



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2024 – 07:11 AM EDT

PDB ID : 3S52  
Title : Crystal structure of a putative fumarylacetoacetate hydrolase family protein from *Yersinia pestis* CO92  
Authors : Nocek, B.; Zhou, M.; Grimshaw, S.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2011-05-20  
Resolution : 2.01 Å(reported)

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

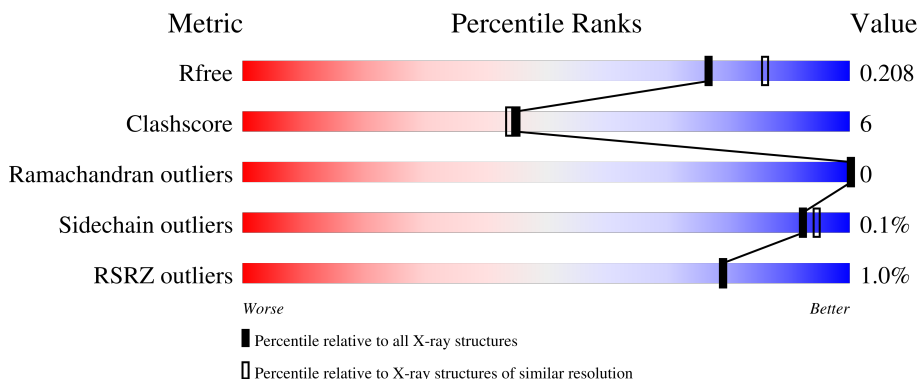
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.01 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))
$R_{free}$	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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 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	221	
1	B	221	
1	C	221	
1	D	221	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7146 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 Putative fumarylacetoacetate hydrolase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	Se	0	0	0
			1661	1056	287	308	3	7			
1	B	211	Total	C	N	O	S	Se	0	0	0
			1612	1027	279	297	3	6			
1	C	217	Total	C	N	O	S	Se	0	2	0
			1665	1057	289	310	3	6			
1	D	208	Total	C	N	O	S	Se	0	0	0
			1560	996	268	287	3	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8D0F9
A	-1	ASN	-	expression tag	UNP Q8D0F9
A	0	ALA	-	expression tag	UNP Q8D0F9
B	-2	SER	-	expression tag	UNP Q8D0F9
B	-1	ASN	-	expression tag	UNP Q8D0F9
B	0	ALA	-	expression tag	UNP Q8D0F9
C	-2	SER	-	expression tag	UNP Q8D0F9
C	-1	ASN	-	expression tag	UNP Q8D0F9
C	0	ALA	-	expression tag	UNP Q8D0F9
D	-2	SER	-	expression tag	UNP Q8D0F9
D	-1	ASN	-	expression tag	UNP Q8D0F9
D	0	ALA	-	expression tag	UNP Q8D0F9

- 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	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		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	192	Total	O	0	0
			192	192		
4	B	120	Total	O	0	0
			120	120		
4	C	175	Total	O	0	0
			175	175		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	135	Total 135	O 135	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.

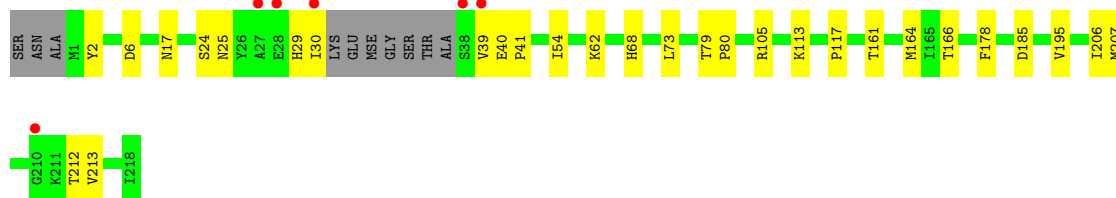
- Molecule 1: Putative fumarylacetoacetate hydrolase family protein

Chain A: 




