

# Full wwPDB X-ray Structure Validation Report (i)

#### Dec 17, 2023 – 03:23 AM EST

PDB ID	:	3NSG
Title	:	Crystal Structure of OmpF, an Outer Membrane Protein from Salmonella
		typhi
Authors	:	Balasubramaniam, D.; Arockiasamy, A.; Sharma, A.; Krishnaswamy, S.
Deposited on	:	2010-07-01
Resolution	:	2.79  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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
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)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.79 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	А	341	35%	48%	16%		
1	В	341	39%	52%	9% •		
1	С	341	3%	49%	11% •		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	А	350	-	-	-	Х
2	SO4	А	361	-	-	Х	-
2	SO4	А	369	-	-	-	Х
2	SO4	В	343	-	-	-	Х
2	SO4	В	344	-	-	-	Х
2	SO4	В	345	-	-	Х	-
2	SO4	В	351	-	-	-	Х
2	SO4	В	362	-	-	-	Х
2	SO4	С	359	-	-	-	Х
2	SO4	С	370	-	-	Х	-
3	GOL	А	378	-	-	-	Х
3	GOL	В	365	-	-	Х	-
3	GOL	В	371	-	-	-	Х
3	GOL	В	373	-	-	-	Х
3	GOL	В	374	-	-	-	Х
3	GOL	С	1325	_	-	-	Х
3	GOL	С	375	-	-	Х	-
3	GOL	С	376	_	_	-	Х
3	GOL	С	379	_	_	-	Х
4	LDA	А	385	_	_	-	Х
4	LDA	A	389	-	-	_	Х
4	LDA	В	381	_	_	_	X
4	LDA	С	385	_	_	_	X
5	TAM	A	390	_	_	Х	X
6	FLC	А	392	-	Х	-	Х
6	FLC	С	388	_	_	Х	-



# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9432 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	941	Total	С	Ν	0	Se	0	0	0
		341	2669	1662	453	547	7	0		0
1	D	9.4.1	Total	С	Ν	0	Se	0	0	0
	D	041	2669	1662	453	547	7			0
1	С	341	Total	С	Ν	0	Se	0	0	0
			2669	1662	453	547	7	0	0	

• Molecule 1 is a protein called Outer membrane protein F.

• Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{c cc} \overline{\text{Total}} & O & S \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{c ccc} \hline Total & O & S \\ \hline 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total O S	0	0
			5 $4$ $1$		
2	А	1	$\begin{array}{ccc} 1 \text{ otal } \mathbf{O} & \mathbf{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	A	1	Total O S	0	0
				-	-
2	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	Total O S	0	0
			$\begin{array}{ccc} 5 & 4 & 1 \\ \hline \end{array}$		
2	В	1	$\begin{array}{ccc} 1 \text{otal} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	В	1	Total O S 5 4 1	0	0
			$\begin{array}{ccc} 0 & 4 & 1 \\ \hline \\ Total & O & S \end{array}$		
2	В	1	$\begin{bmatrix} 10ta1 & 0 & 5 \\ 5 & 4 & 1 \end{bmatrix}$	0	0
0	р	1	Total O S	0	0
	D	L	5 4 1	0	0
0	р	1	Total O S	0	0
	В	1	$5 \ 4 \ 1$	0	0
0	D	1	Total O S	0	0
	D	L	$5 \ 4 \ 1$	0	0
0	D	1	Total O S	0	0
	D	L	$5 \ 4 \ 1$	0	0
0	Р	1	Total O S	0	0
	D	L	$5 \ 4 \ 1$	0	0
9	В	1	Total O S	0	0
2	D	T	$5 \ 4 \ 1$	0	0
2	В	1	Total O S	0	0
	D	I	$5 \ 4 \ 1$	0	0
2	В	1	Total O S	0	0
	D	I	5 4 1	0	0
2	В	1	Total O S	0	0
	D	Ŧ	5 4 1	0	0
2	В	1	Total O S	0	0
	D	I	5 4 1	0	0
2	R	1	Total O $\overline{S}$	0	0
		1	5 4 1		0
2	В	1	Total O S	Ο	0
		1	5 4 1	0	0
2	R	1	Total O S	0	0
			5 4 1		



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total O S	0	0
	D	I	5 4 1	0	0
2	В	1	Total O S	0	0
	D	1	5 4 1		0
2	В	1	Total O S	0	0
		_	5 4 1	-	
2	В	1	Total O S	0	0
			5 $4$ $1$		
2	С	1	$\begin{bmatrix} 1 \text{ otal } \mathbf{O} & \mathbf{S} \\ \mathbf{E} & 4 & 1 \end{bmatrix}$	0	0
			$\begin{array}{ccc} 0 & 4 & 1 \\ \hline \\ Total & O & S \end{array}$		
2	С	1	$\begin{array}{c} 10tal \\ 5 \\ 4 \\ 1 \end{array}$	0	0
			Total O S		
2	С	1	5 4 1	0	0
			Total O S		
2	С	1	5 4 1	0	0
	G		Total O S	0	0
2	C	1	5 4 1	0	0
0	C	1	Total O S	0	0
	C	L	5 4 1	0	0
2	С	1	Total O S	0	0
	0	1	5 4 1	0	0
2	С	1	Total O S	0	0
		1	5 4 1	0	0
2	С	1	Total O S	0	0
		_	5 4 1	-	
2	С	1	Total O S	0	0
			5 $4$ $1$		
2	С	1	Total O S	0	0
			$\begin{array}{ccc} 0 & 4 & 1 \\ \hline \\ \hline \\ \hline \\ \\ \hline \\ \\ \\ \\ \\ \\ \\ \\ \\ \\$		
2	С	1	$\begin{array}{c} 10tal \\ 5 \\ 4 \\ 1 \end{array}$	0	0
			Total O S		
2	С	1	5 4 1	0	0
			Total O S		
2	C	1	5 4 1	0	0
	C		Total O S		0
2	C		5 4 1	0	0
0	C	1	Total O S	0	0
2	C		5 4 1	0	U
0	С	1	Total O S	0	0
			5 4 1		U



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
2	С	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

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• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \overline{\text{Total}} & \mathrm{C} & \mathrm{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{c ccc} \hline Total & C & O \\ \hline 6 & 3 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{c ccc} \hline Total & C & O \\ \hline 6 & 3 & 3 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C N O 16 14 1 1	0	0
4	A	1	Total   C   N   O     16   14   1   1	0	0
	Λ	1	16         14         1         1           Total         C         N         O	0	0
4	A	1	16 14 1 1 Total C N O	0	0
4	А	1	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	0	0
4	А	1	Total C N O 16 14 1 1	0	0
4	А	1	$\begin{array}{cccc} \text{Total} & \text{C} & \text{N} & \text{O} \\ 16 & 14 & 1 & 1 \end{array}$	0	0
4	В	1	Total   C   N   O     16   14   1   1	0	0
	В	1	10         14         1         1           Total         C         N         O	0	0
4	D		16 14 1 1	U	U



Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
4	Р	1	Total	С	Ν	0	0	0
4	D	L	16	14	1	1	0	0
4	В	1	Total	С	Ν	Ο	0	0
4	D	T	16	14	1	1	0	0
4	В	1	Total	С	Ν	0	0	0
4	D	T	16	14	1	1	0	0
4	В	1	Total	С	Ν	0	0	0
4	D	T	16	14	1	1	0	0
1	В	1	Total	С	Ν	Ο	0	0
т	D	I	16	14	1	1	0	0
4	С	1	Total	С	Ν	Ο	0	0
	0	T	16	14	1	1	0	0
4	С	1	Total	С	Ν	Ο	0	0
	0	T	16	14	1	1	0	0
4	С	1	Total	С	Ν	Ο	0	0
		I	16	14	1	1	0	0
4	С	1	Total	С	Ν	Ο	0	0
Т		1	16	14	1	1	0	

• Molecule 5 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: C<sub>7</sub>H<sub>17</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atom	S	ZeroOcc	AltConf
5	А	1	Total C 11 7	N O 1 3	0	0
5	А	1	Total C 11 7	N O 1 3	0	0



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf			
5	В	1	Total C N	0	0	0			
			11 7 1	3		-			
5	С	1	Total C N	I O	0	0			
0	U	I	11  7  1	3	0	0			
н	С	1	Total C N	O I	0	0			
5	U	1	11 7 1	3	0	0			
Ľ	С	1	Total C N	Ο	0	0			
5	U	1	11 7 1	3	0	0			

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• Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total         C         O           13         6         7	0	0
6	С	1	Total         C         O           13         6         7	0	0
6	С	1	Total C O 13 6 7	0	0
6	С	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 13  6  7 \end{array}$	0	0

• Molecule 7 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula:  $C_4H_6O_6$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total         C         O           10         4         6	0	0
7	В	1	Total C O 10 4 6	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	134	Total O 134 134	0	0
8	В	115	Total O 115 115	0	0
8	С	138	Total O 138 138	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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: Outer membrane protein F





 $\bullet$  Molecule 1: Outer membrane protein F





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	85.19Å 139.34Å 150.77Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	42.59 - 2.79	Depositor
Resolution (A)	42.59 - 2.79	EDS
% Data completeness	84.1 (42.59-2.79)	Depositor
(in resolution range)	84.1 (42.59-2.79)	EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.44 (at 2.81 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
B B.	0.255 , $0.337$	Depositor
$n, n_{free}$	0.253 , $0.332$	DCC
$R_{free}$ test set	1898 reflections $(4.99\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	45.9	Xtriage
Anisotropy	1.301	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.27, 54.1	EDS
L-test for $twinning^2$	$ < L >=0.42, < L^2>=0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms $(Å^2)$	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: TAM, LDA, SO4, FLC, GOL, TLA

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).

Mal	Chain	Bond	lengths	Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.60	0/2717	0.75	0/3668
1	В	0.61	0/2717	0.75	0/3668
1	С	0.59	0/2717	0.73	0/3668
All	All	0.60	0/8151	0.74	0/11004

There are no bond length outliers.

There are no bond angle outliers.

