



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 11:26 AM EDT

PDB ID : 4YNG  
Title : Twinned pyruvate kinase from E. coli in the T-state  
Authors : Donovan, K.A.; Dobson, R.C.J.  
Deposited on : 2015-03-10  
Resolution : 2.28 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

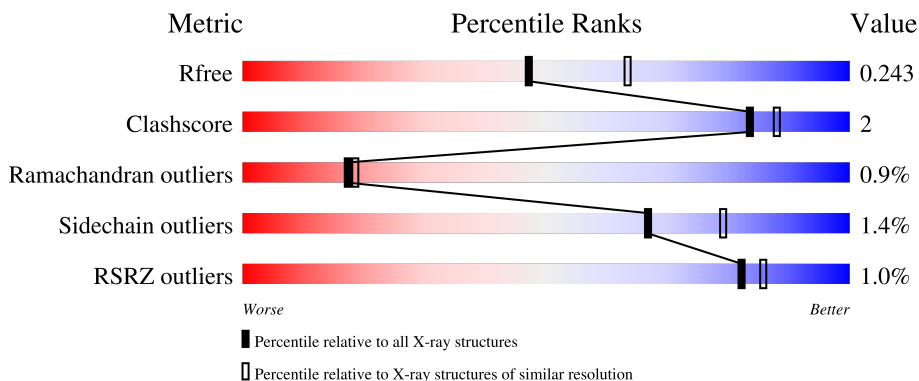
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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))
$R_{free}$	130704	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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  $\geq 3$ , 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	470	90% 8% .
1	B	470	3% 90% 9% .
1	C	470	94% 6% .
1	D	470	92% 7% .
1	E	470	3% 93% 7% .

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Mol	Chain	Length	Quality of chain
1	F	470	 92% 7% ..
1	G	470	 91% 6% ..
1	H	470	 88% 10% .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 59246 atoms, of which 28738 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 I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	465	7095	2184	3593	608	686	24	0	2	0
1	B	464	7060	2173	3572	607	684	24	0	2	0
1	C	467	7145	2195	3625	614	687	24	0	0	0
1	D	463	7057	2168	3580	605	680	24	0	0	0
1	E	470	7171	2204	3631	618	694	24	0	0	0
1	F	465	7092	2182	3595	607	684	24	0	0	0
1	G	463	7061	2173	3574	607	683	24	0	2	0
1	H	463	7044	2167	3568	603	682	24	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

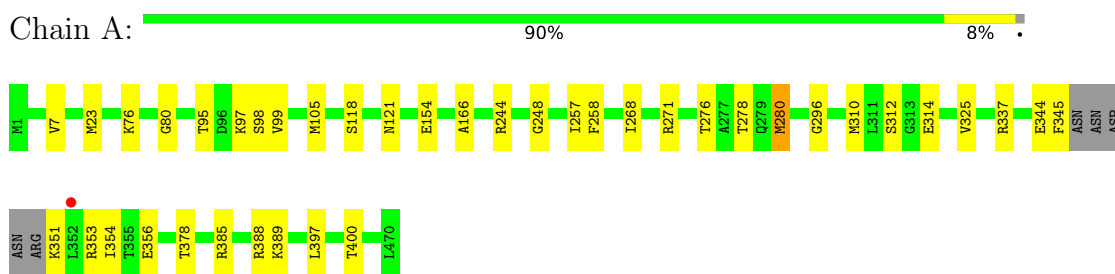
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	303	Total 303	O 303	0	0
3	B	299	Total 299	O 299	0	0
3	C	396	Total 396	O 396	0	0
3	D	425	Total 425	O 425	0	0
3	E	218	Total 218	O 218	0	0
3	F	250	Total 250	O 250	0	0
3	G	288	Total 288	O 288	0	0
3	H	282	Total 282	O 282	0	0

