



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 02:20 PM EDT

PDB ID : 2QTC
Title : E. coli Pyruvate dehydrogenase E1 component E401K mutant with phosphonolactylthiamin diphosphate
Authors : Furey, W.; Arjunan, P.; Chandrasekhar, K.
Deposited on : unknown
Resolution : 1.77 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

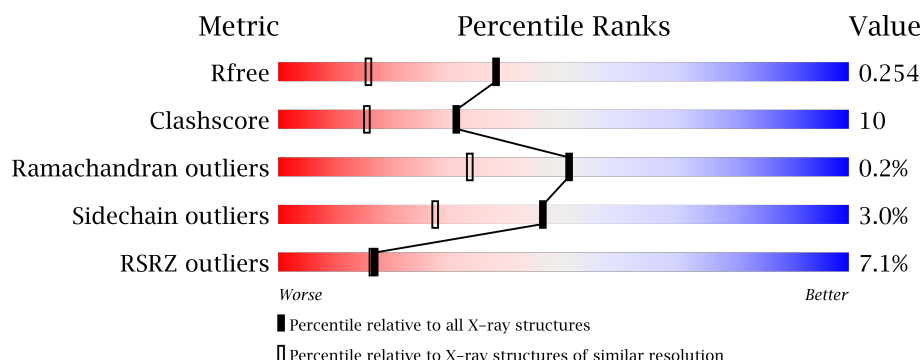
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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}	100719	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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. 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 $\leq 5\%$. 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	 7% 72% 17% • 10%
1	B	886	 6% 75% 14% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13146 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			

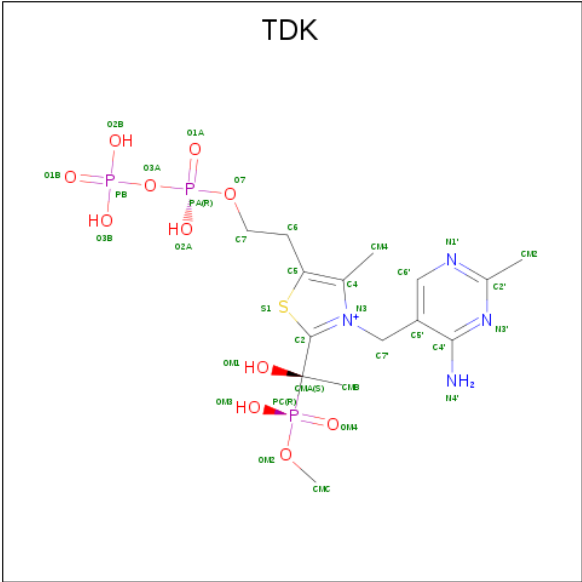
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	LYS	GLU	ENGINEERED MUTATION	UNP P0AFG8
B	401	LYS	GLU	ENGINEERED MUTATION	UNP P0AFG8

- 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 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-[(1S)-1-HYDROXY-1-[(R)-HYDROXY(METHOXY)PHOSPHORYL]ETHYL]-5-(2-[(S)-HYDROXY(PHOSPHONOXY)PHOSPHORYL]OXY)ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: TDK) (formula: C₁₅H₂₆N₄O₁₁P₃S).



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

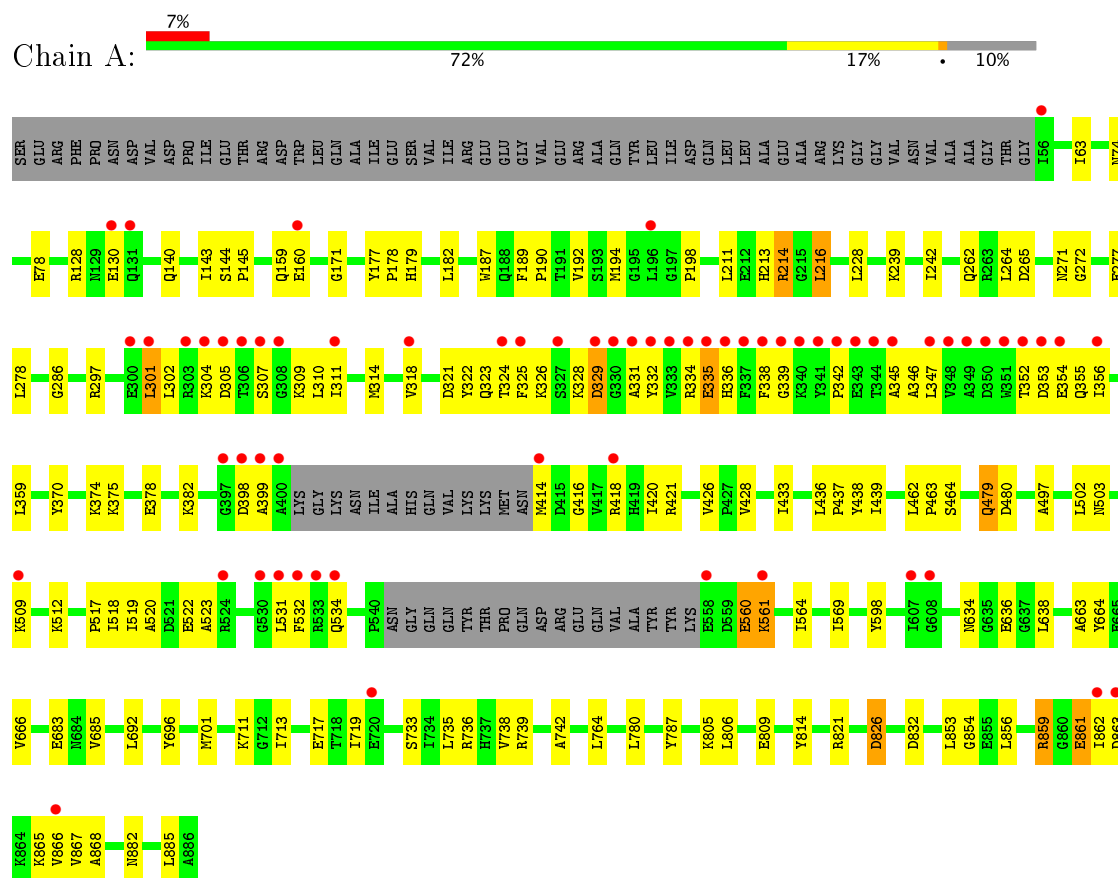
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	186	Total	O	0	0
			186	186		
4	B	208	Total	O	0	0
			208	208		

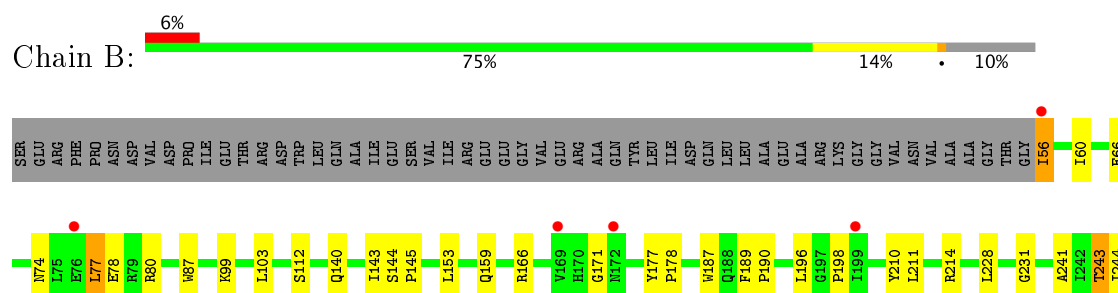
3 Residue-property plots

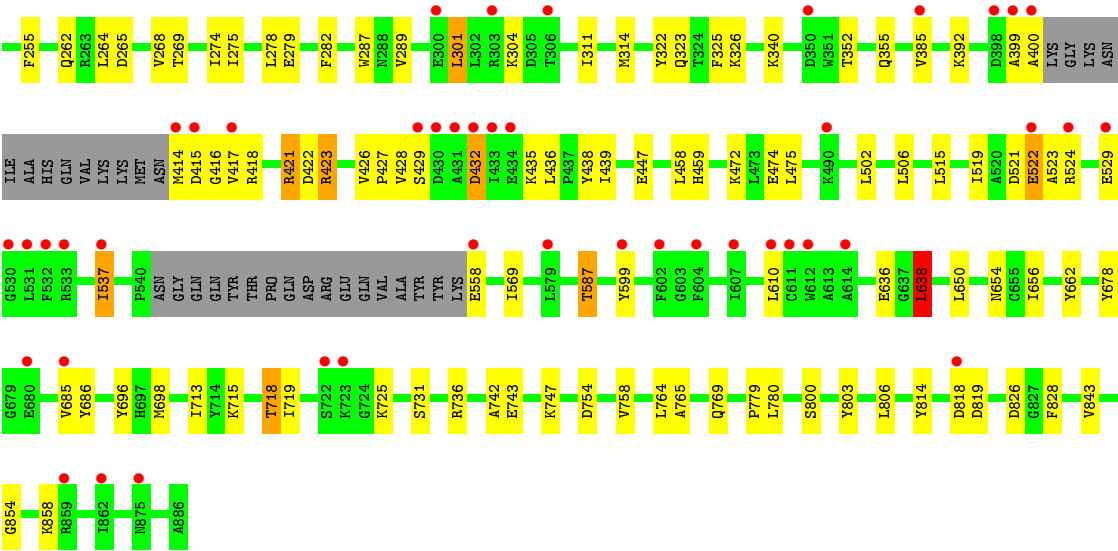
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



- Molecule 1: Pyruvate dehydrogenase E1 component





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.61Å 142.11Å 82.14Å 90.00° 102.68° 90.00°	Depositor
Resolution (Å)	47.53 – 1.77 47.53 – 1.77	Depositor EDS
% Data completeness (in resolution range)	97.1 (47.53-1.77) 90.7 (47.53-1.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 1.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.255 0.225 , 0.254	Depositor DCC
R_{free} test set	8037 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13146	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.55	0/6484	0.74	3/8766 (0.0%)
1	B	0.58	0/6484	0.75	3/8766 (0.0%)
All	All	0.56	0/12968	0.75	6/17532 (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
