



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 03:30 AM GMT

PDB ID : 2E28  
Title : Crystal structure analysis of pyruvate kinase from *Bacillus stearothermophilus*  
Authors : Suzuki, K.  
Deposited on : 2006-11-09  
Resolution : 2.40 Å(reported)

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

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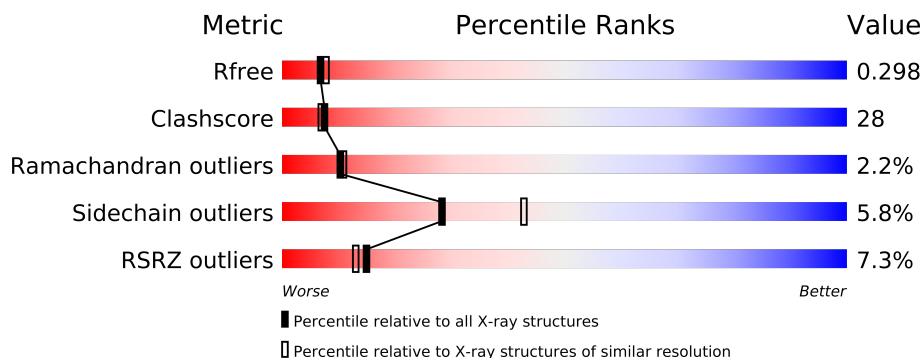
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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  $\geq 3$ , 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	587	

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4522 atoms, of which 4 are hydrogens 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 kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	587	Total	C	H	N	O	S	0	0	0
			4364	2725	4	770	848	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	SER	CYS	ENGINEERED	UNP Q02499
A	268	SER	CYS	ENGINEERED	UNP Q02499

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

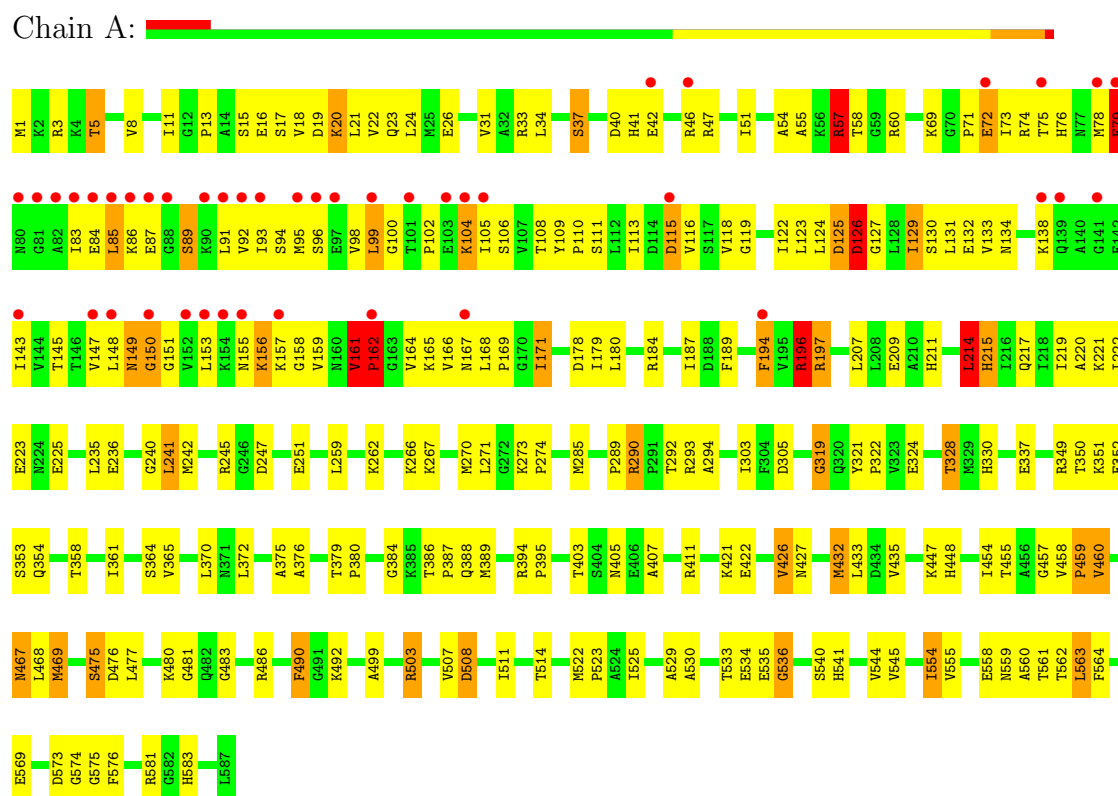
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total 153	O 153	0	0

