Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 06:01 AM EDT

PDB ID	:	2G28
Title	:	E. Coli Pyruvate Dehydrogenase H407A variant Phosphonolactylthiamin Diphosphate Complex
Authors	:	Furey, W.; Arjunan, P.; Chandrasekhar, K.
Deposited on	:	2006-02-15
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 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:

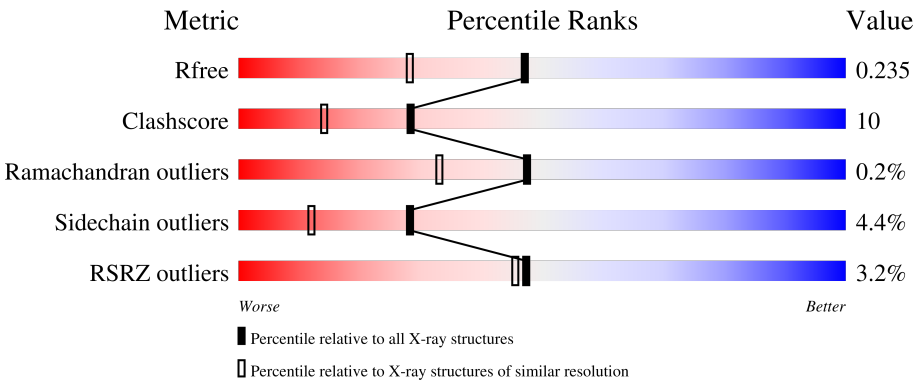
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.85 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))
R_{free}	130704	2469 (1.86-1.86)
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	4% 74% 15% • 10%
1	B	886	2% 76% 13% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13301 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.

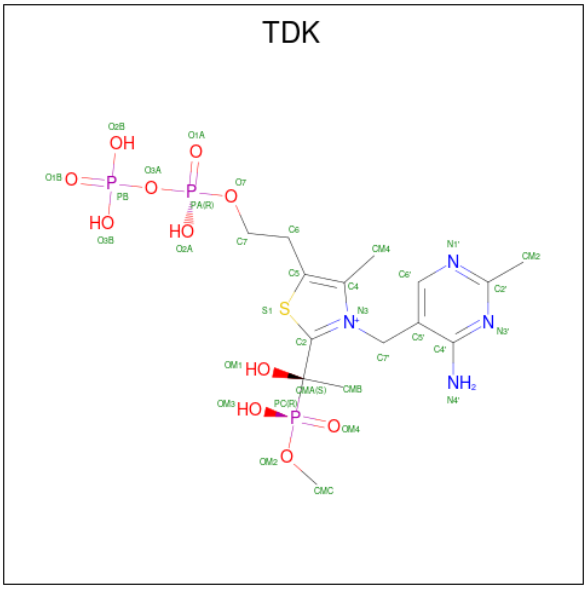
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

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

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

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

- Molecule 3 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-{(1S)-1-HYDROXY-1-[(R)-HYDROXY(METHOXY)PHOSPHORYL]ETHYL}-5-(2-{[(S)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDK) (formula: $C_{15}H_{26}N_4O_{11}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	34	15	4	11	3	1	0	0
			Total	C	N	O	P	S		
3	B	1	34	15	4	11	3	1	0	0

- Molecule 4 is water.

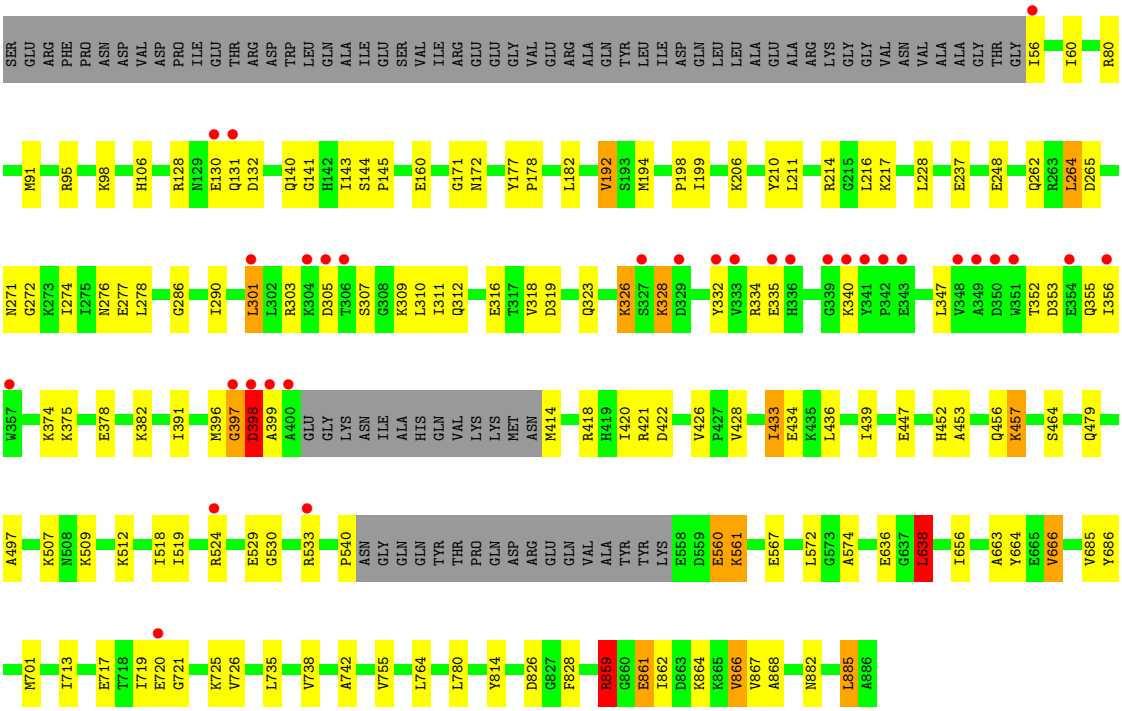
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	278	278	278	0	0
			Total	O		
4	B	271	271	271	0	0

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.

