



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:48 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

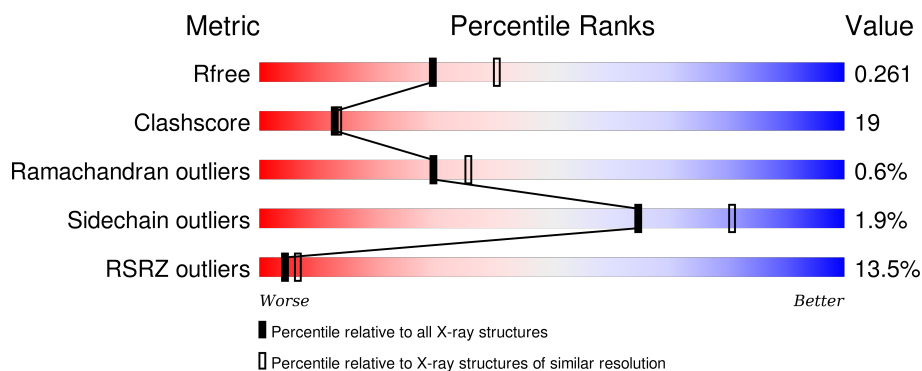
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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. 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	876	

## 2 Entry composition [i](#)

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

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

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).

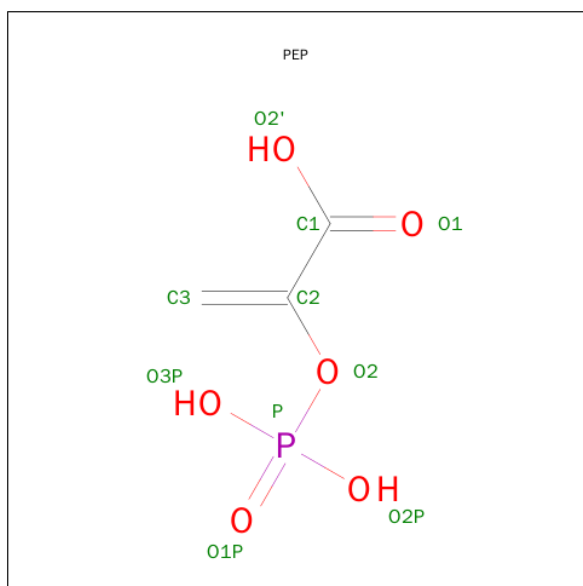
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- 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		

