



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:05 AM GMT

PDB ID : 3KT1  
Title : Crystal structure of Tpa1 from *Saccharomyces cerevisiae*, a component of the messenger ribonucleoprotein complex  
Authors : Kim, H.S.; Kim, H.L.; Kim, K.H.; Kim, D.J.; Lee, S.J.; Yoon, J.Y.; Yoon, H.J.; Lee, H.Y.; Park, S.B.; Kim, S.-J.; Lee, J.Y.; Suh, S.W.  
Deposited on : 2009-11-24  
Resolution : 2.50 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

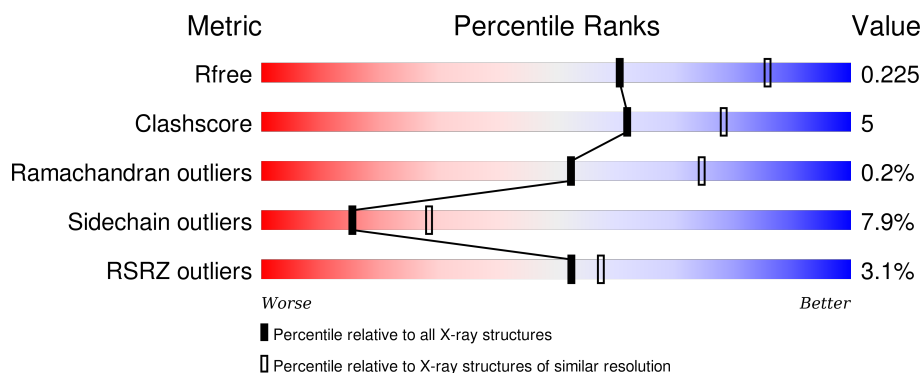
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	633	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4907 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 PKHD-type hydroxylase TPA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4556	2927	762	854	13			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	EXPRESSION TAG	UNP P40032
A	645	LEU	-	EXPRESSION TAG	UNP P40032
A	646	GLU	-	EXPRESSION TAG	UNP P40032
A	647	HIS	-	EXPRESSION TAG	UNP P40032
A	648	HIS	-	EXPRESSION TAG	UNP P40032
A	649	HIS	-	EXPRESSION TAG	UNP P40032
A	650	HIS	-	EXPRESSION TAG	UNP P40032
A	651	HIS	-	EXPRESSION TAG	UNP P40032
A	652	HIS	-	EXPRESSION TAG	UNP P40032

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

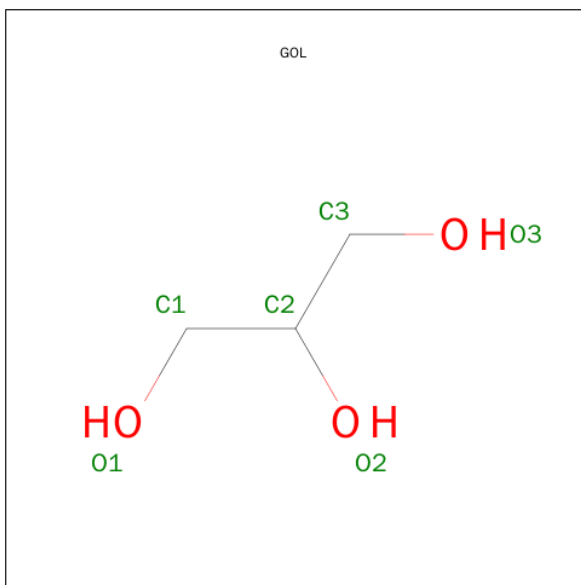
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

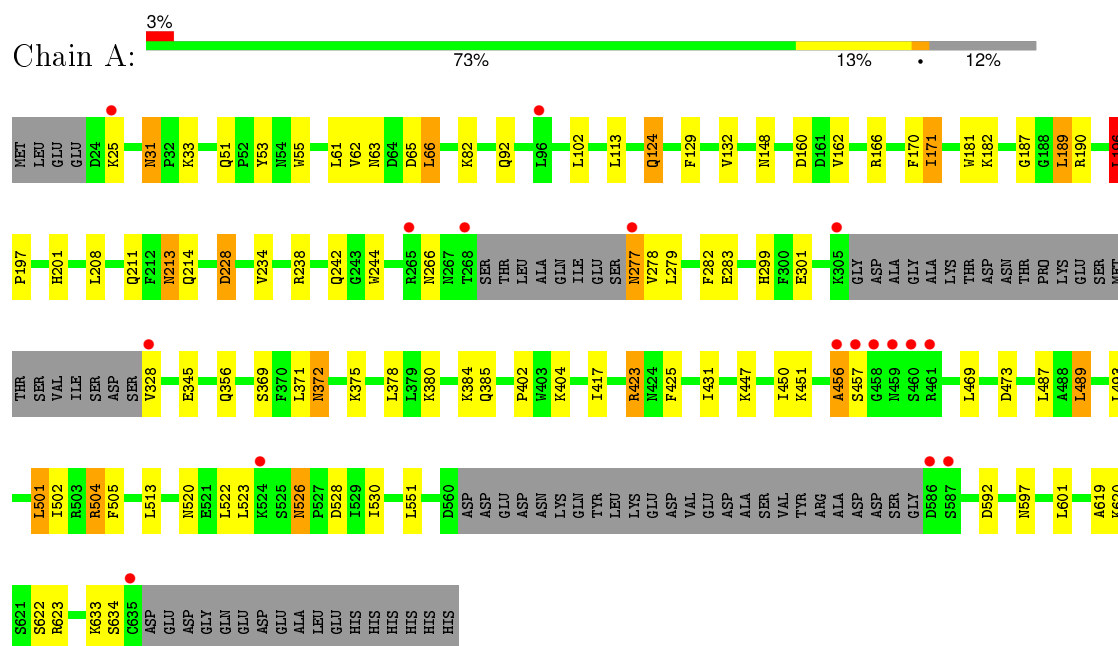
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	324	Total	O	0	0
			324	324		