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	638	LEU	CA-CB-CG	6.89	131.15	115.30
1	A	214	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	171	GLY	N-CA-C	5.66	127.26	113.10
1	A	214	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	171	GLY	N-CA-C	5.54	126.95	113.10
1	B	416	GLY	N-CA-C	-5.17	100.17	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	598	TYR	Sidechain
1	A	814	TYR	Sidechain
1	B	678	TYR	Sidechain
1	B	803	TYR	Sidechain
1	B	814	TYR	Sidechain

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	151	0
1	B	6341	0	6179	125	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	34	0	22	7	0
3	B	34	0	22	6	0
4	A	186	0	0	1	0
4	B	208	0	0	4	0
All	All	13146	0	12402	260	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 (260) 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:B:656:ILE:HG12	1:B:685:VAL:HG21	1.37	1.03
1:A:182:LEU:HD11	1:B:638:LEU:HD23	1.45	0.97
1:B:311:ILE:HA	1:B:314:MET:HE2	1.52	0.91
1:B:800:SER:OG	1:B:843:VAL:HG13	1.71	0.91
1:A:418:ARG:HD2	1:A:433:ILE:HD13	1.52	0.90
1:A:311:ILE:HA	1:A:314:MET:HE3	1.55	0.89
1:B:656:ILE:CG1	1:B:685:VAL:HG21	2.04	0.87
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.06	0.84
1:A:882:ASN:HB3	1:A:885:LEU:HD23	1.59	0.83
1:B:287:TRP:CE3	1:B:385:VAL:HG13	2.13	0.82
1:A:497:ALA:HB1	1:A:666:VAL:HG11	1.60	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:ASN:O	1:B:685:VAL:HG23	1.80	0.81
1:B:311:ILE:HA	1:B:314:MET:CE	2.11	0.80
1:A:182:LEU:CD1	1:B:638:LEU:HD23	2.12	0.79
1:B:696:TYR:CE1	1:B:698:MET:HE1	2.19	0.78
1:A:497:ALA:CB	1:A:666:VAL:HG11	2.14	0.78
1:B:638:LEU:HD22	1:B:828:PHE:HB3	1.65	0.78
1:B:255:PHE:HB2	1:B:385:VAL:HG12	1.66	0.78
1:A:301:LEU:HD12	1:A:310:LEU:HD22	1.67	0.76
1:A:328:LYS:HG3	1:A:332:TYR:CD1	2.22	0.75
1:A:859:ARG:HH11	1:A:859:ARG:HB3	1.51	0.74
1:B:198:PRO:HG3	1:B:228:LEU:HD22	1.70	0.72
1:A:277:GLU:OE2	1:B:243:THR:HG21	1.89	0.72
1:B:698:MET:HE2	1:B:698:MET:HA	1.72	0.72
1:B:696:TYR:HE1	1:B:698:MET:HE1	1.53	0.72
1:A:636:GLU:OE1	3:B:887:TDK:HMC1	1.91	0.70
1:A:503:ASN:OD1	1:A:534:GLN:NE2	2.18	0.70
1:A:286:GLY:O	1:A:382:LYS:HE3	1.93	0.69
1:A:418:ARG:HD2	1:A:433:ILE:CD1	2.23	0.68
1:A:735:LEU:O	1:A:738:VAL:HG22	1.93	0.68
1:A:502:LEU:HD23	1:A:531:LEU:HD11	1.76	0.68
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.30	0.67
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.25	0.67
1:A:418:ARG:HE	1:A:421:ARG:NH2	1.93	0.66
1:A:867:VAL:HG12	1:B:779:PRO:HG3	1.77	0.66
