



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:41 PM GMT

PDB ID : 2G25
Title : E. Coli Pyruvate Dehydrogenase PhosphonolactylthiaminDiphosphate Complex
Authors : Furey, W.; Arjunan, P.; Chandrasekhar, K.
Deposited on : 2006-02-15
Resolution : 2.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

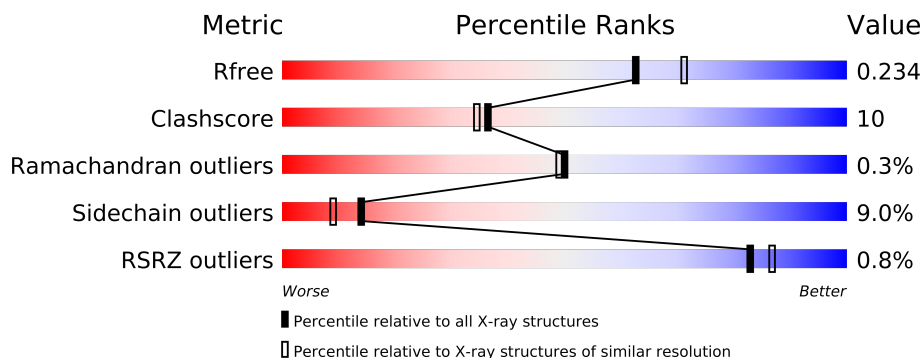
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	886	
1	B	886	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	MG	A	888	-	X
2	MG	B	888	-	X
3	PO4	B	890	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13841 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

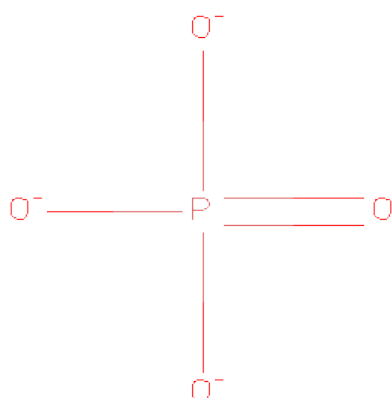
- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	831	Total	C	N	O	S	0	0	0
			6591	4172	1140	1252	27			
1	B	831	Total	C	N	O	S	0	0	0
			6591	4172	1140	1252	27			

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

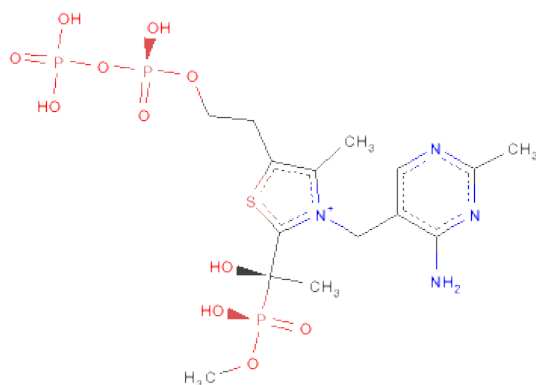
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 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: C₁₅H₂₆N₄O₁₁P₃S).



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

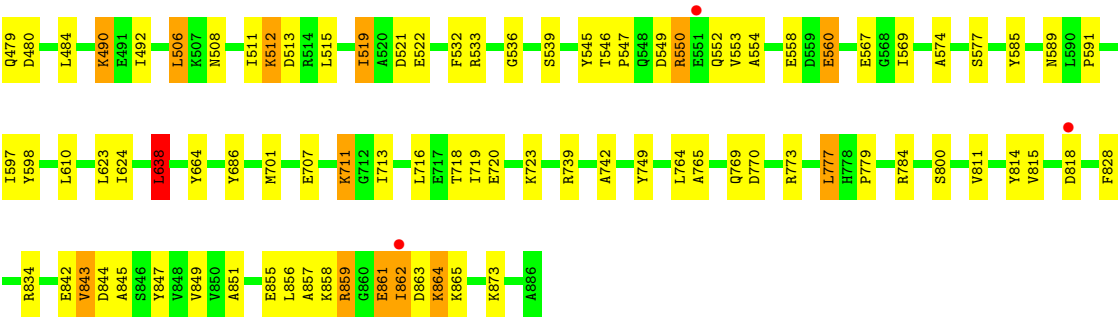
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	273	Total O 273 273	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	291	Total 291	O 291	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.57Å 142.51Å 82.09Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 39.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.0 (8.00-2.10) 93.7 (39.18-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 2.10Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.185 , 0.244 0.180 , 0.234	Depositor DCC
R_{free} test set	4947 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 30.1	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 99699 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13841	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TDK, PO4, 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	0.37	0/6741	0.61	1/9114 (0.0%)
1	B	0.38	0/6741	0.62	2/9114 (0.0%)
All	All	0.37	0/13482	0.62	3/18228 (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	B	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	638	LEU	CA-CB-CG	5.31	127.52	115.30
1	B	638	LEU	CA-CB-CG	5.23	127.34	115.30
1	B	264	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	598	TYR	Sidechain
1	B	686	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6591	0	6422	143	0
