



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:20 PM UTC

PDB ID : 8IAW / pdb_00008iaw
Title : Crystal structure of Streptococcus pneumoniae pyruvate kinase in complex with phosphoenolpyruvate
Authors : Nakashima, R.; Taguchi, A.
Deposited on : 2023-02-09
Resolution : 2.89 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

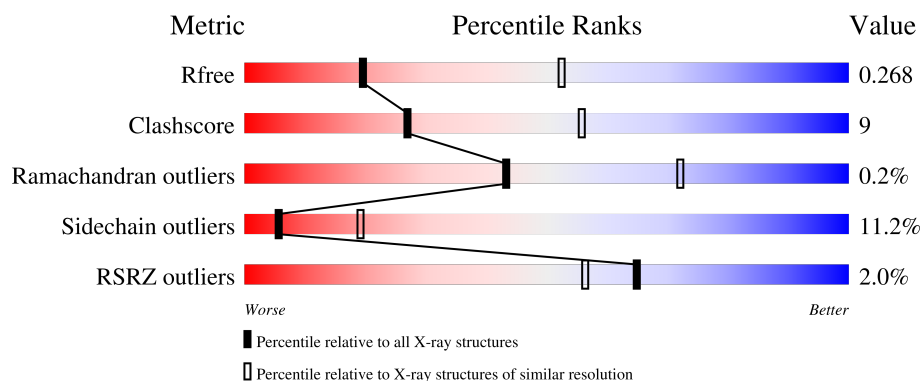
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	521	 2% 72% 20% . .
1	B	521	 2% 73% 22% . .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7753 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 kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			
1	B	501	Total	C	N	O	S	0	0	0
			3840	2399	664	760	17			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8DQ84
A	-18	GLY	-	expression tag	UNP Q8DQ84
A	-17	SER	-	expression tag	UNP Q8DQ84
A	-16	SER	-	expression tag	UNP Q8DQ84
A	-15	HIS	-	expression tag	UNP Q8DQ84
A	-14	HIS	-	expression tag	UNP Q8DQ84
A	-13	HIS	-	expression tag	UNP Q8DQ84
A	-12	HIS	-	expression tag	UNP Q8DQ84
A	-11	HIS	-	expression tag	UNP Q8DQ84
A	-10	HIS	-	expression tag	UNP Q8DQ84
A	-9	SER	-	expression tag	UNP Q8DQ84
A	-8	SER	-	expression tag	UNP Q8DQ84
A	-7	GLY	-	expression tag	UNP Q8DQ84
A	-6	LEU	-	expression tag	UNP Q8DQ84
A	-5	VAL	-	expression tag	UNP Q8DQ84
A	-4	PRO	-	expression tag	UNP Q8DQ84
A	-3	ARG	-	expression tag	UNP Q8DQ84
A	-2	GLY	-	expression tag	UNP Q8DQ84
A	-1	SER	-	expression tag	UNP Q8DQ84
A	0	HIS	-	expression tag	UNP Q8DQ84
B	1	MET	-	initiating methionine	UNP Q8DQ84
B	2	GLY	-	expression tag	UNP Q8DQ84
B	3	SER	-	expression tag	UNP Q8DQ84
B	4	SER	-	expression tag	UNP Q8DQ84
B	5	HIS	-	expression tag	UNP Q8DQ84

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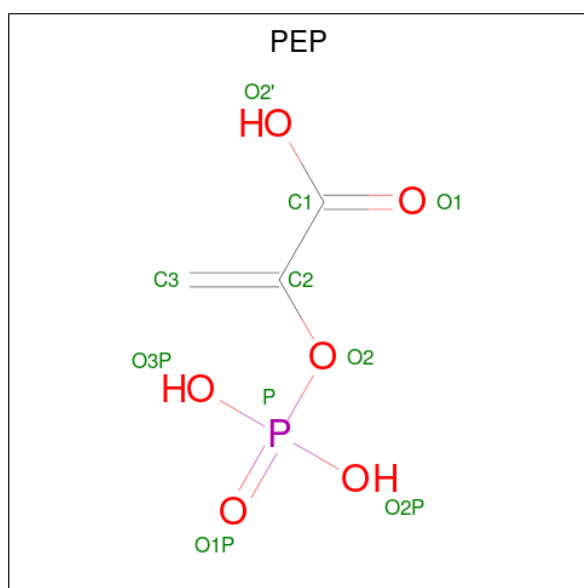
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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP Q8DQ84
B	7	HIS	-	expression tag	UNP Q8DQ84
B	8	HIS	-	expression tag	UNP Q8DQ84
B	9	HIS	-	expression tag	UNP Q8DQ84
B	10	HIS	-	expression tag	UNP Q8DQ84
B	11	SER	-	expression tag	UNP Q8DQ84
B	12	SER	-	expression tag	UNP Q8DQ84
B	13	GLY	-	expression tag	UNP Q8DQ84
B	14	LEU	-	expression tag	UNP Q8DQ84
B	15	VAL	-	expression tag	UNP Q8DQ84
B	16	PRO	-	expression tag	UNP Q8DQ84
B	17	ARG	-	expression tag	UNP Q8DQ84
B	18	GLY	-	expression tag	UNP Q8DQ84
B	19	SER	-	expression tag	UNP Q8DQ84
B	20	HIS	-	expression tag	UNP Q8DQ84

