



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:34 AM UTC

PDB ID : 1VBG / pdb_00001vbg
Title : Pyruvate Phosphate Dikinase from Maize
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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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

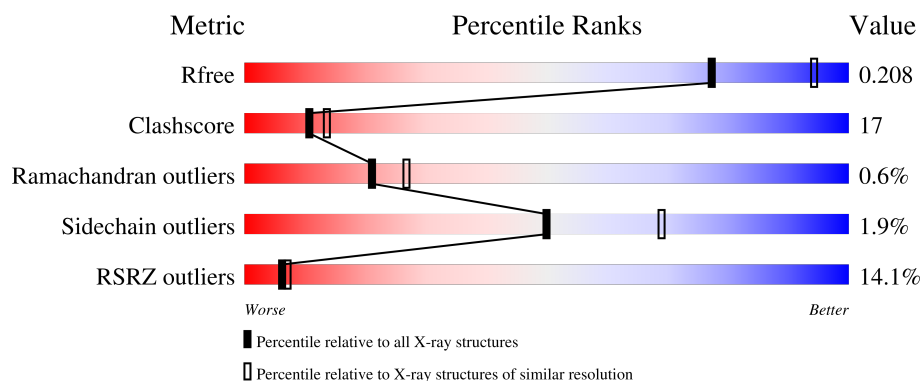
1 Overall quality at a glance

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	14% 71% 26% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6866 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	874	Total	C	N	O	S	0	8	0
			6602	4168	1145	1246	43			

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

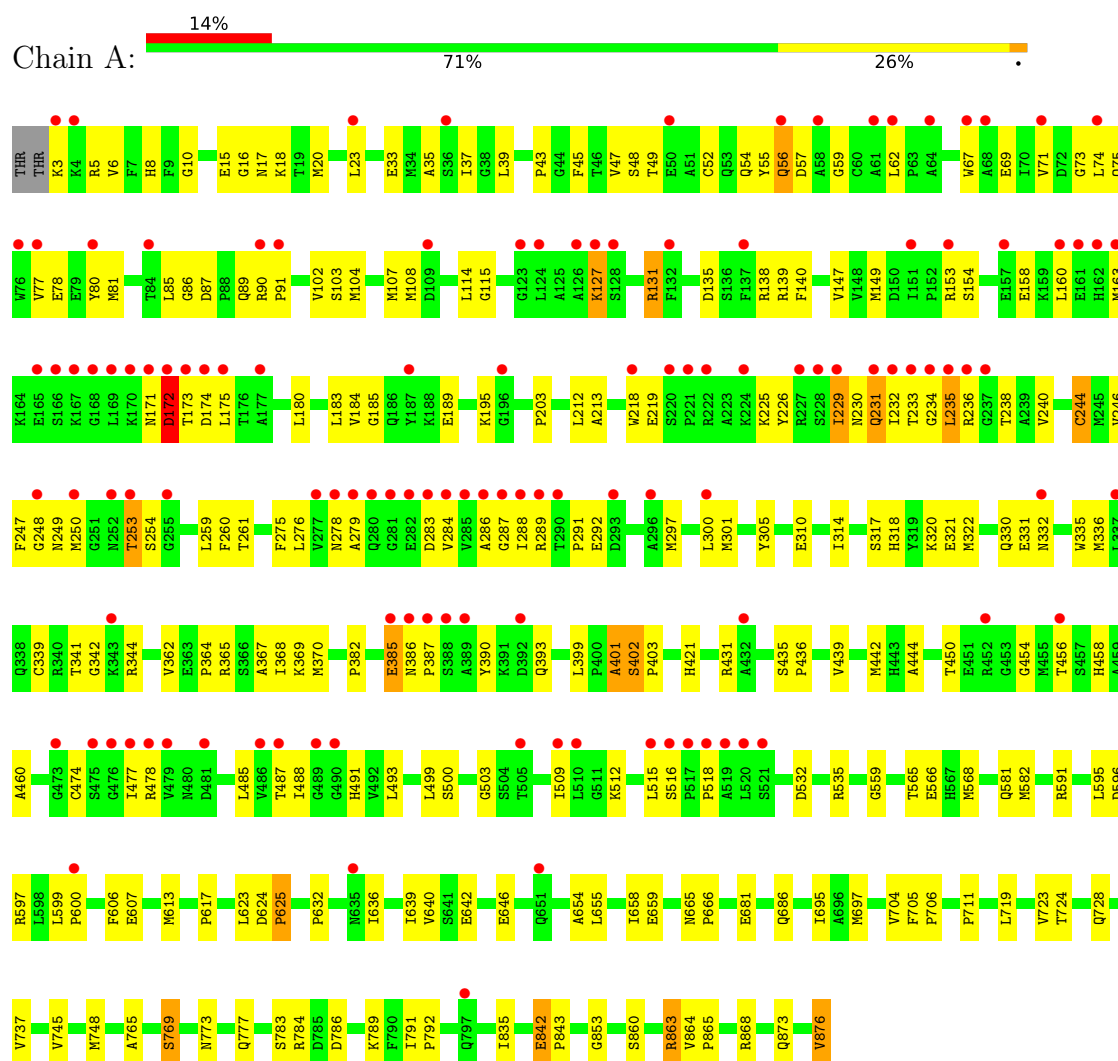
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	248	Total O 248 248	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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,orthophosphate dikinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	108.16Å 100.22Å 108.41Å 90.00° 96.53° 90.00°	Depositor
Resolution (Å)	46.03 – 2.30 46.03 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.03-2.30) 99.8 (46.03-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.237 0.210 , 0.208	Depositor DCC