1	B	6591	0	6422	135	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	0	0
3	B	15	0	0	2	0
4	A	34	0	22	2	0
4	B	34	0	22	4	0
5	A	273	0	0	6	0
5	B	291	0	0	4	0
All	All	13841	0	12888	270	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (270) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:550:ARG:HH11	1:A:550:ARG:HA	1.18	1.06
1:A:309:LYS:HG3	1:A:344:THR:HG23	1.52	0.91
1:A:549:ASP:HB3	1:A:555:TYR:HA	1.53	0.91
1:A:550:ARG:HH11	1:A:550:ARG:CA	1.87	0.88
1:A:550:ARG:NH1	1:A:550:ARG:HA	1.89	0.86
1:B:311:ILE:HA	1:B:314:MET:HE2	1.61	0.82
1:A:91:MET:O	1:A:95:ARG:HG3	1.84	0.77
1:B:506:LEU:HD13	1:B:515:LEU:HD12	1.67	0.77
1:A:507:LYS:HG2	1:A:507:LYS:O	1.84	0.76
1:B:428:VAL:HG12	1:B:439:ILE:HD11	1.67	0.75
1:B:323:GLN:O	1:B:326:LYS:HG3	1.86	0.75
1:A:88:ASN:O	1:A:92:THR:HG23	1.87	0.73
1:A:728:LEU:HD23	1:A:798:VAL:HG13	1.72	0.72
1:A:506:LEU:HD13	1:A:515:LEU:HD12	1.70	0.72
1:B:533:ARG:HE	1:B:554:ALA:H	1.36	0.71
1:A:160:GLU:HG2	1:A:161:GLN:N	2.07	0.69
1:B:707:GLU:O	1:B:711:LYS:HG2	1.93	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:426:VAL:HG12	1:B:428:VAL:HG13	1.77	0.67
4:A:887:TDK:OM4	1:B:106:HIS:HE1	1.78	0.67
1:A:309:LYS:HG2	1:A:343:GLU:HG3	1.76	0.67
1:A:494:THR:OG1	1:A:692:LEU:HG	1.94	0.67
1:B:76:GLU:H	1:B:76:GLU:CD	1.96	0.66
1:A:728:LEU:HD23	1:A:798:VAL:CG1	2.26	0.65
1:A:274:ILE:HG13	1:A:319:ASP:OD2	1.96	0.65
1:A:261:LEU:HD23	1:A:274:ILE:HD11	1.79	0.65
1:B:64:PRO:HB2	1:B:66:GLU:OE2	1.97	0.65
1:A:140:GLN:O	1:A:143:ILE:HG13	1.98	0.64
1:A:400:ALA:HB1	1:A:406:ALA:HA	1.78	0.64
1:A:638:LEU:HD22	1:A:828:PHE:HB3	1.79	0.64
1:A:290:ILE:HD11	1:A:375:LYS:HD2	1.80	0.64
1:A:150:ARG:NH2	5:A:956:HOH:O	2.32	0.63
1:A:832:ASP:OD2	1:B:169:VAL:HB	1.98	0.63
1:A:859:ARG:HD3	1:A:861:GLU:OE2	1.99	0.63
1:A:344:THR:HA	1:A:347:LEU:HD12	1.81	0.62
1:A:301:LEU:HD13	1:A:351:TRP:CZ2	2.34	0.62
1:A:177:TYR:CD2	1:A:192:VAL:HG11	2.35	0.62
1:A:300:GLU:HG3	1:A:301:LEU:N	2.15	0.61
1:A:261:LEU:HD12	1:A:323:GLN:HG2	1.82	0.61
1:A:536:GLY:HA2	1:A:557:LYS:HD2	1.82	0.60
1:A:297:ARG:HB3	1:A:359:LEU:HD23	1.83	0.60
1:B:128:ARG:HG3	1:B:128:ARG:HH11	1.67	0.60
1:B:311:ILE:HA	1:B:314:MET:CE	2.32	0.59
1:A:864:LYS:HE2	1:B:779:PRO:O	2.02	0.59
1:A:434:GLU:CD	1:A:434:GLU:H	2.04	0.59
1:B:326:LYS:HD3	1:B:391:ILE:HG23	1.84	0.59
1:A:304:LYS:HE2	1:A:347:LEU:HD23	1.84	0.59
1:B:287:TRP:CE3	1:B:385:VAL:HG22	2.37	0.58
1:A:309:LYS:HD2	1:A:341:TYR:CG	2.37	0.58
1:B:857:ALA:HB1	1:B:864:LYS:HD3	1.85	0.58
1:A:466:GLN:HG3	1:A:466:GLN:O	2.03	0.58