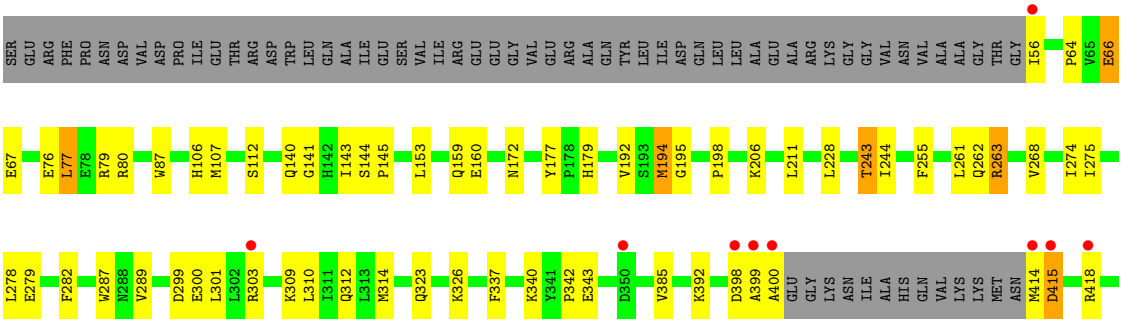
• Molecule 1: Pyruvate dehydrogenase E1 component

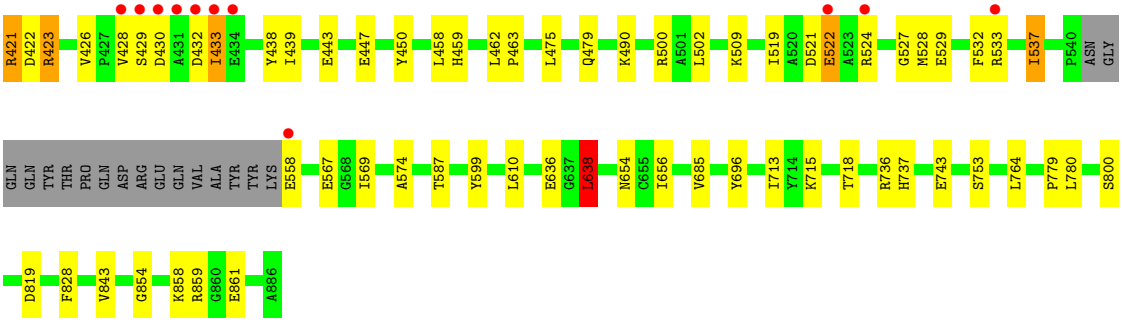
Chain A: 4% 74% 15% • 10%



• Molecule 1: Pyruvate dehydrogenase E1 component

Chain B: 2% 76% 13% • 10%




R421
D422
R423
V426
P427
V428
S429
D430
A431
D432
I433
E434
Y438
I439
E443
E447
Y450
L458
H459
L462
P463
L475
Q479
K490
R500
A501
L502
K509
I519
A520
D521
E522
A523
R524
G527
M528
E529
F532
R533
I537
P540
ASN
GLY
GLN
GLN
TYR
THR
PRO
GLN
ASP
ARG
GLU
GLN
VAL
ALA
TYR
TYR
LYS
E558
E567
G568
I569
A574
T587
Y599
L610
E636
G637
L638
N654
C655
I656
V685
Y696
I713
Y714
K715
T718
R736
H737
E743
S753
L764
P779
L780
S800
D819
F828
V843
G854
K858
R859
G860
E861
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	81.99Å 143.20Å 82.53Å 90.00° 102.61° 90.00°	Depositor
Resolution (Å)	41.77 – 1.85 41.77 – 1.55	Depositor EDS
% Data completeness (in resolution range)	95.2 (41.77-1.85) 79.9 (41.77-1.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.68 (at 1.55Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.216 , 0.240 0.211 , 0.235	Depositor DCC
R_{free} test set	7535 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13301	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: TDK, MG

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	0.50	0/6484	0.73	4/8766 (0.0%)
1	B	0.49	0/6484	0.71	1/8766 (0.0%)
All	All	0.49	0/12968	0.72	5/17532 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	859	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	B	638	LEU	CA-CB-CG	7.74	133.10	115.30
1	A	638	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	859	ARG	NH1-CZ-NH2	5.73	125.70	119.40
1	A	171	GLY	N-CA-C	5.65	127.23	113.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	686	TYR	Sidechain
1	A	814	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6341	0	6179	136	0
1	B	6341	0	6179	116	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	34	0	22	5	0
3	B	34	0	22	5	0
4	A	278	0	0	3	0
4	B	271	0	0	4	0
All	All	13301	0	12402	247	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 10.