R_{free} test set	2546 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6866	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.57	0/6727	0.94	15/9114 (0.2%)

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	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	GLY	N-CA-C	-7.19	104.92	115.63
1	A	625	PRO	N-CA-C	5.83	117.81	110.70
1	A	402	SER	CA-C-N	5.58	125.52	119.78
1	A	402	SER	C-N-CA	5.58	125.52	119.78
1	A	229	ILE	N-CA-C	-5.41	106.15	111.88
1	A	863	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	A	90	ARG	CA-C-N	5.30	125.22	119.76
1	A	90	ARG	C-N-CA	5.30	125.22	119.76
1	A	842	GLU	CA-C-N	5.29	126.45	119.84
1	A	842	GLU	C-N-CA	5.29	126.45	119.84
1	A	535	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	A	342	GLY	N-CA-C	5.19	118.30	111.03
1	A	401	ALA	N-CA-C	5.15	117.63	111.71
1	A	91	PRO	N-CA-C	5.06	119.03	111.14
1	A	253	THR	N-CA-C	-5.04	105.93	113.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	783	SER	Mainchain

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	6602	0	6517	219	0
2	A	1	0	0	0	0
3	A	15	0	0	0	0
4	A	248	0	0	3	0
All	All	6866	0	6517	219	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 17.