### 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 errors 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 kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.97Å 145.97Å 118.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.40 47.78 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.40) 98.4 (47.78-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.17 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.294 0.236 , 0.298	Depositor DCC
$R_{free}$ test set	2552 reflections (9.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 26022 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4522	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: SO4

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	0.65	13/4408 (0.3%)	0.94	35/5969 (0.6%)

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	1	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	196	ARG	C-N	-14.69	1.00	1.34
1	A	33	ARG	C-N	-13.17	1.03	1.34
1	A	104	LYS	C-N	-9.83	1.11	1.34
1	A	184	ARG	C-N	-9.17	1.12	1.34
1	A	486	ARG	C-N	-9.17	1.12	1.34
1	A	499	ALA	C-N	-7.89	1.15	1.34
1	A	490	PHE	C-N	-6.67	1.21	1.33
1	A	167	ASN	C-N	-6.57	1.19	1.34
1	A	126	ASP	C-N	-6.31	1.21	1.33
1	A	426	VAL	C-N	-6.28	1.19	1.34
1	A	161	VAL	C-N	5.89	1.45	1.34
1	A	125	ASP	C-N	-5.38	1.21	1.34
1	A	169	PRO	N-CD	5.29	1.55	1.47

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	PRO	C-N-CA	12.56	148.67	122.30
1	A	104	LYS	O-C-N	-11.59	104.15	122.70
1	A	167	ASN	O-C-N	-11.22	104.75	122.70
1	A	33	ARG	C-N-CA	10.42	147.76	121.70
1	A	486	ARG	CB-CA-C	9.80	130.01	110.40
1	A	33	ARG	O-C-N	-8.92	108.42	122.70
1	A	168	LEU	C-N-CD	8.71	146.70	128.40
1	A	215	HIS	CA-C-N	-8.68	98.10	117.20
1	A	427	ASN	O-C-N	-7.97	109.95	122.70
1	A	104	LYS	CA-C-N	7.51	133.72	117.20
1	A	486	ARG	O-C-N	-7.30	111.01	122.70
1	A	126	ASP	O-C-N	-7.09	111.15	123.20
1	A	167	ASN	CA-C-N	6.71	131.97	117.20
1	A	72	GLU	CB-CA-C	-6.45	97.51	110.40
1	A	554	ILE	CB-CA-C	6.43	124.46	111.60
1	A	162	PRO	N-CA-C	6.28	128.42	112.10
1	A	57	ARG	CB-CA-C	6.27	122.94	110.40
1	A	194	PHE	CB-CG-CD2	6.11	125.08	120.80
1	A	215	HIS	O-C-N	6.10	132.46	122.70
1	A	197	ARG	CB-CA-C	-6.09	98.23	110.40
1	A	34	LEU	CB-CA-C	6.00	121.59	110.20
1	A	169	PRO	CA-N-CD	-5.98	103.13	111.50
1	A	47	ARG	CB-CA-C	5.85	122.10	110.40
1	A	33	ARG	CA-C-N	5.84	130.06	117.20
1	A	427	ASN	CA-C-N	5.80	129.95	117.20
1	A	126	ASP	CA-C-N	5.73	127.65	116.20
1	A	184	ARG	C-N-CA	5.60	135.70	121.70
1	A	196	ARG	O-C-N	-5.54	113.83	122.70
1	A	499	ALA	C-N-CA	5.51	135.47	121.70
1	A	161	VAL	O-C-N	-5.45	110.74	121.10
1	A	72	GLU	CA-C-O	5.45	131.54	120.10
1	A	499	ALA	O-C-N	-5.44	114.00	122.70
1	A	503	ARG	CB-CA-C	5.42	121.24	110.40
1	A	161	VAL	CA-CB-CG2	5.40	119.00	110.90
1	A	194	PHE	CB-CG-CD1	-5.10	117.23	120.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	162	PRO	CA

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	161	VAL	Mainchain
1	A	162	PRO	Mainchain
1	A	214	LEU	Mainchain
1	A	72	GLU	Mainchain

## 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	4360	4	4502	246	1
2	A	5	0	0	0	0
3	A	153	0	0	4	1
All	All	4518	4	4502	246	2

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 28.