1:B:282:PHE:CD2	1:B:385:VAL:HG11	2.30	0.66
1:A:696:TYR:CG	1:A:736:ARG:HD2	2.31	0.66
1:B:854:GLY:O	1:B:858:LYS:HG3	1.98	0.64
1:A:335:GLU:HB3	1:A:336:HIS:HD2	1.62	0.64
1:B:537:ILE:HG23	1:B:558:GLU:HG3	1.78	0.64
1:A:179:HIS:HB3	1:A:182:LEU:HD13	1.79	0.63
1:B:472:LYS:HE3	1:B:474:GLU:OE2	1.99	0.62
1:A:859:ARG:HB3	1:A:859:ARG:NH1	2.15	0.62
1:B:843:VAL:HG12	1:B:843:VAL:O	2.01	0.61
1:A:328:LYS:HB3	1:A:332:TYR:HB3	1.82	0.61
1:A:311:ILE:HD13	1:A:314:MET:HE1	1.82	0.61
1:A:416:GLY:O	1:A:420:ILE:HD12	2.00	0.61
1:B:414:MET:O	1:B:414:MET:HG2	2.01	0.61
1:A:663:ALA:O	1:A:666:VAL:CG1	2.48	0.61
1:A:194:MET:HE2	3:A:887:TDK:C5'	2.31	0.61
1:A:374:LYS:O	1:A:378:GLU:HG3	2.01	0.61
1:B:80:ARG:HD2	1:B:447:GLU:OE2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ILE:HA	1:A:314:MET:CE	2.29	0.60
1:B:587:THR:HG22	4:B:905:HOH:O	2.01	0.60
1:B:719:ILE:HD12	1:B:742:ALA:HB1	1.83	0.60
1:B:587:THR:HG21	4:B:1054:HOH:O	2.01	0.60
1:A:272:GLY:O	1:A:318:VAL:HG22	2.02	0.60
1:B:519:ILE:HD12	1:B:523:ALA:HB2	1.84	0.60
1:B:279:GLU:HG3	1:B:289:VAL:HG21	1.83	0.60
1:A:636:GLU:CD	3:B:887:TDK:HMC1	2.22	0.59
1:A:301:LEU:HD12	1:A:310:LEU:CD2	2.30	0.59
1:A:271:ASN:C	1:A:318:VAL:HG21	2.22	0.59
1:B:282:PHE:CE2	1:B:385:VAL:HG11	2.37	0.59
1:A:329:ASP:OD1	1:A:331:ALA:HB3	2.02	0.59
1:B:56:ILE:HD13	1:B:56:ILE:N	2.18	0.59
1:A:307:SER:OG	1:A:309:LYS:HB2	2.03	0.58
1:A:311:ILE:CA	1:A:314:MET:HE3	2.31	0.58
1:B:429:SER:HB3	1:B:432:ASP:OD1	2.03	0.58
1:A:302:LEU:HD23	1:A:310:LEU:HD23	1.86	0.58
1:B:268:VAL:HB	1:B:274:ILE:HG21	1.86	0.58
1:A:859:ARG:HH11	1:A:859:ARG:CB	2.16	0.58
1:A:418:ARG:HH21	1:A:421:ARG:HH21	1.52	0.58
1:A:194:MET:HE2	3:A:887:TDK:C4'	2.34	0.57
1:A:418:ARG:HH11	1:A:418:ARG:HG3	1.69	0.57
1:A:523:ALA:N	1:B:265:ASP:OD2	2.35	0.57
1:A:265:ASP:OD2	1:B:523:ALA:N	2.37	0.57
1:A:194:MET:HE1	1:B:569:ILE:HG21	1.86	0.57
1:B:399:ALA:O	1:B:400:ALA:HB3	2.04	0.56
1:B:421:ARG:NH1	1:B:422:ASP:OD1	2.38	0.56
1:A:310:LEU:HG	1:A:314:MET:HE2	1.86	0.56
1:A:418:ARG:CZ	1:A:418:ARG:HB3	2.35	0.56
1:A:339:GLY:HA2	1:A:345:ALA:HB2	1.87	0.56
1:A:128:ARG:NH1	1:A:464:SER:OG	2.38	0.56
1:A:370:TYR:OH	1:A:374:LYS:HE3	2.06	0.56
1:A:297:ARG:HH11	1:A:297:ARG:HG2	1.70	0.55
1:A:194:MET:HE1	1:B:569:ILE:CG2	2.36	0.55
1:A:198:PRO:HD3	1:A:228:LEU:CD2	2.37	0.55
1:A:426:VAL:HG12	1:A:428:VAL:HG23	1.88	0.55
3:A:887:TDK:HMC1	1:B:636:GLU:CD	2.27	0.55
1:A:304:LYS:NZ	1:A:347:LEU:O	2.40	0.55
1:A:663:ALA:O	1:A:666:VAL:HG12	2.06	0.55
1:A:334:ARG:HB3	1:A:356:ILE:HD13	1.89	0.55