All (219) 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:108:MET:HE2	1:A:147:VAL:HG12	1.35	1.08
1:A:131:ARG:H	1:A:131:ARG:HD3	1.21	1.02
1:A:365:ARG:HG3	1:A:876:VAL:HG22	1.41	0.98
1:A:695:ILE:HG21	1:A:737:VAL:HG11	1.46	0.94
1:A:17:ASN:H	1:A:20:MET:HE3	1.33	0.93
1:A:623:LEU:H	1:A:686:GLN:HE22	1.20	0.85
1:A:442:MET:HE1	1:A:458:HIS:HE1	1.40	0.84
1:A:777:GLN:HE21	1:A:784:ARG:H	1.27	0.81
1:A:607:GLU:HB3	1:A:697:MET:HE3	1.62	0.81
1:A:226:TYR:O	1:A:230:ASN:HB2	1.81	0.80
1:A:74:LEU:HD12	1:A:75:GLN:N	1.97	0.80
1:A:439:VAL:HA	1:A:442:MET:HE3	1.61	0.78
1:A:87:ASP:OD1	1:A:89:GLN:HG2	1.83	0.78
1:A:596:ASP:O	1:A:600:PRO:HD3	1.82	0.78
1:A:230:ASN:O	1:A:232:ILE:HG13	1.84	0.77
1:A:247:PHE:H	1:A:330:GLN:NE2	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:MET:HE2	1:A:305:TYR:HA	1.67	0.77
1:A:3:LYS:HZ1	1:A:8:HIS:CE1	2.04	0.75
1:A:565:THR:HA	1:A:568:MET:HE3	1.67	0.75
1:A:47:VAL:HB	1:A:240:VAL:CG1	2.17	0.74
1:A:565:THR:HG22	1:A:568:MET:CE	2.18	0.74
1:A:17:ASN:N	1:A:20:MET:HE3	2.03	0.73
1:A:131:ARG:H	1:A:131:ARG:CD	2.00	0.72
1:A:382:PRO:HG3	1:A:518[B]:PRO:HD3	1.71	0.71
1:A:279:ALA:HB1	1:A:283:ASP:OD2	1.90	0.71
1:A:321:GLU:CG	1:A:341:THR:HG23	2.21	0.70
1:A:47:VAL:HB	1:A:240:VAL:HG12	1.73	0.70
1:A:597:ARG:O	1:A:600:PRO:HD2	1.91	0.69
1:A:478:ARG:HB2	1:A:487:THR:HG22	1.74	0.69
1:A:596:ASP:O	1:A:600:PRO:CD	2.39	0.69
1:A:370:MET:HE2	4:A:3118:HOH:O	1.91	0.69
1:A:568:MET:HE1	1:A:606:PHE:CE1	2.28	0.68
1:A:597:ARG:C	1:A:600:PRO:HD2	2.18	0.68
1:A:704:VAL:HG12	1:A:706:PRO:HD3	1.74	0.68
1:A:565:THR:HA	1:A:568:MET:CE	2.24	0.67
1:A:3:LYS:HZ1	1:A:8:HIS:CD2	2.13	0.67
1:A:135:ASP:OD1	1:A:138:ARG:NH1	2.28	0.65
1:A:3:LYS:HB3	1:A:6:VAL:O	1.96	0.65
1:A:624:ASP:HB3	1:A:625:PRO:HD3	1.77	0.65
1:A:321:GLU:HG2	1:A:341:THR:HG23	1.78	0.64
1:A:249:ASN:HA	1:A:278:ASN:HD22	1.63	0.64
1:A:276:LEU:HD11	1:A:289:ARG:HG3	1.79	0.64
1:A:259:LEU:HD12	1:A:259:LEU:C	2.23	0.63
1:A:276:LEU:HD11	1:A:289:ARG:CG	2.28	0.62
1:A:607:GLU:CB	1:A:697:MET:HE3	2.28	0.62
1:A:367:ALA:HA	1:A:370:MET:HE3	1.81	0.62
1:A:225:LYS:HB3	1:A:229:ILE:HD12	1.81	0.61
1:A:74:LEU:O	1:A:78:GLU:HG3	2.00	0.61
