



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 02:49 PM GMT

PDB ID : 1VBH  
Title : Pyruvate Phosphate Dikinase with bound Mg-PEP from Maize  
Authors : Nakanishi, T.; Nakatsu, T.; Matsuoka, M.; Sakata, K.; Kato, H.; RIKEN  
Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2004-02-26  
Resolution : 2.30 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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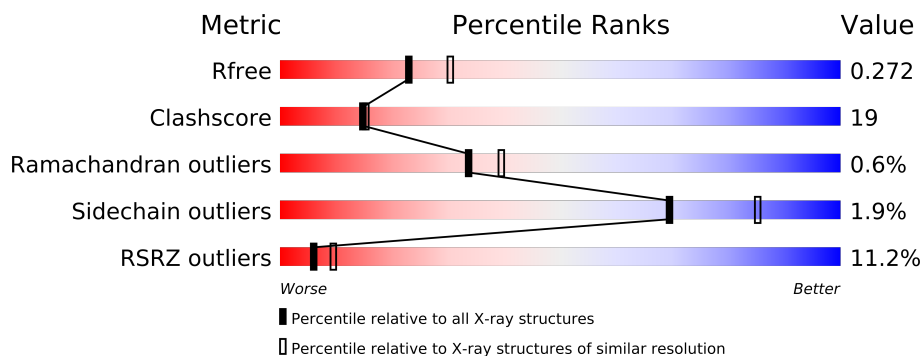
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	876	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6665 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,orthophosphatedikinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	862	6455	4083	1122	1204	46	0	8	0

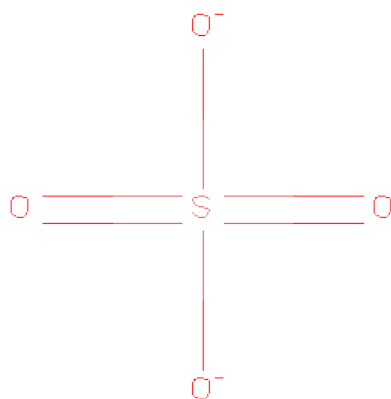
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	819	PHE	LEU	SEE REMARK 999	UNP P11155

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

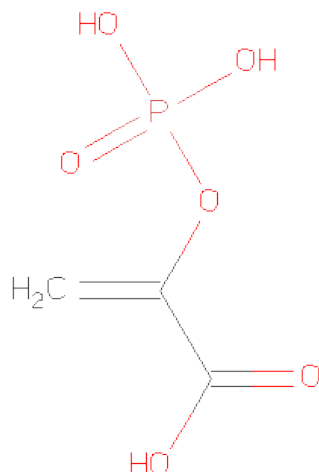
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula:  $C_3H_5O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 5 is water.

