



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:21 PM GMT

PDB ID : 1JTY  
Title : Crystal structure of the multidrug binding transcriptional regulator QacR bound to ethidium  
Authors : Schumacher, M.A.; Miller, M.C.; Grkovic, S.; Brown, M.H.; Skurray, R.A.; Brennan, R.G.  
Deposited on : 2001-08-22  
Resolution : 2.97 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

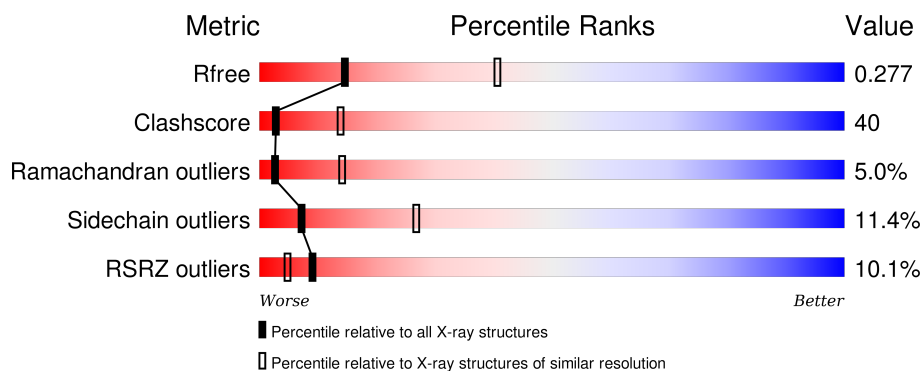
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.97 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))
$R_{free}$	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	194	<div> <div>6%</div> <div>42%</div> <div>45%</div> <div>9%</div> <div>.</div> </div>
1	B	194	<div> <div>20%</div> <div>23%</div> <div>57%</div> <div>15%</div> <div>..</div> </div>
1	D	194	<div> <div>7%</div> <div>35%</div> <div>51%</div> <div>10%</div> <div>..</div> </div>
1	E	194	<div> <div>6%</div> <div>41%</div> <div>45%</div> <div>10%</div> <div>.</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ET	A	205	-	-	X	X
3	SO4	A	799	-	-	-	X
3	SO4	B	1000	-	-	-	X
3	SO4	E	399	-	-	-	X
3	SO4	E	900	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6343 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 HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	D	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	A	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			
1	E	186	Total	C	N	O	S	0	0	0
			1547	998	252	295	2			

There are 32 discrepancies between the modelled and reference sequences:

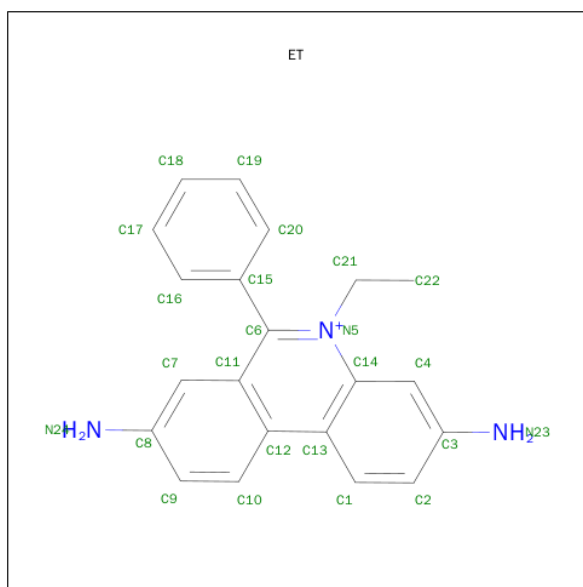
Chain	Residue	Modelled	Actual	Comment	Reference
B	72	ALA	CYS	ENGINEERED	UNP P0A0N4
B	141	SER	CYS	ENGINEERED	UNP P0A0N4
B	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
B	194	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	72	ALA	CYS	ENGINEERED	UNP P0A0N4
D	141	SER	CYS	ENGINEERED	UNP P0A0N4
D	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
D	194	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	72	ALA	CYS	ENGINEERED	UNP P0A0N4
A	141	SER	CYS	ENGINEERED	UNP P0A0N4
A	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	190	HIS	-	EXPRESSION TAG	UNP P0A0N4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
A	194	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	72	ALA	CYS	ENGINEERED	UNP P0A0N4
E	141	SER	CYS	ENGINEERED	UNP P0A0N4
E	189	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	190	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	191	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	192	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	193	HIS	-	EXPRESSION TAG	UNP P0A0N4
E	194	HIS	-	EXPRESSION TAG	UNP P0A0N4

