



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 01:46 PM GMT

PDB ID : 4A0T  
Title : Structure of the carboxy-terminal domain of bacteriophage T7 fibre gp17 containing residues 371-553.  
Authors : Garcia-Doval, C.; Van Raaij, M.J.  
Deposited on : 2011-09-12  
Resolution : 1.90 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>

---

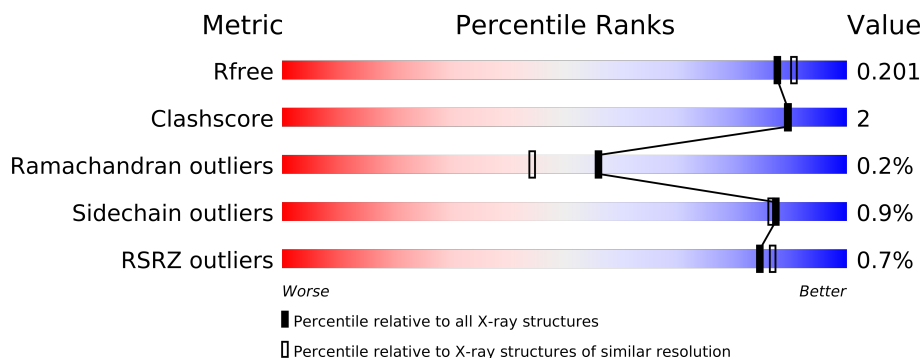
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	227	
1	B	227	
1	C	227	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	TRS	B	1555	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5115 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 TAIL FIBER PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1450	914	263	269	4			
1	B	182	Total	C	N	O	S	0	0	0
			1438	907	261	267	3			
1	C	182	Total	C	N	O	S	0	0	0
			1438	907	261	267	3			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	MET	-	EXPRESSION TAG	UNP P03748
A	328	HIS	-	EXPRESSION TAG	UNP P03748
A	329	HIS	-	EXPRESSION TAG	UNP P03748
A	330	HIS	-	EXPRESSION TAG	UNP P03748
A	331	HIS	-	EXPRESSION TAG	UNP P03748
A	332	HIS	-	EXPRESSION TAG	UNP P03748
A	333	HIS	-	EXPRESSION TAG	UNP P03748
A	334	SER	-	EXPRESSION TAG	UNP P03748
A	335	SER	-	EXPRESSION TAG	UNP P03748
A	336	GLY	-	EXPRESSION TAG	UNP P03748
A	337	LEU	-	EXPRESSION TAG	UNP P03748
A	338	VAL	-	EXPRESSION TAG	UNP P03748
A	339	PRO	-	EXPRESSION TAG	UNP P03748
A	340	ARG	-	EXPRESSION TAG	UNP P03748
A	341	GLY	-	EXPRESSION TAG	UNP P03748
A	342	SER	-	EXPRESSION TAG	UNP P03748
A	343	GLY	-	EXPRESSION TAG	UNP P03748
A	344	MET	-	EXPRESSION TAG	UNP P03748
A	345	LYS	-	EXPRESSION TAG	UNP P03748
A	346	GLU	-	EXPRESSION TAG	UNP P03748
A	347	THR	-	EXPRESSION TAG	UNP P03748
A	348	ALA	-	EXPRESSION TAG	UNP P03748
A	349	ALA	-	EXPRESSION TAG	UNP P03748