All (247) 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:561:LYS:HB2	1:A:561:LYS:NZ	1.77	0.99
1:B:177:TYR:HB3	1:B:192:VAL:HG21	1.43	0.97
1:B:490:LYS:HE2	1:B:500:ARG:HH22	1.29	0.96
1:A:868:ALA:HB2	1:B:780:LEU:HD11	1.46	0.95
1:A:418:ARG:HH21	1:A:421:ARG:HH21	1.13	0.94
1:A:326:LYS:HB3	1:A:326:LYS:NZ	1.82	0.92
1:A:540:PRO:HB3	1:A:560:GLU:HB3	1.53	0.91
1:B:177:TYR:CB	1:B:192:VAL:HG21	2.00	0.91
1:A:177:TYR:CB	1:A:192:VAL:HG21	2.05	0.86
1:A:326:LYS:HD2	1:A:391:ILE:HG23	1.58	0.85
1:A:862:ILE:HD12	1:A:866:VAL:HG22	1.59	0.83
1:B:490:LYS:HE2	1:B:500:ARG:NH2	1.93	0.82
1:A:859:ARG:CB	1:A:859:ARG:HH11	1.93	0.82
1:A:177:TYR:HB3	1:A:192:VAL:HG21	1.64	0.79
1:B:414:MET:O	1:B:414:MET:HG2	1.81	0.79
1:B:177:TYR:HB3	1:B:192:VAL:CG2	2.12	0.79
1:A:418:ARG:NH2	1:A:421:ARG:HH21	1.80	0.78
1:A:290:ILE:HD11	1:A:375:LYS:HD2	1.65	0.78
1:A:561:LYS:HB2	1:A:561:LYS:HZ3	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:TRP:CE3	1:B:385:VAL:HG13	2.19	0.77
1:B:192:VAL:HG23	4:B:903:HOH:O	1.84	0.77
1:B:262:GLN:HG3	1:B:323:GLN:HE21	1.50	0.77
1:B:255:PHE:HB2	1:B:385:VAL:HG12	1.67	0.76
1:A:352:THR:OG1	1:A:355:GLN:HG3	1.86	0.75
1:B:859:ARG:NH1	1:B:861:GLU:OE1	2.20	0.75
1:B:490:LYS:CE	1:B:500:ARG:HH22	1.99	0.75
1:B:421:ARG:NH1	1:B:422:ASP:OD1	2.19	0.74
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.17	0.74
1:A:638:LEU:HD22	1:A:828:PHE:HB3	1.68	0.73
1:B:426:VAL:HG12	1:B:428:VAL:HG12	1.70	0.73
1:A:561:LYS:HB2	1:A:561:LYS:HZ2	1.51	0.73
1:A:862:ILE:HD12	1:A:866:VAL:CG2	2.18	0.73
1:A:326:LYS:HB3	1:A:326:LYS:HZ2	1.53	0.73
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.19	0.73
1:A:540:PRO:CB	1:A:560:GLU:HB3	2.19	0.72
1:A:326:LYS:O	1:A:326:LYS:HG2	1.89	0.72
1:B:421:ARG:HG3	1:B:421:ARG:HH11	1.54	0.72
1:A:530:GLY:HA2	1:A:533:ARG:NH1	2.05	0.71
1:A:859:ARG:NH1	1:A:861:GLU:OE1	2.22	0.71
1:A:720:GLU:HG2	1:A:721:GLY:N	2.06	0.71
1:B:656:ILE:HG12	1:B:685:VAL:HG21	1.73	0.70
1:B:522:GLU:N	1:B:522:GLU:OE1	2.24	0.70
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.72	0.70
1:A:374:LYS:O	1:A:378:GLU:HG3	1.92	0.70
1:A:326:LYS:HB3	1:A:326:LYS:HZ3	1.56	0.70
1:A:312:GLN:O	1:A:316:GLU:HG2	1.93	0.69
1:A:177:TYR:HB3	1:A:192:VAL:CG2	2.21	0.69
1:B:177:TYR:CG	1:B:192:VAL:HG21	2.27	0.69
1:B:656:ILE:CG1	1:B:685:VAL:HG21	2.23	0.69
1:B:715:LYS:HD3	1:B:718:THR:HG22	1.76	0.68
1:B:198:PRO:HG3	1:B:228:LEU:HD22	1.75	0.67
1:A:418:ARG:HE	1:A:421:ARG:NH2	1.91	0.67
1:A:307:SER:OG	1:A:309:LYS:HB2	1.94	0.67
1:A:656:ILE:HG12	1:A:685:VAL:CG2	2.25	0.67
1:B:569:ILE:HD13	3:B:887:TDK:HM43	1.76	0.67
1:A:868:ALA:HB2	1:B:780:LEU:CD1	2.25	0.66
1:B:268:VAL:HB	1:B:274:ILE:HG21	1.77	0.66
1:B:262:GLN:HG3	1:B:323:GLN:NE2	2.10	0.66
1:A:277:GLU:OE2	1:B:243:THR:HG21	1.95	0.66
1:A:859:ARG:HH11	1:A:859:ARG:HB2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:THR:HG23	1:A:355:GLN:CD	2.17	0.65
1:B:282:PHE:CD2	1:B:385:VAL:HG11	2.32	0.65
1:B:141:GLY:HA3	1:B:192:VAL:HG22	1.76	0.65
1:B:800:SER:OG	1:B:843:VAL:HG13	1.95	0.65
1:A:418:ARG:NH2	1:A:422:ASP:OD2	2.29	0.65
1:A:128:ARG:NH1	4:A:1074:HOH:O	2.26	0.64
1:A:177:TYR:CG	1:A:192:VAL:HG21	2.31	0.64
1:A:636:GLU:OE1	3:A:887:TDK:HMC1	1.98	0.64
1:A:140:GLN:O	1:A:143:ILE:HG13	1.99	0.63
1:A:262:GLN:HG2	1:A:323:GLN:NE2	2.13	0.63
1:A:274:ILE:O	1:A:278:LEU:HD13	1.99	0.63
1:A:264:LEU:HG	1:B:522:GLU:OE2	1.98	0.62
1:B:587:THR:HG22	4:B:951:HOH:O	2.00	0.62
1:A:56:ILE:HD13	1:A:276:ASN:HB3	1.82	0.62
1:A:518:ILE:C	1:A:519:ILE:HD12	2.20	0.61
1:A:326:LYS:CD	1:A:391:ILE:HG23	2.30	0.61
1:A:199:ILE:HD13	1:A:572:LEU:HD22	1.81	0.61
1:A:397:GLY:O	1:A:399:ALA:N	2.34	0.61
1:A:859:ARG:NH1	1:A:859:ARG:HB3	2.15	0.60
1:A:663:ALA:O	1:A:666:VAL:HG13	2.00	0.60
1:A:859:ARG:CB	1:A:859:ARG:NH1	2.64	0.60
1:B:587:THR:HG21	4:B:954:HOH:O	2.01	0.60
1:B:263:ARG:HG2	1:B:268:VAL:HG22	1.82	0.60