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	А	2669	0	2464	246	0
1	В	2669	0	2464	219	0
1	С	2669	0	2464	231	0
2	А	135	0	0	6	0
2	В	110	0	0	4	0
2	С	155	0	0	6	0
3	А	84	0	112	4	0
3	В	66	0	88	6	0
3	С	78	0	104	8	0
4	A	96	0	186	6	0



20100						
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	112	0	217	10	0
4	С	64	0	124	15	0
5	А	22	0	34	11	0
5	В	11	0	17	0	0
5	С	33	0	51	12	0
6	А	13	0	5	0	0
6	С	39	0	15	6	0
7	А	10	0	4	0	0
7	В	10	0	4	1	0
8	А	134	0	0	11	0
8	В	115	0	0	7	0
8	С	138	0	0	11	0
All	All	9432	0	8353	687	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 39.

All (687) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:198:ASP:HA	1:A:200:GLN:NE2	1.61	1.13
1:A:21:HIS:CE1	1:A:31:ASN:OD1	2.04	1.11
1:A:107:THR:HG21	1:A:256:GLU:OE1	1.56	1.05
1:A:117:THR:HG23	1:A:118:TRP:H	1.22	1.04
4:B:375:LDA:HM13	4:C:382:LDA:H21	1.38	1.03
5:C:387:TAM:H61	5:C:387:TAM:H51	1.38	1.03
1:A:125:ASN:O	1:A:128:THR:HG23	1.59	1.02
1:A:198:ASP:HA	1:A:200:GLN:HE22	0.84	1.00
1:B:195:ARG:HH12	1:B:206:GLY:HA2	1.26	1.00
5:A:390:TAM:C5	5:A:390:TAM:C4	2.40	0.99
1:C:241:THR:OG1	1:C:323:SER:HB2	1.61	0.99
5:C:387:TAM:H51	5:C:387:TAM:C6	1.93	0.97
1:C:244:ASP:OD1	6:C:388:FLC:HA2	1.64	0.96
5:A:390:TAM:C5	5:A:390:TAM:H41	1.95	0.96
1:A:9:ASN:HB3	1:A:45:THR:HA	1.48	0.95
1:C:128:THR:HG23	1:C:235:MSE:HE1	1.48	0.95
1:C:210:GLU:HB2	1:C:233:ARG:HB2	1.46	0.95
1:A:127:MSE:SE	1:A:154:GLN:OE1	2.34	0.95
1:A:117:THR:CG2	1:A:118:TRP:H	1.79	0.94
1:A:291:ALA:HA	1:A:317:LEU:HD11	1.49	0.94
1:B:139:ASN:HD22	1:B:151:PHE:HE2	1.13	0.94



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:255:LEU:HB3	1:C:275:GLN:HG2	1.47	0.94
1:C:65:ARG:HH11	1:C:65:ARG:CG	1.80	0.93
1:C:178:ALA:HB2	1:C:187:THR:HG23	1.51	0.92
1:B:252:THR:O	1:B:254:ASN:ND2	2.02	0.92
1:C:245:THR:HG22	3:C:375:GOL:H2	1.51	0.92
5:A:390:TAM:C4	5:A:390:TAM:H52	2.02	0.89
1:B:270:ALA:O	1:B:295:GLN:NE2	2.07	0.88
1:B:202:ARG:HB2	1:B:247:GLU:HB3	1.54	0.88
1:C:56:GLN:HB3	1:C:80:PHE:CZ	2.07	0.88
1:C:65:ARG:HH11	1:C:65:ARG:HG2	1.38	0.87
1:A:160:GLN:HA	1:A:168:GLN:HG2	1.58	0.85
1:C:128:THR:CG2	1:C:235:MSE:HE1	2.06	0.85
1:A:21:HIS:HE1	1:A:31:ASN:OD1	1.59	0.85
1:A:127:MSE:HG2	1:A:154:GLN:HE22	1.41	0.85
1:B:76:VAL:H	1:C:70:GLN:HE22	1.25	0.84
1:C:200:GLN:HA	1:C:200:GLN:OE1	1.76	0.84
1:B:1:MSE:O	1:B:2:GLU:HB2	1.77	0.84
1:B:312:TYR:CD2	1:B:333:ALA:HB2	2.13	0.84
5:A:390:TAM:H52	5:A:390:TAM:O4	1.77	0.83
1:C:272:SER:OG	1:C:295:GLN:HG3	1.78	0.83
1:C:26:THR:HG22	1:C:330:ASP:OD2	1.79	0.82
1:A:211:SER:OG	1:A:231:GLU:O	1.97	0.82
1:A:107:THR:CG2	1:A:256:GLU:OE1	2.28	0.82
1:A:115:GLY:O	1:A:120:GLY:HA3	1.81	0.80
1:A:127:MSE:HG2	1:A:154:GLN:NE2	1.97	0.80
1:A:260:GLN:HE21	1:A:270:ALA:HB2	1.46	0.80
1:B:139:ASN:ND2	1:B:142:PHE:HA	1.98	0.79
1:B:158:LYS:HE3	8:B:466:HOH:O	1.82	0.79
1:B:106:TYR:O	1:B:224:TYR:OH	2.00	0.79
1:A:67:GLU:O	1:C:75:LEU:HD22	1.82	0.79
1:B:76:VAL:H	1:C:70:GLN:NE2	1.82	0.78
5:A:390:TAM:O4	5:A:390:TAM:C2	2.30	0.78
1:B:130:ARG:NH2	1:C:67:GLU:OE2	2.16	0.78
5:A:390:TAM:O4	5:A:390:TAM:H21	1.83	0.78
1:C:10:LYS:NZ	1:C:42:LYS:HE2	1.99	0.78
5:A:390:TAM:H41	5:A:390:TAM:H51	1.66	0.77
1:C:77:ARG:O	1:C:95:ARG:HG2	1.83	0.77
1:A:4:TYR:HD1	1:B:1:MSE:HE1	1.48	0.77
1:A:18:VAL:O	1:A:35:THR:HG23	1.84	0.77
1:C:57:TRP:HA	1:C:78:LEU:O	1.84	0.77
1:C:200:GLN:O	1:C:202:ARG:N	2.18	0.76



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:124:ASP:OD1	1:C:66:ALA:HA	1.85	0.76
1:C:112:TYR:HB2	8:C:527:HOH:O	1.85	0.76
1:B:99:ILE:HD11	1:B:176:THR:HG22	1.67	0.76
1:A:93:TYR:OH	1:B:21:HIS:HD2	1.69	0.76
1:C:304:LYS:HE3	1:C:305:ASN:HD21	1.49	0.76
1:A:2:GLU:HA	1:A:12:ASP:HB2	1.68	0.75
1:A:65:ARG:NH1	1:C:162:ASN:OD1	2.18	0.75
1:A:207:ASP:HB3	2:A:361:SO4:O4	1.86	0.75
1:C:302:PHE:HE2	1:C:308:VAL:HG12	1.50	0.75
1:A:88:VAL:HG22	2:A:350:SO4:O3	1.87	0.75
1:B:163:HIS:HB3	1:B:167:SER:HB2	1.69	0.75
1:C:126:TYR:HB2	1:C:235:MSE:HE3	1.67	0.74
1:C:85:TYR:HB3	1:C:88:VAL:HG22	1.69	0.74
1:B:65:ARG:NH2	8:B:492:HOH:O	2.05	0.74
1:A:150:SER:OG	1:A:178:ALA:HB3	1.87	0.74
1:C:99:ILE:HB	1:C:154:GLN:HE21	1.52	0.74
1:B:76:VAL:N	1:C:70:GLN:HE22	1.85	0.74
1:C:65:ARG:HG2	1:C:65:ARG:NH1	1.97	0.74
1:C:98:GLY:HA3	1:C:127:MSE:HA	1.69	0.73
5:A:390:TAM:C5	5:A:390:TAM:O4	2.36	0.73
1:A:337:ILE:CD1	4:A:384:LDA:H122	2.19	0.73
1:B:103:VAL:O	1:B:106:TYR:HB2	1.89	0.72
5:A:390:TAM:H41	5:A:390:TAM:H52	1.62	0.72
1:C:241:THR:OG1	1:C:323:SER:CB	2.38	0.72
1:A:275:GLN:HA	1:A:291:ALA:O	1.89	0.72
1:B:26:THR:HG22	1:B:27:GLY:N	2.04	0.72
2:B:345:SO4:O3	8:B:474:HOH:O	2.08	0.72
1:A:48:ASN:HD22	1:A:49:THR:H	1.35	0.71
1:A:23:TRP:HZ2	4:A:384:LDA:HM13	1.52	0.71
1:B:195:ARG:NH1	1:B:206:GLY:HA2	2.04	0.71
1:C:134:LEU:HD23	1:C:156:GLN:HG3	1.71	0.71
5:C:387:TAM:H61	5:C:387:TAM:C5	2.18	0.71
1:A:204:GLY:O	8:A:485:HOH:O	2.08	0.70
1:A:43:GLY:HA3	1:B:339:TYR:CE2	2.26	0.70
1:C:99:ILE:HB	1:C:154:GLN:HG2	1.73	0.70
1:C:110:ALA:HB3	1:C:114:SER:OG	1.91	0.70
1:B:130:ARG:HH21	1:C:67:GLU:CD	1.93	0.70
1:B:288:ALA:HB1	1:B:320:ASN:HD21	1.56	0.70
1:C:168:GLN:OE1	1:C:196:THR:HG21	1.91	0.70
1:A:32:ALA:HA	4:C:385:LDA:H92	1.74	0.70
1:A:264:ASP:HB2	8:A:510:HOH:O	1.90	0.70