1:A:81:MET:HE2	1:A:244:CYS:SG	2.39	0.61
1:A:456:THR:O	1:A:456:THR:HG22	1.99	0.61
1:A:275:PHE:HE2	1:A:301:MET:HE1	1.65	0.61
1:A:229:ILE:HG22	1:A:229:ILE:O	2.00	0.61
1:A:5:ARG:HD3	1:A:69:GLU:OE2	2.01	0.60
1:A:180:LEU:O	1:A:184:VAL:HG23	2.01	0.60
1:A:246:VAL:HG11	1:A:335:TRP:CD1	2.37	0.60
1:A:163:MET:HG2	1:A:175:LEU:HD21	1.84	0.59
1:A:365:ARG:HG3	1:A:876:VAL:CG2	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:CYS:O	1:A:477:ILE:HG12	2.02	0.59
1:A:33:GLU:OE2	1:A:318:HIS:HE1	1.85	0.59
1:A:108:MET:HE1	1:A:213:ALA:CB	2.32	0.59
1:A:16:GLY:HA2	1:A:20:MET:HE1	1.83	0.59
1:A:625:PRO:HG3	4:A:3246:HOH:O	2.02	0.59
1:A:260:PHE:HD2	1:A:322:MET:HE1	1.67	0.59
1:A:229:ILE:O	1:A:230:ASN:ND2	2.36	0.58
1:A:253:THR:HG22	1:A:332:ASN:N	2.18	0.58
1:A:442:MET:HE1	1:A:458:HIS:CE1	2.31	0.58
1:A:102:VAL:HG12	1:A:103:SER:N	2.19	0.58
1:A:108:MET:CE	1:A:147:VAL:HG12	2.22	0.57
1:A:864:VAL:HB	1:A:865:PRO:HD3	1.86	0.57
1:A:500:SER:HB2	1:A:509:ILE:HB	1.87	0.57
1:A:385:GLU:HG2	1:A:516[A]:SER:HA	1.88	0.56
1:A:127:LYS:CG	1:A:250:MET:HB3	2.35	0.56
1:A:512:LYS:HG3	1:A:512:LYS:O	2.06	0.56
1:A:493:LEU:CD2	1:A:499:LEU:HD13	2.36	0.55
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.72	0.55
1:A:786:ASP:O	1:A:789:LYS:HE2	2.06	0.55
1:A:369:LYS:NZ	1:A:876:VAL:HG13	2.21	0.55
1:A:108:MET:CE	1:A:213:ALA:HB1	2.37	0.55
1:A:655:LEU:O	1:A:659:GLU:HG3	2.07	0.55
1:A:10:GLY:O	1:A:35:ALA:HB1	2.08	0.54
1:A:43:PRO:HG3	1:A:81:MET:HG2	1.90	0.54
1:A:565:THR:HG22	1:A:568:MET:HE1	1.88	0.54
1:A:85:LEU:HG	1:A:203:PRO:HB3	1.90	0.54
1:A:171:ASN:O	1:A:173:THR:N	2.41	0.54
1:A:487:THR:HA	1:A:491:HIS:O	2.08	0.53
1:A:581:GLN:HE22	1:A:597:ARG:HH12	1.55	0.53
1:A:43:PRO:HB3	1:A:80:TYR:CD2	2.44	0.53
1:A:235:LEU:O	1:A:236:ARG:HG2	2.09	0.53
1:A:6:VAL:HG22	1:A:47:VAL:HG22	1.91	0.53
1:A:85:LEU:HG	1:A:203:PRO:CB	2.38	0.53
1:A:172:ASP:C	1:A:174:ASP:H	2.17	0.52
1:A:642:GLU:O	1:A:646:GLU:HG3	2.09	0.52
1:A:104:MET:HE3	1:A:218:TRP:CH2	2.45	0.52
1:A:138:ARG:HD2	1:A:183:LEU:HD23	1.90	0.52
1:A:478:ARG:HB2	1:A:487:THR:CG2	2.38	0.52
1:A:336:MET:HE2	1:A:339:CYS:SG	2.50	0.52
1:A:723:VAL:HG22	1:A:745:VAL:HG11	1.91	0.51