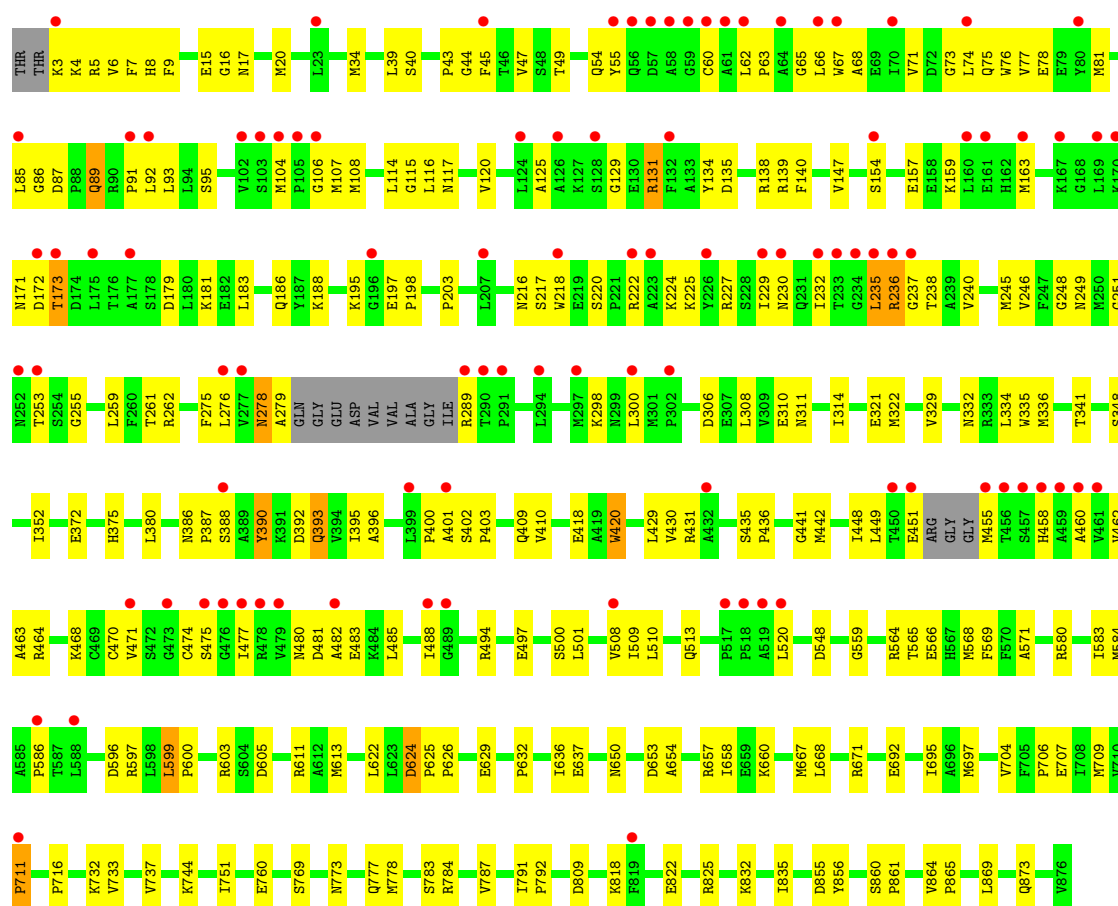
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total	O	0	0
			194	194		

### 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,orthophosphatedikinase

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.34Å 100.51Å 108.16Å 90.00° 98.48° 90.00°	Depositor
Resolution (Å)	45.63 – 2.30 45.62 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.63-2.30) 98.1 (45.62-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.35 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.230 , 0.259 0.243 , 0.272	Depositor DCC
$R_{free}$ test set	2528 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 50481 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6665	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: MG, PEP, 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	0.44	0/6577	0.63	0/8913

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	6455	0	6308	246	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
4	A	10	0	2	2	0
5	A	194	0	0	8	0
All	All	6665	0	6310	246	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 19.