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: C₃H₅O₆P).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

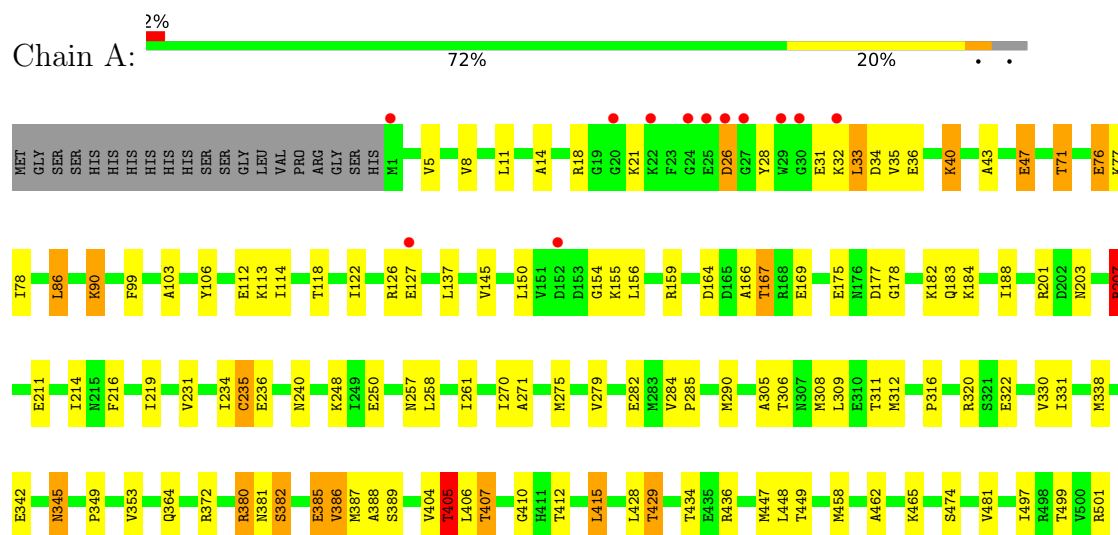
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	15	Total	O	0	0
			15	15		

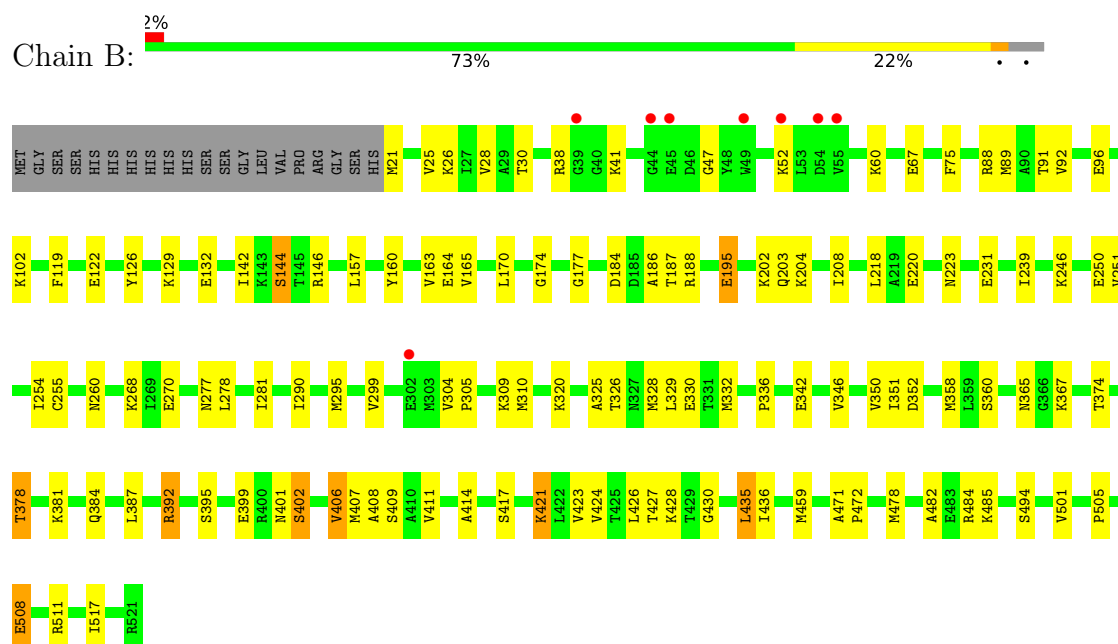
3 Residue-property plots [i](#)

