



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:36 am BST

PDB ID : 2Q3Z  
Title : Transglutaminase 2 undergoes large conformational change upon activation  
Authors : Strop, P.; Pinkas, D.M.; Brunger, A.T.; Khosla, C.  
Deposited on : 2007-05-30  
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

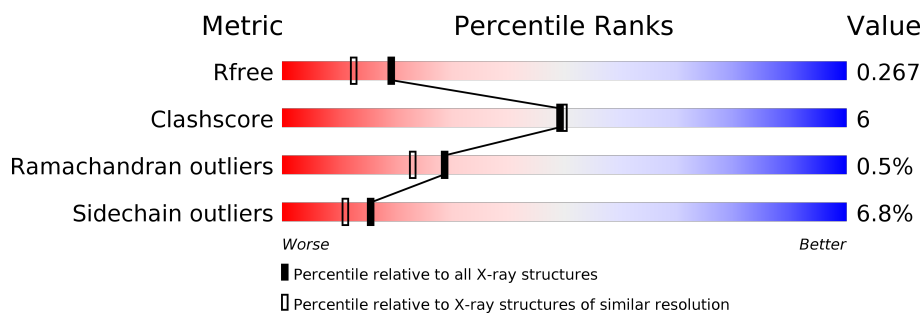
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 respectively. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	687	
2	X	7	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5519 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 Transglutaminase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	655	5186	3282	894	979	31	66	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	GLN	GLU	CONFLICT	UNP P21980
A	186	GLN	GLU	CONFLICT	UNP P21980
A	224	GLY	VAL	CONFLICT	UNP P21980
A	533	THR	ASN	CONFLICT	UNP P21980
A	655	VAL	LEU	CONFLICT	UNP P21980

- Molecule 2 is a protein called Polypeptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	X	7	46	33	6	7	0	0	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		
3	A	1	Total	O	S	0	0
			5	4	1		

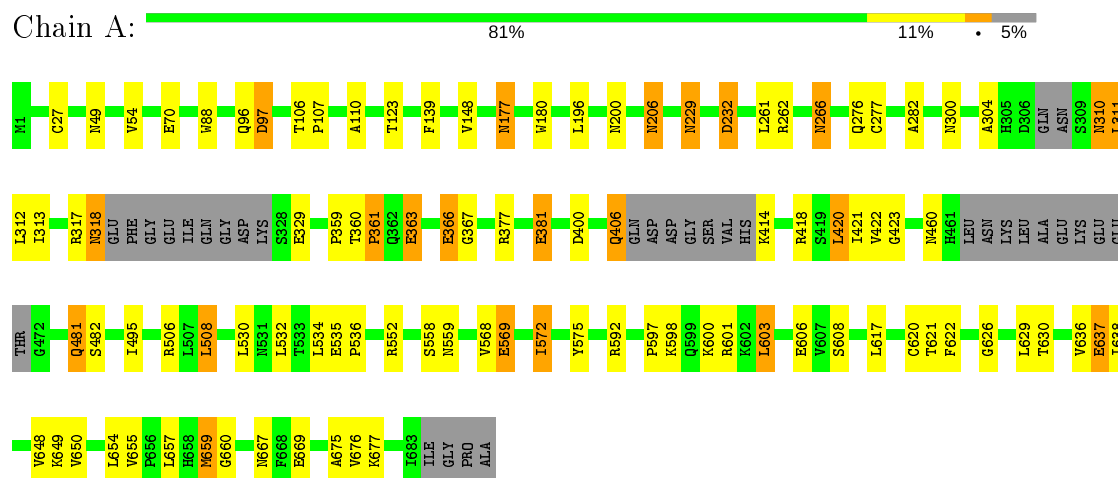
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	262	Total	O	0	0
			262	262		

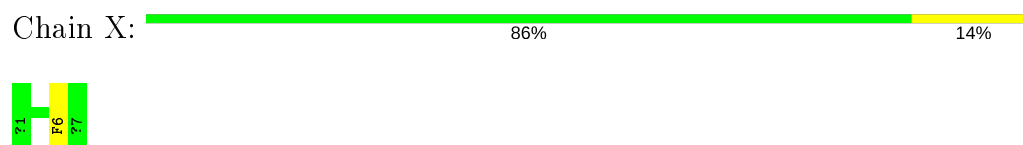
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Transglutaminase 2



