



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:47 PM GMT

PDB ID : 3UR0  
Title : Crystal structures of murine norovirus RNA-dependent RNA polymerase in complex with Suramin  
Authors : Milani, M.; Mastrangelo, E.; Bolognesi, M.  
Deposited on : 2011-11-21  
Resolution : 2.45 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

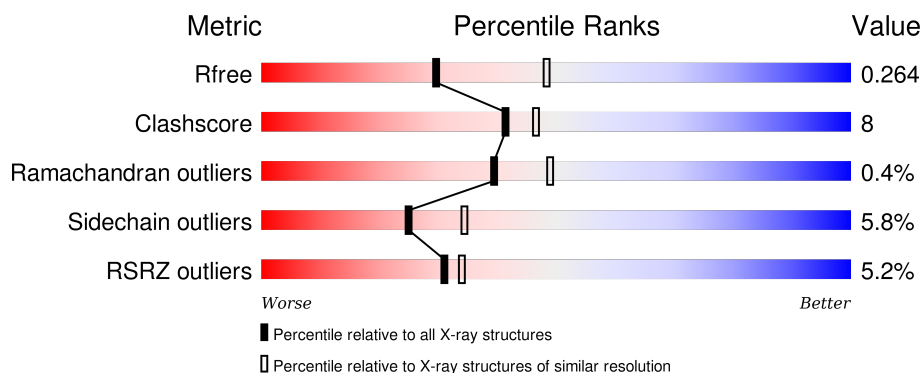
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	515	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>16%</div> <div>• 8%</div> </div> </div>
1	B	515	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 8%</div> </div> </div>
1	C	515	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 8%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12050 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	1	0
			3785	2395	666	699	25			
1	B	476	Total	C	N	O	S	0	2	0
			3792	2402	665	700	25			
1	C	474	Total	C	N	O	S	0	2	0
			3776	2388	663	700	25			

There are 24 discrepancies between the modelled and reference sequences:

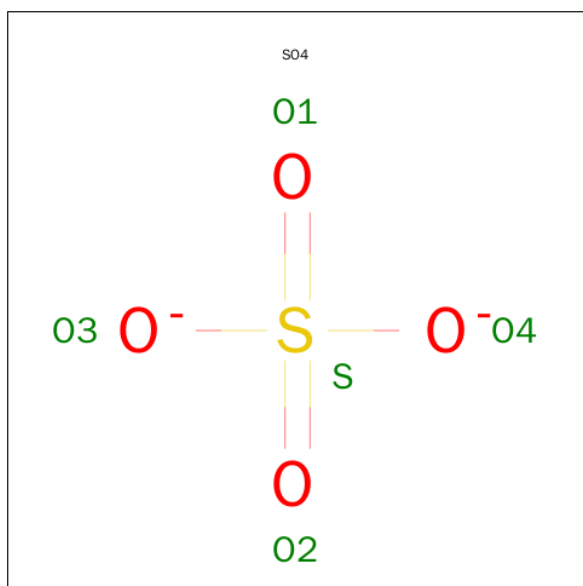
Chain	Residue	Modelled	Actual	Comment	Reference
A	508	LEU	-	EXPRESSION TAG	UNP Q80J95
A	509	GLU	-	EXPRESSION TAG	UNP Q80J95
A	510	HIS	-	EXPRESSION TAG	UNP Q80J95
A	511	HIS	-	EXPRESSION TAG	UNP Q80J95
A	512	HIS	-	EXPRESSION TAG	UNP Q80J95
A	513	HIS	-	EXPRESSION TAG	UNP Q80J95
A	514	HIS	-	EXPRESSION TAG	UNP Q80J95
A	515	HIS	-	EXPRESSION TAG	UNP Q80J95
B	508	LEU	-	EXPRESSION TAG	UNP Q80J95
B	509	GLU	-	EXPRESSION TAG	UNP Q80J95
B	510	HIS	-	EXPRESSION TAG	UNP Q80J95
B	511	HIS	-	EXPRESSION TAG	UNP Q80J95
B	512	HIS	-	EXPRESSION TAG	UNP Q80J95
B	513	HIS	-	EXPRESSION TAG	UNP Q80J95
B	514	HIS	-	EXPRESSION TAG	UNP Q80J95
B	515	HIS	-	EXPRESSION TAG	UNP Q80J95
C	508	LEU	-	EXPRESSION TAG	UNP Q80J95
C	509	GLU	-	EXPRESSION TAG	UNP Q80J95
C	510	HIS	-	EXPRESSION TAG	UNP Q80J95
C	511	HIS	-	EXPRESSION TAG	UNP Q80J95
C	512	HIS	-	EXPRESSION TAG	UNP Q80J95
C	513	HIS	-	EXPRESSION TAG	UNP Q80J95
C	514	HIS	-	EXPRESSION TAG	UNP Q80J95

