



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 01:59 PM GMT

PDB ID : 3ZSO  
Title : Small molecule inhibitors of the LEDGF site of HIV type 1 integrase identified by fragment screening and structure based design  
Authors : Peat, T.S.; Newman, J.; Rhodes, D.I.; Deadman, J.J.; Vandergraaff, N.; Le, G.; Jones, E.D.; Smith, J.A.; Coates, J.A.V.; Thienthong, N.; Dolezal, O.; Ryan, J.H.; Savage, G.P.; Francis, C.L.  
Deposited on : 2011-06-30  
Resolution : 1.75 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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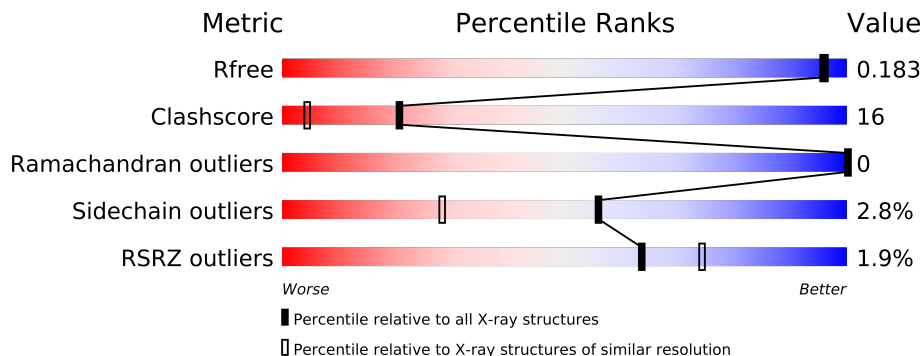
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 1.75 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))
$R_{free}$	66092	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	167	
1	B	167	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1212	-	X
2	SO4	A	1213	-	X
2	SO4	A	1214	-	X
2	SO4	B	1212	-	X
2	SO4	B	1213	-	X
2	SO4	B	1214	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	ACY	A	1217	-	X
3	ACY	B	1215	-	X
5	O2N	A	1219	-	X
5	O2N	B	1217	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2865 atoms, of which 0 are hydrogen and 0 are deuterium.

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 INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	16	0
			1273	816	217	236	4			
1	B	150	Total	C	N	O	S	0	17	0
			1280	819	219	238	4			

There are 26 discrepancies between the modelled and reference sequences:

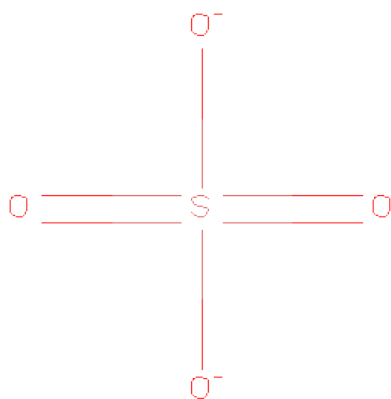
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	MET	-	EXPRESSION TAG	UNP Q76353
A	47	GLY	-	EXPRESSION TAG	UNP Q76353
A	48	SER	-	EXPRESSION TAG	UNP Q76353
A	49	SER	-	EXPRESSION TAG	UNP Q76353
A	50	HIS	-	EXPRESSION TAG	UNP Q76353
A	51	HIS	-	EXPRESSION TAG	UNP Q76353
A	52	HIS	-	EXPRESSION TAG	UNP Q76353
A	53	HIS	-	EXPRESSION TAG	UNP Q76353
A	54	HIS	-	EXPRESSION TAG	UNP Q76353
A	55	HIS	-	EXPRESSION TAG	UNP Q76353
A	56	SER	CYS	ENGINEERED MUTATION	UNP Q76353
A	139	ASP	PHE	ENGINEERED MUTATION	UNP Q76353
A	185	HIS	PHE	ENGINEERED MUTATION	UNP Q76353
B	46	MET	-	EXPRESSION TAG	UNP Q76353
B	47	GLY	-	EXPRESSION TAG	UNP Q76353
B	48	SER	-	EXPRESSION TAG	UNP Q76353
B	49	SER	-	EXPRESSION TAG	UNP Q76353
B	50	HIS	-	EXPRESSION TAG	UNP Q76353
B	51	HIS	-	EXPRESSION TAG	UNP Q76353
B	52	HIS	-	EXPRESSION TAG	UNP Q76353
B	53	HIS	-	EXPRESSION TAG	UNP Q76353
B	54	HIS	-	EXPRESSION TAG	UNP Q76353
B	55	HIS	-	EXPRESSION TAG	UNP Q76353
B	56	SER	CYS	ENGINEERED MUTATION	UNP Q76353
B	139	ASP	PHE	ENGINEERED MUTATION	UNP Q76353

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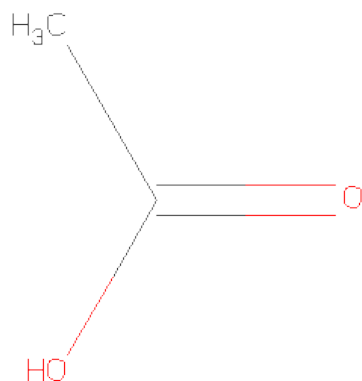
Chain	Residue	Modelled	Actual	Comment	Reference
B	185	HIS	PHE	ENGINEERED MUTATION	UNP Q76353

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (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	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).