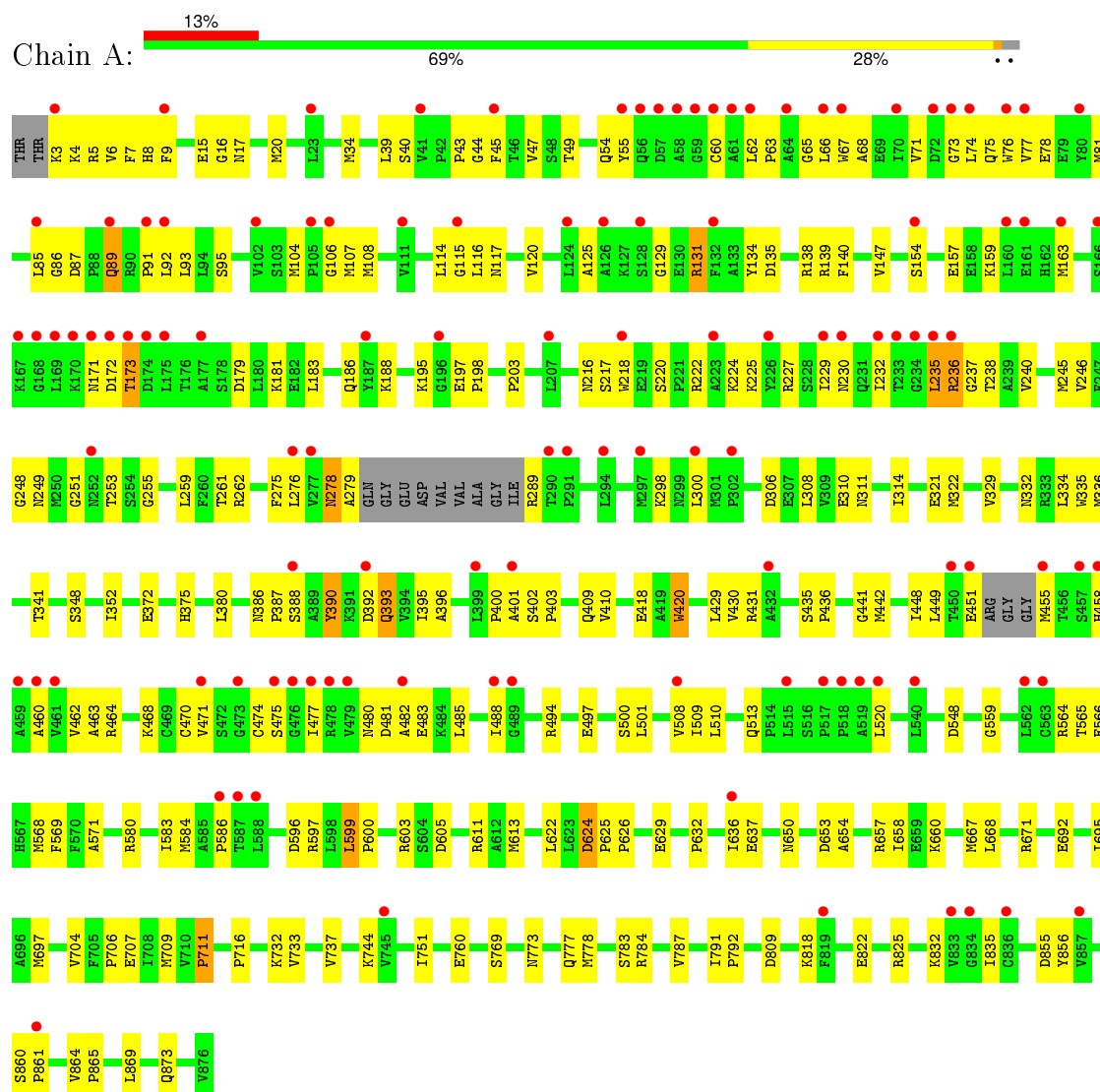
- Molecule 5 is water.

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,orthophosphate dikinase



## 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 0.231 , 0.261	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> )	0.34 , 57.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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 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	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

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 19.

All (246) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLU:H	1:A:375:HIS:CD2	2.13	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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	864/876 (99%)	809 (94%)	50 (6%)	5 (1%)	30	36

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	653/707 (92%)	641 (98%)	12 (2%)	66	82

