



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:23 PM UTC

PDB ID : 4HAO / pdb_00004hao
Title : Crystal Structure of Inorganic Polyphosphate/ATP-NAD Kinase from *Yersinia pestis* CO92
Authors : Kim, Y.; Maltseva, N.; Jedrzejczak, R.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-09-27
Resolution : 2.55 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

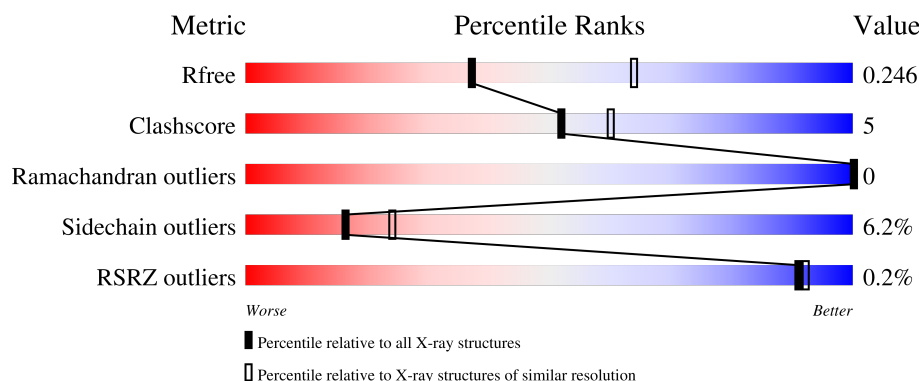
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	304	 78% 14% • 7%
1	B	304	 77% 15% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4553 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.

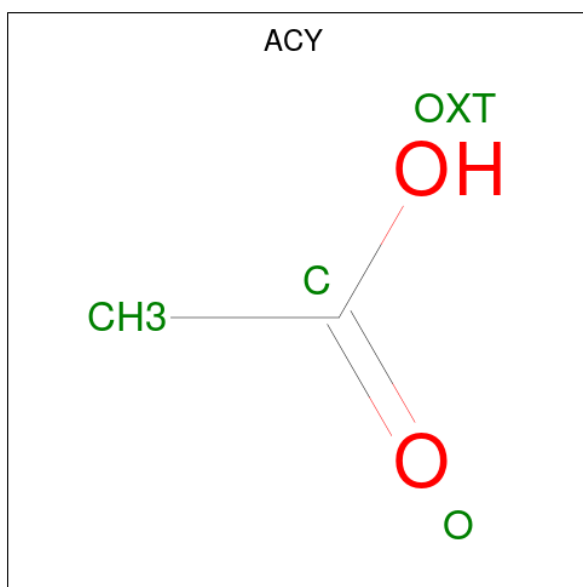
- Molecule 1 is a protein called Probable inorganic polyphosphate/ATP-NAD kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	2	0
			2211	1409	381	415	6			
1	B	284	Total	C	N	O	S	0	3	0
			2236	1423	392	415	6			

There are 22 discrepancies between the modelled and reference sequences:

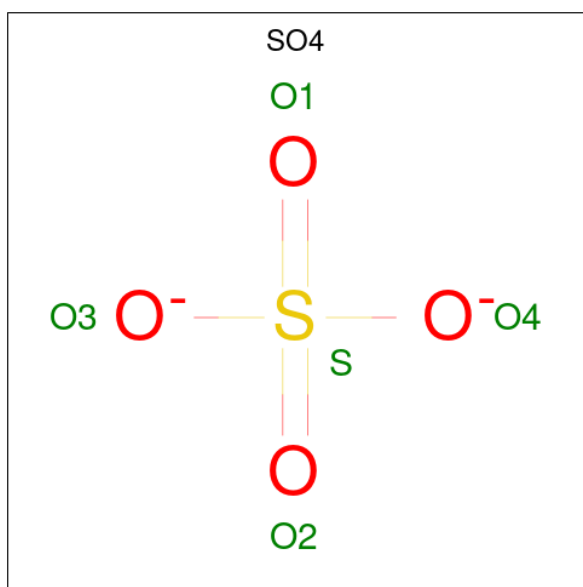
Chain	Residue	Modelled	Actual	Comment	Reference
A	293	GLU	-	expression tag	UNP Q8ZH09
A	294	ASN	-	expression tag	UNP Q8ZH09
A	295	LEU	-	expression tag	UNP Q8ZH09
A	296	TYR	-	expression tag	UNP Q8ZH09
A	297	PHE	-	expression tag	UNP Q8ZH09
A	298	HIS	-	expression tag	UNP Q8ZH09
A	299	HIS	-	expression tag	UNP Q8ZH09
A	300	HIS	-	expression tag	UNP Q8ZH09
A	301	HIS	-	expression tag	UNP Q8ZH09
A	302	HIS	-	expression tag	UNP Q8ZH09
A	303	HIS	-	expression tag	UNP Q8ZH09
B	293	GLU	-	expression tag	UNP Q8ZH09
B	294	ASN	-	expression tag	UNP Q8ZH09
B	295	LEU	-	expression tag	UNP Q8ZH09
B	296	TYR	-	expression tag	UNP Q8ZH09
B	297	PHE	-	expression tag	UNP Q8ZH09
B	298	HIS	-	expression tag	UNP Q8ZH09
B	299	HIS	-	expression tag	UNP Q8ZH09
B	300	HIS	-	expression tag	UNP Q8ZH09
B	301	HIS	-	expression tag	UNP Q8ZH09
B	302	HIS	-	expression tag	UNP Q8ZH09
B	303	HIS	-	expression tag	UNP Q8ZH09