1:A:232:ILE:HG22	1:A:233:THR:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:O	1:A:229:ILE:N	2.43	0.51
1:A:153:ARG:HB2	1:A:153:ARG:NH1	2.25	0.51
1:A:385:GLU:HA	1:A:516[A]:SER:OG	2.11	0.51
1:A:748:MET:HG3	1:A:769:SER:O	2.10	0.51
1:A:399:LEU:CD1	1:A:454:GLY:HA2	2.40	0.51
1:A:127:LYS:HG2	1:A:250:MET:HB3	1.92	0.51
1:A:399:LEU:HD12	1:A:454:GLY:HA2	1.92	0.51
1:A:485:LEU:HD12	1:A:485:LEU:C	2.36	0.51
1:A:234:GLY:O	1:A:235:LEU:C	2.54	0.50
1:A:632:PRO:HG2	1:A:639:ILE:HG23	1.92	0.50
1:A:566:GLU:HG3	1:A:625:PRO:HG3	1.93	0.50
1:A:253:THR:HG22	1:A:253:THR:O	2.12	0.50
1:A:276:LEU:HD13	1:A:291:PRO:HA	1.93	0.50
1:A:532:ASP:OD1	1:A:868:ARG:HD2	2.11	0.50
1:A:108:MET:HE1	1:A:213:ALA:HB1	1.93	0.50
1:A:160:LEU:C	1:A:160:LEU:HD23	2.36	0.50
1:A:300:LEU:C	1:A:301:MET:HG3	2.37	0.50
1:A:107:MET:HE1	1:A:238:THR:HB	1.92	0.49
1:A:5:ARG:HH21	1:A:54:GLN:NE2	2.11	0.49
1:A:369:LYS:HZ2	1:A:876:VAL:HG13	1.76	0.49
1:A:439:VAL:HA	1:A:442:MET:CE	2.38	0.49
1:A:431:ARG:O	1:A:450:THR:HA	2.12	0.49
1:A:104:MET:HG2	1:A:218:TRP:CZ3	2.48	0.49
1:A:261:THR:OG1	1:A:322:MET:HG2	2.13	0.49
1:A:135:ASP:O	1:A:138:ARG:HG2	2.12	0.49
1:A:56:GLN:NE2	1:A:219:GLU:HG2	2.27	0.48
1:A:791:ILE:HB	1:A:792:PRO:HD3	1.95	0.48
1:A:235:LEU:O	1:A:236:ARG:CG	2.61	0.48
1:A:18:LYS:HB3	1:A:33:GLU:HB2	1.94	0.48
1:A:87:ASP:OD1	1:A:89:GLN:CG	2.59	0.48
1:A:114:LEU:C	1:A:114:LEU:HD23	2.39	0.48
1:A:248:GLY:HA2	1:A:254:SER:HB3	1.95	0.48
1:A:3:LYS:HZ2	1:A:15:GLU:CB	2.27	0.48
1:A:364:PRO:O	1:A:368:ILE:HG12	2.14	0.48
1:A:160:LEU:HD23	1:A:160:LEU:O	2.13	0.47
1:A:3:LYS:NZ	1:A:8:HIS:CD2	2.82	0.47
1:A:57:ASP:C	1:A:59:GLY:H	2.22	0.47
1:A:719:LEU:HD21	1:A:765:ALA:HB2	1.96	0.47
1:A:127:LYS:HG3	1:A:250:MET:HB3	1.96	0.47
1:A:62:LEU:HD12	1:A:212:LEU:HD21	1.97	0.47
1:A:17:ASN:ND2	1:A:20:MET:HE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLY:O	1:A:77:VAL:HG23	2.15	0.47
1:A:114:LEU:HD23	1:A:115:GLY:N	2.30	0.47
1:A:493:LEU:HD21	1:A:499:LEU:HD13	1.97	0.46
1:A:67:TRP:O	1:A:71:VAL:HG23	2.15	0.46
1:A:3:LYS:NZ	1:A:15:GLU:CB	2.78	0.46
1:A:596:ASP:O	1:A:600:PRO:HD2	2.15	0.46