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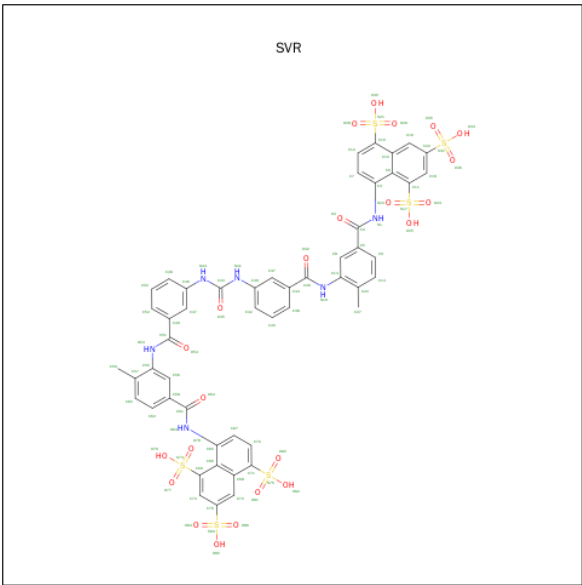
Chain	Residue	Modelled	Actual	Comment	Reference
C	515	HIS	-	EXPRESSION TAG	UNP Q80J95

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

- Molecule 3 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFONIC ACID (three-letter code: SVR) (formula: C<sub>51</sub>H<sub>40</sub>N<sub>6</sub>O<sub>23</sub>S<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			26	12	1	10	3		
3	C	1	Total	C	N	O	S	0	0
			26	12	1	10	3		
3	C	1	Total	C	N	O	S	0	0
			54	33	5	13	3		

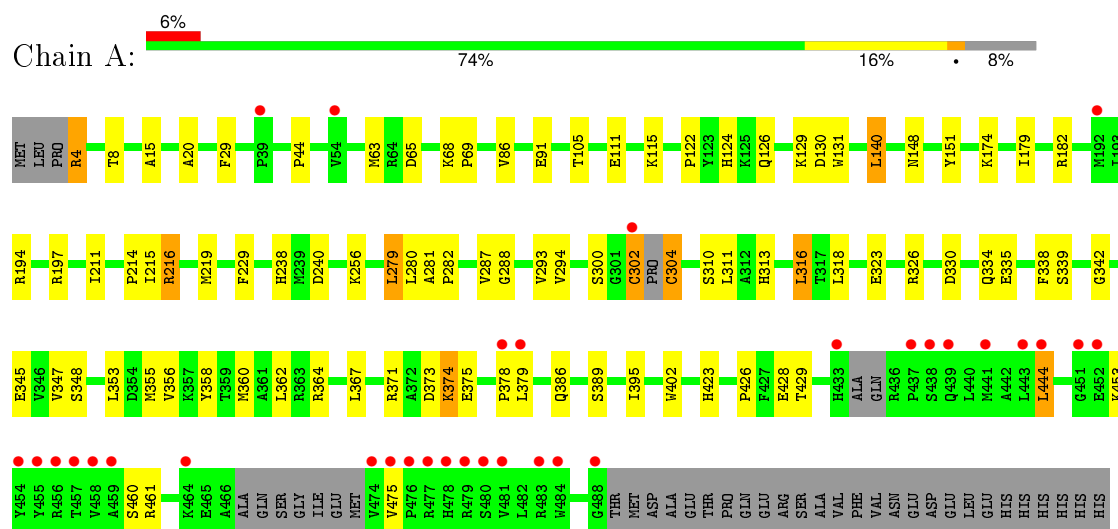
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	166	Total	O	0	0
			166	166		
4	C	217	Total	O	0	0
			217	217		