- Molecule 2 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	1
			8	4	4		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

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



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

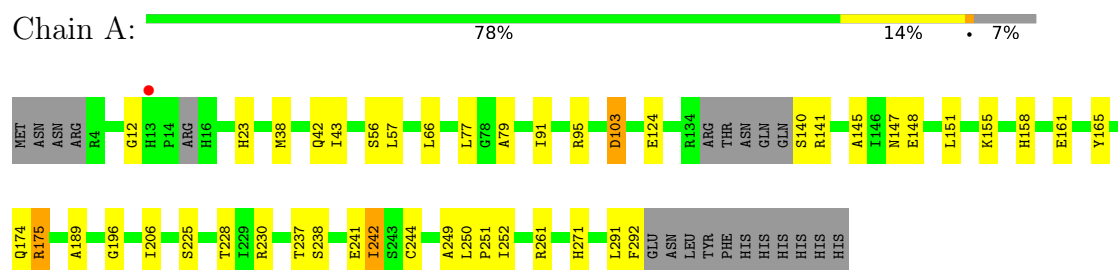
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	30	Total	O	0	0
			30	30		

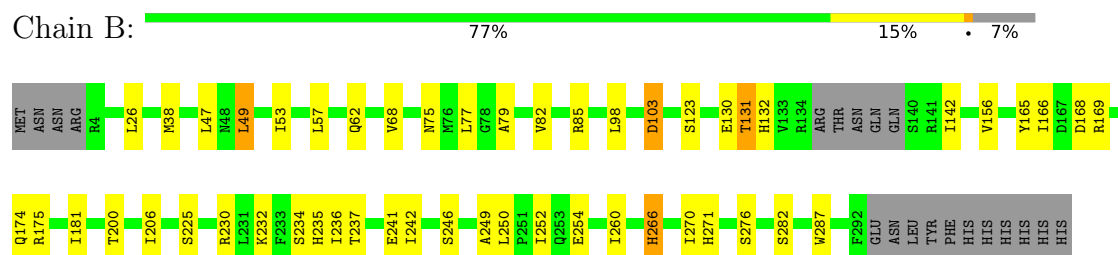
3 Residue-property plots

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: Probable inorganic polyphosphate/ATP-NAD kinase



- Molecule 1: Probable inorganic polyphosphate/ATP-NAD kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	138.09Å 65.16Å 86.39Å 90.00° 124.95° 90.00°	Depositor
Resolution (Å)	33.75 – 2.55 33.75 – 2.55	Depositor EDS
% Data completeness (in resolution range)	98.5 (33.75-2.55) 98.6 (33.75-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1032)	Depositor
R, R_{free}	0.185 , 0.241 0.189 , 0.246	Depositor DCC
R_{free} test set	1046 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4553	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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: ACY, 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	0.53	0/2255	0.88	5/3063 (0.2%)
1	B	0.52	0/2282	0.85	2/3100 (0.1%)
All	All	0.53	0/4537	0.87	7/6163 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	VAL	N-CA-C	5.87	116.34	110.23
1	B	174	GLN	N-CA-C	5.71	117.75	109.07
1	A	189	ALA	N-CA-C	5.63	113.39	108.78
1	A	237	THR	N-CA-C	-5.34	107.42	114.31
1	A	189	ALA	CA-C-O	5.19	120.95	117.94
1	A	196	GLY	CA-C-N	5.08	125.53	120.14
1	A	196	GLY	C-N-CA	5.08	125.53	120.14

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	2211	0	2213	21	0
1	B	2236	0	2244	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	16	0	12	2	0
2	B	32	0	24	3	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	18	0	0	0	0
4	B	30	0	0	2	0
All	All	4553	0	4493	46	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 5.

