.44
1:A:262:GLN:HE21	1:A:392:LYS:HD3	1.82	0.44
1:A:264:LEU:HD12	1:A:265:ASP:OD2	2.18	0.44
1:A:207:PHE:O	1:A:210:TYR:HB3	2.18	0.44
1:A:239:LYS:O	1:A:242:ILE:HG12	2.17	0.44
1:A:634:ASN:HB2	1:A:832:ASP:O	2.17	0.43
1:B:471:GLU:HG2	4:B:915:HOH:O	2.17	0.43
1:B:856:LEU:O	1:B:859:ARG:HG2	2.19	0.43
1:A:302:LEU:HD23	1:A:310:LEU:HD23	1.99	0.43
1:B:426:VAL:CG1	1:B:439:ILE:HD11	2.49	0.43
1:B:434:GLU:OE2	1:B:434:GLU:N	2.46	0.43
1:A:144:SER:OG	1:A:145:PRO:HD3	2.18	0.43
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.48	0.43
1:B:418:ARG:CA	1:B:421:ARG:HG2	2.47	0.43
1:A:178:PRO:HA	1:A:187:TRP:CG	2.53	0.43
1:A:313:LEU:HA	1:A:316:GLU:OE2	2.19	0.43
1:A:323:GLN:OE1	1:A:323:GLN:HA	2.19	0.43
1:B:855:GLU:O	1:B:859:ARG:HD2	2.19	0.43
1:A:128:ARG:NH1	1:A:464:SER:OG	2.52	0.43
1:A:326:LYS:NZ	1:A:392:LYS:H	2.17	0.43
1:A:361:ARG:HD2	1:A:391:ILE:CD1	2.49	0.43
1:A:858:LYS:N	1:A:858:LYS:HD2	2.33	0.42
1:A:436:LEU:N	1:A:437:PRO:CD	2.82	0.42
1:A:593:ILE:HD13	1:A:674:LEU:HD21	2.00	0.42
1:B:199:ILE:H	1:B:199:ILE:HG13	1.50	0.42
1:A:237:GLU:CD	1:B:606:ARG:HH21	2.22	0.42
1:A:363:GLY:O	1:A:369:ILE:HD11	2.19	0.42
1:A:417:VAL:O	1:A:420:ILE:HG12	2.19	0.42
1:A:850:VAL:HG21	1:A:876:ILE:HD12	2.02	0.42
1:A:328:LYS:HG3	1:A:332:TYR:CE2	2.55	0.42
1:B:428:VAL:HG13	1:B:428:VAL:O	2.20	0.42
1:B:435:LYS:O	1:B:435:LYS:HG2	2.20	0.42
1:A:420:ILE:HG13	1:A:421:ARG:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:GLU:HG3	1:B:574:ALA:HA	2.02	0.42
1:B:644:HIS:HB3	1:B:804:MET:HE1	2.02	0.42
1:A:74:ASN:O	1:A:78:GLU:HG3	2.20	0.41
1:B:264:LEU:HD12	1:B:265:ASP:OD1	2.20	0.41
1:B:593:ILE:HD13	1:B:674:LEU:HD21	2.01	0.41
1:A:194:MET:HE1	3:A:887:TPP:H72	2.02	0.41
1:A:806:LEU:HD11	1:B:806:LEU:HD11	2.01	0.41
1:A:298:TRP:CE2	1:A:359:LEU:HB3	2.56	0.41
1:A:421:ARG:HD2	1:A:421:ARG:C	2.40	0.41
1:B:309:LYS:CB	1:B:343:GLU:HG3	2.51	0.41
1:B:772:GLU:OE2	1:B:772:GLU:HA	2.21	0.41
1:A:189:PHE:HA	1:A:190:PRO:HD3	1.78	0.41
1:B:723:LYS:CD	1:B:723:LYS:N	2.84	0.41
1:A:560:GLU:HG2	1:A:561:LYS:CD	2.50	0.41
1:A:593:ILE:HD13	1:A:674:LEU:CD2	2.50	0.41
1:B:737:HIS:HD2	4:B:1022:HOH:O	2.03	0.41
1:B:423:ARG:CZ	1:B:423:ARG:HB2	2.51	0.41
1:B:529:GLU:HA	1:B:532:PHE:CD2	2.56	0.41
1:A:334:ARG:HB3	1:A:356:ILE:HD13	2.03	0.41
1:B:74:ASN:CG	1:B:77:LEU:HB2	2.41	0.41
1:B:414:MET:CE	1:B:434:GLU:HG3	2.49	0.41
1:B:819:ASP:OD1	1:B:855:GLU:HG2	2.21	0.41
1:A:456:GLN:CA	1:A:456:GLN:HE21	2.34	0.40
1:A:736:ARG:NH1	1:A:737:HIS:CE1	2.89	0.40
1:B:65:VAL:HG13	1:B:66:GLU:N	2.36	0.40
1:B:634:ASN:HB2	1:B:832:ASP:O	2.21	0.40
1:A:264:LEU:CD1	1:A:265:ASP:OD2	2.69	0.40
1:B:310:LEU:O	1:B:314:MET:HG3	2.22	0.40
1:B:395:GLY:CA	1:B:423:ARG:HD3	2.51	0.40
1:B:520:ALA:O	1:B:521:ASP:HB3	2.22	0.40
1:B:726:VAL:HG12	1:B:796:PRO:HG2	2.02	0.40
1:B:111:GLN:HG3	1:B:396:MET:CE	2.52	0.40
1:B:262:GLN:HA	1:B:267:PRO:HA	2.02	0.40
1:A:334:ARG:HB3	1:A:356:ILE:CD1	2.51	0.40
1:B:309:LYS:HD2	1:B:341:TYR:CG	2.56	0.40
1:B:846:SER:HB2	1:B:874:PHE:HB3	2.02	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	795/886 (90%)	760 (96%)	34 (4%)	1 (0%)	51	36
1	B	795/886 (90%)	752 (95%)	38 (5%)	5 (1%)	25	12
All	All	1590/1772 (90%)	1512 (95%)	72 (4%)	6 (0%)	34	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	ASN
1	B	394	TYR
1	B	397	GLY
1	B	396	MET
1	A	397	GLY
1	B	428	VAL