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:ARG:HD3	1:A:131:ARG:H	1.21	1.02
1:A:509:ILE:HD12	1:A:509:ILE:H	1.25	1.00
1:A:777:GLN:NE2	1:A:784:ARG:H	1.62	0.97
1:A:777:GLN:HE21	1:A:784:ARG:H	1.04	0.93
1:A:74:LEU:HD12	1:A:75:GLN:N	1.88	0.88
1:A:429:LEU:HD21	1:A:431:ARG:HG3	1.58	0.84
1:A:387:PRO:HA	1:A:390:TYR:CE2	2.13	0.84
1:A:596:ASP:O	1:A:600:PRO:HD3	1.77	0.84
1:A:787:VAL:HG22	1:A:791:ILE:HG12	1.60	0.82
1:A:477:ILE:CG1	1:A:488:ILE:HG12	2.09	0.81
1:A:16:GLY:HA2	1:A:20:MET:HE1	1.61	0.80
1:A:253:THR:HG22	1:A:332:ASN:N	1.98	0.79
1:A:195:LYS:HE2	1:A:195:LYS:HA	1.63	0.78
1:A:396:ALA:HB3	1:A:508:VAL:CG2	2.15	0.76
1:A:396:ALA:HB3	1:A:508:VAL:HG21	1.66	0.76
1:A:668:LEU:HD21	1:A:778[B]:MET:CE	2.16	0.76
1:A:40:SER:H	1:A:311:ASN:HD21	1.31	0.75
1:A:401:ALA:HB1	1:A:460:ALA:CB	2.17	0.75
1:A:372:GLU:H	1:A:375:HIS:HD2	1.33	0.74
1:A:668:LEU:HD21	1:A:778[B]:MET:SD	2.28	0.74
1:A:566:GLU:HG3	1:A:625:PRO:HG3	1.71	0.72
1:A:67:TRP:O	1:A:71:VAL:HG23	1.90	0.71
1:A:249:ASN:HA	1:A:278:ASN:ND2	2.06	0.71
1:A:5:ARG:NH2	1:A:63:PRO:HB2	2.06	0.70
1:A:777:GLN:HE21	1:A:784:ARG:N	1.85	0.70
1:A:276:LEU:HD22	1:A:279:ALA:HB3	1.72	0.69
1:A:509:ILE:HD12	1:A:509:ILE:N	2.04	0.69
1:A:559:GLY:HA2	1:A:613:MET:CE	2.23	0.69
1:A:474:CYS:O	1:A:477:ILE:HG22	1.93	0.68
1:A:431:ARG:HH11	1:A:431:ARG:HG2	1.58	0.68
1:A:626:PRO:HD2	1:A:629:GLU:OE2	1.94	0.68
1:A:321:GLU:CG	1:A:341:THR:HG23	2.24	0.67
1:A:787:VAL:HG22	1:A:791:ILE:CG1	2.25	0.67
1:A:188:LYS:HB3	5:A:3177:HOH:O	1.94	0.67
1:A:87:ASP:OD1	1:A:89:GLN:HG3	1.93	0.67
1:A:520:LEU:O	1:A:520:LEU:HD23	1.94	0.67
1:A:154:SER:HA	1:A:157:GLU:HG2	1.75	0.66
1:A:509:ILE:CD1	1:A:509:ILE:H	2.00	0.66
1:A:401:ALA:HB1	1:A:460:ALA:HB2	1.78	0.66
1:A:3:LYS:HZ1	1:A:8:HIS:CE1	2.13	0.66
1:A:380:LEU:HD13	1:A:865:PRO:HG2	1.77	0.66
1:A:458:HIS:O	1:A:462:VAL:HG23	1.96	0.65
1:A:372:GLU:H	1:A:375:HIS:CD2	2.13	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:ASN:HA	1:A:278:ASN:HD22	1.60	0.65
1:A:125:ALA:HA	1:A:129:GLY:O	1.96	0.65
1:A:259:LEU:C	1:A:259:LEU:HD12	2.18	0.64
1:A:390:TYR:HA	1:A:393:GLN:NE2	2.12	0.64
1:A:624:ASP:O	1:A:671[A]:ARG:HB2	1.96	0.64