All (246) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:162:PRO:HG3	1:A:251:GLU:CD	1.34	1.47
1:A:162:PRO:CG	1:A:251:GLU:CD	1.86	1.41
1:A:162:PRO:HG2	1:A:251:GLU:CG	1.51	1.40
1:A:162:PRO:HG2	1:A:251:GLU:CB	1.73	1.19
1:A:162:PRO:CG	1:A:251:GLU:OE2	1.89	1.17
1:A:535:GLU:HG3	1:A:536:GLY:H	0.98	1.13
1:A:162:PRO:HG3	1:A:251:GLU:OE2	1.48	1.11
1:A:162:PRO:CG	1:A:251:GLU:CG	2.30	1.06
1:A:197:ARG:NH2	3:A:642:HOH:O	1.97	0.97
1:A:40:ASP:OD1	1:A:42:GLU:HG2	1.67	0.94
1:A:535:GLU:HG3	1:A:536:GLY:N	1.82	0.94
1:A:534:GLU:OE2	1:A:561:THR:HG22	1.66	0.94
1:A:197:ARG:CZ	3:A:642:HOH:O	2.16	0.93
1:A:162:PRO:HG2	1:A:251:GLU:HB3	1.48	0.92
1:A:535:GLU:CG	1:A:536:GLY:H	1.74	0.92
1:A:222:ILE:HG12	1:A:241:LEU:HD21	1.50	0.91
1:A:476:ASP:HB2	1:A:581:ARG:NH1	1.86	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:15:SER:HA	1:A:20:LYS:HG2	1.55	0.89
1:A:162:PRO:HG2	1:A:251:GLU:CD	1.66	0.88
1:A:57:ARG:HB2	1:A:57:ARG:HH21	1.37	0.88
1:A:116:VAL:HG11	1:A:143:ILE:HD12	1.56	0.86
1:A:3:ARG:HE	1:A:330:HIS:HD2	1.24	0.86
1:A:3:ARG:HE	1:A:330:HIS:CD2	1.94	0.85
1:A:71:PRO:HG2	1:A:196:ARG:HH12	1.39	0.85
1:A:476:ASP:HB2	1:A:581:ARG:HH12	1.43	0.83
1:A:129:ILE:HD13	1:A:150:GLY:HA2	1.60	0.81
1:A:365:VAL:HA	1:A:469:MET:HE3	1.62	0.80
1:A:162:PRO:HG3	1:A:251:GLU:OE1	1.81	0.80
1:A:26:GLU:HA	1:A:60:ARG:HH22	1.46	0.79
1:A:133:VAL:HA	1:A:145:THR:HG22	1.63	0.79
1:A:86:LYS:HG2	1:A:87:GLU:H	1.47	0.79
1:A:71:PRO:HG2	1:A:196:ARG:NH1	1.97	0.79
1:A:448:HIS:HD2	1:A:475:SER:HA	1.47	0.78
1:A:459:PRO:O	1:A:460:VAL:HG22	1.85	0.77
1:A:194:PHE:CD2	1:A:223:GLU:OE1	2.37	0.77
1:A:162:PRO:HG2	1:A:251:GLU:HG2	1.64	0.77
1:A:156:LYS:O	1:A:156:LYS:HD2	1.84	0.76
1:A:20:LYS:HE3	1:A:20:LYS:HA	1.69	0.75
1:A:447:LYS:HD3	1:A:448:HIS:N	2.00	0.75
1:A:78:MET:HB3	1:A:83:ILE:HG12	1.67	0.74
1:A:559:ASN:HB3	1:A:562:THR:CG2	2.19	0.72
1:A:40:ASP:OD1	1:A:42:GLU:CG	2.37	0.72
1:A:74:ARG:HG3	1:A:75:THR:H	1.54	0.71
1:A:458:VAL:H	1:A:467:ASN:HD21	1.37	0.71
1:A:18:VAL:O	1:A:22:VAL:HG23	1.89	0.71
1:A:162:PRO:CB	1:A:251:GLU:OE2	2.38	0.70
1:A:432:MET:HE1	1:A:433:LEU:HD23	1.72	0.70
1:A:5:THR:HG23	1:A:337:GLU:OE2	1.91	0.70
1:A:129:ILE:HD11	1:A:147:VAL:HG13	1.74	0.69