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 kinase



• Molecule 1: Pyruvate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.06Å 110.37Å 130.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.89 48.58 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.58-2.89) 99.7 (48.58-2.89)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.241 , 0.273 0.238 , 0.268	Depositor DCC
R_{free} test set	1586 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7753	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0727e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	1.05	0/3885	1.51	6/5238 (0.1%)
1	B	1.04	0/3885	1.49	4/5238 (0.1%)
All	All	1.04	0/7770	1.50	10/10476 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	THR	CB-CA-C	-7.05	94.65	109.38
1	A	26	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	47	GLY	CA-C-N	5.34	127.38	120.44
1	B	47	GLY	C-N-CA	5.34	127.38	120.44
1	A	235	CYS	CA-C-N	5.11	127.08	120.44
1	A	235	CYS	C-N-CA	5.11	127.08	120.44
1	A	47	GLU	CB-CG-CD	5.10	121.27	112.60
1	A	207	ARG	CG-CD-NE	-5.10	100.79	112.00
1	B	511	ARG	CA-C-N	5.02	128.23	121.05
1	B	511	ARG	C-N-CA	5.02	128.23	121.05

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	3840	0	3888	82	1
1	B	3840	0	3885	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	2	1	0
3	B	10	0	2	0	0
4	A	15	0	0	1	0
4	B	15	0	0	0	0
5	A	6	0	0	0	0
5	B	15	0	0	0	0
All	All	7753	0	7777	142	1

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 9.