	<b>A</b> 4 <b>O</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:124:ASP:O	1:B:167:SER:HA	1.91	0.70
1:B:30:LYS:HD3	1:B:31:ASN:H	1.57	0.69
1:A:209:ALA:HA	1:A:234:ASN:HB2	1.74	0.69
1:B:3:ILE:HD11	1:B:13:LEU:HB2	1.75	0.69
1:C:244:ASP:OD1	6:C:388:FLC:CA	2.39	0.69
1:A:77:ARG:HH21	3:A:370:GOL:H32	1.57	0.69
1:C:99:ILE:H	1:C:154:GLN:NE2	1.91	0.69
1:A:217:LYS:CB	1:A:226:ALA:HB2	2.23	0.69
1:A:232:THR:HG21	1:A:236:SER:HB2	1.73	0.69
1:B:156:GLN:OE1	1:B:169:ASN:ND2	2.25	0.69
1:C:263:PHE:HB3	1:C:265:PHE:CE2	2.27	0.69
1:C:306:MSE:CE	1:C:339:TYR:HD1	2.06	0.69
1:A:207:ASP:HB3	2:A:361:SO4:S	2.34	0.68
1:B:258:VAL:HG22	1:B:272:SER:HB2	1.76	0.68
1:C:161:ASP:O	1:C:162:ASN:HB2	1.94	0.68
1:A:205:ASN:HB3	1:A:234:ASN:HD21	1.60	0.67
1:B:153:ILE:HD11	1:B:155:TYR:HE2	1.59	0.67
1:C:245:THR:CG2	3:C:375:GOL:H2	2.24	0.67
1:A:146:VAL:HG21	1:A:149:LEU:HB3	1.75	0.67
1:B:312:TYR:HD2	1:B:333:ALA:HB2	1.56	0.67
1:C:262:GLN:NE2	1:C:268:ARG:HD3	2.10	0.67
1:A:232:THR:HB	1:A:252:THR:HB	1.76	0.67
1:B:21:HIS:O	1:B:334:ALA:HB1	1.95	0.67
1:C:25:THR:HG22	4:C:383:LDA:H41	1.77	0.67
1:C:86:ALA:O	1:C:87:GLU:HB2	1.94	0.67
4:C:384:LDA:H41	4:C:384:LDA:HM13	1.77	0.67
1:A:149:LEU:HA	1:A:178:ALA:O	1.95	0.66
4:B:375:LDA:CM1	4:C:382:LDA:H21	2.21	0.66
1:C:306:MSE:HE2	1:C:339:TYR:HD1	1.59	0.66
1:B:77:ARG:O	1:B:95:ARG:HD2	1.96	0.66
1:A:20:ARG:HG3	1:A:34:GLN:O	1.96	0.66
1:C:99:ILE:N	1:C:154:GLN:NE2	2.44	0.66
1:C:194:LYS:HA	1:C:207:ASP:O	1.96	0.66
1:A:196:THR:O	1:A:199:GLN:HG3	1.95	0.66
1:C:136:THR:HG22	1:C:154:GLN:HB2	1.77	0.65
1:C:304:LYS:HE3	1:C:305:ASN:ND2	2.10	0.65
1:C:99:ILE:HB	1:C:154:GLN:NE2	2.11	0.65
1:C:4:TYR:O	1:C:10:LYS:HA	1.95	0.65
1:A:220:ALA:O	1:A:223:VAL:HG23	1.96	0.65
1:C:26:THR:CG2	1:C:330:ASP:OD2	2.44	0.65
1:B:134:LEU:HD22	1:B:154:GLN:HE21	1.61	0.65



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:162:ASN:CB	1:B:65:ARG:HH11	2.09	0.65
1:C:322:TYR:O	1:C:323:SER:C	2.34	0.65
1:A:4:TYR:CD1	1:B:1:MSE:HE1	2.30	0.65
1:A:104:GLU:OE1	1:A:104:GLU:HA	1.97	0.65
1:B:276:SER:HB2	1:B:291:ALA:HB3	1.78	0.65
1:C:222:ASN:N	1:C:222:ASN:HD22	1.95	0.64
1:A:77:ARG:O	1:A:78:LEU:HD23	1.97	0.64
1:A:117:THR:HA	1:A:326:TYR:CD1	2.33	0.64
1:B:127:MSE:HE1	1:B:174:GLY:HA3	1.79	0.64
1:A:20:ARG:NH1	1:A:36:TYR:CD2	2.65	0.64
1:A:93:TYR:OH	1:B:21:HIS:CD2	2.50	0.64
1:C:111:PRO:HA	2:C:348:SO4:O3	1.97	0.64
1:A:227:ALA:HB2	1:A:257:VAL:HG13	1.80	0.64
1:A:260:GLN:HE21	1:A:270:ALA:CB	2.10	0.64
1:B:99:ILE:HG22	1:B:127:MSE:CE	2.27	0.64
1:C:1:MSE:HB3	1:C:13:LEU:O	1.97	0.64
1:A:19:GLY:HA2	1:A:35:THR:HG23	1.80	0.63
1:A:110:ALA:HB3	1:A:114:SER:CB	2.28	0.63
1:A:204:GLY:O	1:A:206:GLY:N	2.31	0.63
1:B:120:GLY:O	1:B:122:TYR:N	2.27	0.63
1:A:91:ILE:HA	1:A:136:THR:O	1.99	0.63
1:A:57:TRP:HA	1:A:78:LEU:O	1.99	0.63
1:B:108:ASP:HA	1:B:114:SER:HB2	1.81	0.63
1:C:10:LYS:HZ1	1:C:42:LYS:HE2	1.62	0.63
1:C:315:ASN:N	1:C:331:ASP:OD1	2.23	0.63
1:A:117:THR:CG2	1:A:118:TRP:N	2.49	0.63
3:B:368:GOL:O2	8:B:414:HOH:O	2.16	0.63
1:B:101:TYR:CD2	1:B:101:TYR:O	2.51	0.63
1:A:302:PHE:HE2	1:A:308:VAL:HG12	1.64	0.62
1:C:207:ASP:OD1	1:C:208:ARG:HG2	1.98	0.62
1:A:4:TYR:O	1:A:10:LYS:HA	2.00	0.62
1:A:35:THR:HG22	1:A:36:TYR:N	2.13	0.62
1:A:161:ASP:HB2	8:A:461:HOH:O	1.98	0.62
1:A:299:THR:OG1	1:A:301:TYR:CE2	2.53	0.62
1:C:65:ARG:HD3	1:C:65:ARG:N	2.15	0.62
1:B:181:PHE:HB2	2:B:354:SO4:S	2.39	0.61
1:C:198:ASP:C	1:C:200:GLN:H	2.03	0.61
1:A:131:ALA:HB3	1:A:134:LEU:HD21	1.82	0.61
1:A:168:GLN:HB3	1:A:196:THR:HG21	1.82	0.61
1:A:202:ARG:HA	1:A:202:ARG:NE	2.15	0.61
1:B:327:VAL:O	1:B:327:VAL:CG2	2.49	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
4:B:377:LDA:H61	4:B:379:LDA:H71	1.82	0.61
1:C:241:THR:HG1	1:C:323:SER:HB2	1.65	0.61
1:B:20:ARG:HD2	1:B:34:GLN:HB3	1.82	0.61
1:C:48:ASN:HD21	1:C:51:LEU:HB2	1.64	0.61
1:B:192:ASN:ND2	1:B:210:GLU:OE2	2.34	0.61
1:B:206:GLY:O	1:B:207:ASP:HB2	2.00	0.61
1:C:50:ASP:HB3	1:C:85:TYR:CE1	2.36	0.61
1:C:19:GLY:HA2	1:C:35:THR:HG23	1.82	0.60
1:C:70:GLN:O	1:C:73:SER:HB2	2.01	0.60
1:A:189:ALA:O	1:A:212:ARG:HA	2.02	0.60
1:C:8:GLY:HA3	8:C:538:HOH:O	2.01	0.60
1:A:65:ARG:CZ	1:C:162:ASN:OD1	2.49	0.60
1:A:117:THR:HG23	1:A:118:TRP:N	2.04	0.60
1:A:260:GLN:NE2	1:A:270:ALA:HB2	2.16	0.60
1:A:1:MSE:HB2	1:A:341:PHE:HB2	1.84	0.60
1:A:82:GLY:C	1:A:83:LEU:HD23	2.21	0.60
1:A:251:LYS:O	1:A:278:GLY:HA2	2.02	0.60
1:B:30:LYS:HD3	1:B:31:ASN:N	2.16	0.60
1:A:26:THR:HB	1:A:330:ASP:HB3	1.83	0.59
1:B:139:ASN:OD1	3:B:365:GOL:H11	2.02	0.59
1:B:158:LYS:NZ	1:B:160:GLN:OE1	2.33	0.59
1:A:85:TYR:CD1	1:A:88:VAL:HG21	2.37	0.59
5:C:393:TAM:H62	8:C:484:HOH:O	2.01	0.59
1:A:22:VAL:HG21	1:A:112:TYR:CZ	2.38	0.59
1:B:139:ASN:HD21	1:B:142:PHE:HA	1.67	0.59
1:C:202:ARG:HB3	8:C:500:HOH:O	2.02	0.59
1:C:260:GLN:HB3	1:C:270:ALA:HA	1.85	0.59
1:A:110:ALA:HB3	1:A:114:SER:HB3	1.84	0.59
6:C:391:FLC:HG2	5:C:393:TAM:HN2	1.68	0.59
1:C:134:LEU:CD2	1:C:156:GLN:HG3	2.33	0.58
1:C:104:GLU:HG2	1:C:118:TRP:CZ2	2.38	0.58
1:C:116:GLU:OE2	1:C:313:ARG:NH1	2.31	0.58
1:C:272:SER:OG	1:C:295:GLN:CG	2.51	0.58
1:A:127:MSE:CG	1:A:154:GLN:HE22	2.13	0.58
1:A:131:ALA:HB3	1:A:134:LEU:HD11	1.85	0.58
1:B:231:GLU:OE2	1:B:233:ARG:NH2	2.35	0.58
1:C:157:GLY:HA2	1:C:171:ASP:OD2	2.03	0.58
1:A:299:THR:HG1	1:A:301:TYR:HE2	1.50	0.58
1:A:48:ASN:HD22	1:A:49:THR:N	2.00	0.58
1:B:99:ILE:HG22	1:B:127:MSE:HE3	1.84	0.58
1:C:306:MSE:CE	1:C:339:TYR:CD1	2.87	0.58