1:A:432:MET:O	1:A:432:MET:HE2	1.93	0.69
1:A:189:PHE:CD1	1:A:217:GLN:HB2	2.29	0.68
1:A:54:ALA:O	1:A:58:THR:HG22	1.94	0.68
1:A:511:ILE:HD12	1:A:530:ALA:HB3	1.76	0.67
1:A:83:ILE:HG22	1:A:84:GLU:N	2.10	0.67
1:A:171:ILE:HD13	1:A:171:ILE:H	1.60	0.67
1:A:481:GLY:C	1:A:554:ILE:HD11	2.15	0.67
1:A:98:VAL:HG22	1:A:106:SER:HB3	1.76	0.66
1:A:57:ARG:HB2	1:A:57:ARG:NH2	2.07	0.66
1:A:292:THR:HG22	1:A:294:ALA:H	1.59	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:490:PHE:O	1:A:511:ILE:CG1	2.44	0.66
1:A:83:ILE:HG22	1:A:84:GLU:H	1.61	0.65
1:A:222:ILE:CG1	1:A:241:LEU:HD21	2.26	0.64
1:A:241:LEU:HD23	1:A:242:MET:H	1.62	0.64
1:A:490:PHE:O	1:A:511:ILE:HG12	1.96	0.64
1:A:459:PRO:O	1:A:460:VAL:HG13	1.97	0.64
1:A:133:VAL:HG22	1:A:143:ILE:HD11	1.79	0.64
1:A:157:LYS:HE2	1:A:157:LYS:HA	1.78	0.64
1:A:161:VAL:N	1:A:162:PRO:HD3	2.13	0.63
1:A:492:LYS:HG2	1:A:569:GLU:OE1	1.99	0.62
1:A:351:LYS:O	1:A:352:GLU:HG2	1.98	0.62
1:A:458:VAL:HA	1:A:459:PRO:C	2.20	0.61
1:A:221:LYS:HG2	1:A:242:MET:HB3	1.83	0.61
1:A:354:GLN:HA	1:A:354:GLN:HE21	1.64	0.61
1:A:26:GLU:HA	1:A:60:ARG:NH2	2.16	0.61
1:A:361:ILE:HG13	1:A:467:ASN:HA	1.81	0.61
1:A:575:GLY:O	1:A:576:PHE:HB2	2.00	0.61
1:A:384:GLY:O	1:A:387:PRO:HD2	2.01	0.60
1:A:321:TYR:HB3	1:A:324:GLU:HB2	1.81	0.60
1:A:83:ILE:HG23	1:A:102:PRO:HG3	1.83	0.60
1:A:354:GLN:HA	1:A:354:GLN:NE2	2.16	0.60
1:A:477:LEU:HD21	1:A:480:LYS:HE2	1.84	0.60
1:A:73:ILE:O	1:A:159:VAL:HB	2.01	0.60
1:A:241:LEU:HD23	1:A:242:MET:N	2.16	0.60
1:A:525:ILE:HG21	1:A:545:VAL:HG11	1.82	0.60
1:A:235:LEU:HB3	1:A:271:LEU:CD1	2.32	0.59
1:A:8:VAL:HG22	1:A:31:VAL:HB	1.84	0.59
1:A:74:ARG:HG3	1:A:75:THR:N	2.16	0.59
1:A:125:ASP:HA	1:A:157:LYS:HB3	1.83	0.59
1:A:162:PRO:CG	1:A:251:GLU:HB3	2.25	0.58
1:A:73:ILE:HG13	1:A:109:TYR:HB2	1.84	0.58
1:A:507:VAL:HG12	1:A:508:ASP:H	1.68	0.58
1:A:132:GLU:HG2	1:A:148:LEU:HD11	1.86	0.58
1:A:60:ARG:HH21	1:A:60:ARG:HG3	1.69	0.57
1:A:235:LEU:HB3	1:A:271:LEU:HD12	1.86	0.57
1:A:1:MET:HE2	3:A:699:HOH:O	2.04	0.57
1:A:162:PRO:CG	1:A:251:GLU:HG2	2.26	0.56
1:A:476:ASP:CB	1:A:581:ARG:HH12	2.17	0.56
1:A:93:ILE:HB	1:A:143:ILE:HG23	1.89	0.55
1:A:468:LEU:C	1:A:468:LEU:HD23	2.26	0.55