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	LYS	-	EXPRESSION TAG	UNP P03748
A	351	PHE	-	EXPRESSION TAG	UNP P03748
A	352	GLU	-	EXPRESSION TAG	UNP P03748
A	353	ARG	-	EXPRESSION TAG	UNP P03748
A	354	GLN	-	EXPRESSION TAG	UNP P03748
A	355	HIS	-	EXPRESSION TAG	UNP P03748
A	356	MET	-	EXPRESSION TAG	UNP P03748
A	357	ASP	-	EXPRESSION TAG	UNP P03748
A	358	SER	-	EXPRESSION TAG	UNP P03748
A	359	PRO	-	EXPRESSION TAG	UNP P03748
A	360	ASP	-	EXPRESSION TAG	UNP P03748
A	361	LEU	-	EXPRESSION TAG	UNP P03748
A	362	GLY	-	EXPRESSION TAG	UNP P03748
A	363	THR	-	EXPRESSION TAG	UNP P03748
A	364	ASP	-	EXPRESSION TAG	UNP P03748
A	365	ASP	-	EXPRESSION TAG	UNP P03748
A	366	ASP	-	EXPRESSION TAG	UNP P03748
A	367	ASP	-	EXPRESSION TAG	UNP P03748
A	368	LYS	-	EXPRESSION TAG	UNP P03748
A	369	ALA	-	EXPRESSION TAG	UNP P03748
A	370	MET	-	EXPRESSION TAG	UNP P03748
B	327	MET	-	EXPRESSION TAG	UNP P03748
B	328	HIS	-	EXPRESSION TAG	UNP P03748
B	329	HIS	-	EXPRESSION TAG	UNP P03748
B	330	HIS	-	EXPRESSION TAG	UNP P03748
B	331	HIS	-	EXPRESSION TAG	UNP P03748
B	332	HIS	-	EXPRESSION TAG	UNP P03748
B	333	HIS	-	EXPRESSION TAG	UNP P03748
B	334	SER	-	EXPRESSION TAG	UNP P03748
B	335	SER	-	EXPRESSION TAG	UNP P03748
B	336	GLY	-	EXPRESSION TAG	UNP P03748
B	337	LEU	-	EXPRESSION TAG	UNP P03748
B	338	VAL	-	EXPRESSION TAG	UNP P03748
B	339	PRO	-	EXPRESSION TAG	UNP P03748
B	340	ARG	-	EXPRESSION TAG	UNP P03748
B	341	GLY	-	EXPRESSION TAG	UNP P03748
B	342	SER	-	EXPRESSION TAG	UNP P03748
B	343	GLY	-	EXPRESSION TAG	UNP P03748
B	344	MET	-	EXPRESSION TAG	UNP P03748
B	345	LYS	-	EXPRESSION TAG	UNP P03748
B	346	GLU	-	EXPRESSION TAG	UNP P03748
B	347	THR	-	EXPRESSION TAG	UNP P03748