1:B:233:MET:O	1:B:239:LYS:HE3	2.04	0.58
1:A:821:ARG:HD2	1:A:855:GLU:CG	2.34	0.58
1:B:86:ARG:NH1	3:B:889:PO4:O2	2.37	0.58
1:B:863:ASP:OD1	1:B:865:LYS:HG3	2.05	0.57
1:B:323:GLN:HA	1:B:326:LYS:HE3	1.86	0.57
1:A:536:GLY:HA3	1:A:557:LYS:NZ	2.18	0.57
1:A:502:LEU:HA	1:A:505:MET:CE	2.34	0.57
1:A:400:ALA:HB2	1:A:409:VAL:HG21	1.85	0.57
1:A:851:ALA:O	1:A:855:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:550:ARG:HH12	1:A:555:TYR:HB2	1.70	0.57
1:B:638:LEU:HD22	1:B:828:PHE:HB3	1.87	0.57
1:A:863:ASP:OD1	1:A:863:ASP:N	2.35	0.57
1:B:90:ILE:CG2	1:B:94:LEU:HD22	2.36	0.56
1:A:532:PHE:O	1:A:536:GLY:HA2	2.06	0.56
1:A:106:HIS:HE1	4:B:887:TDK:OM4	1.87	0.56
1:B:506:LEU:CD1	1:B:515:LEU:HD12	2.36	0.56
1:A:550:ARG:NH1	1:A:555:TYR:HB2	2.21	0.55
1:A:692:LEU:HD22	1:A:733:SER:HB3	1.88	0.55
1:A:863:ASP:O	1:A:866:VAL:HB	2.07	0.55
1:A:197:GLY:N	1:A:198:PRO:HD2	2.21	0.55
1:B:856:LEU:HB3	1:B:862:ILE:HG13	1.89	0.55
1:B:326:LYS:HE2	1:B:361:ARG:NH1	2.22	0.55
1:B:72:PRO:HG3	1:B:370:TYR:CE1	2.42	0.55
1:A:656:ILE:HD11	1:A:685:VAL:HG21	1.89	0.55
1:A:512:LYS:HG3	1:A:513:ASP:N	2.21	0.55
1:A:855:GLU:O	1:A:859:ARG:HG3	2.06	0.55
1:A:508:ASN:O	1:A:512:LYS:HB3	2.07	0.54
1:A:113:SER:HB3	1:A:258:ASN:ND2	2.22	0.54
1:B:177:TYR:HB3	1:B:178:PRO:CD	2.37	0.54
1:B:765:ALA:O	1:B:769:GLN:HG3	2.07	0.54
1:A:450:TYR:O	1:A:454:GLN:HG2	2.07	0.54
1:A:622:PHE:CE1	1:A:677:MET:HE1	2.43	0.54
1:A:821:ARG:HD2	1:A:855:GLU:HG2	1.89	0.54
1:B:664:TYR:CG	1:B:701:MET:HB2	2.42	0.54
1:B:477:SER:O	1:B:480:ASP:HB2	2.07	0.54
1:B:532:PHE:O	1:B:536:GLY:HA2	2.07	0.53
1:B:326:LYS:HG2	1:B:361:ARG:NH2	2.22	0.53
1:B:140:GLN:O	1:B:143:ILE:HG13	2.09	0.53
1:B:859:ARG:HG3	1:B:861:GLU:HB2	1.90	0.53
1:B:197:GLY:N	1:B:198:PRO:HD2	2.24	0.53
1:A:502:LEU:HA	1:A:505:MET:HE2	1.91	0.53
1:A:528:MET:O	1:A:531:LEU:HB2	2.10	0.52
1:B:533:ARG:NH1	1:B:533:ARG:HB3	2.24	0.52
1:B:400:ALA:HB2	1:B:409:VAL:HG21	1.92	0.52
1:B:533:ARG:NE	1:B:554:ALA:H	2.05	0.52
1:A:547:PRO:O	1:A:550:ARG:HB2	2.10	0.51
1:A:160:GLU:HG3	1:A:172:ASN:ND2	2.26	0.51
1:A:82:ARG:O	1:A:86:ARG:HG3	2.11	0.51
1:A:304:LYS:HE2	1:A:347:LEU:CD2	2.40	0.51
1:A:334:ARG:NE	1:A:353:ASP:OD1	2.44	0.51
1:B:128:ARG:HG2	1:B:133:GLY:HA2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:539:SER:O	1:A:560:GLU:HA	2.11	0.50
1:B:326:LYS:HE2	1:B:361:ARG:HH12	1.75	0.50
1:A:420:ILE:HG13	1:A:421:ARG:N	2.26	0.50
5:A:893:HOH:O	1:B:192:VAL:HG22	2.10	0.50
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.92	0.50