1:B:421:ARG:HG2	1:B:433:ILE:HD11	1.84	0.60
1:A:453:ALA:O	1:A:457:LYS:HD3	2.02	0.60
1:A:418:ARG:NE	1:A:421:ARG:NH2	2.49	0.60
1:A:418:ARG:HB3	1:A:418:ARG:CZ	2.31	0.59
1:A:656:ILE:CG1	1:A:685:VAL:HG21	2.32	0.59
1:B:696:TYR:HB3	1:B:736:ARG:NH1	2.17	0.58
1:A:567:GLU:HG3	1:A:574:ALA:HA	1.85	0.58
1:B:430:ASP:OD1	1:B:430:ASP:O	2.21	0.58
1:B:80:ARG:HD2	1:B:447:GLU:OE2	2.03	0.58
1:B:282:PHE:CE2	1:B:385:VAL:HG11	2.39	0.58
1:A:271:ASN:C	1:A:318:VAL:HG21	2.25	0.58
1:A:859:ARG:HH11	1:A:859:ARG:HB3	1.69	0.58
1:B:426:VAL:HG13	1:B:439:ILE:HD11	1.85	0.58
1:A:290:ILE:CD1	1:A:375:LYS:HD2	2.34	0.58
1:A:130:GLU:HG3	1:A:131:GLN:NE2	2.18	0.57
1:B:421:ARG:NH1	1:B:421:ARG:HG3	2.18	0.57
1:B:638:LEU:HD22	1:B:828:PHE:HB3	1.86	0.57
1:A:334:ARG:HB3	1:A:356:ILE:CD1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:ASP:OD2	1:B:418:ARG:HD3	2.04	0.57
1:B:696:TYR:HB3	1:B:736:ARG:HH11	1.70	0.57
1:A:262:GLN:HG2	1:A:323:GLN:HE21	1.69	0.56
1:B:854:GLY:O	1:B:858:LYS:HG3	2.04	0.56
1:B:261:LEU:HD23	1:B:274:ILE:HD11	1.86	0.56
1:A:206:LYS:HG2	4:A:1128:HOH:O	2.06	0.56
1:A:265:ASP:OD1	1:B:521:ASP:O	2.24	0.56
1:A:323:GLN:HA	1:A:326:LYS:NZ	2.21	0.56
1:B:429:SER:HB3	1:B:432:ASP:OD2	2.05	0.55
1:B:528:MET:O	1:B:532:PHE:HD2	1.90	0.55
1:B:279:GLU:HG3	1:B:289:VAL:HG21	1.88	0.55
1:B:414:MET:O	1:B:414:MET:CG	2.54	0.55
1:A:636:GLU:CD	3:A:887:TDK:HMC1	2.27	0.55
1:A:301:LEU:CD1	1:A:347:LEU:HD13	2.37	0.54
1:A:656:ILE:HG12	1:A:685:VAL:HG22	1.88	0.54
1:A:656:ILE:HG12	1:A:685:VAL:HG21	1.88	0.54
1:B:522:GLU:OE1	1:B:522:GLU:CA	2.55	0.54
1:A:735:LEU:O	1:A:738:VAL:HG22	2.07	0.54
1:A:352:THR:HG23	1:A:355:GLN:OE1	2.07	0.54
1:A:418:ARG:NH2	1:A:421:ARG:NH2	2.55	0.54
1:A:507:LYS:HA	1:A:507:LYS:HE2	1.90	0.54
1:A:237:GLU:HG2	1:A:572:LEU:HD11	1.90	0.53
1:B:656:ILE:HG12	1:B:685:VAL:HG22	1.87	0.53
1:A:262:GLN:CG	1:A:323:GLN:NE2	2.71	0.53
1:A:426:VAL:HG13	1:A:439:ILE:CD1	2.39	0.53
3:B:887:TDK:H7'1	3:B:887:TDK:OM1	2.08	0.53
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.90	0.53
1:B:66:GLU:CD	1:B:66:GLU:H	2.12	0.52
1:B:342:PRO:HD2	1:B:343:GLU:OE2	2.10	0.52
1:B:140:GLN:O	1:B:143:ILE:HG13	2.09	0.52
1:B:527:GLY:HA2	1:B:529:GLU:OE2	2.09	0.52
1:B:261:LEU:HA	1:B:274:ILE:CD1	2.38	0.52
1:A:720:GLU:HG2	1:A:721:GLY:H	1.74	0.52
1:A:286:GLY:O	1:A:382:LYS:HE3	2.09	0.51
1:A:426:VAL:HG12	1:A:428:VAL:HG23	1.92	0.51
1:A:509:LYS:HA	1:A:512:LYS:HE3	1.92	0.51
1:A:540:PRO:CA	1:A:560:GLU:HB3	2.40	0.51
1:A:272:GLY:O	1:A:318:VAL:HG23	2.11	0.51
1:A:80:ARG:HD2	1:A:447:GLU:OE2	2.11	0.50
1:B:843:VAL:CG1	1:B:843:VAL:O	2.58	0.50
1:A:882:ASN:HB3	1:A:885:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LYS:HE3	1:B:312:GLN:NE2	2.26	0.50
1:B:310:LEU:O	1:B:314:MET:HG3	2.12	0.50
1:A:106:HIS:HE1	3:B:887:TDK:OM4	1.93	0.49
1:B:537:ILE:C	1:B:537:ILE:HD13	2.32	0.49
1:A:98:LYS:HE2	1:A:436:LEU:HD12	1.95	0.49
1:B:261:LEU:HA	1:B:274:ILE:HD11	1.93	0.49
1:B:198:PRO:HG3	1:B:228:LEU:CD2	2.42	0.49
1:B:636:GLU:CD	3:B:887:TDK:HMC1	2.34	0.48
1:A:396:MET:O	1:A:397:GLY:C	2.51	0.48
3:A:887:TDK:OM1	3:A:887:TDK:H7'1	2.13	0.48
1:B:426:VAL:HG13	1:B:439:ILE:CD1	2.44	0.48
1:B:160:GLU:HG2	1:B:172:ASN:OD1	2.13	0.48
1:B:843:VAL:O	1:B:843:VAL:HG12	2.13	0.48
1:A:326:LYS:O	1:A:326:LYS:CG	2.61	0.47
1:A:452:HIS:O	1:A:456:GLN:HG2	2.14	0.47
1:B:112:SER:HB3	1:B:392:LYS:HA	1.97	0.47
1:B:64:PRO:HG2	1:B:67:GLU:HG3	1.96	0.46
1:A:206:LYS:HD2	1:A:248:GLU:HG3	1.96	0.46
1:B:569:ILE:CD1	3:B:887:TDK:HM43	2.44	0.46
1:A:518:ILE:O	1:A:519:ILE:HD12	2.16	0.46
1:B:743:GLU:OE1	1:B:743:GLU:HA	2.16	0.46
1:A:272:GLY:O	1:A:318:VAL:CG2	2.63	0.46
3:A:887:TDK:OM4	1:B:106:HIS:HE1	1.98	0.46
1:B:244:ILE:N	1:B:244:ILE:HD12	2.31	0.46
1:B:274:ILE:HG13	1:B:275:ILE:N	2.31	0.46
1:A:328:LYS:HG3	1:A:332:TYR:CD1	2.52	0.45
1:A:656:ILE:HD11	1:A:685:VAL:HG21	1.97	0.45