1:A:5:ARG:HH22	1:A:63:PRO:HB2	1.61	0.64
1:A:596:ASP:O	1:A:600:PRO:CD	2.44	0.64
1:A:310:GLU:O	1:A:314:ILE:HG12	1.98	0.64
1:A:251:GLY:C	5:A:3095:HOH:O	2.35	0.63
1:A:695:ILE:HG21	1:A:737:VAL:HG21	1.80	0.63
1:A:751:ILE:HD13	1:A:778[A]:MET:SD	2.39	0.62
1:A:508:VAL:HG23	1:A:508:VAL:O	1.99	0.61
1:A:603:ARG:NH1	1:A:692:GLU:OE1	2.30	0.61
1:A:597:ARG:O	1:A:600:PRO:HD2	2.01	0.59
1:A:494:ARG:O	1:A:497:GLU:HG3	2.02	0.59
1:A:321:GLU:HG2	1:A:341:THR:HG23	1.83	0.59
1:A:429:LEU:HD23	1:A:429:LEU:C	2.23	0.59
1:A:485:LEU:HB3	1:A:494:ARG:HG2	1.84	0.59
1:A:17:ASN:H	1:A:20:MET:HE3	1.67	0.59
1:A:624:ASP:O	1:A:671[B]:ARG:HB2	2.01	0.59
1:A:429:LEU:CD2	1:A:431:ARG:HG3	2.32	0.58
1:A:89:GLN:C	1:A:91:PRO:HD3	2.23	0.58
1:A:74:LEU:O	1:A:78:GLU:HG3	2.03	0.58
1:A:429:LEU:HD23	1:A:430:VAL:N	2.18	0.57
1:A:380:LEU:CD1	1:A:865:PRO:HG2	2.33	0.57
1:A:733:VAL:O	1:A:737:VAL:HG12	2.05	0.57
1:A:387:PRO:HA	1:A:390:TYR:CZ	2.40	0.57
1:A:599:LEU:HB3	1:A:600:PRO:HD3	1.86	0.57
1:A:654:ALA:O	1:A:658:ILE:HG13	2.04	0.57
1:A:154:SER:HA	1:A:157:GLU:CD	2.25	0.56
1:A:154:SER:HA	1:A:157:GLU:CG	2.35	0.56
1:A:5:ARG:CZ	1:A:54:GLN:HE22	2.19	0.56
1:A:251:GLY:CA	5:A:3095:HOH:O	2.54	0.56
1:A:73:GLY:O	1:A:77:VAL:HG23	2.06	0.56
1:A:55:TYR:O	1:A:60:CYS:HA	2.06	0.55
1:A:62:LEU:HD23	1:A:63:PRO:O	2.06	0.55
1:A:455:MET:O	1:A:464:ARG:NH2	2.39	0.55
1:A:78:GLU:HG2	1:A:92:LEU:CD2	2.37	0.55
1:A:235:LEU:O	1:A:236:ARG:HB3	2.07	0.55
1:A:43:PRO:HG3	1:A:81:MET:HG2	1.89	0.55
1:A:235:LEU:O	1:A:236:ARG:CB	2.55	0.54
1:A:172:ASP:O	1:A:173:THR:HB	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:17:ASN:N	1:A:20:MET:HE3	2.23	0.54
1:A:864:VAL:HB	1:A:865:PRO:HD3	1.89	0.54
1:A:435:SER:HB2	1:A:436:PRO:HD2	1.88	0.54
1:A:107:MET:HE2	1:A:238:THR:HB	1.89	0.54
1:A:480:ASN:O	1:A:483:GLU:O	2.24	0.54
1:A:227:ARG:HD3	1:A:235:LEU:HD12	1.88	0.54
1:A:611[A]:ARG:NH1	1:A:697:MET:SD	2.80	0.54
1:A:197:GLU:HB2	1:A:198:PRO:HD2	1.88	0.54
1:A:71:VAL:O	1:A:74:LEU:HG	2.07	0.53
1:A:566:GLU:CD	1:A:625:PRO:HD3	2.29	0.53
1:A:513:GLN:HA	1:A:513:GLN:HE21	1.73	0.53
1:A:636:ILE:HG23	1:A:637:GLU:N	2.24	0.53
1:A:568:MET:CE	1:A:605:ASP:HB3	2.39	0.53