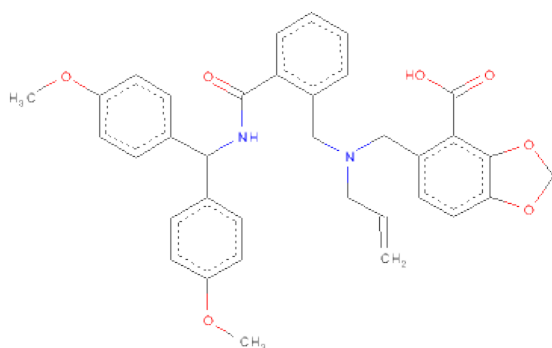


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is 5-{{(2-{{[BIS(4-METHOXYPHENYL)METHYL]CARBAMOYL}}BENZYL)(PROP-2-EN-1-YL)AMINO]METHYL}-1,3-BENZODIOXOLE-4-CARBOXYLICACID (three-letter code: O2N) (formula: C<sub>35</sub>H<sub>34</sub>N<sub>2</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			44	35	2	7		
5	B	1	Total	C	N	O	0	0
			44	35	2	7		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total	O	0	0
			89	89		
6	B	77	Total	O	0	0
			77	77		

### 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.

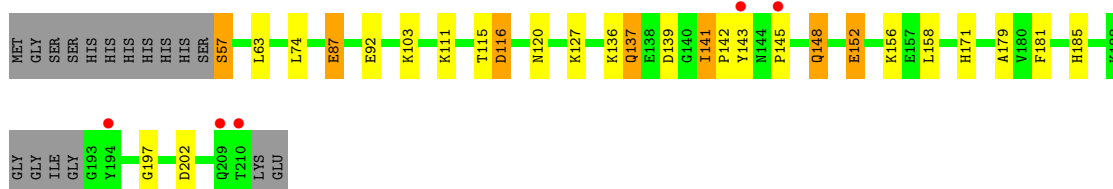
#### • Molecule 1: INTEGRASE

Chain A: 



#### • Molecule 1: INTEGRASE

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.06Å 71.06Å 67.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.54 – 1.75 45.33 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.54-1.75) 99.9 (45.33-1.75)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.17 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.163 , 0.209 0.158 , 0.183	Depositor DCC
$R_{free}$ test set	1930 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.6	EDS
Estimated twinning fraction	0.034 for -h,-k,l 0.488 for h,-h-k,-l 0.034 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 38119 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: O2N, NA, ACY, 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	1.23	4/1322 (0.3%)	1.04	1/1795 (0.1%)
1	B	1.25	2/1332 (0.2%)	1.04	1/1806 (0.1%)
All	All	1.24	6/2654 (0.2%)	1.04	2/3601 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	131	TRP	CZ3-CH2	5.52	1.48	1.40
1	A	61	TRP	CE3-CZ3	5.45	1.47	1.38
1	B	87[A]	GLU	CG-CD	5.27	1.59	1.51
1	B	87[B]	GLU	CG-CD	5.27	1.59	1.51
1	A	87[A]	GLU	CG-CD	5.02	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	116	ASP	CB-CG-OD2	-5.26	113.57	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1273	0	1297	31	0
1	B	1280	0	1306	42	0
2	A	20	0	0	1	0
2	B	20	0	0	2	0
3	A	12	0	9	20	0
3	B	4	0	3	2	0
4	A	1	0	0	1	0
4	B	1	0	0	2	0
5	A	44	0	33	5	0
5	B	44	0	33	5	0
6	A	89	0	0	8	0
6	B	77	0	0	13	0
All	All	2865	0	2681	84	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 84 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141[B]:ILE:HD12	1:A:142:PRO:HD2	1.28	1.10
1:B:111:LYS:HD3	6:B:2003:HOH:O	1.66	0.96
5:B:1217:O2N:H302	6:B:2063:HOH:O	1.68	0.93
5:A:1219:O2N:H302	6:A:2075:HOH:O	1.69	0.93
3:A:1215:ACY:OXT	1:B:87[B]:GLU:OE1	1.88	0.92

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	162/167 (97%)	159 (98%)	3 (2%)	0	100	100
1	B	163/167 (98%)	161 (99%)	2 (1%)	0	100	100
All	All	325/334 (97%)	320 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	140/137 (102%)	138 (99%)	2 (1%)	78	62
1	B	141/137 (103%)	136 (96%)	5 (4%)	48	19
All	All	281/274 (103%)	274 (98%)	7 (2%)	56	33