*Continued on next page...*

*Continued from previous page...*

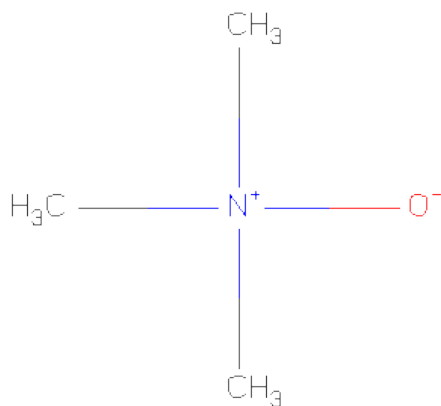
Chain	Residue	Modelled	Actual	Comment	Reference
B	348	ALA	-	EXPRESSION TAG	UNP P03748
B	349	ALA	-	EXPRESSION TAG	UNP P03748
B	350	LYS	-	EXPRESSION TAG	UNP P03748
B	351	PHE	-	EXPRESSION TAG	UNP P03748
B	352	GLU	-	EXPRESSION TAG	UNP P03748
B	353	ARG	-	EXPRESSION TAG	UNP P03748
B	354	GLN	-	EXPRESSION TAG	UNP P03748
B	355	HIS	-	EXPRESSION TAG	UNP P03748
B	356	MET	-	EXPRESSION TAG	UNP P03748
B	357	ASP	-	EXPRESSION TAG	UNP P03748
B	358	SER	-	EXPRESSION TAG	UNP P03748
B	359	PRO	-	EXPRESSION TAG	UNP P03748
B	360	ASP	-	EXPRESSION TAG	UNP P03748
B	361	LEU	-	EXPRESSION TAG	UNP P03748
B	362	GLY	-	EXPRESSION TAG	UNP P03748
B	363	THR	-	EXPRESSION TAG	UNP P03748
B	364	ASP	-	EXPRESSION TAG	UNP P03748
B	365	ASP	-	EXPRESSION TAG	UNP P03748
B	366	ASP	-	EXPRESSION TAG	UNP P03748
B	367	ASP	-	EXPRESSION TAG	UNP P03748
B	368	LYS	-	EXPRESSION TAG	UNP P03748
B	369	ALA	-	EXPRESSION TAG	UNP P03748
B	370	MET	-	EXPRESSION TAG	UNP P03748
C	327	MET	-	EXPRESSION TAG	UNP P03748
C	328	HIS	-	EXPRESSION TAG	UNP P03748
C	329	HIS	-	EXPRESSION TAG	UNP P03748
C	330	HIS	-	EXPRESSION TAG	UNP P03748
C	331	HIS	-	EXPRESSION TAG	UNP P03748
C	332	HIS	-	EXPRESSION TAG	UNP P03748
C	333	HIS	-	EXPRESSION TAG	UNP P03748
C	334	SER	-	EXPRESSION TAG	UNP P03748
C	335	SER	-	EXPRESSION TAG	UNP P03748
C	336	GLY	-	EXPRESSION TAG	UNP P03748
C	337	LEU	-	EXPRESSION TAG	UNP P03748
C	338	VAL	-	EXPRESSION TAG	UNP P03748
C	339	PRO	-	EXPRESSION TAG	UNP P03748
C	340	ARG	-	EXPRESSION TAG	UNP P03748
C	341	GLY	-	EXPRESSION TAG	UNP P03748
C	342	SER	-	EXPRESSION TAG	UNP P03748
C	343	GLY	-	EXPRESSION TAG	UNP P03748
C	344	MET	-	EXPRESSION TAG	UNP P03748
C	345	LYS	-	EXPRESSION TAG	UNP P03748

*Continued on next page...*

Continued from previous page...

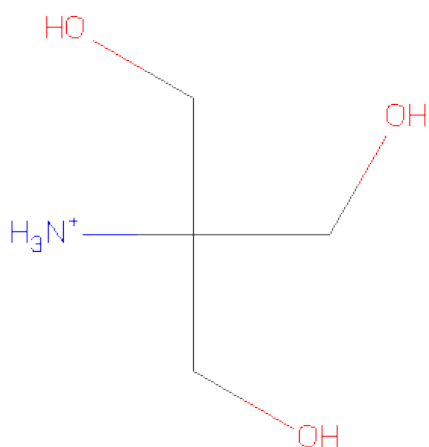
Chain	Residue	Modelled	Actual	Comment	Reference
C	346	GLU	-	EXPRESSION TAG	UNP P03748
C	347	THR	-	EXPRESSION TAG	UNP P03748
C	348	ALA	-	EXPRESSION TAG	UNP P03748
C	349	ALA	-	EXPRESSION TAG	UNP P03748
C	350	LYS	-	EXPRESSION TAG	UNP P03748
C	351	PHE	-	EXPRESSION TAG	UNP P03748
C	352	GLU	-	EXPRESSION TAG	UNP P03748
C	353	ARG	-	EXPRESSION TAG	UNP P03748
C	354	GLN	-	EXPRESSION TAG	UNP P03748
C	355	HIS	-	EXPRESSION TAG	UNP P03748
C	356	MET	-	EXPRESSION TAG	UNP P03748
C	357	ASP	-	EXPRESSION TAG	UNP P03748
C	358	SER	-	EXPRESSION TAG	UNP P03748
C	359	PRO	-	EXPRESSION TAG	UNP P03748
C	360	ASP	-	EXPRESSION TAG	UNP P03748
C	361	LEU	-	EXPRESSION TAG	UNP P03748
C	362	GLY	-	EXPRESSION TAG	UNP P03748
C	363	THR	-	EXPRESSION TAG	UNP P03748
C	364	ASP	-	EXPRESSION TAG	UNP P03748
C	365	ASP	-	EXPRESSION TAG	UNP P03748
C	366	ASP	-	EXPRESSION TAG	UNP P03748
C	367	ASP	-	EXPRESSION TAG	UNP P03748
C	368	LYS	-	EXPRESSION TAG	UNP P03748
C	369	ALA	-	EXPRESSION TAG	UNP P03748
C	370	MET	-	EXPRESSION TAG	UNP P03748

- Molecule 2 is TRIMETHYLAMINE OXIDE (three-letter code: TMO) (formula: C<sub>3</sub>H<sub>9</sub>NO).