1:A:400:PRO:HG2	1:A:455:MET:SD	2.48	0.53
1:A:85:LEU:HG	1:A:203:PRO:HB3	1.91	0.53
1:A:732:LYS:NZ	5:A:3161:HOH:O	2.41	0.53
1:A:569:PHE:C	1:A:571:ALA:H	2.12	0.53
1:A:159:LYS:HD3	1:A:186:GLN:HB3	1.91	0.52
1:A:8:HIS:CE1	1:A:76:TRP:CZ2	2.98	0.52
1:A:225:LYS:O	1:A:229:ILE:HG13	2.09	0.52
1:A:509:ILE:HG22	1:A:510:LEU:N	2.24	0.52
1:A:401:ALA:HB3	1:A:470:CYS:O	2.10	0.52
1:A:227:ARG:HA	1:A:232:ILE:HD12	1.92	0.52
1:A:650:ASN:ND2	1:A:653:ASP:H	2.08	0.52
1:A:16:GLY:HA2	1:A:20:MET:CE	2.38	0.52
1:A:131:ARG:N	1:A:131:ARG:HD3	2.06	0.51
1:A:138:ARG:HD2	1:A:183:LEU:HD23	1.90	0.51
1:A:78:GLU:HG2	1:A:92:LEU:HD22	1.91	0.51
1:A:395:ILE:O	1:A:396:ALA:HB2	2.10	0.51
1:A:500:SER:HB2	1:A:509:ILE:HB	1.93	0.51
1:A:668:LEU:CD2	1:A:778[B]:MET:CE	2.88	0.51
1:A:246:VAL:HG11	1:A:335:TRP:CD1	2.46	0.51
1:A:869:LEU:O	1:A:873:GLN:HG3	2.11	0.51
1:A:777:GLN:NE2	1:A:784:ARG:N	2.46	0.51
1:A:449:LEU:HD12	1:A:471:VAL:O	2.11	0.50
1:A:104:MET:HE1	1:A:227:ARG:HH21	1.75	0.50
1:A:107:MET:HE2	1:A:218:TRP:CE3	2.47	0.50
1:A:481:ASP:O	1:A:482:ALA:C	2.50	0.50
1:A:171:ASN:O	1:A:173:THR:HG22	2.11	0.50
1:A:230:ASN:HB2	1:A:232:ILE:CG1	2.42	0.49
1:A:134:TYR:CE2	1:A:181:LYS:HE2	2.48	0.49
1:A:860:SER:HB2	1:A:861:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:773:ASN:HB2	4:A:3000:PEP:C1	2.42	0.49
1:A:163:MET:HE2	1:A:179:ASP:HB3	1.93	0.49
1:A:580:ARG:CZ	1:A:632:PRO:HG3	2.42	0.49
1:A:232:ILE:HG22	1:A:235:LEU:HD21	1.94	0.49
1:A:117:ASN:OD1	1:A:120:VAL:HG23	2.13	0.49
1:A:818:LYS:O	1:A:822:GLU:HG3	2.12	0.49
1:A:513:GLN:NE2	1:A:513:GLN:HA	2.28	0.48
1:A:564:ARG:HH21	4:A:3000:PEP:P	2.36	0.48
1:A:566:GLU:CB	1:A:625:PRO:CG	2.92	0.48
1:A:251:GLY:HA3	5:A:3095:HOH:O	2.13	0.48
1:A:386:ASN:OD1	1:A:388:SER:HB3	2.12	0.48
1:A:611[A]:ARG:NH1	1:A:611[A]:ARG:HB2	2.29	0.48
1:A:463:ALA:HB1	1:A:468:LYS:O	2.14	0.48
1:A:707:GLU:HG2	1:A:744:LYS:HB2	1.96	0.48
1:A:431:ARG:NH1	1:A:431:ARG:HG2	2.28	0.47
1:A:107:MET:CE	1:A:218:TRP:CZ3	2.97	0.47
1:A:49:THR:OG1	1:A:236:ARG:HD3	2.13	0.47
1:A:188:LYS:O	5:A:3177:HOH:O	2.20	0.47
1:A:485:LEU:C	1:A:485:LEU:HD12	2.34	0.47
1:A:509:ILE:HG22	1:A:510:LEU:H	1.80	0.47
1:A:451:GLU:CB	1:A:477:ILE:CG2	2.92	0.47