1:A:185:GLY:O	1:A:189:GLU:HG3	2.15	0.46
1:A:568:MET:HE1	1:A:606:PHE:CZ	2.49	0.46
1:A:16:GLY:HA2	1:A:20:MET:CE	2.46	0.46
1:A:565:THR:HG22	1:A:568:MET:HE3	1.96	0.46
1:A:52:CYS:O	1:A:55:TYR:HB3	2.16	0.46
1:A:86:GLY:HA3	1:A:203:PRO:HG2	1.97	0.46
1:A:636:ILE:O	1:A:640:VAL:HG23	2.15	0.46
1:A:43:PRO:CG	1:A:81:MET:HG2	2.46	0.45
1:A:365:ARG:CG	1:A:876:VAL:HG22	2.29	0.45
1:A:276:LEU:HD11	1:A:289:ARG:HG2	1.97	0.45
1:A:860:SER:OG	1:A:863:ARG:HG2	2.17	0.45
1:A:5:ARG:NH2	1:A:54:GLN:HE22	2.14	0.45
1:A:297:MET:HE2	1:A:305:TYR:CA	2.40	0.45
1:A:654:ALA:O	1:A:658:ILE:HG13	2.17	0.45
1:A:86:GLY:CA	1:A:203:PRO:HG2	2.46	0.45
1:A:331:GLU:O	1:A:332:ASN:HB2	2.15	0.45
1:A:487:THR:HG23	1:A:487:THR:O	2.15	0.45
1:A:310:GLU:O	1:A:314:ILE:HG13	2.16	0.45
1:A:724:THR:O	1:A:728:GLN:HG3	2.17	0.45
1:A:230:ASN:O	1:A:231:GLN:C	2.60	0.45
1:A:773:ASN:HD21	1:A:784:ARG:HH11	1.65	0.44
1:A:138:ARG:CG	1:A:139:ARG:N	2.80	0.44
1:A:477:ILE:HG22	1:A:488:ILE:HG23	1.99	0.44
1:A:387:PRO:HA	1:A:390:TYR:CE2	2.53	0.44
1:A:362:VAL:HG21	1:A:370:MET:HE1	1.99	0.44
1:A:108:MET:HE1	1:A:213:ALA:HB3	2.00	0.44
1:A:260:PHE:CD2	1:A:322:MET:HE1	2.49	0.44
1:A:515[A]:LEU:HD23	1:A:515[A]:LEU:HA	1.81	0.44
1:A:607:GLU:CG	1:A:697:MET:HE3	2.47	0.44
1:A:317:SER:O	1:A:320:LYS:HE2	2.18	0.43
1:A:107:MET:HE1	1:A:238:THR:CB	2.48	0.43
1:A:218:TRP:HH2	1:A:235:LEU:HD13	1.83	0.43
1:A:235:LEU:O	1:A:236:ARG:CB	2.67	0.43
1:A:286:ALA:HB3	1:A:288:ILE:HG13	2.00	0.43
1:A:87:ASP:OD1	1:A:87:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:PRO:HG3	1:A:518[B]:PRO:CD	2.45	0.43
1:A:172:ASP:C	1:A:174:ASP:N	2.72	0.42
1:A:559:GLY:HA2	1:A:613:MET:HE2	2.01	0.42
1:A:102:VAL:CG1	1:A:103:SER:N	2.82	0.42
1:A:149:MET:O	1:A:195:LYS:HE3	2.19	0.42
1:A:477:ILE:HA	1:A:487:THR:O	2.20	0.42
1:A:8:HIS:HA	1:A:45:PHE:HA	2.00	0.42
1:A:114:LEU:HA	1:A:140:PHE:CE1	2.55	0.42
1:A:387:PRO:HA	1:A:390:TYR:CD2	2.54	0.42
1:A:559:GLY:HA2	1:A:613:MET:CE	2.49	0.42
1:A:368:ILE:HG22	1:A:873:GLN:HG2	2.02	0.42
1:A:386:ASN:C	1:A:386:ASN:ND2	2.78	0.42
1:A:853:GLY:HA3	4:A:3216:HOH:O	2.20	0.42
1:A:108:MET:CE	1:A:213:ALA:CB	2.96	0.42
1:A:591:ARG:NH1	1:A:681:GLU:OE2	2.53	0.42