All (142) 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:429:THR:HG21	1:A:434:THR:HG22	1.61	0.83
1:B:426:LEU:HD22	1:B:478:MET:HG2	1.64	0.80
1:A:429:THR:HG21	1:A:434:THR:CG2	2.18	0.74
1:B:218:LEU:HD21	1:B:223:ASN:HD22	1.54	0.73
1:B:309:LYS:HE3	1:B:392:ARG:HH11	1.55	0.71
1:A:406:LEU:HD22	1:A:458:MET:HG2	1.71	0.71
1:B:332:MET:HE3	1:B:336:PRO:O	1.91	0.69
1:A:342:GLU:H	1:A:342:GLU:CD	2.01	0.69
1:A:106:TYR:CD1	1:A:126:ARG:HG3	2.27	0.68
1:B:325:ALA:HB1	1:B:358:MET:HE2	1.76	0.68
1:B:295:MET:O	1:B:299:VAL:HG22	1.95	0.67
1:A:248:LYS:HE2	1:A:250:GLU:OE2	1.95	0.67
1:B:268:LYS:HE2	1:B:270:GLU:OE2	1.95	0.66
1:B:223:ASN:HD22	1:B:254:ILE:HD11	1.60	0.66
1:B:328:MET:HE3	1:B:346:VAL:HG22	1.76	0.66
1:A:312:MET:HE3	1:A:316:PRO:O	1.95	0.66
1:B:351:ILE:HG22	1:B:392:ARG:HH21	1.61	0.65
1:A:275:MET:O	1:A:279:VAL:HG22	1.97	0.65
1:B:309:LYS:CE	1:B:392:ARG:HH11	2.11	0.64
1:A:305:ALA:HB1	1:A:338:MET:HE2	1.80	0.64
1:B:96:GLU:OE1	1:B:102:LYS:HA	1.99	0.63
1:B:75:PHE:CE1	1:B:89:MET:HG2	2.34	0.62
1:A:126:ARG:NH2	1:A:127:GLU:OE2	2.31	0.62
1:B:170:LEU:HB3	1:B:174:GLY:HA2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:THR:OG1	1:A:410:GLY:N	2.34	0.61
1:B:351:ILE:CG2	1:B:392:ARG:HH21	2.15	0.60
1:A:387:MET:HE1	1:B:517:ILE:HG13	1.84	0.59
1:B:329:LEU:HD23	1:B:342:GLU:HB3	1.85	0.59
1:A:203:ASN:HD22	1:A:234:ILE:HD11	1.66	0.59
1:A:150:LEU:HB3	1:A:154:GLY:HA2	1.85	0.58
1:B:223:ASN:ND2	1:B:254:ILE:HD11	2.17	0.58
1:A:497:ILE:HG13	1:B:407:MET:HE1	1.84	0.58
1:A:203:ASN:ND2	1:A:234:ILE:HD11	2.20	0.57
1:B:38:ARG:O	1:B:41:LYS:HB2	2.05	0.56
1:A:257:ASN:O	1:A:261:ILE:HG13	2.05	0.56
1:A:407:THR:OG1	1:A:410:GLY:CA	2.53	0.56
1:A:90:LYS:HE2	1:A:201:ARG:NH1	2.21	0.56
1:A:86:LEU:HD12	1:A:216:PHE:HB2	1.87	0.56
1:A:405:THR:CG2	1:A:412:THR:CG2	2.83	0.56
1:B:26:LYS:HD2	1:B:459:MET:O	2.07	0.55
1:A:497:ILE:CG1	1:B:407:MET:HE1	2.36	0.55
1:A:331:ILE:HG22	1:A:372:ARG:NH2	2.22	0.54
1:B:277:ASN:O	1:B:281:ILE:HG13	2.06	0.54
1:B:119:PHE:CD2	1:B:144:SER:HB3	2.43	0.54
1:B:309:LYS:NZ	1:B:392:ARG:HH11	2.06	0.54
1:A:167:THR:HB	1:A:169:GLU:HG3	1.89	0.54
1:A:159:ARG:HB2	1:A:175:GLU:OE1	2.08	0.53
1:A:203:ASN:HD21	1:A:207:ARG:NH2	2.05	0.53
1:B:424:VAL:HG11	1:B:482:ALA:HB1	1.89	0.53
1:A:404:VAL:HG11	1:A:462:ALA:HB1	1.91	0.53
1:B:408:ALA:HB2	1:B:435:LEU:CD1	2.38	0.53
1:B:402:SER:O	1:B:406:VAL:HG13	2.08	0.53
1:A:387:MET:HE1	1:B:517:ILE:CG1	2.39	0.53
1:A:164:ASP:OD1	1:A:166:ALA:HB3	2.10	0.52
1:A:235:CYS:HB3	1:A:240:ASN:O	2.10	0.52
1:B:126:TYR:CG	1:B:146:ARG:HG3	2.44	0.52
1:B:160:TYR:CE2	1:B:188:ARG:HA	2.45	0.52
1:B:427:THR:OG1	1:B:430:GLY:N	2.40	0.52
1:A:497:ILE:HD12	1:B:407:MET:HE1	1.92	0.52
1:A:382:SER:O	1:A:386:VAL:HG13	2.10	0.52
1:A:405:THR:HG21	1:A:412:THR:CG2	2.40	0.52
1:B:408:ALA:HB2	1:B:435:LEU:HD13	1.91	0.51
1:A:497:ILE:CD1	1:B:407:MET:HE1	2.40	0.51
1:B:426:LEU:CD2	1:B:472:PRO:HG3	2.41	0.51
1:B:25:VAL:HG21	1:B:350:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LEU:HD13	1:A:178:GLY:HA3	1.92	0.50
1:A:219:ILE:HG12	1:A:231:VAL:HG21	1.94	0.50
1:A:18:ARG:HG3	1:A:28:TYR:CE2	2.46	0.50
1:A:387:MET:HE1	1:B:517:ILE:CD1	2.42	0.49
1:B:427:THR:OG1	1:B:430:GLY:CA	2.59	0.49