1:A:717:GLU:CD	1:A:739:ARG:HH21	2.09	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:GLU:CD	1:B:264:LEU:HD22	2.27	0.55
1:B:843:VAL:CG1	1:B:843:VAL:O	2.55	0.54
1:A:264:LEU:HD12	1:B:522:GLU:OE1	2.07	0.54
1:A:418:ARG:NE	1:A:421:ARG:NH2	2.55	0.54
1:A:334:ARG:HB3	1:A:356:ILE:CD1	2.37	0.54
1:A:518:ILE:C	1:A:519:ILE:HD12	2.27	0.54
1:B:301:LEU:HD12	1:B:304:LYS:HE2	1.90	0.54
1:A:140:GLN:O	1:A:143:ILE:HG13	2.08	0.54
1:A:328:LYS:HG3	1:A:332:TYR:CG	2.43	0.53
1:B:587:THR:CG2	4:B:1054:HOH:O	2.55	0.53
1:B:696:TYR:HB3	1:B:736:ARG:NH1	2.23	0.53
1:B:654:ASN:O	1:B:685:VAL:CG2	2.56	0.53
1:A:311:ILE:HD13	1:A:314:MET:CE	2.39	0.53
1:A:561:LYS:NZ	1:A:561:LYS:HB2	2.24	0.53
1:B:506:LEU:HD23	1:B:515:LEU:HD12	1.90	0.52
1:A:859:ARG:NH1	1:A:861:GLU:OE2	2.42	0.52
1:A:868:ALA:HB2	1:B:780:LEU:HD11	1.90	0.52
1:B:696:TYR:HB3	1:B:736:ARG:HH11	1.75	0.52
1:B:198:PRO:HG3	1:B:228:LEU:CD2	2.40	0.52
1:B:698:MET:CE	1:B:698:MET:HA	2.39	0.52
1:A:182:LEU:HD12	1:A:182:LEU:N	2.26	0.51
1:B:685:VAL:HG22	1:B:686:TYR:N	2.25	0.51
1:B:244:ILE:HD12	1:B:244:ILE:H	1.76	0.51
1:B:262:GLN:HG2	1:B:323:GLN:HE21	1.75	0.51
1:A:305:ASP:OD1	1:A:305:ASP:C	2.49	0.51
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.92	0.51
1:A:663:ALA:O	1:A:666:VAL:HG13	2.11	0.51
1:A:634:ASN:HB2	1:A:832:ASP:O	2.11	0.51
1:A:863:ASP:O	1:A:866:VAL:HG22	2.11	0.51
1:A:414:MET:O	1:A:418:ARG:HG2	2.11	0.51
1:B:428:VAL:HG13	1:B:428:VAL:O	2.11	0.51
1:B:432:ASP:N	1:B:432:ASP:OD1	2.43	0.51
1:A:522:GLU:OE1	1:B:264:LEU:HD22	2.11	0.50
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.92	0.50
1:B:352:THR:OG1	1:B:355:GLN:HG3	2.12	0.50
1:B:524:ARG:HD2	1:B:529:GLU:OE2	2.12	0.50
1:B:241:ALA:HB1	1:B:244:ILE:HD13	1.94	0.50
1:A:272:GLY:O	1:A:318:VAL:CG2	2.60	0.50
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.93	0.50
1:A:735:LEU:HD12	1:A:738:VAL:CG2	2.42	0.49
1:B:112:SER:HB3	1:B:392:LYS:HA	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ILE:N	1:B:244:ILE:HD12	2.26	0.49
1:A:321:ASP:O	1:A:324:THR:HB	2.12	0.49
1:B:262:GLN:CG	1:B:323:GLN:NE2	2.75	0.49
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.43	0.49
1:A:502:LEU:HD23	1:A:531:LEU:CD1	2.42	0.49
1:A:806:LEU:HD11	1:B:806:LEU:HD11	1.95	0.49
1:A:853:LEU:O	1:A:862:ILE:HD11	2.12	0.49
1:B:650:LEU:C	1:B:650:LEU:HD12	2.33	0.49
1:B:323:GLN:O	1:B:326:LYS:HG3	2.13	0.48
1:B:255:PHE:CB	1:B:385:VAL:HG12	2.40	0.48
1:B:656:ILE:CD1	1:B:685:VAL:HG21	2.43	0.48
1:B:269:THR:OG1	1:B:274:ILE:HG23	2.13	0.48
1:A:178:PRO:HA	1:A:187:TRP:CG	2.48	0.48