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

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Mol	Chain	Res	Type
1	A	393	GLN
1	A	420	TRP
1	A	599	LEU
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 molecules 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	5,9,9	1.63	1 (20%)	8,13,13	1.13	2 (25%)
3	SO4	A	3001	-	4,4,4	0.22	0	6,6,6	0.08	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	-	0/5/9/9	0/0/0/0
3	SO4	A	3001	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3000	PEP	P-O2P	-2.12	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3000	PEP	C1-C2-C3	2.04	124.59	120.97
4	A	3000	PEP	P-O2-C2	2.17	127.79	122.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3000	PEP	2	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, 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%)	0.92	116 (13%) 4 6	19, 51, 81, 94	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	LEU	8.3
1	A	160	LEU	7.0
1	A	74	LEU	7.0
1	A	92	LEU	6.0
1	A	458	HIS	5.3
1	A	399	LEU	5.1
1	A	232	ILE	5.1
1	A	475	SER	5.0
1	A	59	GLY	4.9
1	A	67	TRP	4.9
1	A	388	SER	4.8
1	A	459	ALA	4.6
1	A	518	PRO	4.6
1	A	91	PRO	4.6
1	A	61	ALA	4.4
1	A	460	ALA	4.4
1	A	169	LEU	4.3
1	A	477	ILE	4.2
1	A	223	ALA	4.1
1	A	80	TYR	4.0
1	A	85	LEU	4.0
1	A	45	PHE	3.9
1	A	229	ILE	3.9
1	A	520	LEU	3.9
1	A	457	SER	3.9
1	A	488	ILE	3.9
1	A	102	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	476	GLY	3.8
1	A	432	ALA	3.7
1	A	70	ILE	3.7
1	A	473	GLY	3.7
1	A	207	LEU	3.7
1	A	586	PRO	3.7
1	A	478	ARG	3.6
1	A	163	MET	3.6
1	A	175	LEU	3.6
1	A	60	CYS	3.6
1	A	66	LEU	3.6
1	A	479	VAL	3.5
1	A	170	LYS	3.4
1	A	519	ALA	3.4
1	A	489	GLY	3.4
1	A	471	VAL	3.3
1	A	77	VAL	3.3
1	A	124	LEU	3.3
1	A	233	THR	3.2
1	A	132	PHE	3.2
1	A	218	TRP	3.2
1	A	455	MET	3.2
1	A	252	ASN	3.2
1	A	55	TYR	3.2
1	A	57	ASP	3.1
1	A	105	PRO	3.1
1	A	226	TYR	3.1
1	A	64	ALA	3.0
1	A	62	LEU	3.0
1	A	290	THR	3.0
1	A	277	VAL	3.0
1	A	276	LEU	3.0
1	A	236	ARG	3.0
1	A	302	PRO	2.9
1	A	73	GLY	2.9
1	A	234	GLY	2.9
1	A	76	TRP	2.8
1	A	58	ALA	2.8
1	A	291	PRO	2.8
1	A	172	ASP	2.8
1	A	401	ALA	2.8
1	A	111	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	562	LEU	2.7
1	A	819[A]	PHE	2.7
1	A	128	SER	2.7
1	A	167	LYS	2.7
1	A	173	THR	2.7
1	A	23	LEU	2.7
1	A	294	LEU	2.6
1	A	836[A]	CYS	2.6
1	A	300	LEU	2.6
1	A	168	GLY	2.6
1	A	154	SER	2.6
1	A	177	ALA	2.6
1	A	450	THR	2.6
1	A	515	LEU	2.5
1	A	517	PRO	2.5
1	A	230	ASN	2.5
1	A	9	PHE	2.5
1	A	392	ASP	2.5
1	A	106	GLY	2.4
1	A	196	GLY	2.4
1	A	166	SER	2.4
1	A	297	MET	2.4
1	A	833	VAL	2.4
1	A	171	ASN	2.3
1	A	540	LEU	2.3
1	A	508	VAL	2.3
1	A	857	VAL	2.3
1	A	72	ASP	2.3
1	A	41	VAL	2.2
1	A	451	GLU	2.2
1	A	834	GLY	2.2
1	A	174	ASP	2.2
1	A	563	CYS	2.2
1	A	588	LEU	2.2
1	A	56	GLN	2.1
1	A	115	GLY	2.1
1	A	89	GLN	2.1
1	A	126	ALA	2.1
1	A	861	PRO	2.1
1	A	187	TYR	2.1
1	A	482	ALA	2.1
1	A	461	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	161	GLU	2.1
1	A	3	LYS	2.1
1	A	636	ILE	2.1
1	A	587	THR	2.0
1	A	745	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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	2000	1/1	0.87	0.21	0.30	38,38,38,38	0
4	PEP	A	3000	10/10	0.96	0.16	-1.44	38,42,45,47	0
3	SO4	A	3001	5/5	0.96	0.12	-	80,80,81,81	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.