1:A:384:GLY:C	1:A:387:PRO:HD2	2.26	0.55
1:A:358:THR:HG22	1:A:389:MET:HG3	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:42:GLU:O	1:A:46:ARG:HG3	2.07	0.55
1:A:93:ILE:HB	1:A:143:ILE:CG2	2.37	0.55
1:A:124:LEU:HA	1:A:158:GLY:O	2.07	0.55
1:A:324:GLU:O	1:A:328:THR:HG23	2.08	0.54
1:A:55:ALA:O	1:A:58:THR:O	2.23	0.54
1:A:21:LEU:HA	1:A:24:LEU:HD23	1.90	0.54
1:A:132:GLU:HG3	1:A:148:LEU:HD21	1.90	0.54
1:A:17:SER:OG	1:A:20:LYS:HB2	2.09	0.53
1:A:20:LYS:O	1:A:24:LEU:HD22	2.08	0.53
1:A:129:ILE:HA	1:A:149:ASN:O	2.09	0.53
1:A:541:HIS:CE1	1:A:545:VAL:HG21	2.44	0.53
1:A:85:LEU:HB3	1:A:147:VAL:HG21	1.91	0.53
1:A:108:THR:HG22	1:A:108:THR:O	2.09	0.53
1:A:535:GLU:CG	1:A:536:GLY:N	2.48	0.53
1:A:490:PHE:CD2	1:A:583:HIS:CG	2.97	0.52
1:A:540:SER:O	1:A:544:VAL:HG23	2.09	0.52
1:A:92:VAL:O	1:A:104:LYS:HA	2.10	0.52
1:A:365:VAL:HA	1:A:469:MET:CE	2.35	0.52
1:A:379:THR:OG1	1:A:387:PRO:HG3	2.10	0.52
1:A:507:VAL:HG12	1:A:508:ASP:N	2.25	0.52
1:A:79:GLU:H	1:A:99:LEU:HD22	1.75	0.51
1:A:514:THR:O	1:A:533:THR:HA	2.10	0.51
1:A:285:MET:SD	1:A:328:THR:HG21	2.51	0.51
1:A:405:ASN:OD1	1:A:407:ALA:N	2.43	0.51
1:A:468:LEU:HD23	1:A:469:MET:N	2.26	0.51
1:A:215:HIS:O	1:A:411:ARG:NH2	2.44	0.51
1:A:432:MET:C	1:A:432:MET:HE2	2.31	0.51
1:A:403:THR:O	1:A:422:GLU:HA	2.10	0.51
1:A:91:LEU:HD12	1:A:131:LEU:HD13	1.93	0.51
1:A:245:ARG:HD3	1:A:245:ARG:H	1.75	0.51
1:A:41:HIS:HE1	1:A:178:ASP:OD2	1.94	0.50
1:A:511:ILE:CD1	1:A:529:ALA:HB3	2.41	0.50
1:A:575:GLY:O	1:A:576:PHE:CB	2.59	0.50
1:A:73:ILE:HD11	1:A:166:VAL:HG11	1.92	0.50
1:A:123:LEU:HB3	1:A:127:GLY:HA2	1.94	0.50
1:A:126:ASP:OD2	1:A:126:ASP:O	2.29	0.50
1:A:358:THR:CG2	1:A:389:MET:HG3	2.41	0.50
1:A:349:ARG:O	1:A:353:SER:HB2	2.12	0.49
1:A:380:PRO:HG2	1:A:432:MET:HE2	1.94	0.49
1:A:394:ARG:N	1:A:395:PRO:HD3	2.27	0.49
1:A:457:GLY:HA2	1:A:467:ASN:ND2	2.27	0.49
1:A:241:LEU:CD2	1:A:242:MET:N	2.76	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:350:THR:O	1:A:353:SER:HB3	2.13	0.49
1:A:267:LYS:HA	1:A:270:MET:HE2	1.93	0.49
1:A:266:LYS:O	1:A:270:MET:HG3	2.12	0.49
1:A:79:GLU:HG3	1:A:83:ILE:HD11	1.94	0.49
1:A:109:TYR:CZ	1:A:166:VAL:HG13	2.48	0.49
1:A:5:THR:HG21	1:A:303:ILE:HD13	1.95	0.49