1:A:497:ALA:HB1	1:A:666:VAL:CG1	2.39	0.48
1:B:66:GLU:CD	1:B:66:GLU:H	2.16	0.48
1:B:765:ALA:O	1:B:769:GLN:HG3	2.14	0.48
1:A:569:ILE:HG12	3:B:887:TDK:HM43	1.95	0.48
3:A:887:TDK:H7'1	3:A:887:TDK:OM1	2.14	0.48
1:B:177:TYR:HB3	1:B:178:PRO:CD	2.43	0.48
1:A:867:VAL:CG1	1:B:779:PRO:HG3	2.44	0.48
1:A:322:TYR:HA	1:A:325:PHE:CD2	2.49	0.48
1:B:262:GLN:HB2	1:B:392:LYS:HD2	1.96	0.48
1:B:506:LEU:CD2	1:B:515:LEU:HD12	2.44	0.48
1:A:663:ALA:HA	1:A:666:VAL:HG12	1.96	0.47
3:B:887:TDK:OM1	3:B:887:TDK:H7'1	2.14	0.47
1:B:696:TYR:CD2	1:B:736:ARG:NH1	2.82	0.47
1:A:736:ARG:HG3	4:A:955:HOH:O	2.14	0.47
1:B:522:GLU:CA	1:B:522:GLU:OE1	2.63	0.47
1:A:342:PRO:O	1:A:346:ALA:HB2	2.15	0.47
1:B:696:TYR:HD2	1:B:736:ARG:NH1	2.13	0.47
1:B:140:GLN:O	1:B:143:ILE:HG13	2.15	0.47
1:A:517:PRO:HB2	1:A:564:ILE:HG12	1.96	0.47
1:A:144:SER:OG	1:A:145:PRO:HD3	2.15	0.47
1:A:509:LYS:HA	1:A:512:LYS:HE3	1.97	0.46
1:B:662:TYR:HD1	1:B:698:MET:CE	2.29	0.46
1:B:189:PHE:HA	1:B:190:PRO:HD3	1.85	0.46
1:A:262:GLN:CG	1:A:323:GLN:NE2	2.79	0.46
1:A:262:GLN:CG	1:A:323:GLN:HE21	2.29	0.45
1:B:392:LYS:HE2	3:B:887:TDK:O2B	2.16	0.45
1:B:458:LEU:O	1:B:459:HIS:HB2	2.17	0.45
1:B:522:GLU:HG2	1:B:599:TYR:CZ	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:ILE:HG23	1:B:558:GLU:HA	1.98	0.45
1:B:60:ILE:CG2	1:B:314:MET:HE3	2.46	0.45
1:B:696:TYR:HD2	1:B:736:ARG:HH11	1.60	0.45
1:A:418:ARG:HH11	1:A:418:ARG:CG	2.29	0.45
1:A:265:ASP:OD2	1:B:521:ASP:O	2.34	0.45
1:B:77:LEU:HD21	1:B:447:GLU:HA	1.98	0.45
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.97	0.45
1:A:328:LYS:HD2	1:A:332:TYR:CD2	2.52	0.45
1:A:638:LEU:C	1:A:638:LEU:HD23	2.37	0.45
1:B:522:GLU:OE1	1:B:522:GLU:HA	2.17	0.45
1:A:277:GLU:OE2	1:B:243:THR:CG2	2.63	0.45
1:A:301:LEU:CD1	1:A:310:LEU:HD22	2.42	0.45
1:A:868:ALA:HB2	1:B:780:LEU:CD1	2.47	0.45
1:B:144:SER:N	1:B:145:PRO:CD	2.80	0.45
1:B:731:SER:HB2	1:B:758:VAL:O	2.16	0.45
1:A:522:GLU:OE2	1:B:264:LEU:CD2	2.64	0.45
1:B:423:ARG:HD3	1:B:423:ARG:O	2.17	0.44
1:A:194:MET:HE3	1:A:194:MET:HB2	1.65	0.44
1:A:194:MET:HE1	3:A:887:TDK:HM43	1.99	0.44
1:A:214:ARG:HB2	1:A:216:LEU:HD22	2.00	0.44
1:A:328:LYS:HG3	1:A:332:TYR:CE1	2.52	0.44
1:A:692:LEU:HD13	1:A:733:SER:HB3	1.99	0.44
1:B:287:TRP:CZ3	1:B:385:VAL:HG13	2.52	0.44
1:B:274:ILE:HG13	1:B:275:ILE:N	2.33	0.44
1:A:297:ARG:HB2	1:A:359:LEU:HD23	1.99	0.44
1:A:519:ILE:CG2	1:A:520:ALA:N	2.81	0.44
1:A:332:TYR:CD1	1:A:332:TYR:O	2.71	0.43
1:A:821:ARG:HH12	1:A:854:GLY:HA3	1.82	0.43
1:B:289:VAL:HG23	1:B:289:VAL:O	2.17	0.43
