



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:06 PM GMT

PDB ID : 1S5M  
Title : Xylose Isomerase in Substrate and Inhibitor Michaelis States: Atomic Resolution Studies of a Metal-Mediated Hydride Shift  
Authors : Fenn, T.D.; Ringe, D.; Petsko, G.A.  
Deposited on : 2004-01-21  
Resolution : 0.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

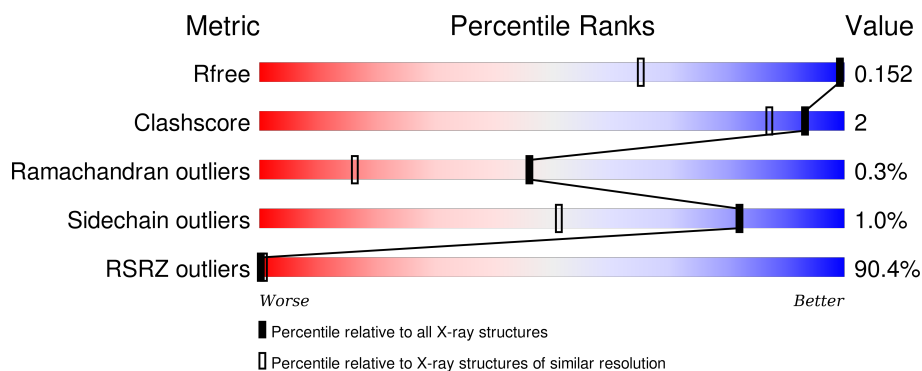
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 0.98 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	1291 (1.10-0.86)
Clashscore	102246	1390 (1.10-0.86)
Ramachandran outliers	100387	1301 (1.10-0.86)
Sidechain outliers	100360	1300 (1.10-0.86)
RSRZ outliers	91569	1295 (1.10-0.86)

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	386	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6830 atoms, of which 3140 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 Xylose isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	386	6378	2036	3128	589	615	10	0	45	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	ILE	THR	SEE REMARK 999	UNP P15587

- Molecule 2 is alpha-D-glucose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	24	6	12	6	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Na	0	0
			2	2		

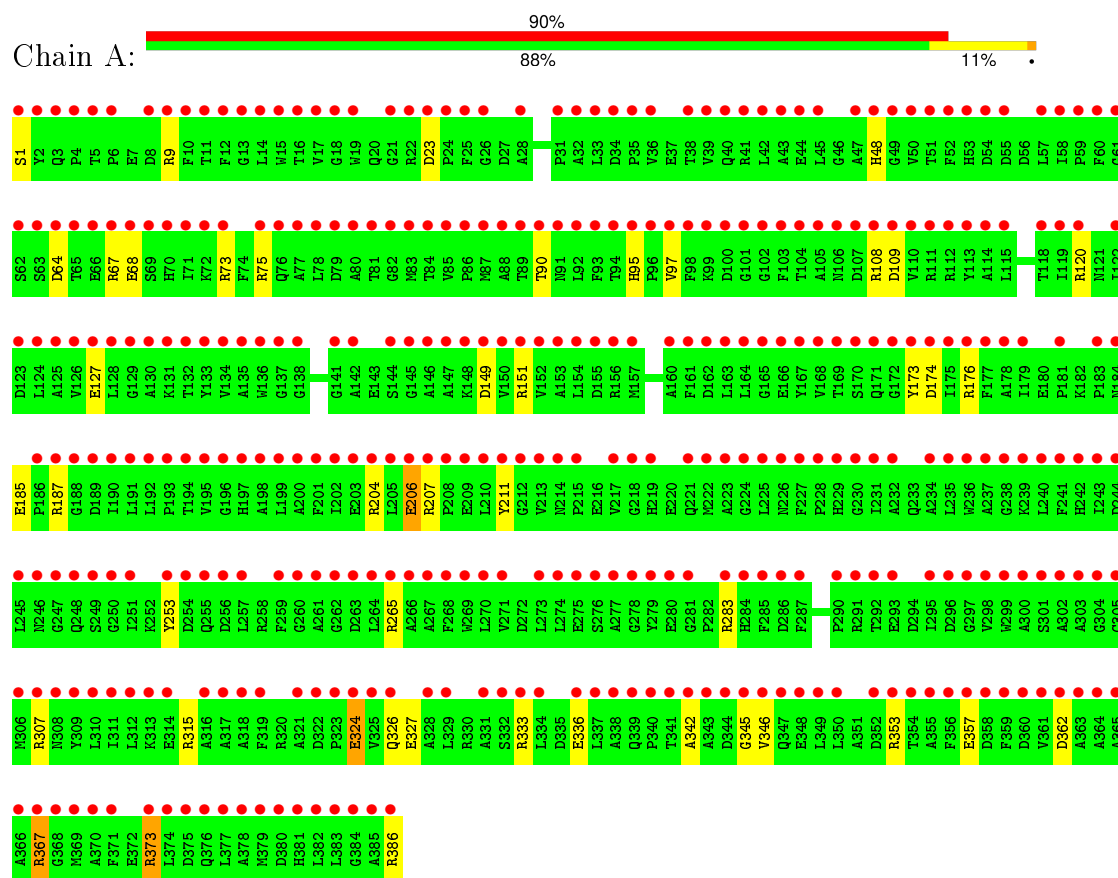
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	411	Total	O	0	13
			424	424		