- Molecule 2 is ETHIDIUM (three-letter code: ET) (formula:  $C_{21}H_{20}N_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			24	21	3		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

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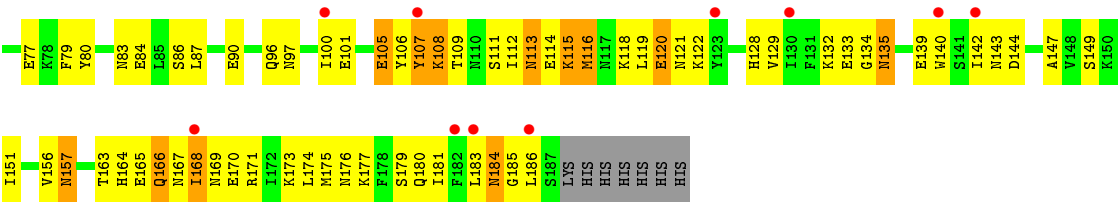
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

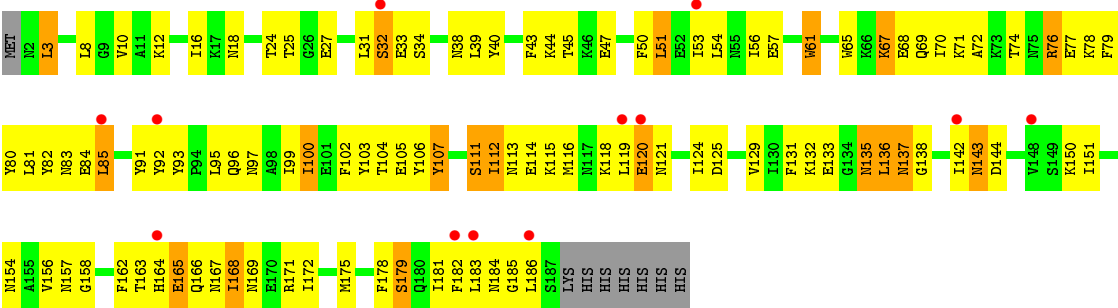
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	O	0	0
			18	18		
4	B	10	Total	O	0	0
			10	10		
4	D	7	Total	O	0	0
			7	7		
4	E	11	Total	O	0	0
			11	11		







● Molecule 1: HYPOTHETICAL TRANSCRIPTIONAL REGULATOR IN QACA 5'REGION



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.00 Å   172.00 Å   95.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	83.16 – 2.97 83.16 – 2.97	Depositor EDS
% Data completeness (in resolution range)	73.6 (83.16-2.97) 73.6 (83.16-2.97)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.96 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.239   ,   0.291 0.230   ,   0.277	Depositor DCC
$R_{free}$ test set	2192 reflections (9.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.1	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 89.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 22060 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ET, 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	0.45	0/1578	0.62	0/2126
1	B	0.40	0/1578	0.61	0/2126
1	D	0.50	2/1578 (0.1%)	0.74	3/2126 (0.1%)
1	E	0.43	0/1578	0.62	0/2126
All	All	0.44	2/6312 (0.0%)	0.65	3/8504 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	187	SER	N-CA	6.76	1.59	1.46
1	D	186	LEU	CA-C	5.20	1.66	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	187	SER	N-CA-C	6.41	128.32	111.00
1	D	164	HIS	N-CA-CB	-5.90	99.98	110.60
1	D	187	SER	CA-C-O	5.40	131.44	120.10