3:B:887:TDK:N4'	3:B:887:TDK:OM1	2.47	0.43
1:B:262:GLN:CG	1:B:323:GLN:HE21	2.31	0.43
1:B:74:ASN:O	1:B:78:GLU:HG3	2.19	0.43
1:A:569:ILE:HD12	1:B:231:GLY:C	2.39	0.43
1:A:189:PHE:HA	1:A:190:PRO:HD3	1.88	0.43
1:A:74:ASN:O	1:A:78:GLU:HG3	2.18	0.43
1:B:178:PRO:HA	1:B:187:TRP:CG	2.54	0.43
1:B:696:TYR:CD1	1:B:698:MET:CE	3.02	0.43
1:A:334:ARG:HA	1:A:338:PHE:HB2	2.00	0.43
1:B:725:LYS:HE3	1:B:754:ASP:OD2	2.19	0.43
1:A:262:GLN:HG3	1:A:323:GLN:NE2	2.34	0.43
1:B:143:ILE:HD12	1:B:143:ILE:C	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:LYS:HD3	1:B:718:THR:HG22	2.01	0.43
1:A:497:ALA:HB3	1:A:666:VAL:HG11	1.98	0.43
1:A:805:LYS:HG3	1:A:826:ASP:OD1	2.19	0.43
1:A:462:LEU:HB2	1:A:463:PRO:HA	2.01	0.42
1:A:194:MET:CE	3:A:887:TDK:C4'	2.97	0.42
1:A:479:GLN:HG2	1:A:480:ASP:N	2.34	0.42
1:A:663:ALA:HA	1:A:666:VAL:CG1	2.50	0.42
1:A:664:TYR:CG	1:A:701:MET:HB2	2.53	0.42
1:A:711:LYS:HD2	1:A:787:TYR:CE1	2.54	0.42
1:A:711:LYS:HD2	1:A:787:TYR:CZ	2.53	0.42
1:A:198:PRO:HD3	1:A:228:LEU:HD22	2.00	0.42
1:A:302:LEU:HD21	1:A:314:MET:CE	2.50	0.42
1:A:352:THR:HG1	1:A:355:GLN:CD	2.23	0.42
1:B:262:GLN:HE21	1:B:323:GLN:HE22	1.67	0.42
1:B:301:LEU:HD12	1:B:301:LEU:HA	1.90	0.42
1:A:213:HIS:HB3	1:A:560:GLU:HB2	2.01	0.42
1:A:63:ILE:HD11	1:A:375:LYS:HD2	2.01	0.42
1:A:159:GLN:HG3	1:A:438:TYR:CD2	2.55	0.42
1:A:436:LEU:N	1:A:437:PRO:CD	2.82	0.41
1:B:435:LYS:O	1:B:436:LEU:C	2.59	0.41
1:B:743:GLU:O	1:B:747:LYS:HG2	2.20	0.41
1:A:532:PHE:CD1	1:A:532:PHE:N	2.88	0.41
1:A:856:LEU:HB2	1:A:862:ILE:HG12	2.02	0.41
1:B:415:ASP:OD1	1:B:418:ARG:HD3	2.21	0.41
1:A:336:HIS:CD2	1:A:336:HIS:N	2.89	0.41
1:A:352:THR:O	1:A:355:GLN:N	2.52	0.41
1:B:427:PRO:HG2	1:B:439:ILE:HD13	2.02	0.41
1:A:865:LYS:HB2	1:A:865:LYS:HE3	1.76	0.41
1:A:561:LYS:HB2	1:A:561:LYS:HZ2	1.86	0.41
1:B:399:ALA:O	1:B:400:ALA:CB	2.68	0.41
1:A:239:LYS:O	1:A:242:ILE:HG12	2.20	0.41
1:A:806:LEU:HA	1:A:809:GLU:HB2	2.03	0.41
3:A:887:TDK:H62	1:B:569:ILE:HD11	2.03	0.40
1:A:178:PRO:HA	1:A:187:TRP:CD2	2.56	0.40
1:B:103:LEU:O	1:B:166:ARG:HD3	2.22	0.40
1:B:153:LEU:HA	1:B:153:LEU:HD12	1.93	0.40
1:B:87:TRP:CD2	1:B:426:VAL:HG11	2.56	0.40
1:A:304:LYS:HE2	1:A:347:LEU:CD2	2.50	0.40
1:B:322:TYR:HA	1:B:325:PHE:CD2	2.56	0.40
1:A:352:THR:C	1:A:354:GLU:N	2.75	0.40
1:A:418:ARG:NH1	1:A:418:ARG:CG	2.84	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:GLU:HG2	1:A:685:VAL:HG13	2.02	0.40
1:B:210:TYR:CZ	1:B:214:ARG:HD3	2.57	0.40
1:B:99:LYS:HE3	4:B:1087:HOH:O	2.22	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%)	762 (96%)	30 (4%)	3 (0%)	38	21