All (46) 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:B:131:THR:HG22	1:B:260:ILE:HG12	1.67	0.77
1:A:161:GLU:HG2	1:A:175:ARG:HG3	1.77	0.66
1:A:141:ARG:HH12	1:A:251:PRO:HD2	1.60	0.66
1:A:56:SER:HA	2:A:403:ACY:H3	1.81	0.63
1:A:206:ILE:HD12	1:A:225:SER:HA	1.82	0.61
1:B:242:ILE:HG12	1:B:252:ILE:HD11	1.82	0.61
1:B:123:SER:HB3	1:B:270:ILE:HG22	1.82	0.61
1:B:282:SER:HB2	1:B:287:TRP:HB2	1.83	0.60
1:B:103:ASP:OD2	1:B:271:HIS:ND1	2.31	0.59
1:A:165:TYR:HB2	1:A:230:ARG:HB2	1.84	0.58
1:A:241:GLU:HB3	1:A:249:ALA:HB1	1.84	0.58
1:B:234:SER:OG	1:B:235:HIS:N	2.32	0.57
1:B:168:ASP:OD1	1:B:230:ARG:NH2	2.37	0.57
1:A:155:LYS:HG2	1:A:158:HIS:HB2	1.86	0.57
1:B:26:LEU:HD21	1:B:68:VAL:HG11	1.88	0.55
1:B:206:ILE:HD12	1:B:225:SER:HA	1.90	0.53
1:A:242:ILE:HD13	1:A:252:ILE:HD11	1.90	0.53
1:A:42[A]:GLN:OE1	1:A:42[A]:GLN:N	2.37	0.53
1:B:232:LYS:NZ	4:B:529:HOH:O	2.39	0.52
1:A:57:LEU:HD21	1:A:79:ALA:HA	1.92	0.52
1:B:165:TYR:HB2	1:B:230:ARG:HB3	1.93	0.51
1:A:23:HIS:CD2	1:A:43:ILE:HD13	2.46	0.50
1:B:169:ARG:HA	2:B:409:ACY:H3	1.92	0.49
1:B:241:GLU:HB3	1:B:249:ALA:HB1	1.93	0.48
1:B:57:LEU:HD21	1:B:79:ALA:HA	1.95	0.48
1:A:145:ALA:HB2	1:A:244:CYS:HB3	1.97	0.47
1:A:103:ASP:OD2	1:A:271:HIS:ND1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HA	1:A:242:ILE:HD12	1.97	0.47
1:B:82:VAL:HA	1:B:85:ARG:NH1	2.30	0.46
1:B:181:ILE:HD13	1:B:260:ILE:HD12	1.98	0.44
1:B:131:THR:CG2	1:B:260:ILE:HG12	2.44	0.44
1:B:49:LEU:O	1:B:49:LEU:HD12	2.18	0.43
1:A:147:ASN:HB3	1:A:148:GLU:OE1	2.18	0.43
1:A:38:MET:HE2	1:A:38:MET:HB3	1.91	0.43
1:A:66:LEU:HD11	1:A:91:ILE:HG22	2.01	0.43
1:B:132:HIS:CE1	1:B:142:ILE:HG12	2.54	0.42
1:B:266:HIS:CD2	1:B:266:HIS:N	2.87	0.42
1:B:38:MET:HE2	1:B:38:MET:HB3	1.95	0.42
2:B:402:ACY:O	4:B:519:HOH:O	2.22	0.42
1:A:155:LYS:HE3	1:A:158:HIS:HB2	2.02	0.41
1:A:174:GLN:HE22	2:A:401[B]:ACY:H2	1.85	0.41
1:A:12:GLY:O	1:A:43:ILE:HD11	2.21	0.41
1:B:246:SER:OG	2:B:407:ACY:O	2.34	0.41
1:A:95:ARG:HE	1:A:95:ARG:HB2	1.54	0.40
1:B:77:LEU:HD12	1:B:77:LEU:HA	1.89	0.40
1:B:26:LEU:HD12	1:B:26:LEU:HA	1.84	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	279/304 (92%)	271 (97%)	8 (3%)	0	100	100
1	B	283/304 (93%)	273 (96%)	10 (4%)	0	100	100
All	All	562/608 (92%)	544 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	242/261 (93%)	230 (95%)	12 (5%)	22	33
1	B	244/261 (94%)	226 (93%)	18 (7%)	13	18
All	All	486/522 (93%)	456 (94%)	30 (6%)	16	24