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:291:ALA:HA	1:C:317:LEU:HD12	1.84	0.58	
1:C:306:MSE:HE1	1:C:339:TYR:CD1	2.39	0.58	
1:B:123:THR:O	1:B:130:ARG:O	2.22	0.58	
1:B:164:SER:O	1:B:166:ASN:N	2.37	0.58	
1:C:99:ILE:H	1:C:154:GLN:HE21	1.49	0.58	
1:C:335:VAL:HG22	1:C:336:GLY:N	2.19	0.57	
1:B:26:THR:CG2	1:B:27:GLY:N	2.66	0.57	
1:A:201:ASP:OD1	1:A:202:ARG:HG2	2.04	0.57	
1:B:118:TRP:CG	1:B:119:GLY:N	2.72	0.57	
1:A:162:ASN:CG	1:B:65:ARG:NH1	2.58	0.57	
1:A:299:THR:OG1	1:A:301:TYR:HE2	1.88	0.57	
1:B:233:ARG:O	1:B:250:ASN:HA	2.04	0.57	
1:A:33:ASP:H	4:C:385:LDA:H111	1.68	0.57	
1:A:244:ASP:O	1:A:245:THR:CB	2.53	0.57	
1:B:297:GLY:HA3	1:B:311:ASP:HA	1.86	0.57	
1:A:87:GLU:O	1:A:143:PHE:HD1	1.88	0.57	
1:A:302:PHE:CE2	1:A:308:VAL:HG12	2.39	0.57	
1:C:49:THR:HB	2:C:370:SO4:O3	2.04	0.57	
1:C:212:ARG:HG2	1:C:231:GLU:HB3	1.86	0.57	
1:C:282:ASN:O	1:C:322:TYR:HE2	1.87	0.57	
1:A:337:ILE:HD13	4:A:384:LDA:H122	1.86	0.57	
1:B:202:ARG:HB2	1:B:247:GLU:CB	2.31	0.57	
1:A:117:THR:CG2	1:A:118:TRP:HD1	2.18	0.56	
1:B:43:GLY:HA3	1:C:339:TYR:OH	2.06	0.56	
1:B:113:PHE:HD1	1:B:116:GLU:OE1	1.89	0.56	
1:C:234:ASN:O	1:C:248:MSE:HG2	2.06	0.56	
1:B:116:GLU:O	1:B:121:ALA:HB2	2.06	0.56	
1:B:313:ARG:NH2	1:B:327:VAL:HB	2.20	0.56	
1:C:111:PRO:HB3	1:C:309:TRP:CD1	2.41	0.56	
1:A:267:LEU:HD12	1:A:268:ARG:H	1.71	0.56	
1:B:61:THR:HG22	1:B:74:ASN:HB3	1.87	0.56	
1:A:33:ASP:OD1	1:A:35:THR:N	2.39	0.56	
1:B:197:ASN:O	1:B:200:GLN:HG3	2.07	0.56	
1:B:293:TYR:CE2	1:B:327:VAL:HG21	2.41	0.56	
1:B:64:ASP:OD2	1:B:65:ARG:HD3	2.05	0.55	
4:C:383:LDA:HM23	8:C:423:HOH:O	2.05	0.55	
1:C:111:PRO:HD3	8:C:476:HOH:O	2.05	0.55	
1:B:124:ASP:OD1	1:C:66:ALA:CA	2.53	0.55	
1:B:202:ARG:CB	1:B:247:GLU:HB3	2.33	0.55	
1:C:117:THR:OG1	1:C:118:TRP:N	2.39	0.55	
1:A:177:MSE:O	1:A:187:THR:HG22	2.07	0.55	



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:142:PHE:O	1:B:145:LEU:HB2	2.06	0.55
1:B:320:ASN:C	1:B:322:TYR:N	2.58	0.55
4:B:377:LDA:H31	4:B:379:LDA:H62	1.89	0.55
1:C:309:TRP:NE1	8:C:527:HOH:O	2.29	0.55
1:B:1:MSE:N	1:B:13:LEU:O	2.31	0.55
1:B:23:TRP:CD1	1:B:31:ASN:OD1	2.60	0.55
1:B:8:GLY:O	1:B:9:ASN:HB2	2.06	0.55
1:C:198:ASP:O	1:C:200:GLN:N	2.40	0.55
1:A:23:TRP:CZ2	4:A:384:LDA:HM13	2.38	0.54
1:B:66:ALA:O	1:B:70:GLN:HG3	2.08	0.54
1:A:70:GLN:NE2	1:C:76:VAL:H	2.05	0.54
1:A:217:LYS:HB3	1:A:226:ALA:HB2	1.89	0.54
1:B:139:ASN:HB3	1:B:151:PHE:CE2	2.42	0.54
1:C:281:LEU:HD13	1:C:281:LEU:H	1.71	0.54
1:A:117:THR:CG2	1:A:118:TRP:CD1	2.90	0.54
1:B:77:ARG:NH2	2:B:345:SO4:O4	2.33	0.54
1:A:25:THR:HB	1:A:331:ASP:O	2.08	0.54
1:A:131:ALA:CB	1:A:134:LEU:HD21	2.38	0.54
1:A:248:MSE:O	1:A:249:ALA:O	2.25	0.54
4:B:375:LDA:HM13	4:C:382:LDA:C2	2.25	0.54
1:C:98:GLY:HA3	1:C:127:MSE:CA	2.37	0.54
1:C:103:VAL:HG11	1:C:213:ALA:HB1	1.90	0.54
1:A:2:GLU:HA	1:A:12:ASP:CB	2.38	0.54
1:A:202:ARG:HD2	1:A:245:THR:CG2	2.38	0.54
1:A:1:MSE:HB3	1:A:341:PHE:HD2	1.73	0.54
1:A:78:LEU:CD2	1:A:130:ARG:HG2	2.37	0.54
1:A:195:ARG:HH21	1:A:248:MSE:HB2	1.72	0.54
1:C:93:TYR:HA	1:C:134:LEU:O	2.07	0.54
1:A:146:VAL:HG11	1:A:149:LEU:HB3	1.88	0.54
1:B:313:ARG:O	1:B:313:ARG:HG3	2.07	0.54
1:A:74:ASN:OD1	1:C:59:TYR:OH	2.14	0.54
1:A:117:THR:HA	1:A:326:TYR:CE1	2.43	0.54
1:C:240:ASN:O	1:C:243:THR:O	2.26	0.54
1:A:5:ASN:ND2	1:A:10:LYS:HB2	2.23	0.53
1:B:89:GLY:HA2	3:B:365:GOL:H12	1.90	0.53
1:B:239:GLU:OE1	1:B:246:VAL:HG13	2.07	0.53
1:B:315:ASN:HD21	1:B:317:LEU:HB3	1.73	0.53
5:C:387:TAM:H32	3:C:392:GOL:O2	2.07	0.53
1:A:47:ILE:HD11	1:B:306:MSE:HG2	1.91	0.53
1:A:172:GLY:HA3	1:A:193:SER:OG	2.08	0.53
1:A:207:ASP:HB3	2:A:361:SO4:O2	2.08	0.53



	<b>A A A</b>	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:306:MSE:HE1	1:B:339:TYR:CD1	2.43	0.53
1:C:23:TRP:CZ3	4:C:383:LDA:H82	2.43	0.53
1:A:101:TYR:CD1	1:A:104:GLU:HB3	2.43	0.53
1:B:169:ASN:ND2	8:B:401:HOH:O	2.40	0.53
1:A:110:ALA:HB3	1:A:114:SER:HB2	1.90	0.53
1:C:21:HIS:CG	4:C:384:LDA:H31	2.43	0.53
1:B:196:THR:HG22	1:B:198:ASP:H	1.74	0.53
1:B:306:MSE:CE	1:B:339:TYR:HD1	2.21	0.53
1:A:207:ASP:OD1	1:A:208:ARG:N	2.42	0.53
1:B:89:GLY:HA3	1:B:137:TYR:CE1	2.43	0.53
1:C:48:ASN:N	1:C:48:ASN:HD22	2.07	0.53
1:A:262:GLN:HG2	8:A:522:HOH:O	2.08	0.53
1:A:300:TYR:HE1	8:A:516:HOH:O	1.92	0.53
1:B:327:VAL:O	1:B:327:VAL:HG22	2.08	0.53
1:A:53:GLY:HA3	1:B:306:MSE:HE3	1.91	0.52
1:A:296:ALA:O	1:A:312:TYR:N	2.40	0.52
1:B:126:TYR:CE1	1:B:169:ASN:HB2	2.43	0.52
1:B:127:MSE:HE1	1:B:174:GLY:CA	2.38	0.52
1:A:232:THR:HB	1:A:252:THR:CB	2.38	0.52
1:B:53:GLY:C	1:C:306:MSE:HE3	2.29	0.52
1:B:145:LEU:HD12	4:B:376:LDA:H61	1.91	0.52
1:C:108:ASP:HA	1:C:114:SER:HB3	1.91	0.52
1:A:172:GLY:HA2	1:A:193:SER:HA	1.92	0.52
1:A:277:LYS:HG3	1:A:288:ALA:O	2.08	0.52
1:A:291:ALA:CA	1:A:317:LEU:HD11	2.33	0.52
1:B:2:GLU:HB3	3:B:364:GOL:H12	1.89	0.52
1:A:117:THR:HG22	1:A:118:TRP:CD1	2.44	0.52
1:B:250:ASN:O	1:B:251:LYS:O	2.28	0.52
1:B:261:TYR:O	1:B:269:PRO:HD2	2.10	0.52
1:C:255:LEU:HB3	1:C:275:GLN:CG	2.31	0.52
1:C:309:TRP:CD1	1:C:309:TRP:C	2.83	0.52
1:A:178:ALA:HA	1:A:187:THR:HG22	1.92	0.52
1:A:306:MSE:O	1:A:307:ASN:HB3	2.10	0.52
1:C:18:VAL:HG21	1:C:36:TYR:CZ	2.45	0.52
1:A:217:LYS:HB2	1:A:226:ALA:HB2	1.93	0.51
1:B:54:PHE:HE2	1:B:84:LYS:HB2	1.75	0.51
1:C:18:VAL:HG13	1:C:338:THR:HG22	1.92	0.51
1:A:111:PRO:HG3	1:A:299:THR:HG21	1.93	0.51
1:B:21:HIS:CE1	1:B:31:ASN:HD21	2.26	0.51
1:A:91:ILE:HD12	1:A:92:ASP:N	2.26	0.51
1:B:320:ASN:C	1:B:322:TYR:H	2.13	0.51