1	B	795/886 (90%)	762 (96%)	33 (4%)	0	100	100
All	All	1590/1772 (90%)	1524 (96%)	63 (4%)	3 (0%)	51	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ASP
1	A	399	ALA
1	A	326	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	665/735 (90%)	648 (97%)	17 (3%)	51	33
1	B	665/735 (90%)	642 (96%)	23 (4%)	41	22
All	All	1330/1470 (90%)	1290 (97%)	40 (3%)	46	27

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	GLU
1	A	160	GLU
1	A	192	VAL
1	A	211	LEU
1	A	216	LEU
1	A	278	LEU
1	A	301	LEU
1	A	329	ASP
1	A	335	GLU
1	A	353	ASP
1	A	479	GLN
1	A	560	GLU
1	A	561	LYS
1	A	780	LEU
1	A	826	ASP
1	A	859	ARG
1	A	861	GLU
1	B	56	ILE
1	B	77	LEU
1	B	196	LEU
1	B	211	LEU
1	B	243	THR
1	B	278	LEU
1	B	301	LEU
1	B	340	LYS
1	B	417	VAL
1	B	421	ARG
1	B	423	ARG
1	B	432	ASP
1	B	475	LEU
1	B	502	LEU
1	B	522	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	537	ILE
1	B	587	THR
1	B	610	LEU
1	B	638	LEU
1	B	718	THR
1	B	818	ASP
1	B	819	ASP
1	B	826	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	336	HIS
1	A	479	GLN
1	B	323	GLN
1	B	466	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	26,35,35	1.39	4 (15%)	31,55,55	1.52	7 (22%)
3	TDK	B	887	2	26,35,35	1.31	3 (11%)	31,55,55	1.50	7 (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	-	0/26/35/35	0/2/2/2
3	TDK	B	887	2	-	0/26/35/35	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	887	TDK	PC-OM3	-3.15	1.50	1.56
3	B	887	TDK	C6'-C5'	-3.03	1.31	1.37
3	B	887	TDK	PC-OM3	-2.79	1.50	1.56
3	A	887	TDK	C6'-C5'	-2.38	1.32	1.37
3	A	887	TDK	PC-OM2	2.22	1.59	1.57
3	B	887	TDK	PC-OM2	2.50	1.60	1.57
3	A	887	TDK	PB-O3A	2.72	1.64	1.60

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	887	TDK	OM2-PC-CMA	-2.85	99.17	104.69
3	A	887	TDK	OM2-PC-OM4	-2.80	108.25	114.67
3	B	887	TDK	OM2-PC-OM4	-2.56	108.79	114.67
3	A	887	TDK	OM2-PC-CMA	-2.13	100.55	104.69
3	B	887	TDK	O3B-PB-O1B	2.00	118.34	110.50
3	A	887	TDK	O3B-PB-O1B	2.02	118.39	110.50
3	A	887	TDK	OM3-PC-OM4	2.41	117.20	111.43
3	A	887	TDK	C6'-N1'-C2'	2.44	120.10	115.88
3	B	887	TDK	C6'-N1'-C2'	2.49	120.18	115.88
3	B	887	TDK	OM3-PC-OM4	2.55	117.55	111.43
3	A	887	TDK	C5-C4-N3	2.57	113.04	107.66
3	B	887	TDK	C5-C4-N3	2.63	113.16	107.66
3	B	887	TDK	C6-C5-C4	3.85	130.52	127.43
3	A	887	TDK	C6-C5-C4	4.45	131.00	127.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	887	TDK	7	0
3	B	887	TDK	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.49	65 (8%) 13 12	14, 22, 37, 42	0
