



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 06:03 pm GMT

PDB ID : 2IF2  
Title : Crystal Structure of the Putative Dephospho-CoA Kinase from Aquifex aeolicus, Northeast Structural Genomics Target QR72.  
Authors : Forouhar, F.; Hussain, M.; Seetharaman, J.; Hussain, A.; Wu, M.; Fang, Y.; Cunningham, K.; Ma, L.C.; Xiao, R.; Liu, J.; Baran, M.; Rost, B.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2006-09-19  
Resolution : 3.00 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)

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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

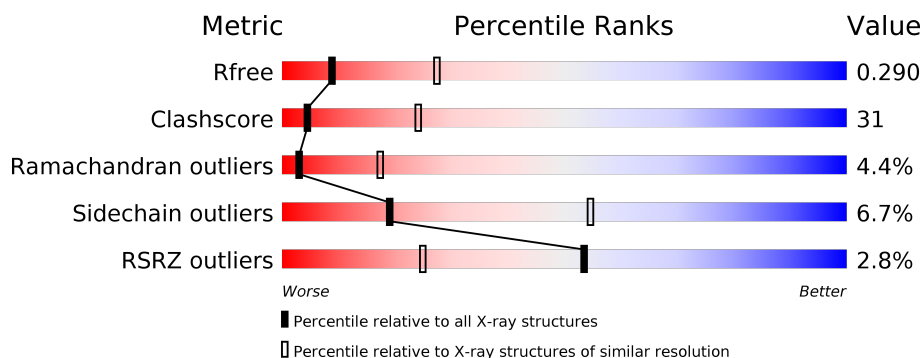
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 39%, yellow 52%, orange 5%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>39%</span> <span>52%</span> <span>• 5%</span> </div> </div>
1	B	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 46%, yellow 43%, orange 6%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>46%</span> <span>43%</span> <span>6%</span> <span>5%</span> </div> </div>
1	C	204	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, green 33%, yellow 41%, orange 6%, grey 20%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>33%</span> <span>41%</span> <span>6%</span> <span>20%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	303	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4567 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 Dephospho-CoA kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	Se	0	0	0
			1598	1022	268	302	2	4			
1	B	194	Total	C	N	O	S	Se	0	0	0
			1598	1022	268	302	2	4			
1	C	163	Total	C	N	O	S	Se	0	0	0
			1345	862	224	253	2	4			

There are 36 discrepancies between the modelled and reference sequences:

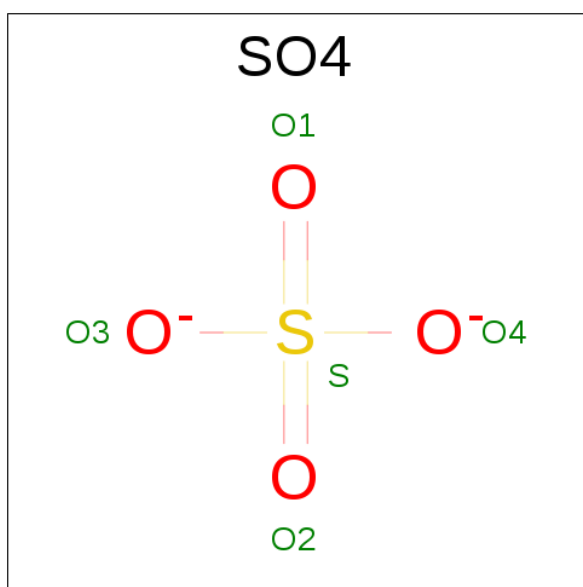
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O67792
A	20	MSE	MET	MODIFIED RESIDUE	UNP O67792
A	146	MSE	MET	MODIFIED RESIDUE	UNP O67792
A	159	MSE	MET	MODIFIED RESIDUE	UNP O67792
A	197	LEU	-	EXPRESSION TAG	UNP O67792
A	198	GLU	-	EXPRESSION TAG	UNP O67792
A	199	HIS	-	EXPRESSION TAG	UNP O67792
A	200	HIS	-	EXPRESSION TAG	UNP O67792
A	201	HIS	-	EXPRESSION TAG	UNP O67792
A	202	HIS	-	EXPRESSION TAG	UNP O67792
A	203	HIS	-	EXPRESSION TAG	UNP O67792
A	204	HIS	-	EXPRESSION TAG	UNP O67792
B	1	MSE	MET	MODIFIED RESIDUE	UNP O67792
B	20	MSE	MET	MODIFIED RESIDUE	UNP O67792
B	146	MSE	MET	MODIFIED RESIDUE	UNP O67792
B	159	MSE	MET	MODIFIED RESIDUE	UNP O67792
B	197	LEU	-	EXPRESSION TAG	UNP O67792
B	198	GLU	-	EXPRESSION TAG	UNP O67792
B	199	HIS	-	EXPRESSION TAG	UNP O67792
B	200	HIS	-	EXPRESSION TAG	UNP O67792
B	201	HIS	-	EXPRESSION TAG	UNP O67792
B	202	HIS	-	EXPRESSION TAG	UNP O67792
B	203	HIS	-	EXPRESSION TAG	UNP O67792