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	103	ASP
1	A	124	GLU
1	A	140	SER
1	A	175	ARG
1	A	228	THR
1	A	238	SER
1	A	242	ILE
1	A	250	LEU
1	A	261	ARG
1	A	291	LEU
1	A	292	PHE
1	B	47	LEU
1	B	49	LEU
1	B	53	ILE
1	B	62	GLN
1	B	75	ASN
1	B	98	LEU
1	B	103	ASP
1	B	130	GLU
1	B	131	THR
1	B	166	ILE
1	B	175	ARG
1	B	200	THR
1	B	236	ILE
1	B	237	THR
1	B	250	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	254	GLU
1	B	266	HIS
1	B	276	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	94	ASN
1	B	16	HIS
1	B	112	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ACY	A	403	-	3,3,3	0.87	0	3,3,3	0.50	0
2	ACY	B	402	-	3,3,3	0.84	0	3,3,3	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACY	B	403	-	3,3,3	0.82	0	3,3,3	0.78	0
2	ACY	A	402	-	3,3,3	0.82	0	3,3,3	0.84	0
3	SO4	B	408	-	4,4,4	0.26	0	6,6,6	0.22	0
2	ACY	B	401	-	3,3,3	0.90	0	3,3,3	0.54	0
2	ACY	B	407	-	3,3,3	0.87	0	3,3,3	0.69	0
2	ACY	B	404	-	3,3,3	0.85	0	3,3,3	0.79	0
2	ACY	B	409	-	3,3,3	0.88	0	3,3,3	0.62	0
2	ACY	A	401[B]	-	3,3,3	0.89	0	3,3,3	0.78	0
2	ACY	B	405	-	3,3,3	0.83	0	3,3,3	0.89	0
2	ACY	B	406	-	3,3,3	0.80	0	3,3,3	0.90	0
3	SO4	A	404	-	4,4,4	0.22	0	6,6,6	0.22	0
2	ACY	A	401[A]	-	3,3,3	0.81	0	3,3,3	0.87	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	ACY	1	0
2	B	402	ACY	1	0
2	B	407	ACY	1	0
2	B	409	ACY	1	0
2	A	401[B]	ACY	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	283/304 (93%)	-0.46	1 (0%) 88 90	24, 56, 91, 128	3 (1%)
1	B	284/304 (93%)	-0.48	0 100 100	16, 58, 93, 114	6 (2%)
All	All	567/608 (93%)	-0.47	1 (0%) 91 92	16, 57, 93, 128	9 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	HIS	2.3

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(Å ²)	Q<0.9
2	ACY	B	402	4/4	0.48	0.22	57,58,59,61	0
2	ACY	B	404	4/4	0.58	0.17	84,84,84,84	0
2	ACY	B	403	4/4	0.64	0.12	87,87,87,87	0
2	ACY	B	401	4/4	0.69	0.13	68,68,69,69	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	408	5/5	0.72	0.10	119,119,119,119	0
2	ACY	B	409	4/4	0.74	0.12	64,64,65,65	0
2	ACY	B	406	4/4	0.74	0.16	82,83,83,83	0
2	ACY	A	403	4/4	0.75	0.11	69,70,70,72	0
2	ACY	A	401[B]	4/4	0.76	0.14	59,59,59,60	4
2	ACY	A	401[A]	4/4	0.76	0.14	60,60,60,60	4
2	ACY	B	405	4/4	0.76	0.12	52,53,53,54	0
2	ACY	B	407	4/4	0.77	0.11	70,71,71,71	0
3	SO4	A	404	5/5	0.86	0.14	98,98,99,99	0
2	ACY	A	402	4/4	0.96	0.07	79,79,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.