1:A:294:TRP:HB3	1:A:298:TRP:CD1	2.47	0.50
1:B:264:LEU:C	1:B:264:LEU:HD12	2.32	0.50
1:B:512:LYS:HG3	1:B:513:ASP:N	2.27	0.50
1:B:287:TRP:HE3	1:B:385:VAL:HG22	1.76	0.50
1:A:773:ARG:HD3	5:A:954:HOH:O	2.11	0.50
1:B:549:ASP:HB2	1:B:552:GLN:HG2	1.94	0.50
1:A:103:LEU:O	1:A:166:ARG:HD3	2.12	0.49
1:A:524:ARG:HG3	1:B:265:ASP:OD1	2.11	0.49
1:B:264:LEU:HD12	1:B:264:LEU:O	2.12	0.49
1:A:585:TYR:O	1:A:589:ASN:HA	2.13	0.49
1:A:502:LEU:HD12	1:A:505:MET:HE3	1.93	0.49
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.42	0.49
1:B:546:THR:O	1:B:546:THR:HG23	2.12	0.49
1:A:177:TYR:CG	1:A:192:VAL:HG11	2.48	0.49
1:B:539:SER:O	1:B:560:GLU:HA	2.12	0.49
1:B:811:VAL:O	1:B:815:VAL:HG23	2.13	0.49
1:B:128:ARG:CG	1:B:128:ARG:HH11	2.26	0.49
1:A:547:PRO:HD2	1:A:550:ARG:HG2	1.95	0.48
1:A:309:LYS:HD2	1:A:341:TYR:CD2	2.48	0.48
1:B:82:ARG:HG2	1:B:86:ARG:NH1	2.29	0.48
1:B:458:LEU:O	1:B:459:HIS:HB2	2.13	0.48
1:A:111:GLN:NE2	1:A:394:TYR:O	2.46	0.48
1:A:126:ARG:HH22	1:A:132:ASP:CG	2.15	0.48
1:B:508:ASN:O	1:B:512:LYS:HB3	2.13	0.48
1:A:274:ILE:HG13	1:A:274:ILE:H	1.46	0.48
1:A:857:ALA:HB1	1:A:864:LYS:HG2	1.95	0.48
1:B:279:GLU:O	1:B:283:GLU:HB2	2.14	0.48
1:B:553:VAL:O	1:B:554:ALA:HB3	2.14	0.48
1:B:199:ILE:HG12	1:B:237:GLU:HB2	1.95	0.48
1:B:547:PRO:O	1:B:550:ARG:HB2	2.14	0.47
1:B:550:ARG:HA	1:B:550:ARG:HD2	1.59	0.47
1:B:490:LYS:HD3	1:B:492:ILE:CG2	2.43	0.47
4:A:887:TDK:H7'1	4:A:887:TDK:OM1	2.14	0.47
1:A:304:LYS:NZ	1:A:347:LEU:O	2.44	0.47
1:A:780:LEU:HD23	1:B:864:LYS:HB2	1.95	0.47
1:B:569:ILE:HD11	4:B:887:TDK:H62	1.97	0.47
1:B:274:ILE:HG13	1:B:319:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:164:ASN:HB3	1:B:173:GLY:HA2	1.97	0.47
1:A:421:ARG:CG	1:A:428:VAL:HG13	2.45	0.46
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.96	0.46
1:A:206:LYS:HD2	1:A:248:GLU:HG3	1.96	0.46
1:A:312:GLN:O	1:A:316:GLU:HG2	2.15	0.46
1:B:428:VAL:CG1	1:B:439:ILE:HD11	2.40	0.46
1:A:654:ASN:O	1:A:685:VAL:HG22	2.15	0.46
1:B:547:PRO:HG2	1:B:550:ARG:HD3	1.96	0.46
1:B:842:GLU:HA	1:B:847:TYR:CE2	2.50	0.46
1:A:352:THR:HG23	1:A:355:GLN:OE1	2.16	0.46
1:B:533:ARG:HB3	1:B:533:ARG:CZ	2.46	0.46
1:A:493:SER:HB2	1:A:692:LEU:HD12	1.98	0.46
1:A:536:GLY:O	1:A:564:ILE:HG23	2.16	0.46
1:B:177:TYR:HB3	1:B:178:PRO:HD2	1.97	0.46
1:A:328:LYS:HG2	1:A:332:TYR:CD2	2.50	0.46
1:A:400:ALA:HB1	1:A:406:ALA:CA	2.45	0.46
1:B:178:PRO:HA	1:B:187:TRP:CG	2.51	0.46
1:A:531:LEU:HD12	1:A:531:LEU:HA	1.80	0.45
1:A:550:ARG:HD3	1:A:550:ARG:C	2.36	0.45
1:B:506:LEU:O	1:B:512:LYS:NZ	2.48	0.45