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	1547	0	1536	120	0
1	B	1547	0	1536	155	0
1	D	1547	0	1536	128	0
1	E	1547	0	1536	132	0
2	A	24	0	20	9	0
3	A	35	0	0	1	0
3	B	15	0	0	0	0
3	D	10	0	0	1	0
3	E	25	0	0	2	0
4	A	18	0	0	1	0
4	B	10	0	0	1	0
4	D	7	0	0	0	0
4	E	11	0	0	0	0
All	All	6343	0	6164	500	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 40.

The worst 5 of 500 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:165:GLU:HB3	1:E:103:TYR:CE1	1.57	1.37
1:D:165:GLU:CB	1:E:103:TYR:HE1	1.54	1.21
1:D:21:ASN:HD22	1:D:21:ASN:N	1.40	1.10
1:E:168:ILE:H	1:E:168:ILE:HD12	1.16	1.09
1:A:113:ASN:HA	1:A:116:MET:HB2	1.39	1.02

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	184/194 (95%)	160 (87%)	22 (12%)	2 (1%)	17	57
1	B	184/194 (95%)	131 (71%)	38 (21%)	15 (8%)	1	4
1	D	184/194 (95%)	150 (82%)	24 (13%)	10 (5%)	2	12
1	E	184/194 (95%)	141 (77%)	33 (18%)	10 (5%)	2	12
All	All	736/776 (95%)	582 (79%)	117 (16%)	37 (5%)	3	14

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	LEU
1	B	41	TYR
1	B	110	ASN
1	B	144	ASP
1	D	71	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	169/177 (96%)	148 (88%)	21 (12%)	6	23
1	B	169/177 (96%)	144 (85%)	25 (15%)	4	16
1	D	169/177 (96%)	153 (90%)	16 (10%)	11	36
1	E	169/177 (96%)	154 (91%)	15 (9%)	12	40
All	All	676/708 (96%)	599 (89%)	77 (11%)	7	27

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	88	THR
1	A	39	LEU
1	E	120	GLU
1	D	90	GLU
1	D	165	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	167	ASN
1	A	83	ASN
1	E	121	ASN
1	A	42	HIS
1	A	96	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 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	ET	A	205	-	26,27,27	3.63	15 (57%)	33,39,39	1.65	6 (18%)
3	SO4	A	299	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	A	499	-	4,4,4	0.20	0	6,6,6	0.12	0
3	SO4	A	699	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	A	799	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	A	800	-	4,4,4	0.21	0	6,6,6	0.14	0
3	SO4	A	801	-	4,4,4	0.20	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	A	802	-	4,4,4	0.18	0	6,6,6	0.09	0
3	SO4	B	1000	-	4,4,4	0.19	0	6,6,6	0.14	0
3	SO4	B	195	-	4,4,4	0.23	0	6,6,6	0.16	0
3	SO4	B	199	-	4,4,4	0.22	0	6,6,6	0.07	0
3	SO4	D	195	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	D	999	-	4,4,4	0.21	0	6,6,6	0.08	0
3	SO4	E	399	-	4,4,4	0.16	0	6,6,6	0.09	0
3	SO4	E	899	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	E	900	-	4,4,4	0.24	0	6,6,6	0.14	0
3	SO4	E	901	-	4,4,4	0.20	0	6,6,6	0.07	0
3	SO4	E	902	-	4,4,4	0.22	0	6,6,6	0.10	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	ET	A	205	-	-	0/6/6/6	0/4/4/4
3	SO4	A	299	-	-	0/0/0/0	0/0/0/0
3	SO4	A	499	-	-	0/0/0/0	0/0/0/0
3	SO4	A	699	-	-	0/0/0/0	0/0/0/0
3	SO4	A	799	-	-	0/0/0/0	0/0/0/0
3	SO4	A	800	-	-	0/0/0/0	0/0/0/0
3	SO4	A	801	-	-	0/0/0/0	0/0/0/0
3	SO4	A	802	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1000	-	-	0/0/0/0	0/0/0/0
3	SO4	B	195	-	-	0/0/0/0	0/0/0/0
3	SO4	B	199	-	-	0/0/0/0	0/0/0/0
3	SO4	D	195	-	-	0/0/0/0	0/0/0/0
3	SO4	D	999	-	-	0/0/0/0	0/0/0/0
3	SO4	E	399	-	-	0/0/0/0	0/0/0/0
3	SO4	E	899	-	-	0/0/0/0	0/0/0/0
3	SO4	E	900	-	-	0/0/0/0	0/0/0/0
3	SO4	E	901	-	-	0/0/0/0	0/0/0/0
3	SO4	E	902	-	-	0/0/0/0	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	205	ET	C6-C11	-2.72	1.38	1.43
2	A	205	ET	C10-C12	2.12	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	205	ET	C19-C20	2.14	1.43	1.38
2	A	205	ET	C13-C14	2.23	1.45	1.41
2	A	205	ET	C10-C9	2.39	1.41	1.36