### 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: Xylose isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.86Å 92.97Å 98.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 0.98 32.33 – 0.95	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.00-0.98) 88.0 (32.33-0.95)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 0.95Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.111 , 0.129 0.151 , 0.152	Depositor DCC
$R_{free}$ test set	10603 reflections (5.52%)	DCC
Wilson B-factor (Å <sup>2</sup> )	9.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.47 , 61.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 229134 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	6830	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% 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: NA, GLC, MN

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	0.89	5/3323 (0.2%)	1.59	61/4494 (1.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	336	GLU	CB-CG	-9.07	1.34	1.52
1	A	73	ARG	CZ-NH2	7.58	1.43	1.33
1	A	73	ARG	CZ-NH1	7.39	1.42	1.33
1	A	315	ARG	CZ-NH2	6.21	1.41	1.33
1	A	327[A]	GLU	CD-OE2	5.99	1.32	1.25

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ARG	CD-NE-CZ	33.46	170.44	123.60
1	A	204[A]	ARG	CD-NE-CZ	18.35	149.29	123.60
1	A	204[B]	ARG	CD-NE-CZ	18.35	149.29	123.60
1	A	386[A]	ARG	NE-CZ-NH1	16.26	128.43	120.30
1	A	386[B]	ARG	NE-CZ-NH1	16.26	128.43	120.30
1	A	386[A]	ARG	NE-CZ-NH2	-15.78	112.41	120.30
1	A	386[B]	ARG	NE-CZ-NH2	-15.78	112.41	120.30
1	A	373	ARG	NE-CZ-NH2	13.24	126.92	120.30
1	A	9[A]	ARG	NE-CZ-NH2	-13.19	113.70	120.30
1	A	9[A]	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	A	127	GLU	OE1-CD-OE2	11.31	136.87	123.30
1	A	367	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	A	211	TYR	CB-CG-CD2	11.04	127.63	121.00
1	A	120	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	A	315	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	315	ARG	NE-CZ-NH1	8.90	124.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207[A]	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	A	187	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	A	120	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	A	265[A]	ARG	CD-NE-CZ	7.59	134.23	123.60
1	A	265[B]	ARG	CD-NE-CZ	7.59	134.23	123.60
1	A	357	GLU	OE1-CD-OE2	-7.59	114.19	123.30
1	A	176[A]	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	A	176[B]	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	A	149	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	174[A]	ASP	CB-CG-OD1	-6.93	112.07	118.30
1	A	174[B]	ASP	CB-CG-OD1	-6.93	112.07	118.30
1	A	174[A]	ASP	O-C-N	-6.91	111.65	122.70
1	A	174[B]	ASP	O-C-N	-6.91	111.65	122.70
1	A	373	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	A	346	VAL	CA-CB-CG1	6.84	121.17	110.90
1	A	75	ARG	CD-NE-CZ	6.84	133.17	123.60
1	A	324[A]	GLU	OE1-CD-OE2	6.82	131.49	123.30
1	A	324[B]	GLU	OE1-CD-OE2	6.82	131.49	123.30
1	A	108	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	204[A]	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	204[B]	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	67	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	211	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	A	353	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	174[A]	ASP	N-CA-CB	-6.17	99.49	110.60
1	A	174[B]	ASP	N-CA-CB	-6.17	99.49	110.60
1	A	187	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	64	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	A	151[A]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	151[B]	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	206[A]	GLU	OE1-CD-OE2	-5.89	116.24	123.30
1	A	206[B]	GLU	OE1-CD-OE2	-5.89	116.24	123.30
1	A	75	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	A	173[A]	TYR	CB-CG-CD1	5.76	124.46	121.00
1	A	173[B]	TYR	CB-CG-CD1	5.76	124.46	121.00
1	A	253	TYR	CB-CG-CD1	5.69	124.41	121.00
1	A	73	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	A	67	ARG	CD-NE-CZ	-5.65	115.69	123.60
1	A	315	ARG	CD-NE-CZ	-5.60	115.76	123.60
1	A	108	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	307	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	367	ARG	NH1-CZ-NH2	5.48	125.43	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ASP	CB-CA-C	5.45	121.29	110.40
1	A	362	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	109	ASP	CB-CG-OD1	5.04	122.83	118.30