1:A:289:PRO:HG3	1:A:321:TYR:CZ	2.48	0.49
1:A:83:ILE:HD12	1:A:102:PRO:HD3	1.95	0.49
1:A:113:ILE:HD11	1:A:138:LYS:HA	1.95	0.49
1:A:563:LEU:HD12	1:A:564:PHE:CE1	2.48	0.49
1:A:483:GLY:HA3	1:A:574:GLY:O	2.12	0.49
1:A:534:GLU:HG2	1:A:560:ALA:HB3	1.95	0.48
1:A:365:VAL:CA	1:A:469:MET:HE3	2.39	0.48
1:A:79:GLU:HA	1:A:99:LEU:HD21	1.95	0.48
1:A:116:VAL:CG2	1:A:133:VAL:HG21	2.43	0.48
1:A:321:TYR:N	1:A:322:PRO:HD3	2.28	0.48
1:A:75:THR:O	1:A:156:LYS:HA	2.13	0.48
1:A:559:ASN:HB3	1:A:562:THR:HG22	1.93	0.48
1:A:180:LEU:HD21	1:A:211:HIS:CD2	2.48	0.48
1:A:116:VAL:HG21	1:A:133:VAL:HG21	1.96	0.47
1:A:13:PRO:HA	1:A:16:GLU:OE2	2.14	0.47
1:A:432:MET:HE1	1:A:454:ILE:HG21	1.96	0.47
1:A:563:LEU:HD12	1:A:564:PHE:CD1	2.49	0.47
1:A:86:LYS:HG2	1:A:87:GLU:OE2	2.15	0.47
1:A:324:GLU:O	1:A:328:THR:CG2	2.62	0.47
1:A:426:VAL:HG11	1:A:435:VAL:HG21	1.97	0.47
1:A:219:ILE:HD12	1:A:240:GLY:HA3	1.97	0.47
1:A:448:HIS:CD2	1:A:475:SER:HA	2.37	0.47
1:A:78:MET:HE1	1:A:153:LEU:HD23	1.97	0.47
1:A:5:THR:CG2	1:A:337:GLU:OE2	2.62	0.47
1:A:267:LYS:HA	1:A:270:MET:CE	2.45	0.47
1:A:78:MET:HE1	1:A:153:LEU:CD2	2.45	0.47
1:A:459:PRO:O	1:A:460:VAL:CG2	2.60	0.46
1:A:375:ALA:O	1:A:376:ALA:HB2	2.15	0.46
1:A:319:GLY:HA3	3:A:613:HOH:O	2.16	0.46
1:A:541:HIS:O	1:A:545:VAL:HG23	2.15	0.46
1:A:179:ILE:HG21	1:A:207:LEU:HD23	1.98	0.46
1:A:503:ARG:HG3	1:A:503:ARG:NH1	2.30	0.46
1:A:161:VAL:HG12	1:A:164:VAL:HG12	1.97	0.46
1:A:129:ILE:HD12	1:A:130:SER:N	2.30	0.46
1:A:89:SER:HB2	1:A:147:VAL:CG2	2.45	0.46
1:A:222:ILE:HG12	1:A:241:LEU:CD2	2.34	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:83:ILE:CG2	1:A:84:GLU:H	2.29	0.45
1:A:78:MET:HE3	1:A:83:ILE:HG13	1.98	0.45
1:A:122:ILE:C	1:A:123:LEU:HD12	2.37	0.45
1:A:559:ASN:O	1:A:562:THR:HG22	2.17	0.45
1:A:511:ILE:HD11	1:A:529:ALA:HB3	1.97	0.45
1:A:292:THR:HG22	1:A:293:ARG:N	2.30	0.45
1:A:194:PHE:CE2	1:A:223:GLU:OE1	2.68	0.45
1:A:83:ILE:CG2	1:A:84:GLU:N	2.79	0.44
1:A:554:ILE:HD12	1:A:555:VAL:N	2.32	0.44
1:A:75:THR:HG22	1:A:76:HIS:N	2.32	0.44
1:A:223:GLU:HB3	1:A:247:ASP:HB3	1.99	0.44
1:A:79:GLU:HB3	1:A:99:LEU:HD13	2.00	0.44
1:A:119:GLY:N	1:A:133:VAL:O	2.43	0.44
1:A:481:GLY:CA	1:A:554:ILE:HD11	2.47	0.44