1:B:800:SER:OG	1:B:843:VAL:HG22	2.16	0.45
1:B:842:GLU:HA	1:B:847:TYR:CD2	2.50	0.45
1:B:834:ARG:HD2	3:B:890:PO4:O3	2.15	0.45
1:B:245:ALA:HA	1:B:250:LEU:HD12	1.97	0.45
1:B:90:ILE:HG22	1:B:94:LEU:HD22	1.98	0.45
1:A:543:GLN:NE2	1:A:547:PRO:HG3	2.32	0.45
1:A:466:GLN:CG	1:A:466:GLN:O	2.65	0.45
1:A:878:ALA:HA	1:B:777:LEU:HG	1.99	0.45
1:B:844:ASP:HB2	5:B:1085:HOH:O	2.15	0.45
1:A:143:ILE:HD12	1:A:143:ILE:O	2.17	0.45
1:A:857:ALA:HA	1:A:862:ILE:HG13	1.98	0.45
1:A:466:GLN:HE22	1:A:589:ASN:HB2	1.80	0.45
1:B:723:LYS:HD3	1:B:749:TYR:O	2.17	0.45
1:A:458:LEU:O	1:A:459:HIS:HB2	2.17	0.45
1:B:361:ARG:HG2	1:B:389:HIS:ND1	2.32	0.45
1:A:471:GLU:OE2	1:A:591:PRO:HD2	2.17	0.45
1:B:193:SER:HB3	1:B:196:LEU:HD12	1.99	0.44
1:A:564:ILE:HG13	1:A:565:LEU:N	2.32	0.43
1:A:314:MET:HA	1:A:322:TYR:OH	2.17	0.43
1:B:723:LYS:HE3	1:B:862:ILE:HD13	1.99	0.43
1:A:838:ARG:HB3	1:A:844:ASP:HB3	2.00	0.43
1:B:106:HIS:HD2	5:B:1142:HOH:O	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:719:ILE:HD13	1:B:742:ALA:HB1	2.01	0.43
1:B:85:ILE:CG1	1:B:153:LEU:HD23	2.49	0.43
1:A:323:GLN:HE22	1:A:392:LYS:H	1.65	0.43
1:B:213:HIS:ND1	1:B:560:GLU:OE1	2.51	0.43
1:A:144:SER:N	1:A:145:PRO:CD	2.82	0.43
1:A:195:GLY:O	1:A:198:PRO:HG2	2.19	0.43
1:B:856:LEU:HB3	1:B:861:GLU:HB3	2.00	0.43
1:B:773:ARG:HD3	5:B:970:HOH:O	2.18	0.43
1:B:539:SER:HB2	1:B:558:GLU:HG2	2.01	0.43
1:B:63:ILE:HG23	1:B:67:GLU:OE2	2.19	0.43
1:B:851:ALA:O	1:B:855:GLU:HG3	2.19	0.43
1:A:374:LYS:HA	1:A:374:LYS:HD3	1.73	0.42
1:A:323:GLN:NE2	1:A:392:LYS:H	2.17	0.42
1:B:864:LYS:HD3	1:B:864:LYS:N	2.34	0.42
4:B:887:TDK:N4'	4:B:887:TDK:OM1	2.45	0.42
1:B:79:ARG:NH2	1:B:424:PHE:HA	2.34	0.42
1:A:453:ALA:O	1:A:457:LYS:HD3	2.19	0.42
1:B:63:ILE:HG23	1:B:67:GLU:CD	2.39	0.42
1:A:725:LYS:NZ	1:A:754:ASP:OD2	2.51	0.42
1:A:711:LYS:HD2	1:A:787:TYR:CD1	2.54	0.42
1:A:638:LEU:HD12	1:A:638:LEU:C	2.39	0.42
1:B:177:TYR:CD2	1:B:192:VAL:HG11	2.54	0.42
1:B:549:ASP:O	1:B:552:GLN:HG2	2.19	0.42
1:A:328:LYS:N	1:A:328:LYS:HD3	2.33	0.42
1:B:125:PHE:HB3	1:B:462:LEU:HD21	2.01	0.42
1:B:597:ILE:HA	1:B:624:ILE:O	2.20	0.42
1:B:144:SER:N	1:B:145:PRO:CD	2.83	0.42
1:B:522:GLU:OE2	4:B:887:TDK:H6'	2.20	0.42
1:A:635:GLY:HA3	1:B:103:LEU:O	2.19	0.42
1:A:323:GLN:OE1	1:A:323:GLN:HA	2.20	0.41
1:B:856:LEU:O	1:B:859:ARG:HG2	2.20	0.41
1:A:512:LYS:HG3	1:A:513:ASP:H	1.85	0.41
1:A:320:GLY:HA3	1:B:545:TYR:CD2	2.54	0.41
1:A:538:TYR:HB2	1:A:562:GLY:O	2.19	0.41
1:B:81:ILE:HA	1:B:441:PHE:HZ	1.85	0.41
1:B:711:LYS:HA	1:B:711:LYS:HD2	1.72	0.41