1	B	801/886 (90%)	0.41	49 (6%) 22 21	12, 20, 31, 41	0
All	All	1602/1772 (90%)	0.45	114 (7%) 17 16	12, 21, 35, 42	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	ALA	12.2
1	B	414	MET	8.8
1	B	400	ALA	8.4
1	A	400	ALA	8.1
1	A	349	ALA	7.1
1	A	339	GLY	7.0
1	A	341	TYR	6.1
1	A	56	ILE	5.9
1	A	342	PRO	5.8
1	A	332	TYR	5.8
1	B	431	ALA	5.4
1	B	56	ILE	5.3
1	B	533	ARG	5.1
1	A	306	THR	4.9
1	A	398	ASP	4.9
1	A	327	SER	4.8
1	A	340	LYS	4.7
1	A	351	TRP	4.6
1	A	348	VAL	4.6
1	A	333	VAL	4.6
1	A	399	ALA	4.5
1	A	418	ARG	4.3
1	B	398	ASP	4.3
1	B	415	ASP	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	336	HIS	4.2
1	A	305	ASP	4.1
1	A	524	ARG	4.1
1	A	325	PHE	4.0
1	A	330	GLY	3.9
1	A	304	LYS	3.9
1	A	720	GLU	3.6
1	A	345	ALA	3.6
1	A	533	ARG	3.5
1	A	347	LEU	3.5
1	B	434	GLU	3.4
1	B	532	PHE	3.3
1	A	301	LEU	3.3
1	A	329	ASP	3.3
1	B	432	ASP	3.3
1	A	335	GLU	3.3
1	A	338	PHE	3.3
1	A	356	ILE	3.3
1	B	607	ILE	3.2
1	A	862	ILE	3.1
1	A	130	GLU	3.1
1	A	354	GLU	3.1
1	A	350	ASP	3.0
1	A	558	GLU	3.0
1	A	530	GLY	3.0
1	B	429	SER	3.0
1	A	353	ASP	3.0
1	A	866	VAL	2.9
1	B	537	ILE	2.9
1	B	604	PHE	2.8
1	B	524	ARG	2.8
1	A	531	LEU	2.8
1	A	308	GLY	2.7
1	A	311	ILE	2.7
1	B	529	GLU	2.6
1	B	172	ASN	2.6
1	A	561	LYS	2.6
1	B	300	GLU	2.6
1	A	344	THR	2.6
1	A	303	ARG	2.6
1	B	430	ASP	2.6
1	A	343	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	397	GLY	2.6
1	B	490	LYS	2.6
1	B	599	TYR	2.6
1	B	611	CYS	2.6
1	A	131	GLN	2.6
1	B	530	GLY	2.5
1	B	531	LEU	2.5
1	B	875	ASN	2.5
1	A	307	SER	2.5
1	B	303	ARG	2.5
1	B	680	GLU	2.5
1	B	722	SER	2.4
1	B	859	ARG	2.4
1	B	558	GLU	2.4
1	B	818	ASP	2.4
1	A	318	VAL	2.4
1	A	331	ALA	2.4
1	B	522	GLU	2.4
1	A	196	LEU	2.3
1	A	607	ILE	2.3
1	B	433	ILE	2.3
1	A	337	PHE	2.3
1	B	612	TRP	2.3
1	B	602	PHE	2.3
1	B	685	VAL	2.3
1	A	509	LYS	2.3
1	A	160	GLU	2.2
1	A	352	THR	2.2
1	B	610	LEU	2.2
1	B	199	ILE	2.2
1	B	723	LYS	2.2
1	B	862	ILE	2.2
1	A	334	ARG	2.2
1	A	300	GLU	2.1
1	B	350	ASP	2.1
1	B	579	LEU	2.1
1	A	534	GLN	2.1
1	A	324	THR	2.1
1	B	306	THR	2.1
1	B	76	GLU	2.0
1	A	608	GLY	2.0
1	B	614	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	532	PHE	2.0
1	B	417	VAL	2.0
1	A	863	ASP	2.0
1	A	414	MET	2.0
1	B	169	VAL	2.0
1	B	385	VAL	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 carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	TDK	B	887	34/34	0.86	0.17	1.40	20,23,27,27	0
3	TDK	A	887	34/34	0.87	0.15	0.36	22,25,28,28	0
2	MG	B	888	1/1	0.98	0.04	-2.30	19,19,19,19	0
2	MG	A	888	1/1	0.97	0.05	-3.22	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.