### 3 Residue-property plots [i](#)

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: PKHD-type hydroxylase TPA1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	136.32Å 136.32Å 79.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.50) 99.8 (19.98-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.13 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.181 , 0.231 0.182 , 0.225	Depositor DCC
$R_{free}$ test set	1505 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 35.5	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29786 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4907	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: GOL, FE, 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	0.52	2/4668 (0.0%)	0.61	4/6307 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	GLU	CB-CG	-5.46	1.41	1.52
1	A	170	PHE	CD2-CE2	-5.12	1.29	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	189	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	501	LEU	CA-CB-CG	5.19	127.25	115.30
1	A	171	ILE	CB-CA-C	-5.07	101.46	111.60

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	4556	0	4490	49	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	20	0	0	0	0
4	A	6	0	8	1	0
5	A	324	0	0	8	1
All	All	4907	0	4498	49	1

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 5.

All (49) 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:201:HIS:CD2	5:A:946:HOH:O	2.17	0.96
1:A:124:GLN:H	1:A:124:GLN:HE21	1.14	0.95
1:A:181:TRP:H	1:A:211:GLN:HE22	1.17	0.93
1:A:63:ASN:HD22	1:A:66:LEU:H	1.25	0.81
1:A:266:ASN:HB3	5:A:803:HOH:O	1.82	0.78
1:A:201:HIS:HD2	5:A:946:HOH:O	1.56	0.78
1:A:238:ARG:NH1	5:A:827:HOH:O	2.18	0.75
1:A:371:LEU:H	1:A:597:ASN:HD21	1.35	0.73
1:A:423:ARG:HG2	1:A:425:PHE:CZ	2.31	0.65
1:A:551:LEU:HD13	1:A:619:ALA:HA	1.81	0.63
1:A:372:ASN:ND2	1:A:375:LYS:H	1.97	0.63
1:A:62:VAL:H	1:A:213:ASN:HD21	1.49	0.60
1:A:31:ASN:HD22	1:A:33:LYS:H	1.50	0.60
1:A:182:LYS:NZ	5:A:973:HOH:O	2.35	0.59
1:A:447:LYS:HE2	1:A:473:ASP:OD2	2.02	0.59
1:A:372:ASN:C	1:A:372:ASN:HD22	2.07	0.57
1:A:402:PRO:HG3	1:A:450:ILE:HD11	1.88	0.56
1:A:63:ASN:HD21	1:A:65:ASP:HB2	1.70	0.55
1:A:345:GLU:HB2	5:A:703:HOH:O	2.07	0.54
1:A:196:LEU:HB2	1:A:197:PRO:HD2	1.90	0.53
1:A:520:ASN:HB3	1:A:523:LEU:HD13	1.91	0.53
1:A:522:LEU:HB3	1:A:523:LEU:HD12	1.91	0.51
1:A:504:ARG:HD3	1:A:622:SER:OG	2.09	0.51
1:A:380:LYS:HG2	1:A:384:LYS:HD2	1.94	0.50
1:A:92:GLN:HA	1:A:148:ASN:HD22	1.78	0.49
1:A:187:GLY:O	1:A:238:ARG:NH2	2.45	0.48
1:A:456:ALA:HA	1:A:457:SER:C	2.34	0.48
1:A:371:LEU:H	1:A:597:ASN:ND2	2.07	0.47
1:A:447:LYS:NZ	4:A:658:GOL:H2	2.31	0.45
1:A:277:ASN:HB2	5:A:872:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ARG:HD3	1:A:622:SER:CB	2.46	0.45
1:A:196:LEU:HB2	1:A:197:PRO:CD	2.47	0.45
1:A:63:ASN:ND2	1:A:66:LEU:H	2.02	0.44
1:A:404:LYS:HE3	1:A:423:ARG:HB2	1.98	0.44
1:A:530:ILE:HD11	1:A:634:SER:HB3	1.99	0.44
1:A:53:TYR:O	1:A:55:TRP:HD1	2.00	0.44
1:A:526:ASN:HD22	1:A:528:ASP:H	1.66	0.43
1:A:160:ASP:OD1	1:A:162:VAL:HG12	2.19	0.42
1:A:211:GLN:H	1:A:214:GLN:HE21	1.67	0.42
1:A:505:PHE:HB2	1:A:623:ARG:HB3	2.01	0.42
1:A:242:GLN:HG3	5:A:904:HOH:O	2.19	0.42
1:A:282:PHE:HD1	1:A:431:ILE:HG21	1.83	0.42
1:A:211:GLN:H	1:A:214:GLN:NE2	2.17	0.42
1:A:190:ARG:HB2	1:A:228:ASP:OD2	2.19	0.42
1:A:372:ASN:HD21	1:A:375:LYS:H	1.68	0.42
1:A:166:ARG:HD3	1:A:244:TRP:CD1	2.55	0.41
1:A:301:GLU:OE2	1:A:633:LYS:NZ	2.42	0.41
1:A:356:GLN:NE2	1:A:489:LEU:HD22	2.36	0.41
1:A:417:ILE:HB	1:A:502:ILE:HB	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:856:HOH:O	5:A:863:HOH:O[3_455]	1.96	0.24