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	137	GLN
1	B	152	GLU
1	B	141	ILE
1	A	188	LYS
1	B	148	GLN

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	137	GLN
1	B	148	GLN
1	B	171	HIS
1	A	209	GLN
1	B	155	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	A	1211	-	4,4,4	0.74	0	6,6,6	0.94	0
2	SO4	A	1212	-	4,4,4	0.60	0	6,6,6	0.78	0
2	SO4	A	1213	-	4,4,4	1.29	0	6,6,6	0.75	0
2	SO4	A	1214	4	4,4,4	0.50	0	6,6,6	0.42	0
3	ACY	A	1215	-	3,3,3	1.41	1 (33%)	3,3,3	1.06	0
3	ACY	A	1216	-	3,3,3	1.31	1 (33%)	3,3,3	1.11	0
3	ACY	A	1217	-	3,3,3	0.47	0	3,3,3	1.56	0
5	O2N	A	1219	-	48,48,48	1.27	4 (8%)	66,66,66	1.74	15 (22%)
2	SO4	B	1211	-	4,4,4	0.76	0	6,6,6	1.45	2 (33%)
2	SO4	B	1212	-	4,4,4	0.37	0	6,6,6	0.71	0
2	SO4	B	1213	-	4,4,4	1.45	1 (25%)	6,6,6	0.81	0
2	SO4	B	1214	4	4,4,4	0.21	0	6,6,6	0.65	0
3	ACY	B	1215	-	3,3,3	0.79	0	3,3,3	0.82	0
5	O2N	B	1217	-	48,48,48	1.19	4 (8%)	66,66,66	1.74	16 (24%)

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	1211	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1212	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1213	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1214	4	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACY	A	1215	-	-	0/0/0/0	0/0/0/0
3	ACY	A	1216	-	-	0/0/0/0	0/0/0/0
3	ACY	A	1217	-	-	0/0/0/0	0/0/0/0
5	O2N	A	1219	-	-	0/35/41/41	0/3/5/5
2	SO4	B	1211	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1212	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1213	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1214	4	-	0/0/0/0	0/0/0/0
3	ACY	B	1215	-	-	0/0/0/0	0/0/0/0
5	O2N	B	1217	-	-	0/35/41/41	0/3/5/5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1219	O2N	C33-N37	5.11	1.57	1.47
5	B	1217	O2N	C33-N37	4.59	1.56	1.47
5	A	1219	O2N	C32-N37	2.73	1.52	1.47
5	A	1219	O2N	C27-N36	2.63	1.40	1.34
5	A	1219	O2N	C10-C5	2.52	1.43	1.38

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1217	O2N	C9-C18-C35	4.37	128.62	120.71
5	B	1217	O2N	C14-C9-C18	4.34	125.80	121.20
5	A	1219	O2N	O42-C22-C16	-4.12	123.91	128.02
5	B	1217	O2N	C9-C14-C24	-4.04	114.34	119.76
5	A	1219	O2N	C26-C34-N37	3.96	117.39	113.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	150/167 (89%)	-0.31	1 (0%) 84 91	12, 20, 47, 59	20 (13%)
1	B	150/167 (89%)	-0.31	5 (3%) 44 53	13, 21, 47, 58	20 (13%)
All	All	300/334 (89%)	-0.31	6 (2%) 64 73	12, 20, 48, 59	40 (13%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	TYR	3.8
1	B	210	THR	3.5
1	B	143	TYR	3.4
1	B	145	PRO	3.0
1	B	209	GLN	2.6

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	1214	5/5	0.15	9.66	27,39,45,46	5
3	ACY	A	1217	4/4	0.12	5.85	47,48,49,50	0
2	SO4	A	1214	5/5	0.15	4.98	33,44,47,50	5
2	SO4	A	1213	5/5	0.14	4.51	35,36,44,48	5
5	O2N	A	1219	44/44	0.13	3.65	18,26,34,37	44
3	ACY	B	1215	4/4	0.12	3.55	42,43,44,44	0
2	SO4	B	1213	5/5	0.14	3.41	33,34,46,48	5
2	SO4	A	1212	5/5	0.10	2.74	22,26,28,31	5
2	SO4	B	1212	5/5	0.09	2.48	24,29,31,36	5
5	O2N	B	1217	44/44	0.12	2.29	19,26,33,36	44
3	ACY	A	1216	4/4	0.12	1.60	29,30,32,33	0
2	SO4	A	1211	5/5	0.10	0.81	28,28,35,38	5
2	SO4	B	1211	5/5	0.08	0.21	28,31,37,41	5
3	ACY	A	1215	4/4	0.09	0.17	28,29,29,31	0
4	NA	A	1218	1/1	0.04	-2.62	48,48,48,48	0
4	NA	B	1216	1/1	0.04	-3.03	45,45,45,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.