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	665/735 (90%)	649 (98%)	16 (2%)	49	33
1	B	665/735 (90%)	636 (96%)	29 (4%)	28	12
All	All	1330/1470 (90%)	1285 (97%)	45 (3%)	37	19

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	A	153	LEU
1	A	172	ASN
1	A	192	VAL
1	A	274	ILE
1	A	278	LEU
1	A	323	GLN
1	A	335	GLU
1	A	374	LYS
1	A	382	LYS
1	A	398	ASP
1	A	560	GLU
1	A	638	LEU
1	A	685	VAL
1	A	867	VAL
1	A	885	LEU
1	B	76	GLU
1	B	77	LEU
1	B	95	ARG
1	B	172	ASN
1	B	192	VAL
1	B	199	ILE
1	B	234	ASP
1	B	250	LEU
1	B	262	GLN
1	B	278	LEU
1	B	334	ARG
1	B	382	LYS
1	B	414	MET
1	B	423	ARG
1	B	430	ASP
1	B	432	ASP
1	B	475	LEU
1	B	519	ILE
1	B	522	GLU
1	B	572	LEU
1	B	638	LEU
1	B	723	LYS
1	B	725	LYS
1	B	758	VAL
1	B	776	MET
1	B	777	LEU
1	B	812	ARG

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Mol	Chain	Res	Type
1	B	818	ASP
1	B	859	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	131	GLN
1	A	355	GLN
1	A	456	GLN
1	A	737	HIS
1	A	875	ASN
1	B	106	HIS
1	B	503	ASN
1	B	534	GLN
1	B	737	HIS
1	B	875	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TPP	A	887	2	22,27,27	1.72	6 (27%)	29,40,40	1.05	1 (3%)
3	TPP	B	887	2	22,27,27	1.75	6 (27%)	29,40,40	1.05	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
3	TPP	A	887	2	-	3/16/17/17	0/2/2/2
3	TPP	B	887	2	-	1/16/17/17	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TPP	C6-C5	-3.76	1.49	1.50
3	A	887	TPP	C6-C5	-3.56	1.49	1.50
3	A	887	TPP	C4'-N3'	3.55	1.40	1.35
3	B	887	TPP	C4'-N3'	3.50	1.40	1.35
3	B	887	TPP	C5'-C4'	3.32	1.48	1.42
3	A	887	TPP	C5'-C4'	3.24	1.48	1.42
3	B	887	TPP	C2'-N1'	2.70	1.38	1.34
3	A	887	TPP	C2'-N1'	2.53	1.38	1.34
3	B	887	TPP	C4-N3	2.38	1.41	1.39
3	A	887	TPP	C4-N3	2.24	1.41	1.39
3	A	887	TPP	C7'-N3	2.09	1.52	1.48
3	B	887	TPP	C6'-N1'	2.01	1.38	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	887	TPP	C6'-N1'-C2'	2.46	120.14	115.96
3	A	887	TPP	C6'-N1'-C2'	2.42	120.08	115.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