## 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	549/633 (87%)	531 (97%)	17 (3%)	1 (0%)	52 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	456	ALA

### 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	507/573 (88%)	467 (92%)	40 (8%)	15	28

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	31	ASN
1	A	51	GLN
1	A	61	LEU
1	A	66	LEU
1	A	82	LYS
1	A	102	LEU
1	A	113	LEU
1	A	124	GLN
1	A	129	PHE
1	A	132	VAL
1	A	171	ILE
1	A	189	LEU
1	A	196	LEU
1	A	208	LEU
1	A	213	ASN
1	A	228	ASP
1	A	234	VAL
1	A	277	ASN
1	A	278	VAL
1	A	279	LEU
1	A	299	HIS
1	A	328	VAL
1	A	369	SER

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Mol	Chain	Res	Type
1	A	372	ASN
1	A	378	LEU
1	A	385	GLN
1	A	423	ARG
1	A	451	LYS
1	A	469	LEU
1	A	487	LEU
1	A	489	LEU
1	A	493	LEU
1	A	501	LEU
1	A	504	ARG
1	A	513	LEU
1	A	526	ASN
1	A	592	ASP
1	A	601	LEU
1	A	620	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	40	GLN
1	A	54	ASN
1	A	63	ASN
1	A	92	GLN
1	A	98	ASN
1	A	112	ASN
1	A	124	GLN
1	A	148	ASN
1	A	211	GLN
1	A	213	ASN
1	A	214	GLN
1	A	249	GLN
1	A	295	HIS
1	A	299	HIS
1	A	340	GLN
1	A	358	GLN
1	A	372	ASN
1	A	385	GLN
1	A	390	GLN
1	A	438	ASN
1	A	499	GLN

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Mol	Chain	Res	Type
1	A	526	ASN
1	A	597	ASN

### 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 ⓘ

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	$\# Z  > 2$
3	SO4	A	654	-	4,4,4	0.26	0	6,6,6	0.19	0
3	SO4	A	655	-	4,4,4	0.27	0	6,6,6	0.18	0
3	SO4	A	656	-	4,4,4	0.18	0	6,6,6	0.12	0
3	SO4	A	657	-	4,4,4	0.21	0	6,6,6	0.16	0
4	GOL	A	658	-	5,5,5	0.30	0	5,5,5	0.46	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
3	SO4	A	654	-	-	0/0/0/0	0/0/0/0
3	SO4	A	655	-	-	0/0/0/0	0/0/0/0
3	SO4	A	656	-	-	0/0/0/0	0/0/0/0
3	SO4	A	657	-	-	0/0/0/0	0/0/0/0
4	GOL	A	658	-	-	0/4/4/4	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	658	GOL	1	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	557/633 (87%)	-0.41	17 (3%) 52 57	15, 25, 51, 61	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	VAL	7.4
1	A	456	ALA	4.3
1	A	586	ASP	4.1
1	A	96	LEU	3.9
1	A	635	CYS	3.9
1	A	277	ASN	3.9
1	A	305	LYS	3.8
1	A	457	SER	3.5
1	A	458	GLY	2.8
1	A	459	ASN	2.8
1	A	25	LYS	2.5
1	A	268	THR	2.5
1	A	265	ARG	2.4
1	A	587	SER	2.2
1	A	460	SER	2.1
1	A	461	ARG	2.1
1	A	524	LYS	2.1

### 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	657	5/5	0.90	0.18	1.30	65,66,66,66	0
3	SO4	A	655	5/5	0.99	0.08	-1.23	28,28,28,28	5
2	FE	A	653	1/1	0.97	0.05	-2.27	43,43,43,43	0
3	SO4	A	654	5/5	0.97	0.20	-	54,55,56,56	0
3	SO4	A	656	5/5	0.90	0.25	-	54,55,55,56	0
4	GOL	A	658	6/6	0.76	0.27	-	57,58,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.