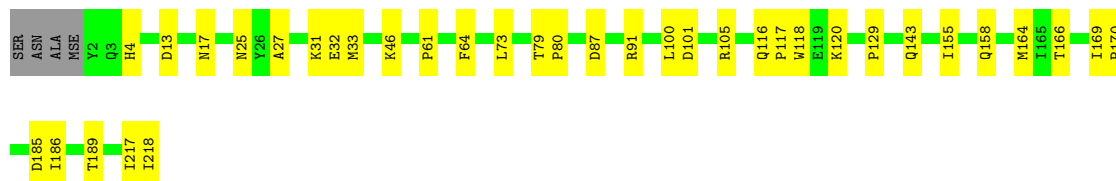
- Molecule 1: Putative fumarylacetoacetate hydrolase family protein

Chain B: 




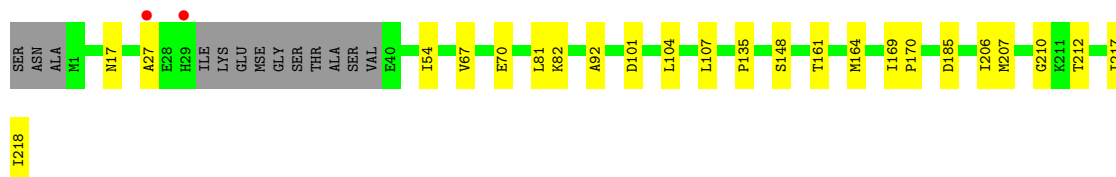
- Molecule 1: Putative fumarylacetoacetate hydrolase family protein

Chain C: 



- Molecule 1: Putative fumarylacetoacetate hydrolase family protein

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.17Å 92.14Å 157.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.80 – 2.01 36.80 – 2.01	Depositor EDS
% Data completeness (in resolution range)	86.9 (36.80-2.01) 92.3 (36.80-2.01)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.01Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.160 , 0.211 0.165 , 0.208	Depositor DCC
$R_{free}$ test set	3035 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7146	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: CL, 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	0.40	0/1688	0.59	0/2277
1	B	0.36	0/1639	0.58	0/2213
1	C	0.39	0/1698	0.60	0/2292
1	D	0.37	0/1587	0.58	0/2148
All	All	0.38	0/6612	0.59	0/8930

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	1661	0	1680	13	0
1	B	1612	0	1629	21	0
1	C	1665	0	1678	29	0
1	D	1560	0	1550	17	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	192	0	0	1	0
4	B	120	0	0	1	0
4	C	175	0	0	2	0
4	D	135	0	0	2	0
All	All	7146	0	6537	76	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 6.