1:A:382:SER:OG	1:A:385:GLU:HG2	2.12	0.49
1:A:349:PRO:O	1:A:353:VAL:HG23	2.13	0.49
1:B:239:ILE:HG12	1:B:251:VAL:HG21	1.93	0.49
1:A:86:LEU:HD12	1:A:216:PHE:CB	2.42	0.49
1:B:255:CYS:HB3	1:B:260:ASN:O	2.11	0.49
1:A:405:THR:HG23	1:A:412:THR:HG21	1.95	0.49
1:A:380:ARG:O	1:B:417:SER:HB3	2.13	0.49
1:A:5:VAL:HG21	1:A:330:VAL:HG22	1.95	0.48
1:A:499:THR:O	1:A:501:ARG:NH1	2.45	0.48
1:A:407:THR:OG1	1:A:410:GLY:HA2	2.13	0.48
1:B:304:VAL:N	1:B:305:PRO:CD	2.76	0.48
1:A:33:LEU:C	1:A:33:LEU:HD12	2.38	0.48
1:B:126:TYR:CD1	1:B:146:ARG:HG3	2.49	0.48
1:A:405:THR:CG2	1:A:412:THR:HG21	2.44	0.48
1:A:284:VAL:N	1:A:285:PRO:CD	2.76	0.47
1:A:106:TYR:CG	1:A:126:ARG:HG3	2.50	0.47
1:A:407:THR:OG1	4:A:603:SO4:O3	2.27	0.47
1:A:387:MET:HE1	1:B:517:ILE:HD12	1.97	0.47
1:A:8:VAL:HG12	1:A:338:MET:HG3	1.96	0.47
1:B:423:VAL:HG11	1:B:436:ILE:HG21	1.97	0.47
1:B:505:PRO:HG2	1:B:508:GLU:HB2	1.97	0.46
1:B:421:LYS:HA	1:B:421:LYS:HE2	1.97	0.46
1:A:309:LEU:HD23	1:A:322:GLU:HB3	1.98	0.46
1:B:88:ARG:O	1:B:92:VAL:HG23	2.16	0.46
1:A:8:VAL:O	1:A:338:MET:HA	2.15	0.46
1:A:342:GLU:OE2	1:A:342:GLU:N	2.40	0.46
1:A:405:THR:HG21	1:A:412:THR:HB	1.97	0.46
1:B:330:GLU:HA	1:B:330:GLU:OE1	2.17	0.45
1:A:497:ILE:HD12	1:B:407:MET:CE	2.45	0.45
1:B:28:VAL:O	1:B:358:MET:HA	2.17	0.45
1:A:203:ASN:OD1	1:A:207:ARG:NH2	2.41	0.44
1:A:14:ALA:HB2	1:A:345:ASN:HA	1.99	0.44
1:A:271:ALA:HB1	3:A:602:PEP:C1	2.48	0.44
1:A:33:LEU:HD12	1:A:34:ASP:N	2.33	0.44
1:A:43:ALA:O	1:A:47:GLU:HG3	2.18	0.44
1:B:352:ASP:OD1	1:B:392:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:VAL:HG13	1:A:71:THR:HG23	2.00	0.43
1:A:258:LEU:CD2	1:A:290:MET:HE2	2.48	0.43
1:B:204:LYS:HA	1:B:204:LYS:HD2	1.85	0.43
1:A:258:LEU:HD23	1:A:290:MET:CE	2.49	0.43
1:A:311:THR:HG23	1:A:322:GLU:OE1	2.18	0.43
1:A:388:ALA:HB2	1:A:415:LEU:HD13	1.99	0.43
1:B:426:LEU:HD23	1:B:472:PRO:HG3	2.01	0.43
1:B:352:ASP:OD1	1:B:392:ARG:CZ	2.66	0.43
1:B:471:ALA:HA	1:B:472:PRO:HD3	1.92	0.43
1:A:405:THR:HG23	1:A:412:THR:CG2	2.49	0.43
1:B:223:ASN:ND2	1:B:254:ILE:CD1	2.80	0.43
1:A:331:ILE:CG2	1:A:372:ARG:NH2	2.82	0.43
1:A:429:THR:CG2	1:A:434:THR:CG2	2.91	0.43
1:B:278:LEU:CD2	1:B:310:MET:HE3	2.49	0.43
1:A:99:PHE:HB2	1:A:103:ALA:O	2.19	0.42
1:B:30:THR:OG1	1:B:360:SER:HA	2.19	0.42
1:B:374:THR:O	1:B:378:THR:OG1	2.34	0.42
1:A:40:LYS:HE3	1:A:78:ILE:HG21	2.01	0.42
1:B:381:LYS:O	1:B:384:GLN:HG2	2.19	0.42
1:B:184:ASP:OD1	1:B:186:ALA:HB3	2.20	0.42
1:A:167:THR:CB	1:A:169:GLU:HG3	2.49	0.42
1:B:485:LYS:HA	1:B:485:LYS:HD2	1.88	0.41
1:A:404:VAL:CG1	1:A:462:ALA:HB1	2.48	0.41
1:B:424:VAL:CG1	1:B:482:ALA:HB1	2.50	0.41
1:A:428:LEU:HD23	1:A:447:MET:HB3	2.01	0.41
1:A:342:GLU:CD	1:A:342:GLU:N	2.72	0.41
1:B:75:PHE:CZ	1:B:89:MET:HG2	2.55	0.41
1:A:465:LYS:HA	1:A:465:LYS:HD2	1.86	0.41
1:B:177:GLY:C	1:B:195:GLU:HG3	2.46	0.41
1:A:203:ASN:CG	1:A:207:ARG:HH21	2.27	0.41
1:B:427:THR:OG1	1:B:430:GLY:HA2	2.21	0.41
1:A:18:ARG:O	1:A:21:LYS:HB2	2.21	0.41
1:B:411:VAL:O	1:B:414:ALA:HB3	2.21	0.41
1:A:76:GLU:OE1	1:A:436:ARG:NH2	2.55	0.40
1:A:11:LEU:HD23	1:A:11:LEU:HA	1.78	0.40
1:B:119:PHE:CE2	1:B:144:SER:HB3	2.57	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ARG:NH2	1:A:372:ARG:NH2[2_545]	2.14	0.06