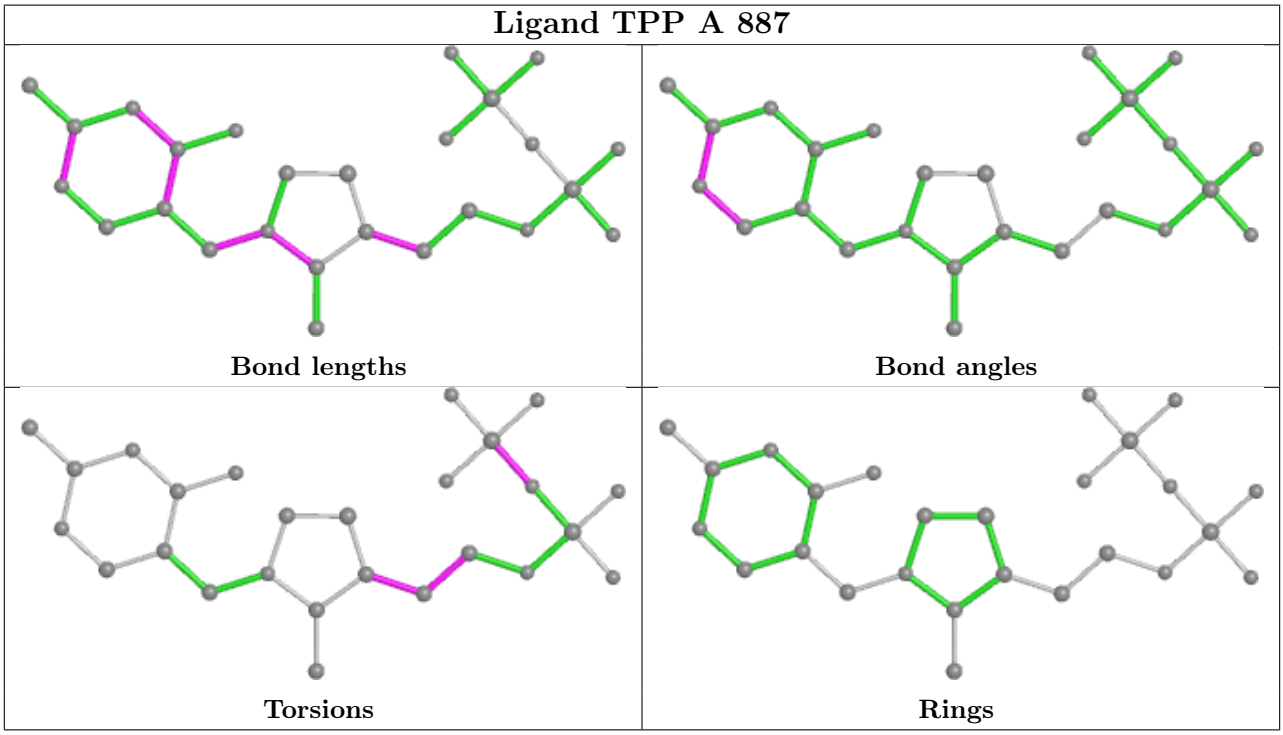
Mol	Chain	Res	Type	Atoms
3	A	887	TPP	C4-C5-C6-C7
3	A	887	TPP	C5-C6-C7-O7
3	A	887	TPP	PA-O3A-PB-O2B
3	B	887	TPP	PA-O3A-PB-O2B

There are no ring outliers.

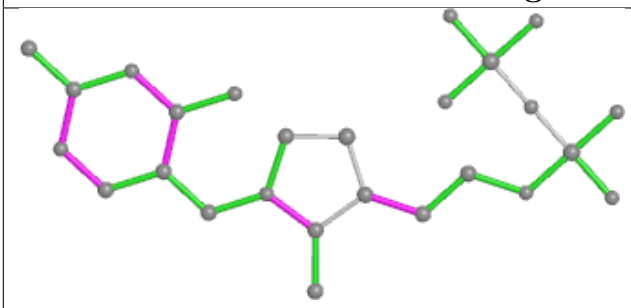
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	887	TPP	2	0
3	B	887	TPP	2	0