1:A:457:GLY:O	1:A:460:VAL:HA	2.17	0.43
1:A:490:PHE:HB2	1:A:583:HIS:ND1	2.32	0.43
1:A:386:THR:HB	1:A:387:PRO:HD3	2.01	0.43
1:A:109:TYR:CZ	1:A:111:SER:HB2	2.53	0.43
1:A:37:SER:OG	1:A:69:LYS:HG3	2.18	0.43
1:A:21:LEU:HD13	1:A:51:ILE:HD13	2.00	0.43
1:A:380:PRO:HG2	1:A:432:MET:CE	2.48	0.43
1:A:109:TYR:C	1:A:111:SER:H	2.22	0.43
1:A:262:LYS:HG2	1:A:305:ASP:OD1	2.17	0.43
1:A:180:LEU:HD21	1:A:211:HIS:NE2	2.34	0.43
1:A:76:HIS:HD2	1:A:106:SER:OG	2.00	0.43
1:A:447:LYS:HD3	1:A:448:HIS:H	1.80	0.43
1:A:573:ASP:OD1	1:A:575:GLY:O	2.36	0.43
1:A:388:GLN:HE21	1:A:388:GLN:HB3	1.54	0.43
1:A:94:SER:C	1:A:96:SER:H	2.23	0.43
1:A:379:THR:HG22	1:A:455:THR:HG23	2.01	0.43
1:A:74:ARG:HD2	1:A:156:LYS:O	2.19	0.42
1:A:84:GLU:O	1:A:151:GLY:O	2.37	0.42
1:A:379:THR:HG22	1:A:455:THR:CG2	2.49	0.42
1:A:123:LEU:HD12	1:A:123:LEU:N	2.34	0.42
1:A:118:VAL:HG13	1:A:134:ASN:O	2.19	0.42
1:A:91:LEU:C	1:A:91:LEU:HD13	2.39	0.42
1:A:290:ARG:HH11	1:A:290:ARG:HB2	1.83	0.42
1:A:155:ASN:O	1:A:156:LYS:HG3	2.20	0.42
1:A:122:ILE:O	1:A:131:LEU:N	2.51	0.42
1:A:129:ILE:CD1	1:A:147:VAL:HG13	2.46	0.42
1:A:95:MET:HA	1:A:95:MET:HE2	2.01	0.42
1:A:96:SER:O	1:A:98:VAL:HG13	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:LYS:HA	1:A:274:PRO:HD3	1.91	0.42
1:A:432:MET:CE	1:A:454:ILE:HG21	2.50	0.42
1:A:20:LYS:O	1:A:23:GLN:HB2	2.20	0.41
1:A:458:VAL:HA	1:A:460:VAL:N	2.34	0.41
1:A:171:ILE:H	1:A:171:ILE:CD1	2.32	0.41
1:A:133:VAL:CG2	1:A:143:ILE:HD11	2.48	0.41
1:A:209:GLU:HA	1:A:214:LEU:HG	2.02	0.41
1:A:220:ALA:O	1:A:241:LEU:HD23	2.21	0.41
1:A:162:PRO:HB2	1:A:225:GLU:OE2	2.20	0.41
1:A:115:ASP:O	1:A:164:VAL:HG21	2.21	0.41
1:A:11:ILE:HD12	1:A:21:LEU:HD21	2.02	0.41
1:A:79:GLU:HG3	1:A:100:GLY:O	2.21	0.41
1:A:73:ILE:N	1:A:73:ILE:HD12	2.36	0.41
1:A:522:MET:HB2	1:A:523:PRO:HD3	2.02	0.40
1:A:187:ILE:HD12	1:A:189:PHE:O	2.21	0.40
1:A:490:PHE:O	1:A:511:ILE:HG13	2.20	0.40
1:A:79:GLU:HA	1:A:99:LEU:CD2	2.52	0.40
1:A:100:GLY:HA2	1:A:105:ILE:HA	2.04	0.40
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.93	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:737:HOH:O	3:A:737:HOH:O[12_566]	1.53	0.67
1:A:364:SER:OG	1:A:364:SER:OG[10_665]	1.87	0.33