1:A:131:ARG:CD	1:A:131:ARG:H	2.04	0.47
1:A:154:SER:O	1:A:157:GLU:HG2	2.15	0.47
1:A:261:THR:OG1	1:A:322:MET:HG2	2.15	0.47
1:A:7:PHE:O	1:A:45:PHE:HA	2.15	0.47
1:A:135:ASP:OD1	1:A:138:ARG:NH1	2.48	0.46
1:A:138:ARG:CG	1:A:139:ARG:N	2.78	0.46
1:A:3:LYS:HB3	1:A:6:VAL:O	2.15	0.46
1:A:114:LEU:HA	1:A:140:PHE:CE1	2.50	0.46
1:A:321:GLU:HG3	1:A:341:THR:HG23	1.96	0.46
1:A:3:LYS:HD2	1:A:15:GLU:CB	2.46	0.46
1:A:95:SER:HB3	1:A:245:MET:SD	2.56	0.46
1:A:791:ILE:HB	1:A:792:PRO:HD3	1.97	0.45
1:A:401:ALA:CB	1:A:460:ALA:HB2	2.46	0.45
1:A:220:SER:O	1:A:224:LYS:HG3	2.17	0.45
1:A:47:VAL:HB	1:A:240:VAL:HB	1.99	0.45
1:A:704:VAL:HG12	1:A:706:PRO:HD3	1.98	0.45
1:A:278:ASN:C	1:A:278:ASN:HD22	2.18	0.45
1:A:5:ARG:NH2	1:A:66:LEU:HB2	2.31	0.45
1:A:660:LYS:HB2	1:A:660:LYS:HE3	1.80	0.45
1:A:442:MET:HE3	1:A:448:ILE:HG21	1.99	0.45
1:A:311:ASN:HB3	1:A:336:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:856:TYR:C	1:A:856:TYR:CD1	2.90	0.45
1:A:71:VAL:HA	1:A:74:LEU:HG	1.98	0.45
1:A:650:ASN:HD21	1:A:653:ASP:H	1.64	0.45
1:A:163:MET:HE2	1:A:179:ASP:CB	2.47	0.45
1:A:255:GLY:HA3	1:A:275:PHE:CZ	2.52	0.45
1:A:108:MET:HG3	1:A:147:VAL:CG1	2.46	0.44
1:A:667[B]:MET:CE	1:A:783:SER:HA	2.48	0.44
1:A:548:ASP:OD2	5:A:3150:HOH:O	2.21	0.44
1:A:3:LYS:HZ1	1:A:8:HIS:CD2	2.34	0.44
1:A:3:LYS:NZ	1:A:8:HIS:CD2	2.85	0.44
1:A:348:SER:O	1:A:352:ILE:HG13	2.17	0.44
1:A:393:GLN:HE21	1:A:393:GLN:N	2.15	0.44
1:A:597:ARG:C	1:A:600:PRO:HD2	2.38	0.44
1:A:85:LEU:HG	1:A:203:PRO:CB	2.48	0.44
1:A:716:PRO:HG3	1:A:760:GLU:HB3	2.00	0.44
1:A:709:MET:SD	1:A:769:SER:HB3	2.57	0.44
1:A:566:GLU:CG	1:A:625:PRO:HG3	2.45	0.44
1:A:106:GLY:N	1:A:222:ARG:HD3	2.33	0.44
1:A:259:LEU:O	1:A:259:LEU:HD12	2.18	0.43
1:A:624:ASP:H	1:A:625:PRO:CD	2.31	0.43
1:A:624:ASP:H	1:A:625:PRO:HD2	1.83	0.43
1:A:583:ILE:HG22	1:A:583:ILE:O	2.17	0.43
1:A:409:GLN:NE2	1:A:420:TRP:HE1	2.16	0.43
1:A:832:LYS:HE3	5:A:3036:HOH:O	2.17	0.43
1:A:114:LEU:HD23	1:A:114:LEU:C	2.39	0.43
1:A:773:ASN:O	1:A:777:GLN:HG3	2.19	0.43
1:A:108:MET:H	1:A:217:SER:CB	2.31	0.43
1:A:329:VAL:O	1:A:329:VAL:HG13	2.18	0.43
1:A:298:LYS:C	1:A:300:LEU:H	2.22	0.43
1:A:276:LEU:HD21	1:A:289:ARG:HD3	2.01	0.43