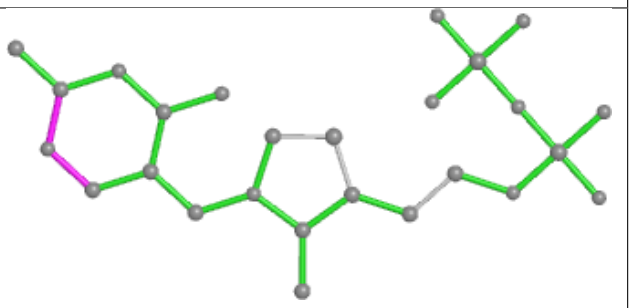
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



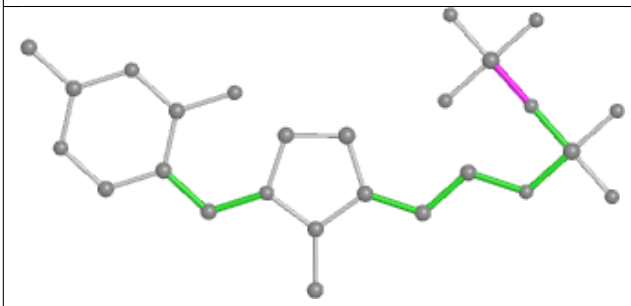
Ligand TPP B 887



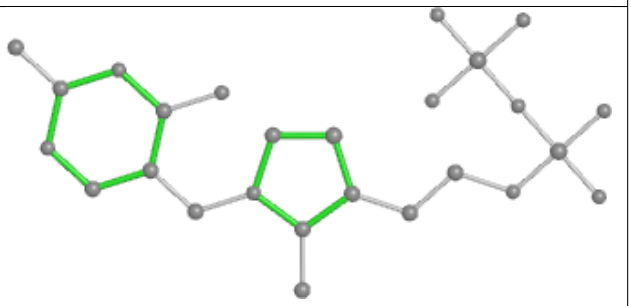
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	-0.04	28 (3%)	44	41	7, 17, 44, 79	0
1	B	801/886 (90%)	-0.01	42 (5%)	27	26	7, 16, 40, 86	0
All	All	1602/1772 (90%)	-0.02	70 (4%)	34	33	7, 16, 43, 86	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	ALA	18.6
1	A	400	ALA	15.0
1	B	400	ALA	11.8
1	B	398	ASP	9.4
1	B	414	MET	9.1
1	A	399	ALA	8.5
1	B	415	ASP	7.5
1	B	416	GLY	7.4
1	A	398	ASP	6.8
1	B	428	VAL	6.4
1	B	420	ILE	6.2
1	B	433	ILE	5.8
1	B	397	GLY	5.7
1	A	349	ALA	5.3
1	B	395	GLY	5.1
1	B	417	VAL	5.0
1	A	397	GLY	4.8
1	B	396	MET	4.7
1	B	436	LEU	4.5
1	B	434	GLU	4.3
1	B	432	ASP	4.2
1	B	430	ASP	4.1
1	B	418	ARG	4.1
1	B	431	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	351	TRP	3.9
1	B	427	PRO	3.9
1	A	533	ARG	3.8
1	A	326	LYS	3.8
1	B	423	ARG	3.8
1	B	393	GLY	3.6
1	B	424	PHE	3.6
1	A	341	TYR	3.6
1	B	56	ILE	3.4
1	A	414	MET	3.3
1	A	354	GLU	3.3
1	B	533	ARG	3.3
1	B	429	SER	3.2
1	B	818	ASP	3.2
1	B	394	TYR	3.1
1	B	171	GLY	3.1
1	A	336	HIS	3.1
1	B	426	VAL	3.0
1	B	422	ASP	3.0
1	A	332	TYR	2.9
1	A	304	LYS	2.8
1	B	306	THR	2.8
1	A	56	ILE	2.6
1	A	818	ASP	2.6
1	A	350	ASP	2.5
1	B	421	ARG	2.5
1	B	437	PRO	2.4
1	B	425	ASN	2.4
1	A	333	VAL	2.4
1	B	532	PHE	2.3
1	B	199	ILE	2.3
1	A	352	THR	2.3
1	A	331	ALA	2.3
1	A	330	GLY	2.2
1	B	304	LYS	2.2
1	B	360	ASN	2.2
1	A	340	LYS	2.2
1	A	415	ASP	2.2
1	A	860	GLY	2.2
1	B	419	HIS	2.1
1	A	305	ASP	2.1
1	B	79	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	344	THR	2.1
1	B	435	LYS	2.0
1	A	130	GLU	2.0
1	A	355	GLN	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)