#### • Molecule 2: Polypeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.67Å 71.67Å 309.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 36.12 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.00) 95.8 (36.12-1.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.228 , 0.266 0.228 , 0.267	Depositor DCC
$R_{free}$ test set	4103 reflections (6.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NH2, ONL, ACE, 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	0.64	2/5297 (0.0%)	0.72	2/7186 (0.0%)
2	X	0.61	0/35	1.01	0/47
All	All	0.64	2/5332 (0.0%)	0.72	2/7233 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	329	GLU	CG-CD	-8.21	1.39	1.51
1	A	27	CYS	CB-SG	-5.75	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASP	CB-CG-OD1	-12.76	106.82	118.30
1	A	97	ASP	CB-CG-OD2	-11.78	107.70	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	600	LYS	Peptide
1	A	659	MET	Peptide
1	A	97	ASP	Sidechain

## 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	5186	0	5097	60	0
2	X	46	0	43	4	0
3	A	25	0	0	0	0
4	A	262	0	0	0	0
All	All	5519	0	5140	60	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 6.

All (60) 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:636:VAL:HG21	1:A:650:VAL:HG11	1.49	0.95
1:A:360:THR:HG23	1:A:361:PRO:HD2	1.52	0.92
1:A:360:THR:CG2	1:A:361:PRO:HD2	2.10	0.81
1:A:603:LEU:HD12	1:A:654:LEU:HD12	1.64	0.77
1:A:638:ILE:HD13	1:A:648:VAL:HG21	1.66	0.76
1:A:622:PHE:HB2	1:A:636:VAL:HG22	1.74	0.68
1:A:318:ASN:HD22	1:A:318:ASN:H	1.43	0.64
1:A:54:VAL:HG12	1:A:123:THR:HG23	1.82	0.62
1:A:318:ASN:N	1:A:318:ASN:HD22	1.99	0.60
1:A:569:GLU:CG	1:A:572:ILE:HD12	2.32	0.60
1:A:420:LEU:HD23	2:X:6:PHE:CD2	2.38	0.58
1:A:232:ASP:N	1:A:232:ASP:OD2	2.37	0.57
1:A:569:GLU:HG3	1:A:572:ILE:HD12	1.87	0.57
1:A:304:ALA:HB2	2:X:6:PHE:CD2	2.40	0.57
1:A:568:VAL:HG13	1:A:575:TYR:CE2	2.41	0.55
1:A:139:PHE:HB3	1:A:148:VAL:HG21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:MET:HG3	1:A:660:GLY:N	2.22	0.54
1:A:406:GLN:HA	1:A:406:GLN:HE21	1.71	0.54
1:A:266:ASN:HD22	1:A:266:ASN:N	2.06	0.53
1:A:377:ARG:O	1:A:381:GLU:HB2	2.08	0.53
1:A:420:LEU:HD11	1:A:422:VAL:HG13	1.89	0.53
1:A:311:LEU:HD22	1:A:508:LEU:HD13	1.92	0.52
1:A:667:ASN:HD21	1:A:675:ALA:HA	1.75	0.51
1:A:366:GLU:HG3	1:A:367:GLY:N	2.25	0.51
1:A:318:ASN:N	1:A:318:ASN:ND2	2.59	0.51
1:A:421:ILE:HD12	1:A:421:ILE:N	2.27	0.50
1:A:310:ASN:HB3	1:A:313:ILE:HD12	1.94	0.50
1:A:420:LEU:HD23	2:X:6:PHE:CE2	2.47	0.49
1:A:621:THR:HG22	1:A:637:GLU:HA	1.93	0.49
1:A:506:ARG:HD3	1:A:530:LEU:HD22	1.95	0.49
1:A:229:ASN:OD1	1:A:361:PRO:HD3	2.12	0.49
1:A:420:LEU:CD1	1:A:422:VAL:HG13	2.43	0.48
1:A:300:ASN:OD1	1:A:423:GLY:HA2	2.13	0.47
1:A:495:ILE:HG21	1:A:534:LEU:HD11	1.95	0.47
1:A:88:TRP:CZ3	1:A:106:THR:HG22	2.50	0.47
1:A:481:GLN:HG2	1:A:482:SER:N	2.30	0.47
1:A:535:GLU:HG3	1:A:536:PRO:HD2	1.96	0.47
1:A:304:ALA:HB2	2:X:6:PHE:HD2	1.78	0.47
1:A:262:ARG:O	1:A:266:ASN:ND2	2.48	0.46
1:A:620:CYS:HB2	1:A:638:ILE:HB	1.97	0.45
1:A:107:PRO:HD2	1:A:110:ALA:HB2	1.99	0.45
1:A:229:ASN:HD22	1:A:229:ASN:C	2.21	0.44
1:A:406:GLN:CA	1:A:406:GLN:HE21	2.30	0.44
1:A:276:GLN:O	1:A:277:CYS:C	2.56	0.43
1:A:420:LEU:HD11	1:A:422:VAL:CG1	2.48	0.43
1:A:196:LEU:HD23	1:A:196:LEU:C	2.39	0.43
1:A:608:SER:HB3	1:A:649:LYS:HG2	2.01	0.43
1:A:206:ASN:HD22	1:A:206:ASN:C	2.22	0.43
1:A:506:ARG:NH1	1:A:530:LEU:HD13	2.33	0.42
1:A:49:ASN:ND2	1:A:96:GLN:O	2.51	0.42
1:A:311:LEU:CD2	1:A:508:LEU:HD13	2.49	0.42
1:A:420:LEU:HD22	1:A:421:ILE:N	2.35	0.42
1:A:569:GLU:HG2	1:A:572:ILE:HD12	2.02	0.42
1:A:558:SER:O	1:A:559:ASN:HB2	2.19	0.42
1:A:54:VAL:CG1	1:A:123:THR:HG23	2.49	0.41
1:A:667:ASN:ND2	1:A:677:LYS:HD3	2.35	0.41
1:A:229:ASN:HB3	1:A:359:PRO:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:TRP:CE2	1:A:282:ALA:HB1	2.56	0.40
1:A:592:ARG:HB2	1:A:606:GLU:HB3	2.03	0.40
1:A:177:ASN:N	1:A:177:ASN:ND2	2.69	0.40