1:A:402:SER:HA	1:A:403:PRO:HD2	1.88	0.43
1:A:34:MET:O	1:A:39:LEU:HB2	2.18	0.43
1:A:395:ILE:HG12	1:A:508:VAL:O	2.18	0.43
1:A:400:PRO:C	1:A:455:MET:SD	2.97	0.43
1:A:501:LEU:CD2	1:A:508:VAL:HG12	2.49	0.43
1:A:475:SER:C	1:A:477:ILE:H	2.21	0.43
1:A:114:LEU:HD23	1:A:115:GLY:N	2.33	0.43
1:A:622:LEU:O	1:A:711:PRO:HG3	2.19	0.43
1:A:43:PRO:CG	1:A:81:MET:HG2	2.48	0.42
1:A:253:THR:O	1:A:253:THR:HG22	2.19	0.42
1:A:667[B]:MET:HE1	1:A:783:SER:HA	2.00	0.42
1:A:449:LEU:HB2	1:A:501:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:825:ARG:NH2	1:A:855:ASP:OD2	2.47	0.42
1:A:8:HIS:HA	1:A:45:PHE:HA	2.01	0.42
1:A:565:THR:HA	1:A:568:MET:HG3	2.02	0.42
1:A:410:VAL:HG23	1:A:497:GLU:O	2.19	0.42
1:A:108:MET:HG3	1:A:147:VAL:HG12	2.02	0.42
1:A:418:GLU:HG3	1:A:441:GLY:HA2	2.01	0.42
1:A:4:LYS:O	1:A:4:LYS:HG2	2.20	0.42
1:A:249:ASN:CA	1:A:278:ASN:ND2	2.81	0.42
1:A:9:PHE:N	1:A:44:GLY:O	2.50	0.42
1:A:559:GLY:CA	1:A:613:MET:CE	2.96	0.41
1:A:227:ARG:HG3	1:A:232:ILE:HB	2.01	0.41
1:A:138:ARG:HG2	1:A:139:ARG:N	2.35	0.41
1:A:451:GLU:CB	1:A:477:ILE:HG23	2.50	0.41
1:A:248:GLY:O	1:A:278:ASN:HA	2.20	0.41
1:A:65:GLY:O	1:A:68:ALA:HB3	2.20	0.41
1:A:104:MET:CE	1:A:227:ARG:HH21	2.33	0.41
1:A:261:THR:O	1:A:262:ARG:HG2	2.19	0.41
1:A:86:GLY:HA3	1:A:203:PRO:HG2	2.02	0.41
1:A:93:LEU:HD21	1:A:116:LEU:HD13	2.03	0.41
1:A:62:LEU:HD23	1:A:62:LEU:C	2.41	0.41
1:A:107:MET:CE	1:A:218:TRP:HZ3	2.34	0.41
1:A:253:THR:HG23	1:A:332:ASN:ND2	2.35	0.41
1:A:107:MET:CE	1:A:218:TRP:CE3	3.04	0.41
1:A:259:LEU:C	1:A:259:LEU:CD1	2.87	0.41
1:A:584:MET:SD	1:A:657:ARG:HG2	2.60	0.41
1:A:55:TYR:HE2	1:A:216:ASN:ND2	2.19	0.41
1:A:509:ILE:HG21	1:A:513:GLN:HG3	2.02	0.40
1:A:218:TRP:CE2	1:A:237:GLY:HA2	2.56	0.40
1:A:611[A]:ARG:HH11	1:A:611[A]:ARG:HB2	1.86	0.40
1:A:668:LEU:HD21	1:A:778[B]:MET:HE1	1.98	0.40
1:A:308:LEU:N	1:A:334:LEU:HD22	2.36	0.40
1:A:395:ILE:HD13	1:A:510:LEU:HD13	2.04	0.40
1:A:667[A]:MET:O	1:A:668:LEU:HD23	2.22	0.40
1:A:401:ALA:HB1	1:A:460:ALA:CA	2.51	0.40
1:A:568:MET:HE2	1:A:605:ASP:CB	2.51	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	864/876 (99%)	809 (94%)	50 (6%)	5 (1%)	33 39