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	205	ET	C11-C6-N5	-3.15	114.90	119.47
2	A	205	ET	C20-C15-C16	-2.69	112.47	117.55
2	A	205	ET	C19-C20-C15	2.39	123.71	120.56
2	A	205	ET	C8-C7-C11	2.56	123.61	120.81
2	A	205	ET	C20-C15-C6	3.49	126.11	120.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	205	ET	9	0
3	A	499	SO4	1	0
3	D	195	SO4	1	0
3	E	900	SO4	2	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	186/194 (95%)	0.62	11 (5%) 26 13	52, 72, 112, 138	0
1	B	186/194 (95%)	1.22	38 (20%) 1 1	52, 94, 155, 164	0
1	D	186/194 (95%)	0.74	14 (7%) 17 8	56, 90, 125, 137	0
1	E	186/194 (95%)	0.75	12 (6%) 22 11	49, 78, 109, 116	0
All	All	744/776 (95%)	0.83	75 (10%) 9 5	49, 83, 131, 164	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	HIS	8.7
1	B	112	ILE	7.5
1	B	43	PHE	5.7
1	B	107	TYR	4.6
1	B	40	TYR	4.5

### 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
3	SO4	A	799	5/5	0.68	0.68	8.73	171,171,172,172	0
3	SO4	E	399	5/5	0.89	0.57	4.78	179,179,179,180	0
3	SO4	B	1000	5/5	0.49	0.51	3.71	200,200,200,200	0
2	ET	A	205	24/24	0.86	0.46	2.22	55,59,67,69	0
3	SO4	E	899	5/5	0.81	0.26	0.42	145,146,146,146	0
3	SO4	E	900	5/5	0.81	0.29	0.08	105,105,106,106	0
3	SO4	A	499	5/5	0.88	0.22	-0.56	157,158,158,158	0
3	SO4	A	801	5/5	0.74	0.22	-1.32	167,167,167,167	0
3	SO4	A	802	5/5	0.85	0.17	-1.65	171,171,172,172	0
3	SO4	E	902	5/5	0.82	0.25	-	167,167,167,167	0
3	SO4	A	800	5/5	0.88	0.21	-	157,158,158,158	0
3	SO4	A	299	5/5	0.89	0.25	-	131,131,131,131	0
3	SO4	A	699	5/5	0.56	0.30	-	160,160,161,161	0
3	SO4	D	195	5/5	0.69	0.28	-	187,187,187,187	0
3	SO4	E	901	5/5	0.59	0.19	-	188,188,189,189	0
3	SO4	D	999	5/5	0.79	0.20	-	171,171,171,171	0
3	SO4	B	195	5/5	0.66	0.23	-	200,200,200,200	0
3	SO4	B	199	5/5	0.65	0.28	-	176,176,176,177	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.