## 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	585/587 (100%)	522 (89%)	50 (8%)	13 (2%)	10 11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	LEU
1	A	459	PRO
1	A	460	VAL
1	A	79	GLU
1	A	89	SER
1	A	536	GLY
1	A	115	ASP
1	A	558	GLU
1	A	150	GLY
1	A	85	LEU
1	A	319	GLY
1	A	475	SER
1	A	110	PRO

### 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	469/471 (100%)	442 (94%)	27 (6%)	28 43

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	19	ASP
1	A	20	LYS
1	A	37	SER
1	A	57	ARG
1	A	79	GLU
1	A	99	LEU
1	A	126	ASP
1	A	129	ILE
1	A	149	ASN
1	A	156	LYS
1	A	165	LYS
1	A	171	ILE
1	A	196	ARG
1	A	236	GLU

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	259	LEU
1	A	290	ARG
1	A	328	THR
1	A	370	LEU
1	A	372	LEU
1	A	421	LYS
1	A	432	MET
1	A	467	ASN
1	A	469	MET
1	A	508	ASP
1	A	563	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	50	ASN
1	A	76	HIS
1	A	77	ASN
1	A	134	ASN
1	A	139	GLN
1	A	149	ASN
1	A	230	ASN
1	A	280	GLN
1	A	330	HIS
1	A	331	GLN
1	A	338	GLN
1	A	354	GLN
1	A	388	GLN
1	A	448	HIS
1	A	467	ASN

### 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 ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	588	-	4,4,4	0.22	0	6,6,6	0.09	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
2	SO4	A	588	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	587/587 (100%)	0.24	43 (7%)	15 13	18, 47, 107, 151	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	ASN	7.0
1	A	90	LYS	5.4
1	A	152	VAL	5.4
1	A	86	LYS	4.8
1	A	87	GLU	4.8
1	A	153	LEU	4.7
1	A	75	THR	4.6
1	A	93	ILE	4.6
1	A	83	ILE	4.2
1	A	82	ALA	4.0
1	A	72	GLU	3.9
1	A	79	GLU	3.8
1	A	78	MET	3.8
1	A	96	SER	3.7
1	A	162	PRO	3.7
1	A	139	GLN	3.7
1	A	155	ASN	3.6
1	A	85	LEU	3.5
1	A	138	LYS	3.4
1	A	88	GLY	3.4
1	A	91	LEU	3.4
1	A	99	LEU	3.4
1	A	103	GLU	3.3
1	A	141	GLY	3.2
1	A	81	GLY	3.1
1	A	167	ASN	3.1
1	A	97	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	154	LYS	2.9
1	A	105	ILE	2.8
1	A	104	LYS	2.6
1	A	148	LEU	2.5
1	A	147	VAL	2.5
1	A	84	GLU	2.4
1	A	115	ASP	2.4
1	A	46	ARG	2.4
1	A	95	MET	2.3
1	A	42	GLU	2.3
1	A	143	ILE	2.2
1	A	101	THR	2.2
1	A	157	LYS	2.2
1	A	92	VAL	2.1
1	A	194	PHE	2.0
1	A	150	GLY	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	A	588	5/5	0.16	0.90	38,38,45,49	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.