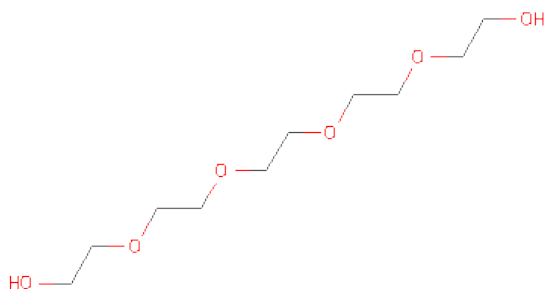
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	3	1	1		
2	B	1	Total	C	N	O	0	0
			5	3	1	1		
2	C	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			12	8	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	292	Total	O	0	0
			292	292		
5	B	241	Total	O	0	0
			241	241		
5	C	221	Total	O	0	0
			221	221		

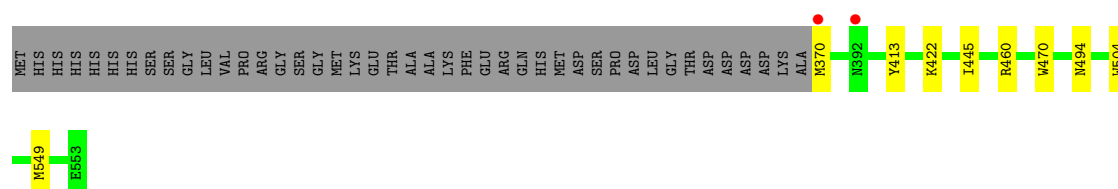


### 3 Residue-property plots i

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.

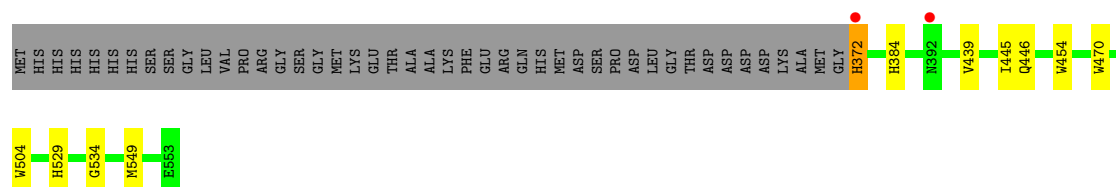
- Molecule 1: TAIL FIBER PROTEIN

Chain A: 



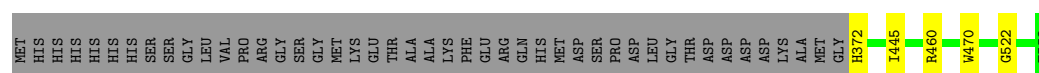
- Molecule 1: TAIL FIBER PROTEIN

Chain B: 



- Molecule 1: TAIL FIBER PROTEIN

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.24Å 86.04Å 118.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 1.90 19.86 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.86-1.90) 100.0 (19.86-1.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.155 , 0.200 0.155 , 0.201	Depositor DCC
$R_{free}$ test set	2111 reflections (4.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.5	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50000 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5115	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: TRS, 1PE, TMO

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	0.74	0/1489	0.67	0/2017
1	B	0.72	0/1477	0.69	0/2002
1	C	0.72	0/1477	0.70	0/2002
All	All	0.72	0/4443	0.69	0/6021

There are no bond length outliers.

There are no bond angle outliers.