1:A:821:ARG:HH12	1:A:854:GLY:HA3	1.85	0.41
1:B:471:GLU:OE2	1:B:591:PRO:HD2	2.20	0.41
1:B:519:ILE:HG12	1:B:519:ILE:O	2.20	0.41
1:A:578:TRP:CD1	1:A:594:PRO:HB2	2.55	0.41
1:B:585:TYR:O	1:B:589:ASN:HA	2.20	0.41
1:B:845:ALA:O	1:B:849:VAL:HG23	2.18	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:245:ALA:HA	1:A:250:LEU:HD12	2.01	0.41
1:A:502:LEU:HA	1:A:505:MET:HE3	2.01	0.41
1:B:777:LEU:HD12	1:B:777:LEU:HA	1.88	0.41
1:B:436:LEU:N	1:B:437:PRO:CD	2.83	0.41
1:A:487:GLU:HG3	1:A:488:GLN:N	2.35	0.41
1:A:273:LYS:HG2	5:A:1079:HOH:O	2.20	0.41
1:B:856:LEU:CB	1:B:862:ILE:HG13	2.51	0.41
1:B:408:GLN:O	1:B:410:LYS:HE2	2.19	0.41
1:B:262:GLN:HA	1:B:267:PRO:HA	2.03	0.41
1:B:511:ILE:HD12	1:B:515:LEU:HD21	2.02	0.41
1:A:569:ILE:HD12	1:B:231:GLY:C	2.40	0.41
1:A:884:ARG:NH2	1:B:770:ASP:OD2	2.54	0.41
1:B:664:TYR:CD1	1:B:701:MET:HB2	2.56	0.41
1:A:471:GLU:HG2	5:A:1116:HOH:O	2.20	0.41
1:B:317:THR:HB	1:B:322:TYR:CE2	2.55	0.41
1:B:91:MET:O	1:B:95:ARG:HG3	2.20	0.41
1:A:92:THR:HG22	1:A:438:TYR:HE1	1.85	0.41
1:B:196:LEU:HA	1:B:199:ILE:HD11	2.02	0.41
1:A:711:LYS:HD3	5:A:1067:HOH:O	2.20	0.41
1:B:189:PHE:HA	1:B:190:PRO:HD3	1.78	0.41
1:B:405:ILE:HG13	1:B:405:ILE:H	1.73	0.41
1:A:550:ARG:O	1:A:550:ARG:HD3	2.20	0.41
1:B:128:ARG:NH1	1:B:128:ARG:CG	2.83	0.41
1:B:177:TYR:CG	1:B:192:VAL:HG11	2.55	0.41
1:A:87:TRP:CD2	1:A:426:VAL:HG11	2.56	0.41
1:A:87:TRP:CE3	1:A:420:ILE:HD11	2.56	0.41
1:B:567:GLU:HG3	1:B:574:ALA:HA	2.03	0.41
1:B:348:VAL:HA	1:B:351:TRP:CD1	2.56	0.41
1:B:716:LEU:HD13	1:B:739:ARG:CZ	2.51	0.41
1:B:164:ASN:CB	1:B:173:GLY:HA2	2.50	0.41
1:A:410:LYS:HB3	1:A:410:LYS:HE3	1.84	0.40
1:B:81:ILE:HA	1:B:441:PHE:CZ	2.57	0.40
1:A:768:GLY:HA2	1:A:786:PRO:HB3	2.02	0.40
1:B:214:ARG:HD3	5:B:1098:HOH:O	2.20	0.40
1:A:716:LEU:HD13	1:A:739:ARG:CZ	2.52	0.40
1:A:158:THR:OG1	1:A:160:GLU:CD	2.59	0.40
1:A:726:VAL:O	1:A:753:SER:HA	2.22	0.40
1:A:627:THR:HB	1:A:633:LEU:HD13	2.03	0.40
1:A:177:TYR:HB2	1:A:192:VAL:HG21	2.04	0.40
1:A:341:TYR:HB2	1:A:344:THR:OG1	2.21	0.40
1:B:90:ILE:HG23	1:B:94:LEU:HD22	2.02	0.40
1:A:385:VAL:HG13	1:A:385:VAL:O	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:263:ARG:HD2	1:B:521:ASP:CG	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	829/886 (94%)	785 (95%)	40 (5%)	4 (0%)	38	33
1	B	829/886 (94%)	790 (95%)	38 (5%)	1 (0%)	59	61
All	All	1658/1772 (94%)	1575 (95%)	78 (5%)	5 (0%)	50	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	553	VAL
1	A	347	LEU
1	A	550	ARG
1	A	398	ASP