1:A:91:MET:O	1:A:95:ARG:HG3	2.17	0.45
1:A:328:LYS:HG3	1:A:332:TYR:CG	2.51	0.45
1:B:522:GLU:HG2	1:B:599:TYR:OH	2.16	0.45
1:B:299:ASP:O	1:B:303:ARG:HB3	2.16	0.45
1:A:397:GLY:O	1:A:398:ASP:C	2.55	0.45
1:B:107:MET:HB2	1:B:107:MET:HE2	1.67	0.45
1:B:415:ASP:OD2	1:B:418:ARG:NH1	2.50	0.45
1:A:717:GLU:HG2	1:A:755:VAL:HB	1.97	0.45
1:A:160:GLU:OE1	1:A:172:ASN:OD1	2.35	0.45
1:A:323:GLN:HA	1:A:326:LYS:HZ1	1.82	0.45
1:A:664:TYR:CG	1:A:701:MET:HB2	2.52	0.44
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.47	0.44
1:B:429:SER:HB3	1:B:432:ASP:CG	2.37	0.44
1:B:76:GLU:CD	1:B:76:GLU:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:PHE:O	1:B:340:LYS:HB2	2.18	0.44
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.99	0.44
1:B:399:ALA:O	1:B:400:ALA:O	2.35	0.44
1:A:60:ILE:HG21	1:A:311:ILE:CD1	2.47	0.44
1:B:309:LYS:HE3	1:B:312:GLN:HE22	1.83	0.43
1:B:529:GLU:HA	1:B:532:PHE:CD2	2.53	0.43
1:B:537:ILE:HG23	1:B:558:GLU:HG3	2.00	0.43
1:B:718:THR:HA	1:B:753:SER:O	2.18	0.43
1:A:130:GLU:HG3	1:A:131:GLN:HE22	1.81	0.43
1:A:352:THR:CG2	1:A:355:GLN:HG3	2.49	0.43
1:B:421:ARG:NH1	1:B:421:ARG:CG	2.79	0.43
1:A:398:ASP:OD1	1:A:398:ASP:N	2.51	0.43
1:A:882:ASN:HB3	1:A:885:LEU:HD23	1.99	0.43
1:B:87:TRP:CZ3	1:B:421:ARG:HB3	2.53	0.43
1:A:128:ARG:NH1	1:A:464:SER:OG	2.47	0.43
1:A:352:THR:HG23	1:A:355:GLN:HG3	2.01	0.43
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.99	0.43
1:B:529:GLU:O	1:B:532:PHE:HB2	2.19	0.43
1:B:656:ILE:CD1	1:B:685:VAL:HG21	2.49	0.43
1:B:528:MET:O	1:B:532:PHE:CD2	2.71	0.43
1:B:779:PRO:HG2	1:B:780:LEU:HD12	2.00	0.43
1:B:737:HIS:HE1	4:B:948:HOH:O	2.01	0.43
1:B:77:LEU:HD13	1:B:450:TYR:CD2	2.53	0.43
1:B:567:GLU:HG3	1:B:574:ALA:HA	2.01	0.43
1:A:60:ILE:HG21	1:A:311:ILE:HD12	2.01	0.42
1:A:328:LYS:HB3	1:A:332:TYR:HB3	2.01	0.42
1:B:195:GLY:C	1:B:198:PRO:HD2	2.39	0.42
1:A:132:ASP:HA	1:A:217:LYS:HE3	2.01	0.42
1:A:198:PRO:HD3	1:A:228:LEU:CD2	2.50	0.42
1:A:305:ASP:HB2	1:A:347:LEU:HD11	2.02	0.42
1:B:654:ASN:O	1:B:685:VAL:HG23	2.19	0.42
1:A:497:ALA:CB	1:A:666:VAL:HG11	2.49	0.42
1:A:663:ALA:O	1:A:666:VAL:CG1	2.67	0.42
1:B:779:PRO:HG2	1:B:780:LEU:CD1	2.49	0.42
1:B:458:LEU:O	1:B:459:HIS:HB2	2.19	0.42
1:A:328:LYS:HB3	1:A:332:TYR:CB	2.50	0.42
4:A:961:HOH:O	1:B:243:THR:HB	2.19	0.42
1:B:610:LEU:C	1:B:610:LEU:HD13	2.40	0.41
1:A:352:THR:HG23	1:A:355:GLN:CG	2.49	0.41
1:B:144:SER:N	1:B:145:PRO:CD	2.83	0.41
1:B:656:ILE:HD11	1:B:685:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:O	1:A:214:ARG:HG2	2.19	0.41
1:A:418:ARG:CZ	1:A:421:ARG:NH2	2.84	0.41
1:B:423:ARG:HD3	1:B:423:ARG:O	2.21	0.41
1:B:426:VAL:CG1	1:B:439:ILE:HD11	2.49	0.41
1:A:334:ARG:HB3	1:A:356:ILE:HD12	2.02	0.41
1:A:638:LEU:HB3	1:B:179:HIS:CE1	2.55	0.41
1:B:398:ASP:C	1:B:400:ALA:H	2.23	0.41
1:A:277:GLU:OE2	1:B:243:THR:CG2	2.65	0.41
1:A:262:GLN:CG	1:A:323:GLN:HE22	2.33	0.41
1:A:864:LYS:O	1:A:867:VAL:HG12	2.21	0.41
1:B:153:LEU:HD12	1:B:153:LEU:HA	1.90	0.41
3:A:887:TDK:N3'	1:B:194:MET:HG3	2.36	0.41
1:A:656:ILE:CD1	1:A:685:VAL:HG21	2.50	0.41
1:B:262:GLN:CG	1:B:323:GLN:HE21	2.25	0.41
1:A:318:VAL:HG22	1:A:319:ASP:N	2.36	0.40
1:A:418:ARG:HD2	1:A:433:ILE:HD12	2.02	0.40
1:A:725:LYS:HD3	1:A:726:VAL:N	2.36	0.40
1:A:144:SER:N	1:A:145:PRO:CD	2.85	0.40
1:A:144:SER:OG	1:A:145:PRO:HD3	2.22	0.40
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.56	0.40
1:A:141:GLY:HA3	1:A:192:VAL:HG22	2.02	0.40
1:A:414:MET:CE	1:A:434:GLU:HA	2.52	0.40
1:B:462:LEU:HB2	1:B:463:PRO:HA	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	795/886 (90%)	763 (96%)	29 (4%)	3 (0%)	34 19
1	B	795/886 (90%)	763 (96%)	32 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1590/1772 (90%)	1526 (96%)	61 (4%)	3 (0%)	47 33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ASP
1	A	397	GLY
1	A	328	LYS