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:195:ARG:HH22	1:C:206:GLY:HA2	1.76	0.51
1:B:166:ASN:OD1	1:B:237:ILE:HD13	2.10	0.51
1:C:170:GLY:HA3	1:C:194:LYS:O	2.10	0.51
3:C:394:GOL:H2	8:C:488:HOH:O	2.11	0.51
1:C:107:THR:CG2	1:C:228:VAL:HG12	2.40	0.51
1:C:317:LEU:HD23	1:C:318:ASP:N	2.26	0.51
1:B:62:LYS:HB2	1:B:73:SER:HB2	1.92	0.51
1:A:70:GLN:HE22	1:C:76:VAL:HG22	1.76	0.51
1:B:42:LYS:NZ	1:B:42:LYS:CB	2.74	0.51
1:B:58:GLU:HB3	1:B:77:ARG:HG3	1.92	0.50
1:B:277:LYS:HE2	4:B:380:LDA:HM13	1.93	0.50
1:B:317:LEU:HD21	1:B:323:SER:OG	2.10	0.50
1:A:25:THR:HG21	1:A:312:TYR:OH	2.12	0.50
1:B:99:ILE:O	1:B:102:ASP:HB2	2.11	0.50
1:B:306:MSE:HE2	1:B:339:TYR:HD1	1.76	0.50
1:C:303:ASN:HB3	1:C:305:ASN:H	1.76	0.50
1:A:140:SER:O	1:A:150:SER:HB3	2.11	0.50
1:A:158:LYS:HE3	1:A:160:GLN:HB3	1.92	0.50
1:B:134:LEU:HD13	1:B:154:GLN:NE2	2.26	0.50
1:B:229:TYR:CE2	1:B:231:GLU:HG3	2.46	0.50
1:C:335:VAL:CG2	1:C:336:GLY:N	2.74	0.50
1:A:99:ILE:O	1:A:102:ASP:HB2	2.12	0.50
1:C:200:GLN:HG2	8:C:458:HOH:O	2.11	0.50
1:A:134:LEU:HD23	1:A:156:GLN:HG3	1.93	0.50
1:C:102:ASP:OD2	1:C:138:ARG:NH2	2.40	0.50
1:B:2:GLU:OE1	1:B:5:ASN:ND2	2.45	0.50
1:C:282:ASN:HA	2:C:365:SO4:O1	2.11	0.50
1:C:313:ARG:CZ	1:C:327:VAL:HG13	2.42	0.50
1:A:20:ARG:NH1	1:A:36:TYR:CE2	2.80	0.50
1:C:9:ASN:O	1:C:10:LYS:CB	2.60	0.50
1:C:222:ASN:N	1:C:222:ASN:ND2	2.60	0.50
1:A:23:TRP:CD2	4:A:388:LDA:H82	2.47	0.49
1:A:91:ILE:HD12	1:A:91:ILE:C	2.32	0.49
1:A:180:GLU:HA	1:A:185:GLY:HA2	1.93	0.49
1:A:195:ARG:HD2	1:A:209:ALA:HB2	1.93	0.49
1:C:281:LEU:HD13	1:C:281:LEU:N	2.27	0.49
1:A:146:VAL:HG23	1:A:147:ASP:N	2.27	0.49
1:B:89:GLY:HA2	3:B:365:GOL:C1	2.42	0.49
1:A:20:ARG:NH1	1:A:36:TYR:HD2	2.10	0.49
1:A:66:ALA:HB3	1:A:69:GLU:OE2	2.12	0.49
1:A:111:PRO:HG3	1:A:299:THR:CG2	2.43	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:267:LEU:HD12	1:A:268:ARG:N	2.28	0.49
1:B:265:PHE:HE1	1:B:267:LEU:HB2	1.77	0.49
7:B:383:TLA:O11	8:B:457:HOH:O	2.20	0.49
1:B:139:ASN:HD21	1:B:143:PHE:N	2.11	0.49
1:B:306:MSE:CE	1:B:339:TYR:CD1	2.96	0.49
1:C:50:ASP:CB	1:C:85:TYR:HE1	2.25	0.49
3:C:375:GOL:O2	5:C:386:TAM:C2	2.60	0.49
1:B:95:ARG:HA	1:B:132:GLY:HA2	1.94	0.49
1:B:307:ASN:ND2	1:B:338:THR:CG2	2.75	0.49
3:C:375:GOL:O2	5:C:386:TAM:H21	2.13	0.49
1:A:57:TRP:CZ2	1:A:59:TYR:HB2	2.48	0.49
1:A:1:MSE:O	1:A:13:LEU:O	2.31	0.49
1:B:127:MSE:CE	1:B:174:GLY:HA3	2.41	0.49
6:C:388:FLC:OG1	6:C:388:FLC:CBC	2.59	0.49
1:C:99:ILE:CB	1:C:154:GLN:HE21	2.23	0.49
1:C:136:THR:HG22	1:C:154:GLN:CB	2.42	0.49
1:C:195:ARG:HH21	1:C:203:ASP:HB3	1.78	0.49
1:C:241:THR:OG1	1:C:323:SER:CA	2.60	0.49
1:A:150:SER:OG	1:A:178:ALA:CB	2.60	0.49
1:A:87:GLU:O	1:A:143:PHE:CD1	2.66	0.49
1:B:26:THR:HG22	1:B:27:GLY:H	1.78	0.49
1:C:128:THR:HG21	1:C:235:MSE:HE1	1.93	0.49
1:C:200:GLN:C	1:C:202:ARG:N	2.66	0.49
1:C:265:PHE:HD2	1:C:265:PHE:H	1.59	0.49
1:A:275:GLN:HB2	1:A:292:LYS:HD2	1.93	0.48
1:C:110:ALA:O	1:C:111:PRO:C	2.48	0.48
1:A:106:TYR:CE2	1:A:217:LYS:HG2	2.47	0.48
1:B:21:HIS:CE1	1:B:31:ASN:ND2	2.81	0.48
4:C:382:LDA:H62	4:C:383:LDA:H111	1.94	0.48
1:B:26:THR:O	1:B:28:ASP:O	2.30	0.48
1:C:15:GLY:HA2	1:C:38:GLN:O	2.14	0.48
1:C:262:GLN:HB2	1:C:268:ARG:HD2	1.96	0.48
1:A:146:VAL:CG2	1:A:149:LEU:H	2.26	0.48
1:B:99:ILE:HG22	1:B:127:MSE:HE2	1.94	0.48
1:C:95:ARG:HH22	1:C:124:ASP:CG	2.16	0.48
1:A:24:THR:HB	1:A:30:LYS:H	1.78	0.48
1:A:69:GLU:OE1	1:C:164:SER:OG	2.31	0.48
1:B:26:THR:CG2	1:B:27:GLY:H	2.27	0.48
1:B:303:ASN:HB3	1:B:305:ASN:H	1.79	0.48
1:A:1:MSE:N	1:A:341:PHE:C	2.67	0.48
1:A:282:ASN:N	1:A:282:ASN:OD1	2.47	0.48



	ti c	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
5:C:386:TAM:H22	5:C:386:TAM:H61	1.23	0.48		
1:A:141:ASP:CG	1:A:144:GLY:H	2.17	0.48		
1:B:21:HIS:O	1:B:334:ALA:CB	2.61	0.48		
1:B:199:GLN:O	1:B:203:ASP:HB3	2.13	0.48		
1:C:187:THR:HG22	1:C:188:ALA:N	2.29	0.48		
1:C:279:LYS:O	1:C:280:GLN:HB2	2.13	0.48		
1:A:95:ARG:NH2	1:A:124:ASP:OD1	2.47	0.48		
1:B:137:TYR:HB3	1:B:153:ILE:HD13	1.96	0.48		
1:C:201:ASP:O	1:C:202:ARG:C	2.51	0.47		
1:A:20:ARG:HH11	1:A:36:TYR:HD2	1.62	0.47		
1:A:238:VAL:HG13	1:A:325:SER:CB	2.43	0.47		
1:A:320:ASN:HB2	1:A:323:SER:HB2	1.96	0.47		
1:B:265:PHE:CE1	1:B:267:LEU:HB2	2.49	0.47		
1:C:65:ARG:HH11	1:C:65:ARG:HG3	1.69	0.47		
1:C:76:VAL:HG23	1:C:95:ARG:HD2	1.94	0.47		
1:A:95:ARG:HG3	1:A:131:ALA:O	2.14	0.47		
1:C:80:PHE:CD2	1:C:96:ASN:ND2	2.82	0.47		
1:C:198:ASP:C	1:C:200:GLN:N	2.66	0.47		
1:C:224:TYR:HB3	1:C:260:GLN:HG3	1.96	0.47		
1:A:292:LYS:O	1:A:316:LEU:N	2.44	0.47		
1:C:322:TYR:O	1:C:323:SER:O	2.32	0.47		
1:A:279:LYS:O	1:A:280:GLN:HB2	2.14	0.47		
1:B:229:TYR:HE2	1:B:231:GLU:HG3	1.78	0.47		
1:C:263:PHE:HB3	1:C:265:PHE:HE2	1.74	0.47		
1:A:244:ASP:O	1:A:245:THR:HB	2.15	0.47		
1:A:18:VAL:HG12	1:A:20:ARG:HG2	1.95	0.47		
1:A:78:LEU:HD21	1:A:130:ARG:HD2	1.97	0.47		
1:A:330:ASP:OD2	1:A:330:ASP:N	2.48	0.47		
1:C:33:ASP:C	1:C:34:GLN:HG2	2.35	0.47		
1:A:76:VAL:HG13	1:B:70:GLN:HE22	1.79	0.47		
1:B:23:TRP:HD1	1:B:31:ASN:OD1	1.97	0.47		
1:B:53:GLY:HA3	1:C:306:MSE:HE3	1.97	0.47		
1:A:70:GLN:HE22	1:C:76:VAL:H	1.63	0.46		
1:A:99:ILE:HG12	1:A:176:THR:HB	1.97	0.46		
1:A:160:GLN:NE2	8:A:476:HOH:O	2.47	0.46		
1:A:238:VAL:HG13	1:A:325:SER:HB3	1.97	0.46		
1:A:154:GLN:HG3	8:A:446:HOH:O	2.14	0.46		
1:A:162:ASN:CB	1:B:65:ARG:NH1	2.77	0.46		
1:C:220:ALA:O	1:C:221:ASN:C	2.53	0.46		
1:A:35:THR:CG2	1:A:36:TYR:N	2.79	0.46		
1:A:119:GLY:HA2	1:A:128:THR:OG1	2.15	0.46		