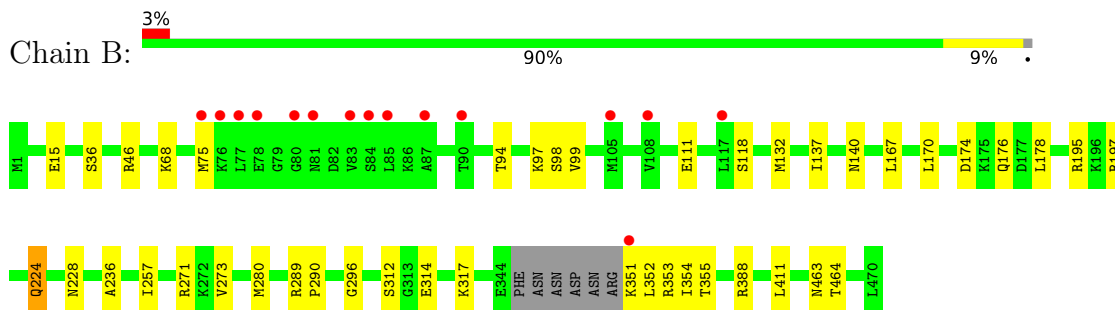
### 3 Residue-property plots [i](#)

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.

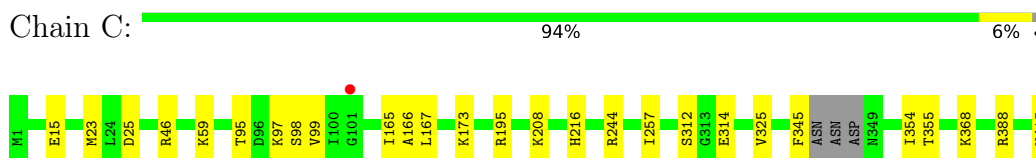
- Molecule 1: Pyruvate kinase I



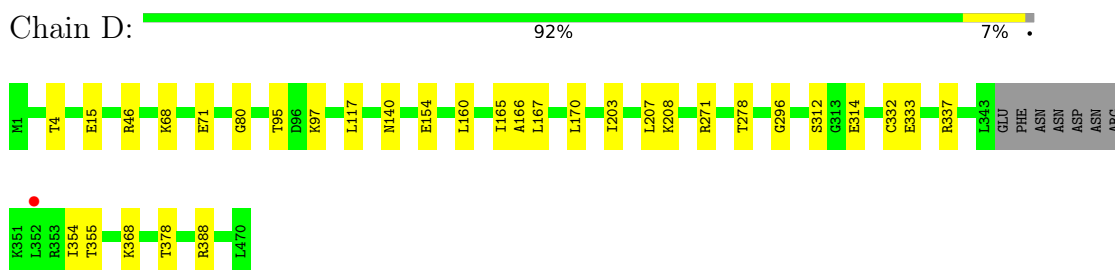
- Molecule 1: Pyruvate kinase I



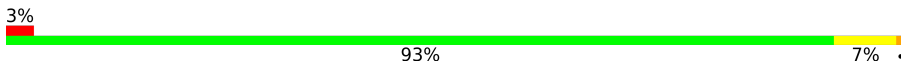
- Molecule 1: Pyruvate kinase I

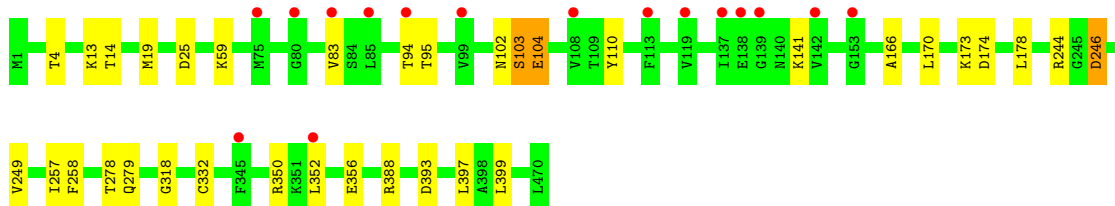


- Molecule 1: Pyruvate kinase I



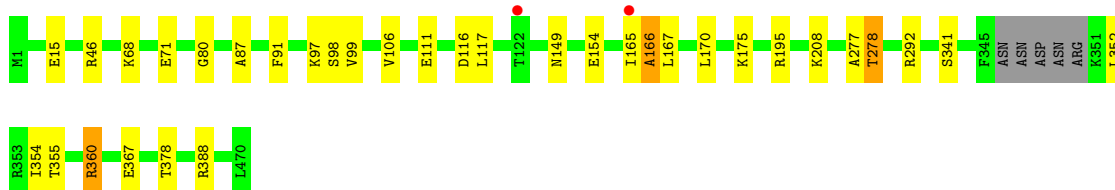
- Molecule 1: Pyruvate kinase I

Chain E:  3% 93% 7%



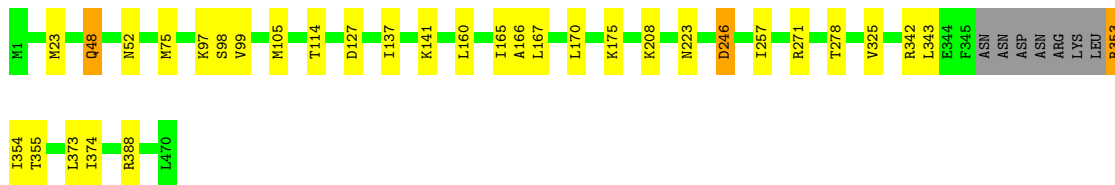
- Molecule 1: Pyruvate kinase I

Chain F:  92% 7%




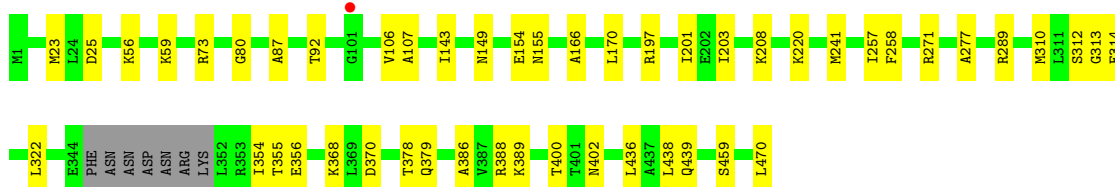
- Molecule 1: Pyruvate kinase I

Chain G:  91% 6%



- Molecule 1: Pyruvate kinase I

Chain H:  88% 10%





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.09Å 74.60Å 241.63Å 90.00° 90.14° 90.00°	Depositor
Resolution (Å)	44.13 – 2.28 44.13 – 2.22	Depositor EDS
% Data completeness (in resolution range)	95.2 (44.13-2.28) 88.6 (44.13-2.22)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.87 (at 2.22Å)	Xtrriage
Refinement program	PHENIX, REFMAC	Depositor
R, $R_{free}$	0.217 , 0.244 0.218 , 0.243	Depositor DCC
$R_{free}$ test set	2329 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtrriage