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%)	635 (96%)	30 (4%)	27 11
1	B	665/735 (90%)	636 (96%)	29 (4%)	28 12
All	All	1330/1470 (90%)	1271 (96%)	59 (4%)	28 12

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	LEU
1	A	192	VAL
1	A	194	MET
1	A	211	LEU
1	A	216	LEU
1	A	264	LEU
1	A	301	LEU
1	A	303	ARG
1	A	310	LEU
1	A	326	LYS
1	A	335	GLU
1	A	340	LYS
1	A	353	ASP
1	A	398	ASP
1	A	420	ILE

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Mol	Chain	Res	Type
1	A	433	ILE
1	A	457	LYS
1	A	479	GLN
1	A	524	ARG
1	A	529	GLU
1	A	560	GLU
1	A	561	LYS
1	A	638	LEU
1	A	666	VAL
1	A	780	LEU
1	A	826	ASP
1	A	859	ARG
1	A	861	GLU
1	A	866	VAL
1	A	885	LEU
1	B	56	ILE
1	B	66	GLU
1	B	77	LEU
1	B	79	ARG
1	B	194	MET
1	B	206	LYS
1	B	211	LEU
1	B	243	THR
1	B	263	ARG
1	B	278	LEU
1	B	300	GLU
1	B	301	LEU
1	B	326	LYS
1	B	415	ASP
1	B	421	ARG
1	B	423	ARG
1	B	433	ILE
1	B	443	GLU
1	B	475	LEU
1	B	479	GLN
1	B	502	LEU
1	B	509	LYS
1	B	519	ILE
1	B	522	GLU
1	B	524	ARG
1	B	533	ARG
1	B	537	ILE

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Mol	Chain	Res	Type
1	B	638	LEU
1	B	819	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	131	GLN
1	A	262	GLN
1	A	323	GLN
1	A	534	GLN
1	B	106	HIS
1	B	312	GLN
1	B	737	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 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	TDK	A	887	2	29,35,35	1.65	4 (13%)	36,55,55	1.68	8 (22%)
3	TDK	B	887	2	29,35,35	1.92	4 (13%)	36,55,55	1.66	8 (22%)

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	TDK	A	887	2	-	2/26/35/35	0/2/2/2
3	TDK	B	887	2	-	2/26/35/35	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TDK	C6-C5	-7.58	1.47	1.50
3	A	887	TDK	C6-C5	-4.91	1.48	1.50
3	A	887	TDK	PB-O1B	3.38	1.61	1.50
3	A	887	TDK	PC-OM3	-3.17	1.50	1.56
3	B	887	TDK	PB-O1B	3.05	1.60	1.50
3	B	887	TDK	PC-OM3	-2.93	1.50	1.56
3	A	887	TDK	C6'-C5'	-2.88	1.31	1.37
3	B	887	TDK	C6'-C5'	-2.58	1.32	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	887	TDK	OM4-PC-CMA	-4.59	108.86	113.53
3	B	887	TDK	C6-C5-C4	4.32	130.90	127.43
3	B	887	TDK	OM4-PC-CMA	-3.94	109.52	113.53
3	A	887	TDK	C6-C5-C4	3.87	130.54	127.43
3	B	887	TDK	O3B-PB-O2B	2.90	118.74	107.64
3	A	887	TDK	O3B-PB-O2B	2.86	118.55	107.64
3	B	887	TDK	OM2-PC-OM4	-2.68	108.79	114.58
3	B	887	TDK	PA-O3A-PB	-2.60	123.89	132.83
3	A	887	TDK	OM2-PC-OM4	-2.58	109.00	114.58
3	A	887	TDK	C5-C4-N3	2.55	112.99	107.66
3	B	887	TDK	C5-C4-N3	2.51	112.90	107.66
3	B	887	TDK	C6'-N1'-C2'	2.49	120.19	115.96
3	A	887	TDK	C6'-N1'-C2'	2.48	120.18	115.96
3	A	887	TDK	OM3-PC-OM4	2.41	117.15	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	887	TDK	OM3-PC-OM4	2.38	117.08	111.34
3	A	887	TDK	PA-O3A-PB	-2.36	124.74	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	887	TDK	CMC-OM2-PC-OM4
3	B	887	TDK	PA-O3A-PB-O2B
3	A	887	TDK	CMC-OM2-PC-OM4
3	A	887	TDK	PA-O3A-PB-O2B

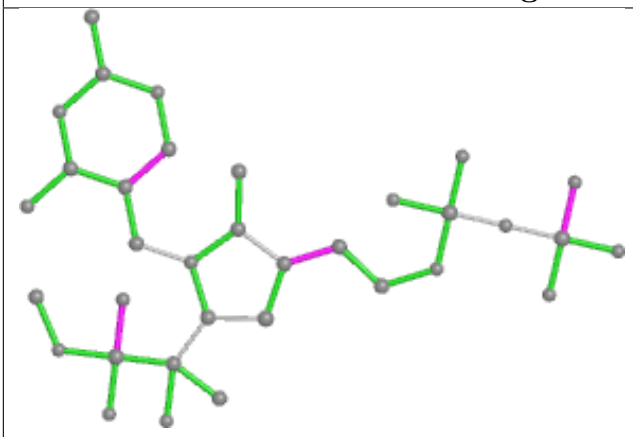
There are no ring outliers.

2 monomers are involved in 10 short contacts:

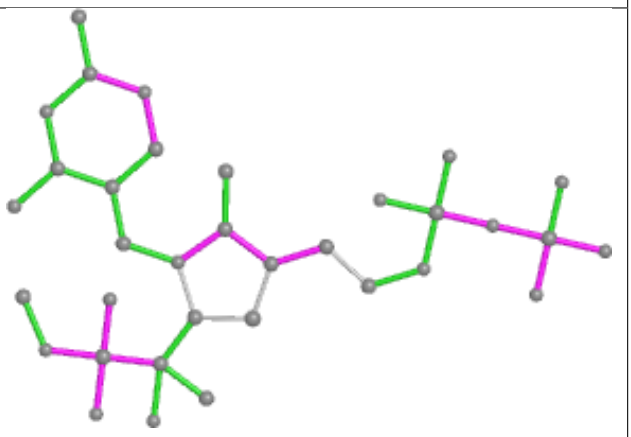
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	887	TDK	5	0
3	B	887	TDK	5	0

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.