		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:A:160:GLN:CA	1:A:168:GLN:HG2	2.39	0.46		
1:A:205:ASN:HB2	1:A:250:ASN:OD1	2.15	0.46		
1:A:279:LYS:HG2	1:A:286:GLY:O	2.15	0.46		
3:A:370:GOL:H12	5:A:390:TAM:O4	2.16	0.46		
1:B:15:GLY:HA2	1:B:38:GLN:O	2.16	0.46		
1:B:196:THR:HB	2:B:348:SO4:O3	2.15	0.46		
1:B:238:VAL:HG11	1:B:290:LEU:HD21	1.98	0.46		
1:A:306:MSE:HE2	1:C:83:LEU:HD21	1.97	0.46		
1:B:141:ASP:HA	1:B:149:LEU:O	2.16	0.46		
1:C:107:THR:HG23	1:C:228:VAL:HG12	1.96	0.46		
1:A:202:ARG:HD2	1:A:245:THR:HG23	1.97	0.46		
1:B:222:ASN:HB3	1:B:262:GLN:O	2.16	0.46		
1:B:320:ASN:O	1:B:322:TYR:N	2.48	0.46		
1:B:97:TYR:CZ	1:B:130:ARG:HD3	2.51	0.46		
1:C:99:ILE:N	1:C:154:GLN:HE21	2.10	0.46		
1:C:158:LYS:HD2	4:C:385:LDA:H61	1.98	0.46		
1:A:9:ASN:CB	1:A:44:GLU:O	2.64	0.46		
1:B:191:SER:O	1:B:210:GLU:HB2	2.15	0.46		
1:C:86:ALA:O	1:C:87:GLU:CB	2.62	0.46		
1:C:120:GLY:O	1:C:122:TYR:N	2.49	0.46		
1:C:182:ASP:HB3	1:C:183:GLY:H	1.57	0.46		
1:A:127:MSE:SE	1:A:154:GLN:CD	3.02	0.46		
1:A:300:TYR:HD2	1:A:301:TYR:N	2.13	0.46		
1:C:9:ASN:O	1:C:44:GLU:O	2.33	0.46		
1:B:75:LEU:HB2	1:C:67:GLU:HG2	1.98	0.46		
1:C:212:ARG:CG	1:C:231:GLU:HB3	2.46	0.46		
1:C:251:LYS:HD2	1:C:280:GLN:HE22	1.81	0.46		
1:A:200:GLN:HE21	1:A:200:GLN:N	2.14	0.46		
1:C:23:TRP:HZ3	1:C:335:VAL:HG12	1.80	0.46		
1:C:263:PHE:CB	1:C:265:PHE:CE2	2.96	0.46		
1:C:103:VAL:HG12	1:C:104:GLU:N	2.31	0.45		
1:B:18:VAL:O	1:B:35:THR:HG23	2.17	0.45		
1:B:30:LYS:HE2	1:B:30:LYS:HA	1.98	0.45		
1:C:103:VAL:O	1:C:106:TYR:HB2	2.16	0.45		
1:C:109:MSE:CE	1:C:268:ARG:NH2	2.79	0.45		
3:A:380:GOL:H31	8:A:500:HOH:O	2.16	0.45		
1:B:203:ASP:OD1	1:B:203:ASP:N	2.48	0.45		
1:B:288:ALA:HB1	1:B:320:ASN:ND2	2.29	0.45		
5:C:393:TAM:H21	5:C:393:TAM:H41	1.61	0.45		
1:B:77:ARG:O	1:B:78:LEU:HD23	2.16	0.45		
1:B:109:MSE:HG3	1:B:224:TYR:CE2	2.51	0.45		



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:164:SER:C	1:B:166:ASN:N	2.70	0.45
1:A:16:LYS:HB3	1:A:340:GLN:HB3	1.98	0.45
1:A:146:VAL:O	1:A:147:ASP:HB2	2.17	0.45
1:B:76:VAL:N	1:C:70:GLN:NE2	2.52	0.45
1:B:89:GLY:HA3	1:B:137:TYR:HE1	1.82	0.45
1:C:244:ASP:CG	6:C:388:FLC:HA2	2.34	0.45
1:B:42:LYS:HZ3	1:B:42:LYS:HB3	1.82	0.45
1:C:56:GLN:HB3	1:C:80:PHE:CE2	2.49	0.45
1:A:18:VAL:O	1:A:35:THR:CG2	2.60	0.45
1:B:7:ASP:O	1:B:9:ASN:ND2	2.50	0.45
1:A:104:GLU:O	1:A:105:SER:C	2.55	0.45
1:A:257:VAL:O	1:A:272:SER:HB2	2.17	0.45
1:A:309:TRP:CD1	1:A:309:TRP:C	2.90	0.45
1:B:91:ILE:HG12	4:C:384:LDA:C12	2.47	0.45
1:C:125:ASN:HA	8:C:477:HOH:O	2.17	0.45
1:C:151:PHE:HB3	1:C:177:MSE:HG3	1.98	0.45
1:C:262:GLN:NE2	1:C:268:ARG:CD	2.76	0.45
1:C:65:ARG:HD3	1:C:65:ARG:H	1.79	0.45
1:B:18:VAL:HG13	1:B:338:THR:HB	2.00	0.44
1:C:76:VAL:CG2	1:C:76:VAL:O	2.65	0.44
1:C:99:ILE:HG21	1:C:174:GLY:HA3	1.99	0.44
1:C:202:ARG:CD	3:C:375:GOL:H31	2.48	0.44
1:A:91:ILE:HD11	4:A:386:LDA:H91	1.98	0.44
1:A:123:THR:O	1:A:129:SER:HB3	2.16	0.44
1:B:75:LEU:HA	1:C:70:GLN:HE21	1.82	0.44
1:B:124:ASP:OD1	1:C:66:ALA:CB	2.66	0.44
1:B:250:ASN:O	1:B:251:LYS:C	2.54	0.44
1:C:127:MSE:HG2	1:C:154:GLN:NE2	2.32	0.44
1:A:202:ARG:HD2	1:A:245:THR:HG21	2.00	0.44
1:C:255:LEU:O	1:C:256:GLU:HG3	2.17	0.44
1:B:20:ARG:HD2	1:B:34:GLN:O	2.17	0.44
1:B:127:MSE:HE1	1:B:174:GLY:N	2.32	0.44
1:C:48:ASN:HB2	2:C:370:SO4:S	2.58	0.44
1:C:74:ASN:O	1:C:75:LEU:HD23	2.17	0.44
1:C:195:ARG:NH2	1:C:206:GLY:HA2	2.31	0.44
1:B:165:ILE:HG23	1:B:198:ASP:HB3	2.00	0.44
1:B:205:ASN:CG	8:B:433:HOH:O	2.56	0.44
1:C:99:ILE:HB	1:C:154:GLN:CG	2.43	0.44
1:A:9:ASN:HB2	8:A:409:HOH:O	2.17	0.44
1:A:238:VAL:O	1:A:246:VAL:HG23	2.17	0.44
1:B:197:ASN:C	1:B:199:GLN:H	2.21	0.44



	to as pagem	Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:43:GLY:HA3	1:C:339:TYR:CZ	2.52	0.44		
1:C:98:GLY:HA2	1:C:154:GLN:HE22	1.82	0.44		
1:C:156:GLN:HE21	1:C:156:GLN:HB3	1.65	0.44		
1:A:43:GLY:HA3	1:B:339:TYR:CZ	2.52	0.44		
1:A:101:TYR:HA	1:A:104:GLU:HB2	2.00	0.44		
1:A:162:ASN:HB3	1:B:65:ARG:HH11	1.83	0.44		
1:A:224:TYR:HE2	1:A:258:VAL:HG11	1.83	0.44		
1:B:76:VAL:HG13	1:C:70:GLN:NE2	2.32	0.44		
1:B:110:ALA:HB3	1:B:114:SER:N	2.33	0.44		
1:B:113:PHE:CD1	1:B:116:GLU:OE1	2.69	0.44		
1:B:313:ARG:NH2	1:B:332:GLN:OE1	2.51	0.44		
1:B:325:SER:O	1:B:326:TYR:CB	2.65	0.44		
1:C:52:THR:O	1:C:84:LYS:N	2.42	0.44		
1:C:60:ARG:NH1	8:C:439:HOH:O	2.51	0.44		
1:C:282:ASN:O	1:C:322:TYR:CE2	2.69	0.44		
1:A:236:SER:HG	1:A:326:TYR:HH	1.65	0.44		
1:C:213:ALA:HA	1:C:230:ALA:HA	1.99	0.44		
1:A:181:PHE:CE1	1:A:184:PHE:HB2	2.53	0.43		
1:A:24:THR:HB	1:A:30:LYS:N	2.33	0.43		
1:C:23:TRP:CZ3	1:C:335:VAL:HG12	2.54	0.43		
1:A:97:TYR:CE1	1:A:130:ARG:HD3	2.54	0.43		
1:B:320:ASN:CB	1:B:323:SER:OG	2.65	0.43		
1:C:20:ARG:HD3	1:C:34:GLN:HB2	2.00	0.43		
1:C:190:TYR:CD1	1:C:191:SER:N	2.87	0.43		
1:A:159:ASN:ND2	2:A:358:SO4:O2	2.52	0.43		
1:B:171:ASP:OD1	1:B:171:ASP:N	2.46	0.43		
1:C:16:LYS:NZ	2:C:343:SO4:O4	2.48	0.43		
1:C:222:ASN:HB3	1:C:262:GLN:O	2.19	0.43		
1:A:217:LYS:HB3	1:A:226:ALA:CB	2.49	0.43		
1:B:141:ASP:OD1	3:B:365:GOL:C3	2.67	0.43		
1:C:244:ASP:OD1	6:C:388:FLC:OB1	2.35	0.43		
5:C:386:TAM:H21	5:C:386:TAM:H42	1.25	0.43		
1:B:84:LYS:HG3	1:B:90:SER:HB3	2.00	0.43		
1:B:158:LYS:HA	1:B:169:ASN:O	2.19	0.43		
1:C:229:TYR:HA	1:C:254:ASN:O	2.19	0.43		
1:A:22:VAL:HG22	1:A:334:ALA:HB2	2.01	0.43		
1:A:239:GLU:HB2	8:A:443:HOH:O	2.17	0.43		
1:B:47:ILE:HD11	1:C:306:MSE:HG2	2.01	0.43		
1:B:170:GLY:HA3	1:B:194:LYS:O	2.18	0.43		
1:B:200:GLN:C	1:B:201:ASP:O	2.56	0.43		
1:B:255:LEU:O	1:B:256:GLU:HG3	2.18	0.43		