Anisotropy	0.318	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 25.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.450 for h,-k,-l	Xtrriage
Reported twinning fraction	0.480 for h,-k,-l	Depositor
Outliers	8 of 213569 reflections (0.004%)	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	59246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.50 % 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 2.3394e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.23	0/3545	0.45	0/4780
1	B	0.24	0/3531	0.47	0/4763
1	C	0.23	0/3555	0.44	0/4790
1	D	0.23	0/3511	0.45	0/4733
1	E	0.24	0/3576	0.47	0/4822
1	F	0.23	0/3532	0.46	0/4761
1	G	0.23	0/3531	0.46	0/4760
1	H	0.23	0/3510	0.47	0/4733
All	All	0.23	0/28291	0.46	0/38142

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 [i](#)

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	3502	3593	3588	21	0
1	B	3488	3572	3560	22	0
1	C	3520	3625	3625	12	0
1	D	3477	3580	3580	15	0
1	E	3540	3631	3631	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3497	3595	3595	18	0
1	G	3487	3574	3560	14	0
1	H	3476	3568	3568	25	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	10	0	0	1	0
2	G	5	0	0	0	0
2	H	10	0	0	1	0
3	A	303	0	0	4	0
3	B	299	0	0	0	0
3	C	396	0	0	1	0
3	D	425	0	0	1	0
3	E	218	0	0	1	0
3	F	250	0	0	0	0
3	G	288	0	0	4	0
3	H	282	0	0	1	0
All	All	30508	28738	28707	138	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 2.