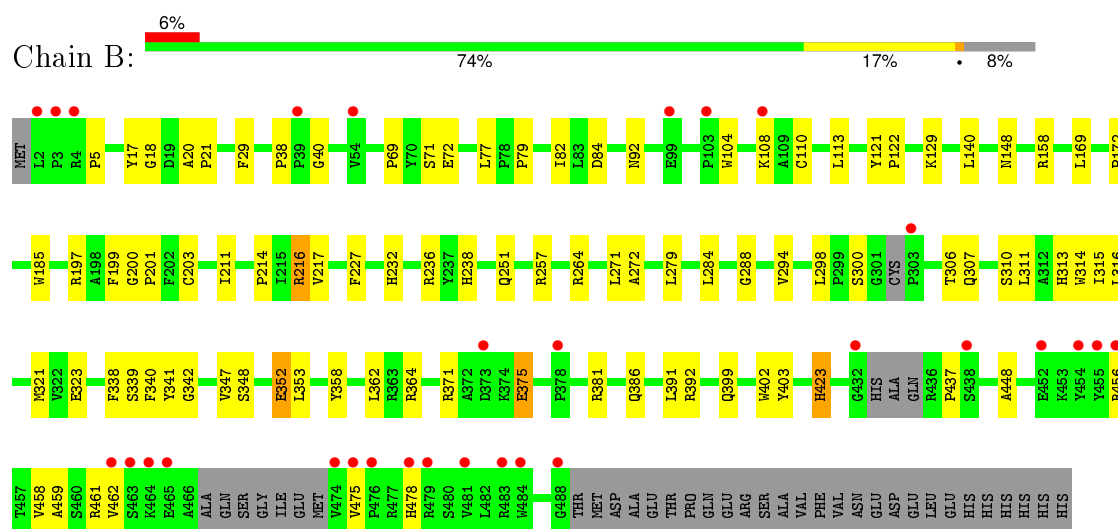
### 3 Residue-property plots

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

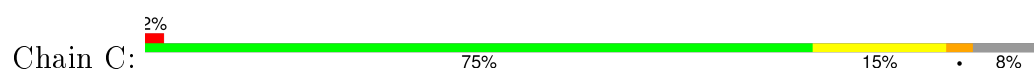
#### • Molecule 1: RNA-dependent RNA polymerase



#### • Molecule 1: RNA-dependent RNA polymerase



#### • Molecule 1: RNA-dependent RNA polymerase



SER	GLY	ILE	GLU	MET	VAL	V475	R326	V327	D328	P329	D330	E335	F338	S339	G342	E345	S348	L353	R364	L367	A372	D373	L391	R392	R393	H423	Q424	N425	P426	F427	E428	G432	HIS	L280	ALA	GLN	R436	P437	S438	A448	E452	R456	R461	S462	K464	E465	A466	A467	GLN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.84Å 196.51Å 109.07Å 90.00° 114.55° 90.00°	Depositor
Resolution (Å)	48.00 – 2.45 48.08 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.00-2.45) 97.4 (48.08-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.199 , 0.268 0.199 , 0.264	Depositor DCC
$R_{free}$ test set	4102 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 82297 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: SVR, 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	0.58	0/3879	0.71	2/5250 (0.0%)
1	B	0.54	0/3890	0.64	0/5267
1	C	0.62	0/3872	0.71	1/5241 (0.0%)
All	All	0.58	0/11641	0.69	3/15758 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	65	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	65	ASP	CB-CG-OD1	5.06	122.85	118.30

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	3785	0	3745	66	0
1	B	3792	0	3760	51	0
1	C	3776	0	3734	68	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	0	0	0
3	B	26	0	6	2	0
3	C	80	0	31	17	0
4	A	173	0	0	6	0
4	B	166	0	0	2	0
4	C	217	0	0	3	0
All	All	12050	0	11276	192	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 8.

The worst 5 of 192 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:C:301:GLY:HA3	1:C:302:CYS:CB	1.56	1.27
1:C:301:GLY:HA3	1:C:302:CYS:HB3	1.24	1.12
1:C:301:GLY:HA3	1:C:302:CYS:HB2	1.35	1.03
1:A:373:ASP:O	1:A:374:LYS:HB2	1.59	0.97
1:C:301:GLY:CA	1:C:302:CYS:CB	2.44	0.93

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	468/515 (91%)	451 (96%)	16 (3%)	1 (0%)	52	64
1	B	470/515 (91%)	449 (96%)	20 (4%)	1 (0%)	52	64
1	C	468/515 (91%)	452 (97%)	12 (3%)	4 (1%)	21	25
All	All	1406/1545 (91%)	1352 (96%)	48 (3%)	6 (0%)	39	49

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	301	GLY
1	A	300	SER
1	B	437	PRO
1	C	242	ASP
1	C	300	SER