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	3250	3128	2961	12	0
2	A	12	12	10	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	424	0	0	7	0
All	All	3690	3140	2971	12	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 2.

All (12) 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:A:283[B]:ARG:CZ	5:A:2413:HOH:O	1.65	1.24
1:A:283[B]:ARG:NH2	5:A:2413:HOH:O	1.58	1.12
1:A:283[B]:ARG:NE	5:A:2413:HOH:O	1.62	1.07
1:A:95:HIS:HD2	1:A:97:VAL:H	1.40	0.68
1:A:48[A]:HIS:HD2	5:A:2324:HOH:O	1.90	0.54
1:A:333:ARG:NH2	1:A:367:ARG:HD3	2.27	0.50
1:A:324[A]:GLU:OE2	1:A:373:ARG:NH2	2.47	0.48
1:A:345:GLY:N	5:A:2410:HOH:O	2.48	0.45
1:A:326[A]:GLN:NE2	5:A:2112:HOH:O	2.52	0.41
1:A:95:HIS:CD2	1:A:97:VAL:H	2.28	0.41
1:A:342:ALA:HB1	5:A:2410:HOH:O	2.20	0.41

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	408/386 (106%)	394 (97%)	13 (3%)	1 (0%)	52 20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU

### 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	326/302 (108%)	323 (99%)	3 (1%)	84 55

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	68	GLU
1	A	90	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	308	ASN
1	A	376	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](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	GLC	A	1001	3	12,12,12	1.34	1 (8%)	17,17,17	2.04	5 (29%)

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	GLC	A	1001	3	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GLC	O5-C1	4.35	1.51	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	GLC	C1-O5-C5	-4.20	105.70	113.47
2	A	1001	GLC	C6-C5-C4	-3.42	104.57	113.02
2	A	1001	GLC	O6-C6-C5	-2.77	102.17	111.33
2	A	1001	GLC	C3-C4-C5	-2.42	105.97	110.20
2	A	1001	GLC	O5-C5-C6	4.37	117.39	106.36