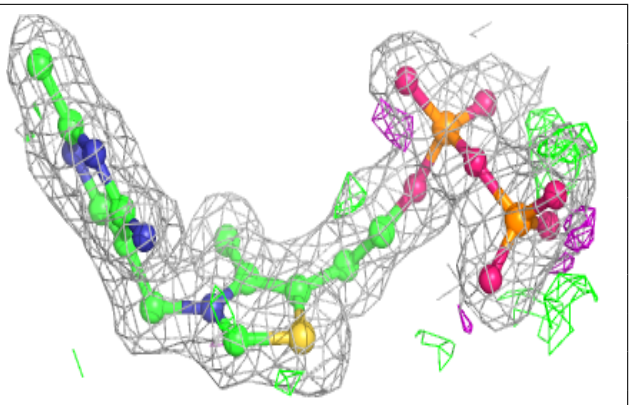
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

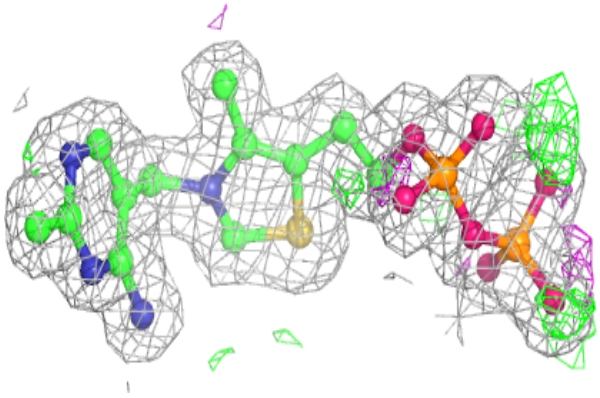
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	888	1/1	0.91	0.14	15,15,15,15	0
2	MG	B	888	1/1	0.92	0.16	15,15,15,15	0
3	TPP	A	887	26/26	0.97	0.10	7,13,18,20	0
3	TPP	B	887	26/26	0.97	0.10	9,13,16,18	0

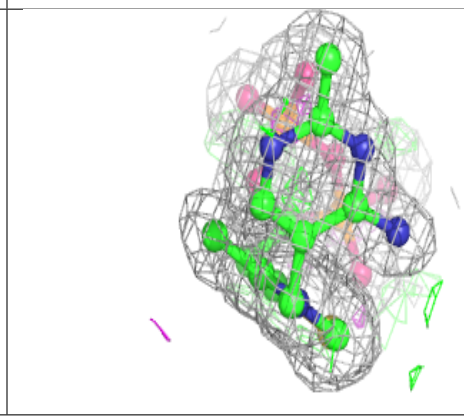
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

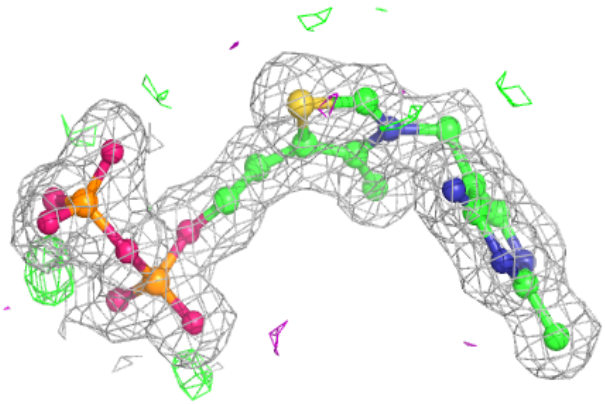


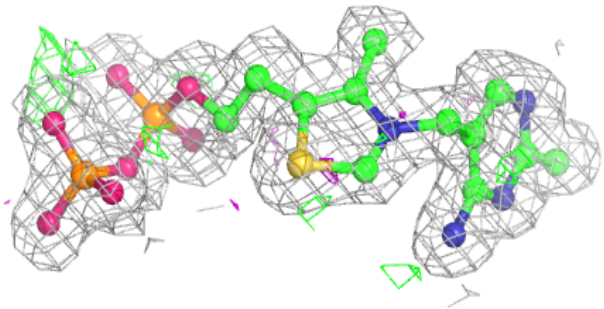


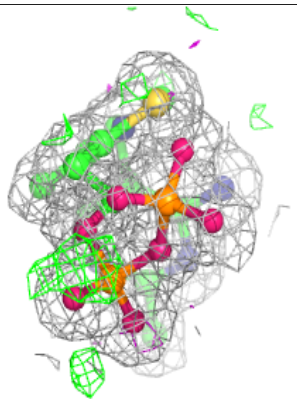


Electron density around TPP B 887:

$2mF_o$-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.