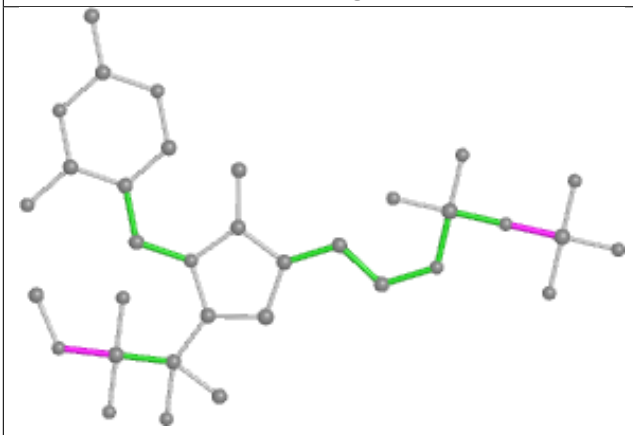
Ligand TDK A 887



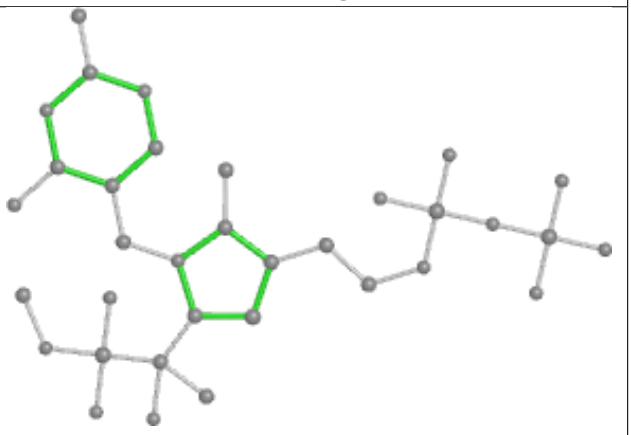
Bond lengths



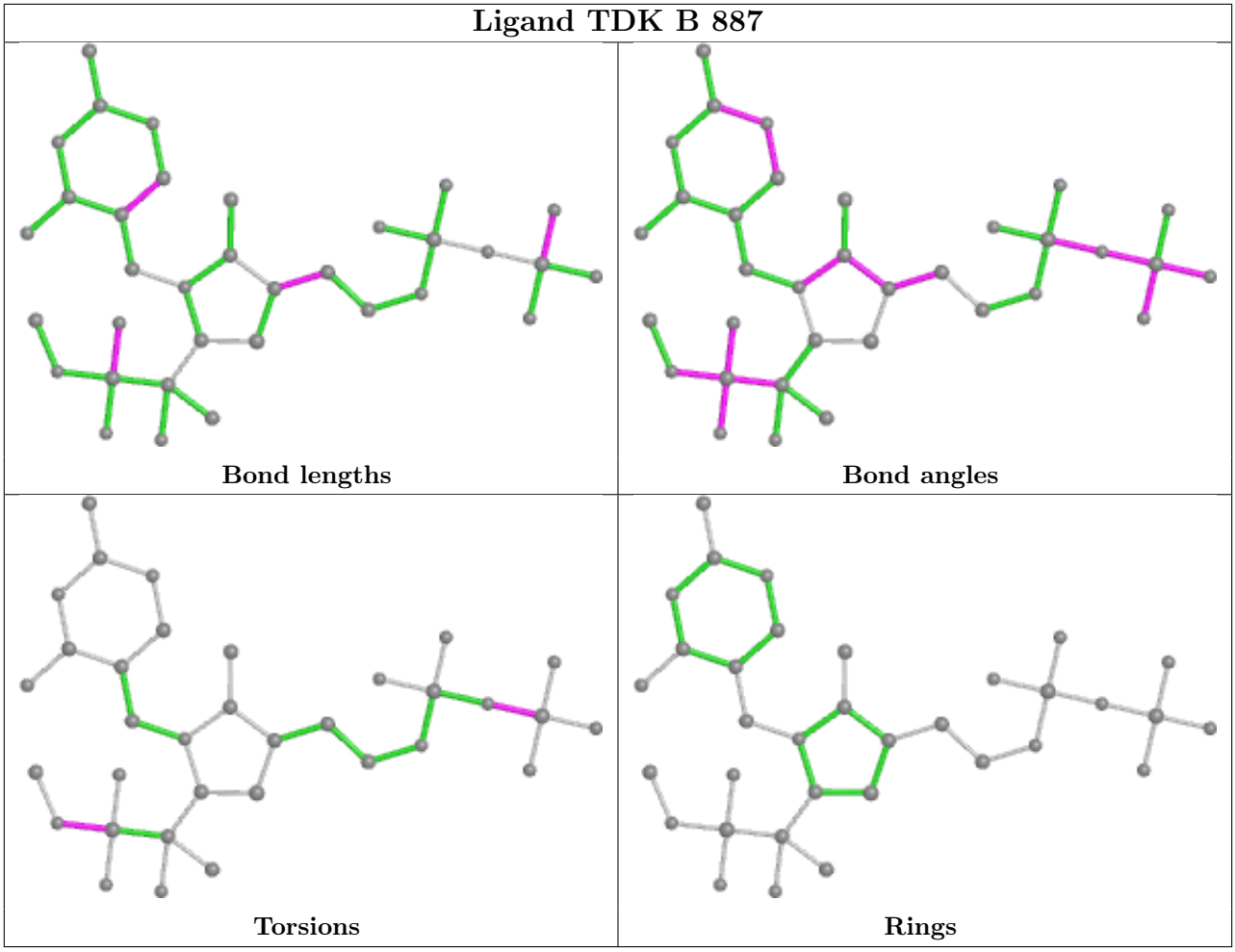
Bond angles



Torsions



Rings



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%)	-0.09	32 (3%)	38	36	14, 20, 31, 34	0
1	B	801/886 (90%)	-0.16	20 (2%)	57	56	12, 20, 29, 38	0
All	All	1602/1772 (90%)	-0.12	52 (3%)	47	45	12, 20, 30, 38	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	400	ALA	9.4
1	B	399	ALA	8.4
1	B	400	ALA	6.8
1	B	398	ASP	6.3
1	B	414	MET	6.1
1	A	399	ALA	5.9
1	A	398	ASP	5.5
1	A	341	TYR	5.4
1	A	349	ALA	4.9
1	B	431	ALA	4.1
1	A	342	PRO	3.9
1	B	56	ILE	3.9
1	A	56	ILE	3.9
1	B	415	ASP	3.8
1	A	327	SER	3.7
1	B	303	ARG	3.6
1	A	339	GLY	3.4
1	A	397	GLY	3.4
1	A	332	TYR	3.3
1	B	533	ARG	3.2
1	B	524	ARG	3.1
1	A	350	ASP	3.0
1	B	428	VAL	2.9
1	B	433	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	720	GLU	2.8
1	A	351	TRP	2.8
1	B	434	GLU	2.8
1	A	336	HIS	2.8