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 ⓘ

### 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	386/386 (100%)	3.53	349 (90%) 0 1	7, 10, 26, 46	0

All (349) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	SER	10.5
1	A	78	LEU	7.8
1	A	385[A]	ALA	7.1
1	A	174[A]	ASP	6.9
1	A	33	LEU	6.8
1	A	173[A]	TYR	6.8
1	A	75	ARG	6.7
1	A	24	PRO	6.7
1	A	76	GLN	6.5
1	A	346	VAL	6.3
1	A	9[A]	ARG	6.0
1	A	163[A]	LEU	6.0
1	A	205[A]	LEU	6.0
1	A	386[A]	ARG	5.9
1	A	36	VAL	5.9
1	A	122	ILE	5.8
1	A	383	LEU	5.7
1	A	169	THR	5.6
1	A	190	ILE	5.5
1	A	299	TRP	5.5
1	A	126	VAL	5.5
1	A	298	VAL	5.5
1	A	356	PHE	5.5
1	A	114	ALA	5.5
1	A	6	PRO	5.5
1	A	276[A]	SER	5.5
1	A	125	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	208	PRO	5.4
1	A	343	ALA	5.4
1	A	382	LEU	5.3
1	A	80	ALA	5.3
1	A	235	LEU	5.3
1	A	65	THR	5.3
1	A	342	ALA	5.2
1	A	329	LEU	5.2
1	A	89	THR	5.2
1	A	243	ILE	5.2
1	A	61	GLY	5.1
1	A	119	ILE	5.1
1	A	25	PHE	5.1
1	A	241	PHE	5.1
1	A	310	LEU	5.1
1	A	178	ALA	5.0
1	A	15	TRP	5.0
1	A	370	ALA	5.0
1	A	267	ALA	4.9
1	A	98	PHE	4.9
1	A	245	LEU	4.9
1	A	269	TRP	4.9
1	A	142	ALA	4.9
1	A	359	PHE	4.8
1	A	266[A]	ALA	4.8
1	A	168	VAL	4.8
1	A	347	GLN	4.8
1	A	157[A]	MET	4.8
1	A	135	ALA	4.7
1	A	113	TYR	4.7
1	A	63	SER	4.7
1	A	202	ILE	4.7
1	A	249[A]	SER	4.7
1	A	210	LEU	4.7
1	A	128	LEU	4.6
1	A	147	ALA	4.6
1	A	28	ALA	4.6
1	A	136	TRP	4.6
1	A	349[A]	LEU	4.6
1	A	217	VAL	4.6
1	A	285	PHE	4.6
1	A	204[A]	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	32	ALA	4.6
1	A	152[A]	VAL	4.5
1	A	361	VAL	4.5
1	A	167	TYR	4.5
1	A	357	GLU	4.5
1	A	45	LEU	4.5
1	A	48[A]	HIS	4.5
1	A	154	LEU	4.5
1	A	161	PHE	4.5
1	A	350	LEU	4.4
1	A	71	ILE	4.4
1	A	10[A]	PHE	4.4
1	A	362	ASP	4.4
1	A	193	PRO	4.4
1	A	68	GLU	4.4
1	A	283[A]	ARG	4.4
1	A	250[A]	GLY	4.3
1	A	287[A]	PHE	4.3
1	A	19	TRP	4.3
1	A	58	ILE	4.3
1	A	153	ALA	4.3
1	A	198	ALA	4.3
1	A	41[A]	ARG	4.3
1	A	31	PRO	4.3
1	A	138	GLY	4.3
1	A	240	LEU	4.3
1	A	59	PRO	4.3
1	A	97	VAL	4.3
1	A	323	PRO	4.3
1	A	277[A]	ALA	4.3
1	A	345	GLY	4.3
1	A	251	ILE	4.3
1	A	101	GLY	4.2
1	A	133	TYR	4.2
1	A	34	ASP	4.2
1	A	192	LEU	4.2
1	A	195	VAL	4.2
1	A	177[A]	PHE	4.1
1	A	50[A]	VAL	4.1
1	A	64	ASP	4.1
1	A	325[A]	VAL	4.1
1	A	88	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	132	THR	4.1