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	499/521 (96%)	486 (97%)	12 (2%)	1 (0%)	43	72
1	B	499/521 (96%)	483 (97%)	15 (3%)	1 (0%)	43	72
All	All	998/1042 (96%)	969 (97%)	27 (3%)	2 (0%)	43	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	THR
1	B	326	THR

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	411/428 (96%)	362 (88%)	49 (12%)	5	16
1	B	411/428 (96%)	368 (90%)	43 (10%)	6	22
All	All	822/856 (96%)	730 (89%)	92 (11%)	6	19

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	31	GLU
1	A	32	LYS
1	A	33	LEU
1	A	36	GLU
1	A	40	LYS
1	A	71	THR
1	A	76	GLU
1	A	77	LYS
1	A	86	LEU
1	A	90	LYS
1	A	112	GLU
1	A	113	LYS
1	A	114	ILE
1	A	118	THR
1	A	122	ILE
1	A	137	LEU
1	A	145	VAL
1	A	155	LYS
1	A	167	THR
1	A	177	ASP
1	A	182	LYS
1	A	183	GLN
1	A	184	LYS
1	A	188	ILE
1	A	207	ARG
1	A	211	GLU
1	A	214	ILE
1	A	236	GLU
1	A	270	ILE
1	A	282	GLU
1	A	308	MET
1	A	320	ARG
1	A	345	ASN
1	A	364	GLN
1	A	380	ARG
1	A	381	ASN
1	A	382	SER
1	A	385	GLU
1	A	386	VAL
1	A	389	SER
1	A	405	THR
1	A	407	THR

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Mol	Chain	Res	Type
1	A	415	LEU
1	A	429	THR
1	A	448	LEU
1	A	449	THR
1	A	474	SER
1	A	481	VAL
1	B	21	MET
1	B	52	LYS
1	B	60	LYS
1	B	67	GLU
1	B	91	THR
1	B	122	GLU
1	B	129	LYS
1	B	132	GLU
1	B	142	ILE
1	B	144	SER
1	B	157	LEU
1	B	163	VAL
1	B	164	GLU
1	B	165	VAL
1	B	187	THR
1	B	195	GLU
1	B	202	LYS
1	B	203	GLN
1	B	208	ILE
1	B	220	GLU
1	B	231	GLU
1	B	246	LYS
1	B	250	GLU
1	B	290	ILE
1	B	320	LYS
1	B	365	ASN
1	B	367	LYS
1	B	378	THR
1	B	387	LEU
1	B	392	ARG
1	B	395	SER
1	B	399	GLU
1	B	401	ASN
1	B	402	SER
1	B	406	VAL
1	B	409	SER