1	B	400	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	691/735 (94%)	624 (90%)	67 (10%)	12	7
1	B	691/735 (94%)	634 (92%)	57 (8%)	17	11
All	All	1382/1470 (94%)	1258 (91%)	124 (9%)	14	9

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	66	GLU
1	A	97	SER
1	A	98	LYS
1	A	126	ARG
1	A	150	ARG
1	A	153	LEU
1	A	160	GLU
1	A	168	GLU
1	A	192	VAL
1	A	216	LEU
1	A	274	ILE
1	A	278	LEU
1	A	297	ARG
1	A	300	GLU
1	A	302	LEU
1	A	306	THR
1	A	323	GLN
1	A	328	LYS
1	A	335	GLU
1	A	340	LYS
1	A	343	GLU
1	A	350	ASP
1	A	354	GLU
1	A	367	LYS
1	A	375	LYS
1	A	382	LYS
1	A	410	LYS
1	A	418	ARG
1	A	420	ILE
1	A	428	VAL
1	A	443	GLU
1	A	446	GLU
1	A	457	LYS
1	A	464	SER
1	A	472	LYS
1	A	486	GLU
1	A	487	GLU
1	A	506	LEU
1	A	507	LYS
1	A	512	LYS
1	A	521	ASP

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Mol	Chain	Res	Type
1	A	531	LEU
1	A	533	ARG
1	A	546	THR
1	A	550	ARG
1	A	551	GLU
1	A	553	VAL
1	A	555	TYR
1	A	560	GLU
1	A	561	LYS
1	A	564	ILE
1	A	638	LEU
1	A	680	GLU
1	A	681	LYS
1	A	685	VAL
1	A	692	LEU
1	A	703	GLU
1	A	818	ASP
1	A	819	ASP
1	A	826	ASP
1	A	835	GLU
1	A	863	ASP
1	A	864	LYS
1	A	865	LYS
1	A	873	LYS
1	A	880	LYS
1	B	60	ILE
1	B	65	VAL
1	B	67	GLU
1	B	68	GLN
1	B	94	LEU
1	B	98	LYS
1	B	128	ARG
1	B	153	LEU
1	B	168	GLU
1	B	192	VAL
1	B	199	ILE
1	B	244	ILE
1	B	264	LEU
1	B	274	ILE
1	B	278	LEU
1	B	297	ARG
1	B	303	ARG

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Mol	Chain	Res	Type
1	B	306	THR
1	B	309	LYS
1	B	326	LYS
1	B	328	LYS
1	B	334	ARG
1	B	385	VAL
1	B	398	ASP
1	B	401	GLU
1	B	403	LYS
1	B	411	LYS
1	B	428	VAL
1	B	430	ASP
1	B	456	GLN
1	B	475	LEU
1	B	479	GLN
1	B	484	LEU
1	B	490	LYS
1	B	506	LEU
1	B	512	LYS
1	B	519	ILE
1	B	550	ARG
1	B	560	GLU
1	B	577	SER
1	B	610	LEU
1	B	623	LEU
1	B	638	LEU
1	B	711	LYS
1	B	718	THR
1	B	720	GLU
1	B	777	LEU
1	B	784	ARG
1	B	814	TYR
1	B	818	ASP
1	B	843	VAL
1	B	858	LYS
1	B	859	ARG
1	B	861	GLU
1	B	862	ILE
1	B	864	LYS
1	B	873	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	A	131	GLN
1	A	159	GLN
1	A	419	HIS
1	A	466	GLN
1	A	552	GLN
1	A	737	HIS
1	B	106	HIS
1	B	448	HIS
1	B	737	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	TDK	A	887	2	34,35,35	1.59	5 (14%)	49,55,55	1.63	9 (18%)
3	PO4	A	889	-	4,4,4	0.22	0	6,6,6	0.33	0
3	PO4	A	890	-	4,4,4	0.26	0	6,6,6	0.33	0
4	TDK	B	887	2	34,35,35	1.54	5 (14%)	49,55,55	1.67	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	B	889	-	4,4,4	0.36	0	6,6,6	0.32	0
3	PO4	B	890	-	4,4,4	0.40	0	6,6,6	0.32	0
3	PO4	B	891	-	4,4,4	0.37	0	6,6,6	0.33	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