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Chain	Residue	Modelled	Actual	Comment	Reference
B	204	HIS	-	EXPRESSION TAG	UNP O67792
C	1	MSE	MET	MODIFIED RESIDUE	UNP O67792
C	20	MSE	MET	MODIFIED RESIDUE	UNP O67792
C	146	MSE	MET	MODIFIED RESIDUE	UNP O67792
C	159	MSE	MET	MODIFIED RESIDUE	UNP O67792
C	197	LEU	-	EXPRESSION TAG	UNP O67792
C	198	GLU	-	EXPRESSION TAG	UNP O67792
C	199	HIS	-	EXPRESSION TAG	UNP O67792
C	200	HIS	-	EXPRESSION TAG	UNP O67792
C	201	HIS	-	EXPRESSION TAG	UNP O67792
C	202	HIS	-	EXPRESSION TAG	UNP O67792
C	203	HIS	-	EXPRESSION TAG	UNP O67792
C	204	HIS	-	EXPRESSION TAG	UNP O67792

- 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	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

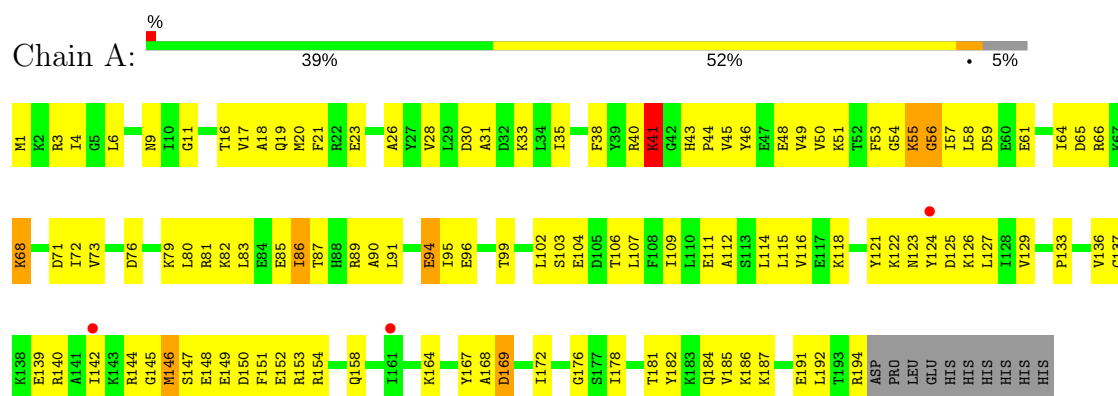
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	5	Total	O	0	0
			5	5		

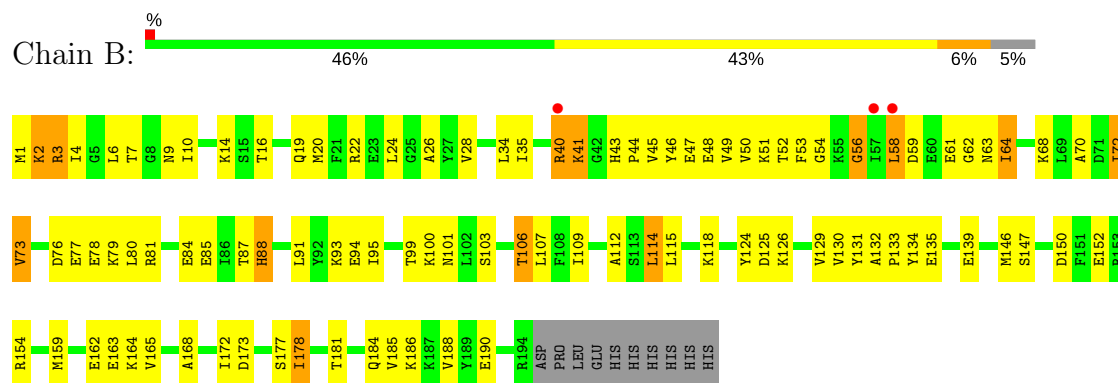
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