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	645/687 (94%)	610 (95%)	32 (5%)	3 (0%)	29	23
2	X	4/7 (57%)	4 (100%)	0	0	100	100
All	All	649/694 (94%)	614 (95%)	32 (5%)	3 (0%)	29	23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	PRO
1	A	597	PRO
1	A	626	GLY

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	570/596 (96%)	531 (93%)	39 (7%)	16	11
2	X	4/4 (100%)	4 (100%)	0	100	100
All	All	574/600 (96%)	535 (93%)	39 (7%)	16	11

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	GLU
1	A	177	ASN
1	A	200	ASN
1	A	206	ASN
1	A	229	ASN
1	A	232	ASP
1	A	261	LEU
1	A	266	ASN
1	A	310	ASN
1	A	311	LEU
1	A	312	LEU
1	A	317	ARG
1	A	318	ASN
1	A	363	GLU
1	A	366	GLU
1	A	381	GLU
1	A	400	ASP
1	A	406	GLN
1	A	414	LYS
1	A	418	ARG
1	A	420	LEU
1	A	460	ASN
1	A	481	GLN
1	A	508	LEU
1	A	532	LEU
1	A	552	ARG
1	A	569	GLU
1	A	572	ILE
1	A	598	LYS
1	A	601	ARG
1	A	603	LEU
1	A	617	LEU

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	630	THR
1	A	637	GLU
1	A	655	VAL
1	A	657	LEU
1	A	669	GLU
1	A	676	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	126	GLN
1	A	134	HIS
1	A	169	GLN
1	A	177	ASN
1	A	206	ASN
1	A	266	ASN
1	A	267	HIS
1	A	318	ASN
1	A	406	GLN
1	A	531	ASN
1	A	573	ASN
1	A	610	GLN
1	A	633	GLN
1	A	662	HIS
1	A	667	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	ONL	X	3	1,2	7,8,9	0.58	0	4,9,11	2.12	1 (25%)

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	ONL	X	3	1,2	-	1/6/7/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	3	ONL	CB-CG-CD	-4.20	110.25	114.57

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	3	ONL	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

5 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	$\# Z  > 2$
3	SO4	A	691	-	4,4,4	0.25	0	6,6,6	0.59	0
3	SO4	A	692	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	688	-	4,4,4	0.14	0	6,6,6	0.38	0
3	SO4	A	690	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	A	689	-	4,4,4	0.16	0	6,6,6	0.31	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.

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.