1	A	329	ASP	2.7
1	B	418	ARG	2.7
1	A	304	LYS	2.7
1	A	348	VAL	2.7
1	B	432	ASP	2.7
1	A	340	LYS	2.7
1	A	533	ARG	2.6
1	A	130	GLU	2.6
1	B	429	SER	2.5
1	B	430	ASP	2.5
1	A	131	GLN	2.4
1	A	357	TRP	2.3
1	A	333	VAL	2.3
1	A	305	ASP	2.3
1	B	522	GLU	2.2
1	B	558	GLU	2.2
1	A	301	LEU	2.2
1	A	343	GLU	2.2
1	B	350	ASP	2.2
1	A	356	ILE	2.1
1	A	306	THR	2.1
1	A	335	GLU	2.1
1	A	524	ARG	2.1
1	A	354	GLU	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,

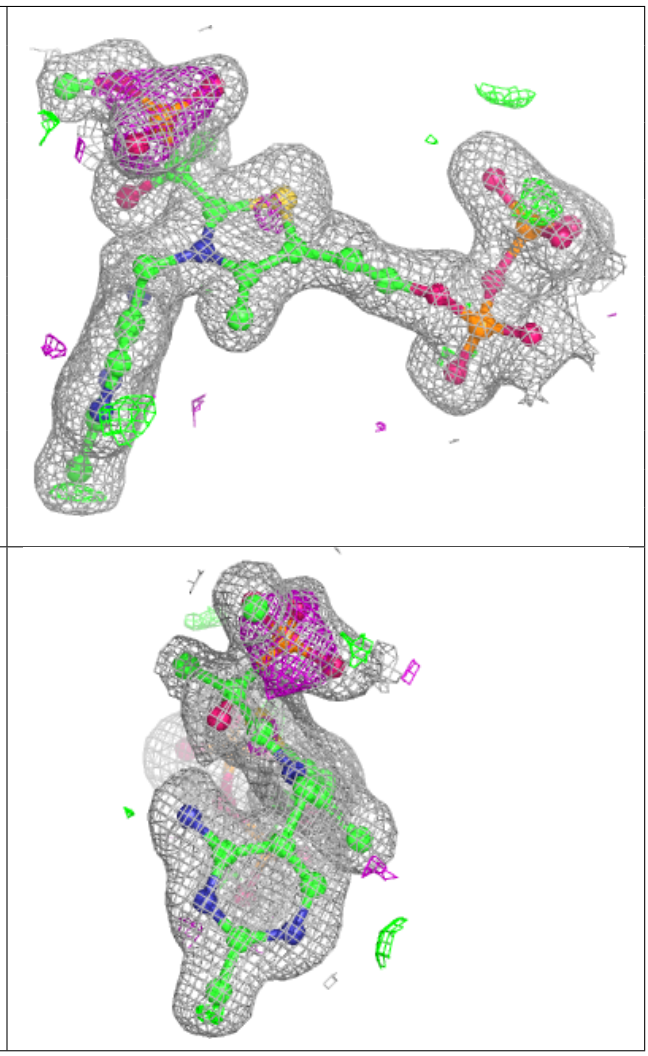
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TDK	A	887	34/34	0.90	0.13	20,23,26,26	0
3	TDK	B	887	34/34	0.92	0.12	19,22,25,25	0
2	MG	A	888	1/1	0.99	0.07	19,19,19,19	0
2	MG	B	888	1/1	0.99	0.10	18,18,18,18	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.

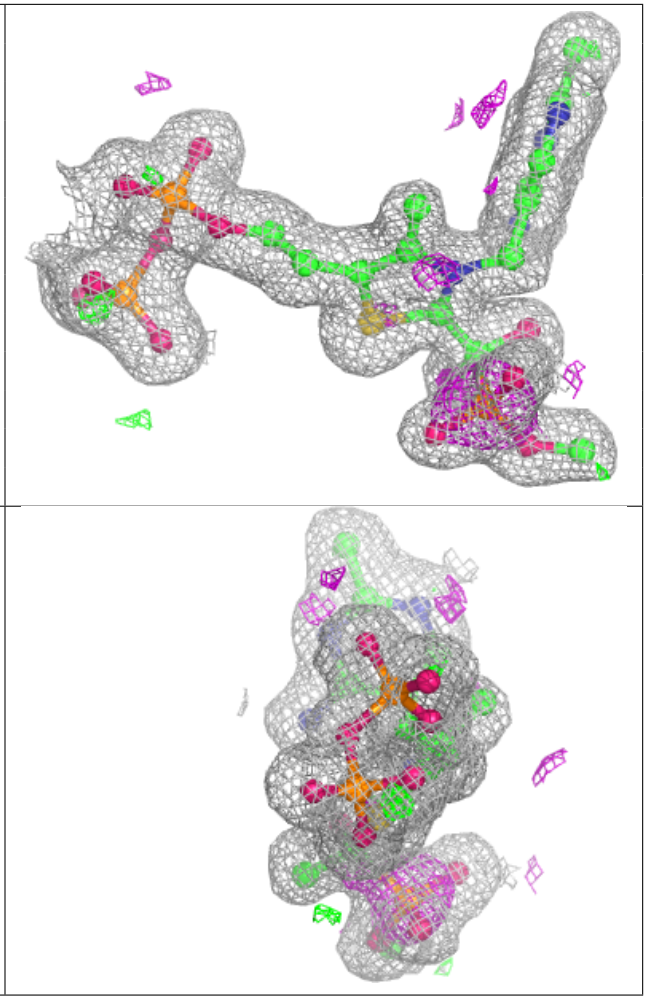
Electron density around TDK A 887:

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 TDK 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.