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	1450	0	1371	11	0
1	B	1438	0	1359	6	0
1	C	1438	0	1359	5	0
2	A	5	0	9	2	0
2	B	5	0	9	0	0
2	C	5	0	9	0	0
3	B	8	0	12	2	0
4	C	12	0	15	0	0
5	A	292	0	0	4	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	241	0	0	1	0
5	C	221	0	0	2	1
All	All	5115	0	4143	19	1

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 2.

The worst 5 of 19 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:494:ASN:HD21	3:B:1555:TRS:H12	1.29	0.97
1:C:460:ARG:NH2	5:C:2084:HOH:O	2.29	0.65
1:A:370:MET:N	5:A:2002:HOH:O	2.32	0.61
1:A:445:ILE:HD11	1:C:445:ILE:HD13	1.85	0.59
1:A:494:ASN:ND2	3:B:1555:TRS:H12	2.11	0.57

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	Distance(Å)	Clash(Å)
5:A:2016:HOH:O	5:C:2129:HOH:O[4_555]	2.18	0.02

## 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	182/227 (80%)	176 (97%)	6 (3%)	0	100	100
1	B	180/227 (79%)	174 (97%)	6 (3%)	0	100	100
1	C	180/227 (79%)	175 (97%)	4 (2%)	1 (1%)	33	19
All	All	542/681 (80%)	525 (97%)	16 (3%)	1 (0%)	56	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	522	GLY

### 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	151/187 (81%)	150 (99%)	1 (1%)	91	90
1	B	150/187 (80%)	148 (99%)	2 (1%)	80	77
1	C	150/187 (80%)	149 (99%)	1 (1%)	91	90
All	All	451/561 (80%)	447 (99%)	4 (1%)	87	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	TRP
1	B	372	HIS
1	B	470	TRP
1	C	470	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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

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$
2	TMO	A	1554	-	4,4,4	1.64	1 (25%)	6,6,6	0.72	0
2	TMO	B	1554	-	4,4,4	1.22	0	6,6,6	0.47	0
3	TRS	B	1555	-	7,7,7	1.08	1 (14%)	9,9,9	1.77	2 (22%)
2	TMO	C	1554	-	4,4,4	1.47	1 (25%)	6,6,6	0.44	0
4	1PE	C	1555	-	11,11,15	1.62	1 (9%)	9,10,14	0.47	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	TMO	A	1554	-	-	0/0/0/0	0/0/0/0
2	TMO	B	1554	-	-	0/0/0/0	0/0/0/0
3	TRS	B	1555	-	-	0/9/9/9	0/0/0/0
2	TMO	C	1554	-	-	0/0/0/0	0/0/0/0
4	1PE	C	1555	-	-	0/9/9/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1555	1PE	C15-C25	-5.08	1.53	1.55
3	B	1555	TRS	C-N	-2.67	1.46	1.50
2	A	1554	TMO	OAE-NAC	2.27	1.47	1.39
2	C	1554	TMO	OAE-NAC	2.22	1.47	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1555	TRS	C3-C-C2	3.16	115.89	110.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1555	TRS	C3-C-C1	-2.89	105.95	110.70

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	184/227 (81%)	-0.48	2 (1%) 77 79	7, 13, 23, 37	0
1	B	182/227 (80%)	-0.42	2 (1%) 77 79	7, 13, 24, 39	0
1	C	182/227 (80%)	-0.54	0 100 100	6, 12, 22, 31	0
All	All	548/681 (80%)	-0.48	4 (0%) 84 87	6, 12, 23, 39	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372	HIS	3.6
1	A	370	MET	2.9
1	B	392	ASN	2.8
1	A	392	ASN	2.7

### 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
3	TRS	B	1555	8/8	0.23	6.69	35,37,38,38	0
2	TMO	C	1554	5/5	0.10	1.94	19,20,20,20	0
2	TMO	A	1554	5/5	0.10	1.60	21,23,24,24	0
4	1PE	C	1555	12/16	0.07	0.86	18,21,25,25	0
2	TMO	B	1554	5/5	0.08	-0.76	21,21,22,22	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.