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Mol	Chain	Res	Type
1	B	421	LYS
1	B	428	LYS
1	B	435	LEU
1	B	484	ARG
1	B	494	SER
1	B	501	VAL
1	B	508	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	HIS
1	A	63	GLN
1	A	362	ASN
1	A	381	ASN
1	A	441	ASN
1	B	82	HIS
1	B	223	ASN
1	B	262	HIS
1	B	273	GLN
1	B	348	ASN
1	B	401	ASN
1	B	461	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	SO4	B	604	-	4,4,4	0.93	0	6,6,6	0.12	0
4	SO4	A	604	-	4,4,4	0.34	0	6,6,6	0.12	0
3	PEP	A	602	2	9,9,9	3.02	3 (33%)	11,13,13	1.90	2 (18%)
4	SO4	A	605	-	4,4,4	0.26	0	6,6,6	0.15	0
4	SO4	A	603	-	4,4,4	0.34	0	6,6,6	0.16	0
4	SO4	B	603	-	4,4,4	0.33	0	6,6,6	0.11	0
3	PEP	B	602	2	9,9,9	3.19	3 (33%)	11,13,13	2.06	4 (36%)
4	SO4	B	605	-	4,4,4	0.29	0	6,6,6	0.11	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
3	PEP	B	602	2	-	3/9/9/9	-
3	PEP	A	602	2	-	3/9/9/9	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	PEP	C2-C1	-8.36	1.41	1.49
3	A	602	PEP	C2-C1	-7.66	1.41	1.49
3	A	602	PEP	C3-C2	3.85	1.42	1.31
3	B	602	PEP	C3-C2	3.43	1.41	1.31
3	B	602	PEP	O2'-C1	-2.34	1.24	1.30
3	A	602	PEP	O2'-C1	-2.20	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	PEP	O2-C2-C3	-4.28	116.68	124.85
3	B	602	PEP	O2-C2-C3	-4.27	116.68	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	602	PEP	C3-C2-C1	4.16	130.41	122.73
3	B	602	PEP	O1-C1-C2	-3.22	116.93	121.79
3	B	602	PEP	C3-C2-C1	2.71	127.74	122.73
3	B	602	PEP	O2'-C1-C2	2.27	117.77	113.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	PEP	O2'-C1-C2-O2
3	A	602	PEP	O1-C1-C2-O2
3	B	602	PEP	O1-C1-C2-O2
3	B	602	PEP	O2'-C1-C2-O2
3	A	602	PEP	C2-O2-P-O1P
3	B	602	PEP	C2-O2-P-O1P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PEP	1	0
4	A	603	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	501/521 (96%)	0.21	12 (2%) 59 50	30, 54, 87, 104	0
1	B	501/521 (96%)	0.07	8 (1%) 70 62	25, 47, 78, 107	0
All	All	1002/1042 (96%)	0.14	20 (1%) 65 56	25, 51, 83, 107	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	30	GLY	5.3
1	B	302	GLU	5.1
1	A	1	MET	3.9
1	A	26	ASP	3.1
1	A	29	TRP	2.7
1	A	27	GLY	2.7
1	A	20	GLY	2.6
1	A	25	GLU	2.4
1	B	39	GLY	2.4
1	B	54	ASP	2.4
1	B	49	TRP	2.3
1	A	24	GLY	2.3
1	A	32	LYS	2.3
1	B	52	LYS	2.3
1	A	127	GLU	2.2
1	A	22	LYS	2.2
1	B	55	VAL	2.1
1	B	44	GLY	2.1
1	B	45	GLU	2.1
1	A	152	ASP	2.1

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
4	SO4	A	604	5/5	0.91	0.10	63,66,75,78	0
4	SO4	B	604	5/5	0.92	0.12	52,54,55,55	0
4	SO4	A	603	5/5	0.96	0.08	42,50,51,51	0
3	PEP	A	602	10/10	0.96	0.10	48,56,72,72	0
4	SO4	B	603	5/5	0.96	0.07	36,36,41,43	0
3	PEP	B	602	10/10	0.96	0.07	44,52,64,69	0
4	SO4	B	605	5/5	0.96	0.09	63,67,73,73	0
4	SO4	A	605	5/5	0.97	0.07	40,41,46,46	0
2	MG	A	601	1/1	0.99	0.04	32,32,32,32	0
2	MG	B	601	1/1	0.99	0.04	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.