		Interatomic	Clash		
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)		
1:B:320:ASN:HB3	1:B:323:SER:OG	2.18	0.43		
1:C:312:TYR:CD1	1:C:333:ALA:HB2	2.54	0.43		
1:B:321:ASP:C	1:B:322:TYR:HD1	2.22	0.43		
1:C:309:TRP:HZ3	1:C:338:THR:CG2	2.31	0.43		
1:A:233:ARG:NH2	2:A:363:SO4:S	2.87	0.42		
1:B:164:SER:C	1:B:166:ASN:H	2.22	0.42		
1:C:174:GLY:HA2	1:C:191:SER:HA	2.01	0.42		
1:A:150:SER:O	1:A:178:ALA:N	2.52	0.42		
1:A:307:ASN:OD1	1:A:307:ASN:C	2.58	0.42		
1:B:164:SER:O	1:B:167:SER:N	2.50	0.42		
1:C:104:GLU:HG2	1:C:118:TRP:CE2	2.54	0.42		
1:A:198:ASP:CA	1:A:200:GLN:NE2	2.55	0.42		
1:A:229:TYR:HA	1:A:254:ASN:O	2.19	0.42		
1:B:320:ASN:ND2	1:B:322:TYR:HB2	2.34	0.42		
5:C:387:TAM:H22	5:C:387:TAM:H41	1.66	0.42		
1:A:78:LEU:HD23	1:A:130:ARG:HG2	2.01	0.42		
1:A:339:TYR:CZ	1:C:43:GLY:HA3	2.55	0.42		
1:B:19:GLY:HA2	1:B:35:THR:HG23	2.00	0.42		
1:C:50:ASP:CB	1:C:85:TYR:CE1	3.00	0.42		
1:C:160:GLN:H	4:C:385:LDA:H81	1.84	0.42		
1:A:208:ARG:HE	1:A:208:ARG:HB2	1.72	0.42		
1:A:211:SER:OG	1:A:232:THR:HA	2.20	0.42		
1:B:56:GLN:CG	1:B:57:TRP:N	2.82	0.42		
1:C:317:LEU:HD23	2:C:364:SO4:O1	2.19	0.42		
1:B:57:TRP:CD1	1:C:37:ALA:HB3	2.55	0.42		
1:A:208:ARG:NH2	3:A:375:GOL:H12	2.34	0.42		
1:B:314:PHE:CZ	4:B:381:LDA:H42	2.55	0.42		
1:C:65:ARG:N	1:C:65:ARG:CD	2.83	0.42		
1:C:190:TYR:HA	1:C:211:SER:O	2.19	0.42		
1:C:199:GLN:HG2	1:C:203:ASP:HB2	2.02	0.42		
1:A:110:ALA:CB	1:A:114:SER:HB2	2.50	0.42		
1:A:268:ARG:O	1:A:298:ALA:HA	2.20	0.42		
1:A:281:LEU:HB2	1:A:322:TYR:OH	2.20	0.42		
5:A:391:TAM:H52	5:A:391:TAM:H12	1.38	0.42		
1:B:196:THR:O	1:B:199:GLN:HG2	2.20	0.42		
1:C:201:ASP:HB3	1:C:246:VAL:O	2.20	0.42		
1:A:66:ALA:HB2	1:C:167:SER:HB3	2.02	0.42		
1:A:95:ARG:HB2	1:B:63:ALA:HB1	2.02	0.42		
1:C:13:LEU:HD12	1:C:40:GLY:O	2.20	0.42		
1:C:58:GLU:HB2	1:C:78:LEU:HD12	2.02	0.42		
1:A:48:ASN:O	1:A:49:THR:C	2.57	0.41		



	A L O	Interatomic	Clash		
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)		
1:A:261:TYR:O	1:A:269:PRO:HD2	2.20	0.41		
1:B:20:ARG:HD2	1:B:34:GLN:CB	2.47	0.41		
1:B:293:TYR:HB3	1:B:315:ASN:HA	2.01	0.41		
1:A:126:TYR:HE2	1:A:248:MSE:CE	2.32	0.41		
1:B:91:ILE:HG12	4:C:384:LDA:H123	2.02	0.41		
1:B:100:VAL:O	1:B:102:ASP:N	2.53	0.41		
1:A:91:ILE:HD13	1:A:135:LEU:HD11	2.02	0.41		
1:C:164:SER:O	1:C:168:GLN:HG3	2.20	0.41		
1:B:100:VAL:C	1:B:102:ASP:N	2.74	0.41		
1:B:91:ILE:HD11	1:B:135:LEU:HD11	2.02	0.41		
1:C:341:PHE:CD2	1:C:341:PHE:C	2.94	0.41		
1:A:241:THR:HG22	1:A:321:ASP:O	2.21	0.41		
1:C:118:TRP:HB3	1:C:254:ASN:ND2	2.35	0.41		
1:A:313:ARG:O	1:A:313:ARG:HG3	2.21	0.41		
1:B:53:GLY:CA	1:C:306:MSE:HE3	2.50	0.41		
1:C:136:THR:HG22	1:C:154:GLN:OE1	2.21	0.41		
1:A:111:PRO:HD2	1:A:311:ASP:OD2	2.20	0.41		
1:B:78:LEU:HA	1:B:95:ARG:HG3	2.03	0.41		
1:C:202:ARG:HD2	3:C:375:GOL:H31	2.03	0.41		
1:C:266:GLY:HA3	1:C:300:TYR:CE1	2.56	0.41		
1:A:194:LYS:HA	1:A:208:ARG:HD3	2.02	0.41		
1:B:22:VAL:HG23	1:B:334:ALA:HB2	2.03	0.41		
1:B:62:LYS:HB2	1:B:73:SER:CB	2.50	0.41		
1:B:93:TYR:CG	1:B:94:GLY:N	2.88	0.41		
1:B:115:GLY:O	1:B:120:GLY:HA3	2.20	0.41		
1:B:254:ASN:N	1:B:254:ASN:HD22	2.19	0.41		
1:B:317:LEU:CD2	1:B:323:SER:OG	2.69	0.41		
1:A:238:VAL:HG12	1:A:239:GLU:H	1.86	0.41		
1:A:262:GLN:O	1:A:262:GLN:HG3	2.19	0.41		
1:B:93:TYR:OH	1:C:33:ASP:OD1	2.39	0.41		
1:B:101:TYR:HB2	1:B:128:THR:O	2.21	0.41		
1:A:11:LEU:O	1:A:12:ASP:HB3	2.21	0.40		
1:A:67:GLU:OE1	1:C:77:ARG:HG2	2.21	0.40		
1:A:142:PHE:CD1	1:A:149:LEU:HD23	2.56	0.40		
1:C:281:LEU:HB2	1:C:322:TYR:CZ	2.56	0.40		
1:A:117:THR:HA	1:A:326:TYR:HD1	1.82	0.40		
1:A:146:VAL:HG23	1:A:147:ASP:H	1.86	0.40		
1:B:226:ALA:O	1:B:257:VAL:HA	2.21	0.40		
1:B:303:ASN:C	1:B:305:ASN:H	2.25	0.40		
1:C:151:PHE:HA	1:C:177:MSE:HA	2.01	0.40		
1:A:30:LYS:HE3	8:A:414:HOH:O	2.21	0.40		



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance $(A)$	overlap (Å)
1:A:162:ASN:CG	1:B:65:ARG:HH12	2.25	0.40
1:B:134:LEU:HD23	1:B:156:GLN:HB2	2.03	0.40
1:B:205:ASN:HB2	1:B:234:ASN:ND2	2.37	0.40
1:B:277:LYS:NZ	4:B:380:LDA:O1	2.45	0.40
4:B:380:LDA:HM22	4:B:380:LDA:H22	1.76	0.40
1:C:21:HIS:NE2	1:C:31:ASN:OD1	2.45	0.40
1:C:39:ILE:HG22	1:C:59:TYR:HB3	2.03	0.40
1:A:91:ILE:CD1	1:A:135:LEU:HD11	2.50	0.40
1:B:68:GLY:C	1:B:69:GLU:HG3	2.41	0.40
1:B:210:GLU:OE1	1:B:212:ARG:NH1	2.55	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	Per	rce	ntiles
1	А	339/341~(99%)	286 (84%)	39 (12%)	14 (4%)		3	9
1	В	339/341~(99%)	285 (84%)	37 (11%)	17 (5%)		2	6
1	С	339/341~(99%)	279 (82%)	41 (12%)	19 (6%)		2	5
All	All	1017/1023~(99%)	850 (84%)	117 (12%)	50 (5%)		2	7

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	113	PHE
1	А	205	ASN
1	А	208	ARG
1	А	245	THR
1	А	249	ALA
1	В	2	GLU
1	В	9	ASN



Mol	Chain	Res	Type
1	В	207	ASP
1	В	251	LYS
1	В	326	TYR
1	С	6	LYS
1	С	9	ASN
1	С	126	TYR
1	С	201	ASP
1	С	202	ARG
1	С	251	LYS
1	С	286	GLY
1	А	114	SER
1	А	197	ASN
1	А	206	GLY
1	В	105	SER
1	В	206	GLY
1	В	283	GLY
1	С	10	LYS
1	С	87	GLU
1	С	199	GLN
1	С	200	GLN
1	С	236	SER
1	С	323	SER
1	А	4	TYR
1	А	7	ASP
1	А	148	GLY
1	А	233	ARG
1	В	240	ASN
1	С	86	ALA
1	С	221	ASN
1	В	7	ASP
1	В	101	TYR
1	В	117	THR
1	В	197	ASN
1	С	4	TYR
1	С	121	ALA
1	С	162	ASN
1	А	126	TYR
1	А	244	ASP
1	В	28	ASP
1	В	127	MSE
1	С	283	GLY
1	В	204	GLY



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Mol	Chain	$\mathbf{Res}$	Type
1	В	327	VAL

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Pe	erce	entil	$\mathbf{es}$
1	А	271/265~(102%)	208~(77%)	63~(23%)		1	2	
1	В	271/265~(102%)	223~(82%)	48 (18%)		2	5	
1	С	271/265~(102%)	216 (80%)	55 (20%)		1	4	
All	All	813/795 (102%)	647 (80%)	166 (20%)		1	4	

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	2	GLU
1	А	4	TYR
1	А	5	ASN
1	А	6	LYS
1	А	9	ASN
1	А	10	LYS
1	А	20	ARG
1	А	24	THR
1	А	46	GLN
1	А	48	ASN
1	А	49	THR
1	А	52	THR
1	А	71	GLN
1	А	74	ASN
1	А	76	VAL
1	А	78	LEU
1	А	83	LEU
1	А	85	TYR
1	А	88	VAL
1	А	91	ILE
1	А	102	ASP