### 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	407/441 (92%)	387 (95%)	20 (5%)	31	43
1	B	409/441 (93%)	385 (94%)	24 (6%)	24	34
1	C	406/441 (92%)	380 (94%)	26 (6%)	22	29
All	All	1222/1323 (92%)	1152 (94%)	70 (6%)	25	35

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	264	ARG
1	B	375	GLU
1	C	353	LEU
1	B	271	LEU
1	B	298	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	232	HIS
1	B	307	GLN
1	C	313	HIS
1	B	238	HIS
1	B	313	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

10 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	516	-	4,4,4	0.15	0	6,6,6	0.37	0
2	SO4	A	517	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	A	518	-	4,4,4	0.12	0	6,6,6	0.11	0
3	SVR	B	516	-	27,27,93	1.53	2 (7%)	37,44,145	1.64	8 (21%)
2	SO4	B	517	-	4,4,4	0.19	0	6,6,6	0.21	0
3	SVR	C	516	-	27,27,93	1.41	4 (14%)	37,44,145	1.36	3 (8%)
3	SVR	C	517	-	58,58,93	2.73	15 (25%)	82,88,145	1.91	14 (17%)
2	SO4	C	518	-	4,4,4	0.27	0	6,6,6	0.58	0
2	SO4	C	519	-	4,4,4	0.36	0	6,6,6	0.27	0
2	SO4	C	520	-	4,4,4	0.20	0	6,6,6	0.16	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	516	-	-	0/0/0/0	0/0/0/0
2	SO4	A	517	-	-	0/0/0/0	0/0/0/0
2	SO4	A	518	-	-	0/0/0/0	0/0/0/0
3	SVR	B	516	-	-	0/22/22/76	0/2/2/8
2	SO4	B	517	-	-	0/0/0/0	0/0/0/0
3	SVR	C	516	-	-	0/22/22/76	0/2/2/8
3	SVR	C	517	-	-	0/46/46/76	0/5/5/8
2	SO4	C	518	-	-	0/0/0/0	0/0/0/0
2	SO4	C	519	-	-	0/0/0/0	0/0/0/0
2	SO4	C	520	-	-	0/0/0/0	0/0/0/0

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	517	SVR	C27-C20	-7.13	1.36	1.51
3	C	517	SVR	C49-C51	-6.23	1.40	1.50
3	B	516	SVR	C69-S73	-5.24	1.70	1.78
3	C	517	SVR	C5-C2	-5.15	1.39	1.50
3	C	517	SVR	C33-C26	-4.33	1.41	1.50

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	517	SVR	C3-N1-C2	-5.86	110.40	128.87
3	C	517	SVR	C16-C10-C15	-4.98	117.49	123.23
3	C	517	SVR	O45-C43-N41	-3.72	117.94	123.58
3	B	516	SVR	C74-C69-S73	-3.56	111.65	117.82
3	C	516	SVR	C72-C68-C71	-3.41	119.30	123.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	516	SVR	2	0
3	C	516	SVR	3	0
3	C	517	SVR	14	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	475/515 (92%)	0.20	33 (6%)	20 21	30, 50, 105, 124	7 (1%)
1	B	476/515 (92%)	0.25	30 (6%)	23 25	36, 58, 102, 124	7 (1%)
1	C	474/515 (92%)	0.00	11 (2%)	64 66	25, 44, 83, 120	7 (1%)
All	All	1425/1545 (92%)	0.15	74 (5%)	31 34	25, 51, 99, 124	21 (1%)

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	481	VAL	7.2
1	A	454	TYR	7.1
1	B	378	PRO	6.1
1	A	39	PRO	6.0
1	A	474	VAL	5.9

### 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	A	518	5/5	0.95	0.23	1.68	124,124,125,127	0
3	SVR	C	516	26/86	0.94	0.20	1.53	82,96,102,104	0
3	SVR	C	517	54/86	0.85	0.22	1.46	87,95,127,130	0
3	SVR	B	516	26/86	0.89	0.21	1.03	112,121,130,131	0
2	SO4	C	519	5/5	0.94	0.15	0.56	92,94,97,98	0
2	SO4	C	518	5/5	0.98	0.13	-0.43	72,79,86,88	0
2	SO4	C	520	5/5	0.95	0.12	-1.22	93,94,96,96	0
2	SO4	A	516	5/5	0.86	0.20	-	112,115,116,116	0
2	SO4	B	517	5/5	0.87	0.19	-	133,134,135,135	0
2	SO4	A	517	5/5	0.84	0.18	-	155,155,155,156	0

## 6.5 Other polymers

There are no such residues in this entry.