1	A	57	LEU	4.1
1	A	199	LEU	4.1
1	A	72	LYS	4.0
1	A	150	VAL	4.0
1	A	303	ALA	4.0
1	A	358	ASP	4.0
1	A	365	ALA	4.0
1	A	124	LEU	4.0
1	A	90	THR	4.0
1	A	227	PHE	4.0
1	A	115	LEU	4.0
1	A	11	THR	4.0
1	A	236	TRP	3.9
1	A	12	PHE	3.9
1	A	305	CYS	3.9
1	A	110	VAL	3.9
1	A	118	THR	3.9
1	A	231	ILE	3.9
1	A	295	ILE	3.9
1	A	191	LEU	3.9
1	A	271	VAL	3.9
1	A	247	GLY	3.9
1	A	367	ARG	3.9
1	A	363	ALA	3.9
1	A	265[A]	ARG	3.9
1	A	257	LEU	3.9
1	A	206[A]	GLU	3.9
1	A	130	ALA	3.9
1	A	270	LEU	3.8
1	A	274	LEU	3.8
1	A	374	LEU	3.8
1	A	213	VAL	3.8
1	A	279	TYR	3.8
1	A	268	PHE	3.8
1	A	371	PHE	3.8
1	A	43	ALA	3.8
1	A	3[A]	GLN	3.8
1	A	16	THR	3.8
1	A	96	PRO	3.8
1	A	264	LEU	3.8
1	A	212	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	223	ALA	3.7
1	A	38	THR	3.7
1	A	104	THR	3.7
1	A	292	THR	3.7
1	A	179	ILE	3.7
1	A	253	TYR	3.7
1	A	145	GLY	3.7
1	A	160	ALA	3.7
1	A	337	LEU	3.7
1	A	47	ALA	3.7
1	A	232	ALA	3.7
1	A	201	PHE	3.7
1	A	194	THR	3.7
1	A	260	GLY	3.7
1	A	211	TYR	3.7
1	A	93	PHE	3.7
1	A	35	PRO	3.6
1	A	2	TYR	3.6
1	A	39	VAL	3.6
1	A	77	ALA	3.6
1	A	218	GLY	3.6
1	A	278	GLY	3.6
1	A	70	HIS	3.6
1	A	324[A]	GLU	3.6
1	A	176[A]	ARG	3.6
1	A	215	PRO	3.6
1	A	134	VAL	3.6
1	A	304	GLY	3.6
1	A	60	PHE	3.6
1	A	44	GLU	3.5
1	A	86	PRO	3.5
1	A	228	PRO	3.5
1	A	51[A]	THR	3.5
1	A	105	ALA	3.5
1	A	312	LEU	3.5
1	A	373	ARG	3.5
1	A	146	ALA	3.5
1	A	302	ALA	3.5
1	A	149	ASP	3.5
1	A	172	GLY	3.5
1	A	368	GLY	3.5
1	A	311	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	21	GLY	3.4
1	A	378	ALA	3.4
1	A	92	LEU	3.4
1	A	131	LYS	3.4
1	A	214	ASN	3.4
1	A	55	ASP	3.4
1	A	200	ALA	3.4
1	A	261	ALA	3.4
1	A	355	ALA	3.4
1	A	334	LEU	3.4
1	A	17	VAL	3.4
1	A	314	GLU	3.4
1	A	73	ARG	3.3
1	A	341	THR	3.3
1	A	181	PRO	3.3
1	A	331	ALA	3.3
1	A	377	LEU	3.3
1	A	22	ARG	3.3
1	A	106	ASN	3.3
1	A	49[A]	GLY	3.3
1	A	280	GLU	3.3
1	A	379	MET	3.3
1	A	319	PHE	3.3
1	A	137	GLY	3.3
1	A	234	ALA	3.3
1	A	144	SER	3.2
1	A	171	GLN	3.2
1	A	164[A]	LEU	3.2
1	A	309	TYR	3.2
1	A	286[A]	ASP	3.2
1	A	69	SER	3.2
1	A	120	ARG	3.2
1	A	52	PHE	3.2
1	A	103	PHE	3.2
1	A	259	PHE	3.2
1	A	364	ALA	3.2
1	A	42	LEU	3.2
1	A	225	LEU	3.2
1	A	187	ARG	3.2
1	A	53	HIS	3.1
1	A	186	PRO	3.1
1	A	151[A]	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	175[A]	ILE	3.1
1	A	381	HIS	3.1
1	A	338	ALA	3.1