1:A:402:SER:HA	1:A:403:PRO:HD2	1.93	0.42
1:A:284:VAL:HG22	1:A:291:PRO:HD3	2.02	0.41
1:A:421:HIS:HB2	1:A:444:ALA:HB1	2.02	0.41
1:A:581:GLN:OE1	1:A:597:ARG:NH1	2.53	0.41
1:A:773:ASN:O	1:A:777:GLN:HG3	2.20	0.41
1:A:401:ALA:HB1	1:A:460:ALA:CB	2.49	0.41
1:A:582:MET:SD	1:A:595:LEU:HD13	2.59	0.41
1:A:37:ILE:HG13	1:A:39:LEU:HG	2.02	0.41
1:A:43:PRO:HG3	1:A:80:TYR:HD2	1.84	0.41
1:A:246:VAL:CG1	1:A:330:GLN:HB2	2.50	0.41
1:A:23:LEU:O	1:A:49:THR:HG23	2.20	0.41
1:A:402:SER:O	1:A:503:GLY:HA3	2.21	0.41
1:A:71:VAL:HA	1:A:74:LEU:HG	2.03	0.41
1:A:108:MET:HE3	1:A:213:ALA:HB1	2.02	0.41
1:A:456:THR:O	1:A:456:THR:CG2	2.67	0.41
1:A:127:LYS:HG3	1:A:250:MET:CB	2.51	0.41
1:A:154:SER:O	1:A:158:GLU:HB2	2.21	0.41
1:A:259:LEU:C	1:A:259:LEU:CD1	2.92	0.40
1:A:842:GLU:HA	1:A:843:PRO:HD3	1.90	0.40
1:A:276:LEU:HD13	1:A:291:PRO:CA	2.51	0.40
1:A:390:TYR:CD1	1:A:390:TYR:C	2.99	0.40
1:A:617:PRO:HA	1:A:705:PHE:HB2	2.03	0.40
1:A:665:ASN:HA	1:A:666:PRO:HD2	1.93	0.40
1:A:435:SER:HB2	1:A:436:PRO:HD2	2.02	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	880/876 (100%)	835 (95%)	40 (4%)	5 (1%)	21 27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	A	235	LEU
1	A	231	GLN
1	A	385	GLU
1	A	48	SER

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	681/707 (96%)	668 (98%)	13 (2%)	50 69

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	127	LYS
1	A	131	ARG
1	A	172	ASP
1	A	244	CYS
1	A	292	GLU

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Mol	Chain	Res	Type
1	A	344	ARG
1	A	393	GLN
1	A	599	LEU
1	A	711	PRO
1	A	769	SER
1	A	835	ILE
1	A	876	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	54	GLN
1	A	216	ASN
1	A	230	ASN
1	A	241	ASN
1	A	252	ASN
1	A	278	ASN
1	A	280	GLN
1	A	318	HIS
1	A	330	GLN
1	A	332	ASN
1	A	386	ASN
1	A	393	GLN
1	A	602	GLN
1	A	665	ASN
1	A	686	GLN
1	A	777	GLN
1	A	802	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	SO4	A	3000	-	4,4,4	0.33	0	6,6,6	0.13	0
3	SO4	A	3001	-	4,4,4	0.38	0	6,6,6	0.15	0
3	SO4	A	3002	-	4,4,4	0.38	0	6,6,6	0.07	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.

No monomer is involved in short contacts.