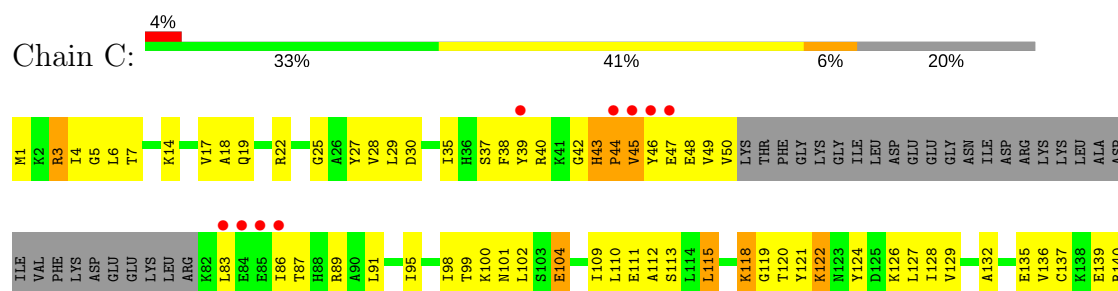
#### • Molecule 1: Dephospho-CoA kinase



#### • Molecule 1: Dephospho-CoA kinase



#### • Molecule 1: Dephospho-CoA kinase



M146	S147	E148	E149	D150	F151	E152	R153	R154	W155	K156	K157	V165	A168	D169	V170	V171	I172	D173	S177	I178	E179	E180	T181	Y182	K183	Q184	V185	K186	K187	V188	Y189	E190	E193	L192	T193	R194	ASP	PRO	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.63Å 97.01Å 121.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.92 – 3.00 48.51 – 2.86	Depositor EDS
% Data completeness (in resolution range)	87.2 (37.92-3.00) 94.8 (48.51-2.86)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.86Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, $R_{free}$	0.235 , 0.284 0.251 , 0.290	Depositor DCC
$R_{free}$ test set	1608 reflections (9.70%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.784	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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, 0.333 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, EDO

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	0.40	0/1620	0.54	0/2162
1	B	0.50	0/1620	0.63	0/2162
1	C	0.48	0/1364	0.59	0/1822
All	All	0.46	0/4604	0.59	0/6146

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	124	TYR	Sidechain

### 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	1598	0	1637	109	0
1	B	1598	0	1637	92	0
1	C	1345	0	1372	90	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	B	4	0	6	1	0
4	A	2	0	0	0	0
4	B	5	0	0	0	0
All	All	4567	0	4652	290	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 31.

The worst 5 of 290 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:178:ILE:H	1:B:178:ILE:HD13	1.12	1.12
1:C:112:ALA:HB3	1:C:115:LEU:HD13	1.48	0.93
1:A:54:GLY:HA3	1:A:57:ILE:HG22	1.56	0.87
1:A:58:LEU:HD23	1:A:58:LEU:H	1.41	0.85
1:A:16:THR:O	1:A:20:MSE:HG3	1.80	0.81

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	192/204 (94%)	158 (82%)	23 (12%)	11 (6%)	2	12
1	B	192/204 (94%)	162 (84%)	23 (12%)	7 (4%)	4	22
1	C	159/204 (78%)	123 (77%)	30 (19%)	6 (4%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	543/612 (89%)	443 (82%)	76 (14%)	24 (4%)	3	17

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	ARG
1	A	55	LYS
1	A	125	ASP
1	B	41	LYS
1	A	41	LYS

### 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	173/179 (97%)	161 (93%)	12 (7%)	18	53
1	B	173/179 (97%)	161 (93%)	12 (7%)	18	53
1	C	146/179 (82%)	137 (94%)	9 (6%)	21	58
All	All	492/537 (92%)	459 (93%)	33 (7%)	19	54

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	58	LEU
1	B	73	VAL
1	C	169	ASP
1	B	59	ASP
1	B	64	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	GLN
1	B	63	ASN

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Mol	Chain	Res	Type
1	B	174	ASN
1	A	174	ASN
1	B	101	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 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	A	301	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	B	302	-	4,4,4	0.34	0	6,6,6	0.11	0
3	EDO	B	304	-	3,3,3	0.57	0	2,2,2	0.64	0
2	SO4	C	303	-	4,4,4	0.33	0	6,6,6	0.17	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
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	302	-	-	0/0/0/0	0/0/0/0
3	EDO	B	304	-	-	0/1/1/1	0/0/0/0
2	SO4	C	303	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	304	EDO	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, 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	190/204 (93%)	-0.01	3 (1%) 72 44	33, 78, 107, 117	0
1	B	190/204 (93%)	-0.19	3 (1%) 72 44	12, 43, 101, 116	0
1	C	159/204 (77%)	0.03	9 (5%) 24 9	21, 49, 140, 148	0
All	All	539/612 (88%)	-0.07	15 (2%) 53 25	12, 62, 117, 148	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	57	ILE	6.7
1	C	46	TYR	3.6
1	A	161	ILE	3.4
1	C	44	PRO	3.3
1	B	58	LEU	3.0

### 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	303	5/5	0.99	0.24	2.06	32,34,36,38	0
3	EDO	B	304	4/4	0.90	0.28	1.55	40,41,41,42	0
2	SO4	B	302	5/5	0.99	0.22	0.69	36,37,38,39	0
2	SO4	A	301	5/5	0.99	0.14	-1.45	43,44,45,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.