All (76) 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:D:161:THR:HB	1:D:164:MSE:HE3	1.63	0.80
1:D:207:MSE:HE2	1:D:210:GLY:HA2	1.67	0.77
1:C:164:MSE:HE2	1:C:166:THR:O	1.90	0.71
1:A:68:HIS:CD2	1:A:105:ARG:HD2	2.27	0.69
1:C:33:MSE:HE1	1:C:105:ARG:NH1	2.13	0.64
1:C:27:ALA:O	1:C:31:LYS:HG3	1.98	0.62
1:D:207:MSE:HE3	1:D:212:THR:OG1	2.01	0.61
1:B:161:THR:HB	1:B:164:MSE:HE3	1.82	0.60
1:B:17:ASN:HB3	1:B:185:ASP:OD1	2.00	0.60
1:A:161:THR:HG22	1:A:164:MSE:HE3	1.83	0.60
1:C:32:GLU:HG3	1:C:33:MSE:CE	2.32	0.59
1:B:206:ILE:HB	1:B:213:VAL:HG23	1.86	0.58
1:D:148:SER:HB3	1:D:207:MSE:HB2	1.85	0.57
1:D:27:ALA:HB3	4:D:639:HOH:O	2.05	0.57
1:C:17[A]:ASN:HB2	1:C:185:ASP:OD1	2.06	0.55
1:C:17[B]:ASN:HB3	1:C:185:ASP:OD1	2.06	0.55
1:C:32:GLU:HG3	1:C:33:MSE:HE3	1.88	0.54
1:C:17[B]:ASN:ND2	4:C:278:HOH:O	2.39	0.54
1:A:206:ILE:HB	1:A:213:VAL:HG23	1.90	0.54
1:D:17:ASN:HB3	1:D:185:ASP:OD1	2.07	0.54
1:B:25:ASN:HD21	1:B:166:THR:H	1.56	0.53
1:B:206:ILE:HB	1:B:213:VAL:CG2	2.39	0.53
1:A:161:THR:CG2	1:A:164:MSE:HE3	2.38	0.53
1:B:24:SER:HB2	1:B:30:ILE:HG12	1.90	0.53
1:C:61:PRO:HB2	1:C:64:PHE:HD2	1.74	0.52
1:C:33:MSE:HE1	1:C:105:ARG:CZ	2.40	0.51
1:D:135:PRO:HD3	4:D:289:HOH:O	2.11	0.50
1:C:100:LEU:HB2	1:C:129:PRO:HG2	1.94	0.49
1:B:207:MSE:HE3	1:B:212:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:THR:CB	1:D:164:MSE:HE3	2.39	0.48
1:A:67:VAL:HG22	1:A:104:LEU:HD23	1.96	0.48
1:B:117:PRO:HD3	1:C:118:TRP:CZ2	2.48	0.48
1:A:68:HIS:CD2	1:A:105:ARG:CD	2.97	0.47
1:B:73:LEU:HD22	1:B:161:THR:HG21	1.97	0.47
1:C:116:GLN:CD	4:C:469:HOH:O	2.54	0.47
1:C:25:ASN:ND2	1:C:164:MSE:HE3	2.30	0.47
1:D:67:VAL:HG22	1:D:104:LEU:CD2	2.44	0.47
1:C:116:GLN:HB3	1:C:117:PRO:HD2	1.96	0.46
1:B:79:THR:HG23	1:B:80:PRO:HD2	1.97	0.46
1:B:113:LYS:HB2	1:B:113:LYS:HE3	1.66	0.46
1:C:32:GLU:HG3	1:C:33:MSE:HE2	1.97	0.46
1:B:24:SER:HB2	1:B:30:ILE:CG1	2.46	0.46
1:C:169:ILE:HB	1:C:170:PRO:CD	2.46	0.46
1:B:39:VAL:HG23	1:B:40:GLU:HG3	1.98	0.46
1:C:79:THR:HG23	1:C:80:PRO:HD2	1.99	0.45
1:D:67:VAL:HG22	1:D:104:LEU:HD23	1.98	0.44
1:A:143:GLN:HE22	1:A:164:MSE:SE	2.50	0.44
1:C:87:ASP:O	1:C:91:ARG:HG3	2.17	0.44
1:A:207:MSE:HE3	4:A:627:HOH:O	2.17	0.44
1:A:67:VAL:HG22	1:A:104:LEU:CD2	2.47	0.44
1:B:54:ILE:HD11	1:B:206:ILE:CD1	2.49	0.43
1:D:81:LEU:HD21	1:D:92:ALA:HB2	1.99	0.43
1:C:155:ILE:CG2	1:C:158:GLN:HG3	2.48	0.43
1:B:41:PRO:HA	4:B:230:HOH:O	2.18	0.43
1:B:68:HIS:CE1	1:B:105:ARG:HD3	2.54	0.43
1:D:217:ILE:O	1:D:218:ILE:CB	2.67	0.43
1:B:178:PHE:CZ	1:C:120:LYS:HD3	2.54	0.42
1:A:164:MSE:CE	1:A:189:THR:OG1	2.67	0.42
1:D:54:ILE:HD11	1:D:206:ILE:HD13	2.01	0.42
1:C:73:LEU:HB3	1:C:189:THR:OG1	2.20	0.42