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	THR
1	A	235	LEU
1	A	236	ARG
1	A	586	PRO
1	A	624	ASP

### 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	653/707 (92%)	641 (98%)	12 (2%)	71 86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	131	ARG
1	A	278	ASN
1	A	306	ASP
1	A	390	TYR
1	A	392	ASP
1	A	393	GLN
1	A	420	TRP
1	A	599	LEU

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Mol	Chain	Res	Type
1	A	711	PRO
1	A	809	ASP
1	A	835	ILE

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	54	GLN
1	A	216	ASN
1	A	252	ASN
1	A	278	ASN
1	A	311	ASN
1	A	318	HIS
1	A	330	GLN
1	A	375	HIS
1	A	393	GLN
1	A	409	GLN
1	A	602	GLN
1	A	650	ASN
1	A	651	GLN
1	A	722	GLN
1	A	764	GLN
1	A	777	GLN

### 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 3 ligands modelled in this entry, 1 is 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$
4	PEP	A	3000	2	9,9,9	3.59	4 (44%)	13,13,13	2.50	3 (23%)
3	SO4	A	3001	-	4,4,4	0.27	0	6,6,6	0.07	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	PEP	A	3000	2	-	0/9/9/9	0/0/0/0
3	SO4	A	3001	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3000	PEP	C2-C1	8.49	1.57	1.49
4	A	3000	PEP	O2'-C1	-4.15	1.17	1.30
4	A	3000	PEP	P-O2	3.55	1.65	1.60
4	A	3000	PEP	P-O2P	-2.08	1.47	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3000	PEP	O2'-C1-C2	7.31	126.69	113.90
4	A	3000	PEP	O1-C1-C2	-3.70	116.09	121.81
4	A	3000	PEP	O2'-C1-O1	-2.71	117.22	123.62

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	862/876 (98%)	0.75	97 (11%) 6 9	19, 51, 81, 94	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	LEU	8.7
1	A	160	LEU	5.9
1	A	74	LEU	5.6
1	A	59	GLY	5.6
1	A	399	LEU	5.6
1	A	458	HIS	5.5
1	A	459	ALA	5.5
1	A	61	ALA	5.3
1	A	232	ILE	5.1
1	A	102	VAL	4.9
1	A	475	SER	4.7
1	A	477	ILE	4.6
1	A	92	LEU	4.6
1	A	58	ALA	4.5
1	A	457	SER	4.4
1	A	518	PRO	4.3
1	A	488	ILE	4.3
1	A	388	SER	4.2
1	A	229	ILE	4.1
1	A	460	ALA	4.0
1	A	432	ALA	4.0
1	A	62	LEU	3.9
1	A	455	MET	3.9
1	A	223	ALA	3.8
1	A	473	GLY	3.8
1	A	277	VAL	3.7
1	A	60	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	218	TRP	3.6
1	A	169	LEU	3.6
1	A	478	ARG	3.5
1	A	91	PRO	3.5
1	A	105	PRO	3.5
1	A	479	VAL	3.5
1	A	236	ARG	3.4
1	A	55	TYR	3.4
1	A	57	ASP	3.3
1	A	106	GLY	3.3
1	A	520	LEU	3.3
1	A	80	TYR	3.3
1	A	476	GLY	3.3
1	A	401	ALA	3.3
1	A	226	TYR	3.2
1	A	45	PHE	3.2
1	A	234	GLY	3.2
1	A	124	LEU	3.2
1	A	233	THR	3.1
1	A	67	TRP	3.1
1	A	85	LEU	3.1
1	A	290	THR	3.1
1	A	302	PRO	3.1
1	A	23	LEU	3.0
1	A	64	ALA	3.0
1	A	471	VAL	3.0
1	A	66	LEU	3.0
1	A	70	ILE	2.9
1	A	252	ASN	2.9
1	A	450	THR	2.9
1	A	172	ASP	2.9
1	A	489	GLY	2.8
1	A	132	PHE	2.8
1	A	154	SER	2.8
1	A	819[A]	PHE	2.8
1	A	451	GLU	2.7
1	A	276	LEU	2.7
1	A	230	ASN	2.7
1	A	175	LEU	2.7
1	A	291	PRO	2.6
1	A	56	GLN	2.6
1	A	461	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	586	PRO	2.5
1	A	170	LYS	2.5
1	A	519	ALA	2.5
1	A	294	LEU	2.4
1	A	222	ARG	2.4
1	A	161	GLU	2.4
1	A	300	LEU	2.4
1	A	173	THR	2.3
1	A	167	LYS	2.3
1	A	237	GLY	2.3
1	A	482	ALA	2.3
1	A	104	MET	2.3
1	A	103	SER	2.3
1	A	128	SER	2.3
1	A	297	MET	2.3
1	A	456	THR	2.2
1	A	508	VAL	2.2
1	A	289	ARG	2.1
1	A	588	LEU	2.1
1	A	517	PRO	2.1
1	A	3	LYS	2.1
1	A	126	ALA	2.1
1	A	196	GLY	2.1
1	A	207	LEU	2.1
1	A	253	THR	2.1
1	A	177	ALA	2.1
1	A	163	MET	2.0
1	A	711	PRO	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	MG	A	2000	1/1	0.21	0.81	38,38,38,38	0
4	PEP	A	3000	10/10	0.15	-1.20	38,42,45,47	0
3	SO4	A	3001	5/5	0.09	-1.88	80,80,81,81	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.