The worst 5 of 138 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:F:97:LYS:NZ	1:F:111:GLU:OE1	2.11	0.83
1:C:25:ASP:OD1	1:C:59:LYS:NZ	2.12	0.83
1:E:25:ASP:OD1	1:E:59:LYS:NZ	2.23	0.72
1:E:13:LYS:NZ	1:E:318:GLY:O	2.23	0.70
1:F:68:LYS:NZ	1:F:71:GLU:OE2	2.25	0.70

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	463/470 (98%)	444 (96%)	14 (3%)	5 (1%)	14	14
1	B	462/470 (98%)	439 (95%)	20 (4%)	3 (1%)	25	29
1	C	463/470 (98%)	445 (96%)	13 (3%)	5 (1%)	14	14
1	D	459/470 (98%)	441 (96%)	12 (3%)	6 (1%)	12	11
1	E	468/470 (100%)	446 (95%)	20 (4%)	2 (0%)	34	40
1	F	461/470 (98%)	441 (96%)	14 (3%)	6 (1%)	12	11
1	G	461/470 (98%)	442 (96%)	14 (3%)	5 (1%)	14	14
1	H	459/470 (98%)	441 (96%)	15 (3%)	3 (1%)	22	25
All	All	3696/3760 (98%)	3539 (96%)	122 (3%)	35 (1%)	17	18

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	SER
1	A	166	ALA
1	B	98	SER
1	C	98	SER
1	C	166	ALA

### 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	384/389 (99%)	377 (98%)	7 (2%)	59	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	382/389 (98%)	375 (98%)	7 (2%)	59	72
1	C	386/389 (99%)	381 (99%)	5 (1%)	69	80
1	D	381/389 (98%)	378 (99%)	3 (1%)	81	90
1	E	388/389 (100%)	383 (99%)	5 (1%)	69	80
1	F	383/389 (98%)	380 (99%)	3 (1%)	81	90
1	G	382/389 (98%)	372 (97%)	10 (3%)	46	60
1	H	380/389 (98%)	376 (99%)	4 (1%)	73	84
All	All	3066/3112 (98%)	3022 (99%)	44 (1%)	67	79

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	360	ARG
1	G	271[A]	ARG
1	F	388	ARG
1	G	127	ASP
1	G	342	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	52	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	SO4	E	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	H	502	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	F	501	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	G	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	H	501	-	4,4,4	0.13	0	6,6,6	0.04	0
2	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.04	0
2	SO4	B	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.05	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	SO4	1	0
2	H	501	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	465/470 (98%)	-0.30	1 (0%) 95 96	15, 24, 35, 50	0
1	B	464/470 (98%)	-0.08	15 (3%) 47 53	15, 24, 62, 83	0
1	C	467/470 (99%)	-0.34	1 (0%) 95 96	14, 21, 33, 66	0
1	D	463/470 (98%)	-0.35	1 (0%) 95 96	13, 20, 30, 52	0
1	E	470/470 (100%)	0.07	16 (3%) 45 50	21, 31, 69, 81	0
1	F	465/470 (98%)	-0.13	2 (0%) 92 94	21, 33, 48, 58	0
1	G	463/470 (98%)	-0.24	0 100 100	21, 28, 36, 60	0
1	H	463/470 (98%)	-0.18	1 (0%) 95 96	22, 31, 42, 52	0
All	All	3720/3760 (98%)	-0.19	37 (0%) 82 86	13, 27, 49, 83	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	137	ILE	7.8
1	E	139	GLY	7.0
1	B	80	GLY	5.1
1	E	75	MET	3.9
1	H	101	GLY	3.7

### 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 monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	501	5/5	0.97	0.12	21,23,26,27	0
2	SO4	D	502	5/5	0.97	0.09	22,22,32,36	0
2	SO4	F	502	5/5	0.97	0.08	50,54,57,59	0
2	SO4	H	502	5/5	0.97	0.09	36,37,47,59	0
2	SO4	D	501	5/5	0.98	0.14	21,23,24,24	0
2	SO4	G	501	5/5	0.98	0.13	30,30,32,34	0
2	SO4	H	501	5/5	0.98	0.09	35,36,36,36	0
2	SO4	B	502	5/5	0.98	0.09	30,33,42,45	0
2	SO4	A	501	5/5	0.99	0.12	23,24,27,27	0
2	SO4	C	501	5/5	0.99	0.11	19,20,20,23	0
2	SO4	E	501	5/5	0.99	0.11	25,25,26,27	0
2	SO4	F	501	5/5	0.99	0.11	29,30,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.