1	A	102	GLY	3.1
1	A	94	THR	3.0
1	A	318	ALA	3.0
1	A	82	GLY	3.0
1	A	123	ASP	3.0
1	A	224	GLY	3.0
1	A	109	ASP	3.0
1	A	40[A]	GLN	3.0
1	A	91	ASN	3.0
1	A	83	MET	3.0
1	A	242	HIS	3.0
1	A	196	GLY	2.9
1	A	317	ALA	2.9
1	A	184	ASN	2.9
1	A	273	LEU	2.9
1	A	354	THR	2.9
1	A	290	PRO	2.9
1	A	230	GLY	2.9
1	A	300	ALA	2.8
1	A	23	ASP	2.8
1	A	244	ASP	2.8
1	A	375	ASP	2.8
1	A	67	ARG	2.8
1	A	84	THR	2.8
1	A	197	HIS	2.8
1	A	360	ASP	2.8
1	A	328	ALA	2.8
1	A	226	ASN	2.8
1	A	340	PRO	2.8
1	A	306	MET	2.8
1	A	297	GLY	2.8
1	A	313	LYS	2.8
1	A	353	ARG	2.8
1	A	111	ARG	2.7
1	A	14	LEU	2.7
1	A	308	ASN	2.7
1	A	79	ASP	2.7
1	A	229	HIS	2.7
1	A	246	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	141	GLY	2.6
1	A	183	PRO	2.6
1	A	339	GLN	2.6
1	A	127	GLU	2.6
1	A	203[A]	GLU	2.6
1	A	384	GLY	2.6
1	A	256	ASP	2.6
1	A	4	PRO	2.6
1	A	5	THR	2.6
1	A	85	VAL	2.6
1	A	336	GLU	2.6
1	A	275	GLU	2.6
1	A	207[A]	ARG	2.6
1	A	316	ALA	2.6
1	A	326[A]	GLN	2.5
1	A	219	HIS	2.5
1	A	87	MET	2.5
1	A	107	ASP	2.5
1	A	81	THR	2.5
1	A	348[A]	GLU	2.5
1	A	188	GLY	2.5
1	A	95	HIS	2.5
1	A	376	GLN	2.5
1	A	62	SER	2.5
1	A	237	ALA	2.4
1	A	99[A]	LYS	2.4
1	A	209	GLU	2.4
1	A	322	ASP	2.4
1	A	238	GLY	2.4
1	A	108	ARG	2.4
1	A	66	GLU	2.4
1	A	26	GLY	2.4
1	A	162	ASP	2.4
1	A	189	ASP	2.4
1	A	296	ASP	2.4
1	A	255	GLN	2.3
1	A	366	ALA	2.3
1	A	221	GLN	2.3
1	A	165	GLY	2.3
1	A	239	LYS	2.3
1	A	54	ASP	2.3
1	A	291	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	369	MET	2.3
1	A	301	SER	2.3
1	A	248	GLN	2.3
1	A	148	LYS	2.3
1	A	13	GLY	2.3
1	A	307	ARG	2.3
1	A	166	GLU	2.3
1	A	100[A]	ASP	2.3
1	A	263	ASP	2.3
1	A	156	ARG	2.2
1	A	321	ALA	2.2
1	A	155	ASP	2.2
1	A	333	ARG	2.2
1	A	18	GLY	2.2
1	A	8	ASP	2.2
1	A	284[A]	HIS	2.2
1	A	112	ARG	2.2
1	A	293	GLU	2.2
1	A	129	GLY	2.2
1	A	170	SER	2.2
1	A	380	ASP	2.1
1	A	344	ASP	2.1
1	A	262	GLY	2.1
1	A	352	ASP	2.1
1	A	332	SER	2.1
1	A	281	GLY	2.0
1	A	254	ASP	2.0
1	A	222	MET	2.0

## 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(Å <sup>2</sup> )	Q<0.9
2	GLC	A	1001	12/12	0.88	0.19	-0.23	10,16,28,32	0
3	MN	A	2002	1/1	1.00	0.17	-1.48	7,7,7,7	1
4	NA	A	2005	1/1	0.94	0.14	-1.77	26,26,26,26	0
4	NA	A	2004	1/1	0.99	0.11	-2.21	19,19,19,19	0
3	MN	A	2001	1/1	1.00	0.17	-2.44	8,8,8,8	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.