1:C:4:HIS:CE1	1:C:186:ILE:HD11	2.55	0.42
1:C:4:HIS:HE1	1:C:186:ILE:HD11	1.85	0.42
1:A:40:GLU:OE1	1:C:13:ASP:OD1	2.38	0.42
1:B:6:ASP:OD1	1:B:6:ASP:C	2.58	0.42
1:C:46:LYS:NZ	1:C:101:ASP:OD1	2.46	0.42
1:D:70:GLU:HB2	1:D:101:ASP:HB3	2.02	0.42
1:C:79:THR:CG2	1:C:80:PRO:HD2	2.50	0.41
1:D:169:ILE:HB	1:D:170:PRO:CD	2.50	0.41
1:C:143:GLN:HE22	1:C:164:MSE:SE	2.53	0.41
1:B:62:LYS:HD2	1:B:62:LYS:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ILE:O	1:C:218:ILE:CB	2.69	0.41
1:A:68:HIS:NE2	1:A:105:ARG:HD3	2.36	0.40
1:B:29:HIS:CE1	1:B:195:VAL:HG21	2.56	0.40
1:A:125:ASP:OD2	1:D:82:LYS:HE2	2.21	0.40
1:D:107:LEU:HD23	1:D:107:LEU:HA	1.84	0.40
1:B:39:VAL:HG23	1:B:40:GLU:H	1.87	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	216/221 (98%)	213 (99%)	3 (1%)	0	100	100
1	B	207/221 (94%)	204 (99%)	3 (1%)	0	100	100
1	C	217/221 (98%)	213 (98%)	4 (2%)	0	100	100
1	D	204/221 (92%)	203 (100%)	1 (0%)	0	100	100
All	All	844/884 (96%)	833 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	178/175 (102%)	178 (100%)	0	100	100
1	B	173/175 (99%)	172 (99%)	1 (1%)	84	88
1	C	179/175 (102%)	179 (100%)	0	100	100
1	D	163/175 (93%)	163 (100%)	0	100	100
All	All	693/700 (99%)	692 (100%)	1 (0%)	92	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	68	HIS
1	B	25	ASN
1	B	29	HIS
1	D	193	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](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\# Z  > 2$
2	SO4	D	219	-	4,4,4	0.23	0	6,6,6	0.31	0
2	SO4	A	220	-	4,4,4	0.25	0	6,6,6	0.25	0
2	SO4	B	219	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	A	219	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	C	219	-	4,4,4	0.25	0	6,6,6	0.30	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 [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	211/221 (95%)	-0.66	0 <b>100</b> <b>100</b>	10, 17, 34, 50	0
1	B	205/221 (92%)	-0.37	6 (2%) 54 53	13, 25, 45, 81	0
1	C	211/221 (95%)	-0.61	0 <b>100</b> <b>100</b>	11, 18, 34, 48	2 (0%)
1	D	202/221 (91%)	-0.39	2 (0%) 79 79	11, 23, 40, 55	0
All	All	829/884 (93%)	-0.51	8 (0%) 79 79	10, 21, 39, 81	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	ILE	3.5
1	B	39	VAL	3.2
1	B	38	SER	3.0
1	B	28	GLU	3.0
1	B	210	GLY	2.5
1	B	27	ALA	2.5
1	D	27	ALA	2.3
1	D	29	HIS	2.2

### 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	A	220	5/5	0.90	0.12	50,52,56,57	0
2	SO4	D	219	5/5	0.91	0.10	41,46,48,52	0
2	SO4	C	219	5/5	0.94	0.08	37,39,41,42	0
3	CL	D	220	1/1	0.95	0.11	63,63,63,63	0
2	SO4	B	219	5/5	0.96	0.09	43,45,48,53	0
2	SO4	A	219	5/5	0.96	0.07	29,30,36,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.