4	TDK	A	887	2	-	0/29/35/35	0/2/2/2
3	PO4	A	889	-	-	0/0/0/0	0/0/0/0
3	PO4	A	890	-	-	0/0/0/0	0/0/0/0
4	TDK	B	887	2	-	0/29/35/35	0/2/2/2
3	PO4	B	889	-	-	0/0/0/0	0/0/0/0
3	PO4	B	890	-	-	0/0/0/0	0/0/0/0
3	PO4	B	891	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	887	TDK	C2-S1	-4.41	1.68	1.73
4	B	887	TDK	PC-OM3	-4.15	1.47	1.56
4	B	887	TDK	C2-S1	-4.14	1.68	1.73
4	A	887	TDK	PC-OM3	-4.08	1.47	1.56
4	B	887	TDK	PB-O1B	2.83	1.60	1.51
4	A	887	TDK	PB-O1B	2.80	1.60	1.51
4	A	887	TDK	C6'-C5'	-2.35	1.32	1.37
4	B	887	TDK	C6'-C5'	-2.16	1.32	1.37
4	B	887	TDK	PC-OM4	-2.12	1.47	1.51
4	A	887	TDK	PB-O3B	-2.03	1.47	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	887	TDK	C2-N3-C4	5.46	114.53	109.76
4	B	887	TDK	C2-N3-C4	5.34	114.42	109.76
4	A	887	TDK	C6-C5-C4	4.80	130.94	127.44
4	B	887	TDK	C6-C5-C4	4.78	130.92	127.44
4	B	887	TDK	PA-O3A-PB	-3.21	122.28	131.68
4	B	887	TDK	O3B-PB-O2B	2.85	118.70	107.61
4	A	887	TDK	O3B-PB-O2B	2.82	118.60	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	887	TDK	C6'-N1'-C2'	2.76	120.52	115.68
4	B	887	TDK	C6'-N1'-C2'	2.62	120.28	115.68
4	A	887	TDK	PA-O3A-PB	-2.54	124.22	131.68
4	B	887	TDK	C5-C4-N3	2.51	112.90	107.66
4	A	887	TDK	C5-C4-N3	2.43	112.73	107.66
4	B	887	TDK	OM4-PC-CMA	-2.35	108.59	113.15
4	A	887	TDK	OM4-PC-CMA	-2.16	108.97	113.15
4	B	887	TDK	OM3-PC-OM4	2.16	117.01	111.74
4	A	887	TDK	OM3-PC-OM4	2.06	116.78	111.74
4	B	887	TDK	OM2-PC-OM4	-2.03	109.34	114.52
4	A	887	TDK	OM2-PC-OM4	-2.03	109.35	114.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	831/886 (93%)	-0.23	11 (1%) 74 78	2, 8, 29, 43	0
1	B	831/886 (93%)	-0.28	3 (0%) 90 92	2, 6, 24, 37	0
All	All	1662/1772 (93%)	-0.25	14 (0%) 83 87	2, 7, 28, 43	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	ASN	3.6
1	A	552	GLN	2.9
1	B	551	GLU	2.8
1	A	354	GLU	2.6
1	A	351	TRP	2.6
1	A	352	THR	2.6
1	A	550	ARG	2.5
1	A	341	TYR	2.5
1	B	862	ILE	2.4
1	A	555	TYR	2.3
1	A	549	ASP	2.2
1	A	551	GLU	2.1
1	A	349	ALA	2.0
1	B	818	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	A	888	1/1	0.17	5.35	10,10,10,10	0
2	MG	B	888	1/1	0.15	3.37	13,13,13,13	0
3	PO4	B	890	5/5	0.13	2.16	23,24,25,27	0
3	PO4	B	891	5/5	0.12	1.94	24,24,27,28	0
3	PO4	A	890	5/5	0.10	0.62	23,24,25,28	0
3	PO4	A	889	5/5	0.10	0.31	12,13,14,16	0
3	PO4	B	889	5/5	0.10	0.10	15,18,20,20	0
4	TDK	B	887	34/34	0.10	-0.19	4,7,15,16	0
4	TDK	A	887	34/34	0.10	-0.40	2,3,13,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.