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	874/876 (99%)	0.63	123 (14%) 6 7	12, 36, 66, 81	8 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	520[A]	LEU	7.9
1	A	517[A]	PRO	6.7
1	A	521[A]	SER	6.3
1	A	286	ALA	6.3
1	A	169	LEU	6.2
1	A	168	GLY	6.1
1	A	518[A]	PRO	5.3
1	A	80	TYR	5.1
1	A	234	GLY	5.1
1	A	284	VAL	4.6
1	A	127	LYS	4.5
1	A	519[A]	ALA	4.4
1	A	229	ILE	4.4
1	A	165	GLU	4.4
1	A	300	LEU	4.3
1	A	285	VAL	4.2
1	A	475	SER	4.2
1	A	160	LEU	4.2
1	A	289	ARG	4.1
1	A	288	ILE	4.1
1	A	161	GLU	4.1
1	A	175	LEU	4.1
1	A	232	ILE	4.0
1	A	290	THR	3.9
1	A	162	HIS	3.9
1	A	481	ASP	3.8
1	A	173	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	170	LYS	3.6
1	A	287	GLY	3.6
1	A	490	GLY	3.6
1	A	235	LEU	3.6
1	A	58	ALA	3.6
1	A	171	ASN	3.5
1	A	386	ASN	3.5
1	A	163	MET	3.4
1	A	233	THR	3.4
1	A	296	ALA	3.4
1	A	432	ALA	3.4
1	A	515[A]	LEU	3.4
1	A	283	ASP	3.3
1	A	128	SER	3.3
1	A	174	ASP	3.3
1	A	157	GLU	3.3
1	A	218	TRP	3.2
1	A	489	GLY	3.2
1	A	177	ALA	3.1
1	A	231	GLN	3.1
1	A	487	THR	3.1
1	A	172	ASP	3.0
1	A	237	GLY	3.0
1	A	473	GLY	3.0
1	A	222	ARG	3.0
1	A	253	THR	3.0
1	A	228	SER	3.0
1	A	476	GLY	3.0
1	A	4	LYS	3.0
1	A	516[A]	SER	3.0
1	A	389	ALA	2.9
1	A	250	MET	2.9
1	A	124	LEU	2.9
1	A	74	LEU	2.9
1	A	153	ARG	2.8
1	A	56	GLN	2.8
1	A	221	PRO	2.8
1	A	282	GLU	2.7
1	A	277	VAL	2.7
1	A	126	ALA	2.6
1	A	3	LYS	2.6
1	A	167	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	280	GLN	2.6
1	A	71	VAL	2.6
1	A	456	THR	2.6
1	A	166	SER	2.6
1	A	90	ARG	2.6
1	A	332	ASN	2.6
1	A	635	ASN	2.6
1	A	509	ILE	2.5
1	A	236	ARG	2.5
1	A	281	GLY	2.5
1	A	651	GLN	2.5
1	A	187	TYR	2.5
1	A	50	GLU	2.4
1	A	220	SER	2.4
1	A	61	ALA	2.4
1	A	196	GLY	2.4
1	A	248	GLY	2.4
1	A	132	PHE	2.4
1	A	151	ILE	2.4
1	A	279	ALA	2.3
1	A	67	TRP	2.3
1	A	23	LEU	2.3
1	A	252	ASN	2.3
1	A	387	PRO	2.3
1	A	486	VAL	2.3
1	A	91	PRO	2.2
1	A	76	TRP	2.2
1	A	797	GLN	2.2
1	A	224	LYS	2.2
1	A	477	ILE	2.2
1	A	77	VAL	2.2
1	A	388	SER	2.2
1	A	68	ALA	2.2
1	A	478	ARG	2.2
1	A	385	GLU	2.2
1	A	64	ALA	2.2
1	A	505	THR	2.2
1	A	452	ARG	2.1
1	A	337	LEU	2.1
1	A	510	LEU	2.1
1	A	479	VAL	2.1
1	A	343	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	109	ASP	2.1
1	A	278	ASN	2.1
1	A	392	ASP	2.1
1	A	137	PHE	2.1
1	A	293	ASP	2.1
1	A	600	PRO	2.1
1	A	123	GLY	2.1
1	A	36	SER	2.1
1	A	62	LEU	2.1
1	A	255	GLY	2.1
1	A	84	THR	2.0
1	A	227	ARG	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	3002	5/5	0.84	0.13	89,89,91,92	0
3	SO4	A	3001	5/5	0.98	0.11	31,37,39,47	0
2	MG	A	2000	1/1	0.99	0.02	14,14,14,14	0
3	SO4	A	3000	5/5	0.99	0.05	22,24,25,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.