Mol	Chain	Res	Type
1	А	104	GLU
1	А	109	MSE
1	А	112	TYR
1	А	117	THR
1	А	123	THR
1	А	128	THR
1	А	145	LEU
1	А	153	ILE
1	А	154	GLN
1	А	156	GLN
1	А	161	ASP
1	А	165	ILE
1	А	167	SER
1	A	171	ASP
1	А	177	MSE
1	А	193	SER
1	А	197	ASN
1	А	198	ASP
1	А	200	GLN
1	А	211	SER
1	А	212	ARG
1	А	223	VAL
1	А	225	LEU
1	А	228	VAL
1	А	235	MSE
1	А	246	VAL
1	А	252	THR
1	А	260	GLN
1	A	264	ASP
1	А	267	LEU
1	А	275	GLN
1	A	281	LEU
1	A	282	ASN
1	A	290	LEU
1	A	299	THR
1	A	300	TYR
1	A	308	VAL
1	A	311	ASP
1	A	313	ARG
1	A	315	ASN
1	A	330	ASP
1	А	335	VAL



Mol Chain		Res	Type
1	В	3	ILE
1	В	4	TYR
1	В	6	LYS
1	В	10	LYS
1	В	13	LEU
1	В	20	ARG
1	В	24	THR
1	В	28	ASP
1	В	30	LYS
1	В	42	LYS
1	В	47	ILE
1	В	52	THR
1	В	65	ARG
1	В	71	GLN
1	В	74	ASN
1	В	76	VAL
1	В	83	LEU
1	В	87	GLU
1	В	92	ASP
1	В	146	VAL
1	В	153	ILE
1	В	171	ASP
1	В	175	TYR
1	В	182	ASP
1	В	187	THR
1	В	191	SER
1	В	193	SER
1	В	208	ARG
1	В	212	ARG
1	В	225	LEU
1	В	241	THR
1	В	242	VAL
1	В	243	THR
1	В	246	VAL
1	В	248	MSE
1	В	257	VAL
1	В	264	ASP
1	В	272	SER
1	В	274	VAL
1	В	276	SER
1	В	289	ASP
1	В	303	ASN



Mol	Chain	Res	Type
1	В	310	VAL
1	В	313	ARG
1	В	321	ASP
1	В	326	TYR
1	В	327	VAL
1	В	338	THR
1	С	10	LYS
1	С	12	ASP
1	С	20	ARG
1	С	28	ASP
1	С	29	SER
1	С	46	GLN
1	С	48	ASN
1	С	49	THR
1	С	52	THR
1	С	64	ASP
1	C	65	ARG
1	С	69	GLU
1	С	75	LEU
1	С	92	ASP
1	С	96	ASN
1	С	105	SER
1	С	117	THR
1	С	145	LEU
1	С	150	SER
1	С	156	GLN
1	С	158	LYS
1	С	163	HIS
1	С	167	SER
1	С	171	ASP
1	С	175	TYR
1	C	198	ASP
1	C	199	GLN
1	C	200	GLN
1	C	202	ARG
1	C	205	ASN
1	C	207	ASP
1	C	212	ARG
1	C	214	VAL
1	C	217	LYS
1	C	222	ASN
1	С	228	VAL



Mol	Chain	Res	Type
1	С	233	ARG
1	С	235	MSE
1	С	243	THR
1	С	245	THR
1	С	248	MSE
1	С	257	VAL
1	С	274	VAL
1	С	275	GLN
1	С	281	LEU
1	С	290	LEU
1	С	303	ASN
1	С	304	LYS
1	С	310	VAL
1	С	313	ARG
1	С	315	ASN
1	С	316	LEU
1	С	319	GLU
1	С	338	THR
1	С	340	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	5	ASN
1	А	9	ASN
1	А	21	HIS
1	А	48	ASN
1	А	70	GLN
1	А	159	ASN
1	А	166	ASN
1	А	200	GLN
1	А	234	ASN
1	А	240	ASN
1	А	260	GLN
1	А	275	GLN
1	А	305	ASN
1	А	315	ASN
1	В	5	ASN
1	В	9	ASN
1	В	21	HIS
1	В	31	ASN
1	В	56	GLN



Mol	Chain	Res	Type
1	В	70	GLN
1	В	154	GLN
1	В	159	ASN
1	В	200	GLN
1	В	282	ASN
1	В	307	ASN
1	В	315	ASN
1	В	320	ASN
1	С	5	ASN
1	С	48	ASN
1	С	56	GLN
1	С	70	GLN
1	С	154	GLN
1	С	156	GLN
1	С	159	ASN
1	С	166	ASN
1	С	169	ASN
1	С	205	ASN
1	С	222	ASN
1	С	254	ASN
1	С	262	GLN
1	С	275	GLN
1	С	280	GLN
1	С	282	ASN
1	С	303	ASN
1	С	305	ASN
1	С	315	ASN

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#### 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 monosaccharides in this entry.



### 5.6 Ligand geometry (i)

147 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).

Mal	Turne	Chain	Dec	Tink	Bond lengths		Bond angles			
1VIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	SO4	С	368	-	4,4,4	0.13	0	$6,\!6,\!6$	0.12	0
3	GOL	С	380	-	$5,\!5,\!5$	0.39	0	$5,\!5,\!5$	0.22	0
4	LDA	А	387	-	12,15,15	1.99	1 (8%)	14,17,17	0.75	1 (7%)
5	TAM	В	382	-	7,10,10	0.56	0	9,12,12	0.36	0
2	SO4	С	371	-	4,4,4	0.14	0	6,6,6	0.09	0
3	GOL	С	394	-	$5,\!5,\!5$	0.36	0	$5,\!5,\!5$	0.59	0
3	GOL	С	377	-	$5,\!5,\!5$	0.41	0	$5,\!5,\!5$	0.29	0
2	SO4	С	357	-	4,4,4	0.13	0	$6,\!6,\!6$	0.20	0
4	LDA	А	389	-	12,15,15	1.97	1 (8%)	14,17,17	0.60	0
2	SO4	В	350	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	А	343	-	4,4,4	0.11	0	6,6,6	0.19	0
2	SO4	С	356	-	4,4,4	0.15	0	6,6,6	0.14	0
3	GOL	С	376	-	$5,\!5,\!5$	0.43	0	$5,\!5,\!5$	0.15	0
2	SO4	С	343	-	4,4,4	0.13	0	6,6,6	0.11	0
5	TAM	А	390	-	7,10,10	0.46	0	9,12,12	0.44	0
3	GOL	А	378	-	$5,\!5,\!5$	0.31	0	$5,\!5,\!5$	0.27	0
2	SO4	В	344	-	4,4,4	0.13	0	$6,\!6,\!6$	0.16	0
2	SO4	В	354	-	4,4,4	0.15	0	$6,\!6,\!6$	0.07	0
2	SO4	В	345	-	4,4,4	0.27	0	$6,\!6,\!6$	0.16	0
3	GOL	В	368	-	$5,\!5,\!5$	0.42	0	$5,\!5,\!5$	0.22	0
2	SO4	А	349	-	4,4,4	0.25	0	$6,\!6,\!6$	0.14	0
2	SO4	А	344	-	4,4,4	0.12	0	$6,\!6,\!6$	0.12	0
4	LDA	В	381	-	$12,\!15,\!15$	1.86	1 (8%)	$14,\!17,\!17$	0.56	0
2	SO4	В	348	-	4,4,4	0.14	0	$6,\!6,\!6$	0.40	0
4	LDA	В	377	-	12,15,15	1.93	1 (8%)	14,17,17	0.71	0
3	GOL	В	367	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.36	0
5	TAM	С	393	-	7,10,10	0.47	0	9,12,12	0.69	0
2	SO4	В	343	-	4,4,4	0.14	0	$6,\!6,\!6$	0.11	0
2	SO4	А	367	-	4,4,4	0.16	0	$6,\!6,\!6$	0.20	0
2	SO4	С	352	-	4,4,4	0.13	0	$6,\!6,\!6$	0.24	0
2	SO4	A	360	-	4,4,4	0.18	0	6,6,6	0.10	0



	T	<u> </u>	Ъ	T · 1	Bo	ond leng	$\mathbf{ths}$	В	ond ang	les
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	GOL	В	374	-	$5,\!5,\!5$	0.41	0	$5,\!5,\!5$	0.15	0
4	LDA	С	385	-	12,15,15	2.00	1 (8%)	$14,\!17,\!17$	0.64	0
2	SO4	С	362	-	4,4,4	0.15	0	6,6,6	0.12	0
6	FLC	С	391	-	12,12,12	1.26	0	17,17,17	5.34	8 (47%)
2	SO4	А	356	-	4,4,4	0.17	0	6,6,6	0.29	0
2	SO4	В	359	-	4,4,4	0.15	0	6,6,6	0.15	0
3	GOL	А	374	-	$5,\!5,\!5$	0.40	0	$5,\!5,\!5$	0.11	0
2	SO4	С	354	-	4,4,4	0.16	0	$6,\!6,\!6$	0.11	0
7	TLA	В	383	-	$9,\!9,\!9$	1.15	0	$12,\!12,\!12$	1.14	0
5	TAM	С	386	-	7,10,10	0.55	0	9,12,12	0.68	0
3	GOL	А	370	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.27	0
2	SO4	В	347	-	4,4,4	0.17	0	$6,\!6,\!6$	0.37	0
2	SO4	В	363	-	4,4,4	0.12	0	$6,\!6,\!6$	0.17	0
2	SO4	A	348	-	4,4,4	0.16	0	$6,\!6,\!6$	0.15	0
4	LDA	В	375	-	$12,\!15,\!15$	2.14	1 (8%)	$14,\!17,\!17$	0.93	1 (7%)
2	SO4	С	351	-	4,4,4	0.18	0	$6,\!6,\!6$	0.21	0
4	LDA	А	388	-	$12,\!15,\!15$	2.00	1 (8%)	$14,\!17,\!17$	0.69	0
2	SO4	В	358	-	4,4,4	0.16	0	$6,\!6,\!6$	0.09	0
2	SO4	С	370	-	4,4,4	0.25	0	$6,\!6,\!6$	0.21	0
4	LDA	С	382	-	12,15,15	2.01	1 (8%)	$14,\!17,\!17$	0.48	0
2	SO4	А	352	-	4,4,4	0.14	0	$6,\!6,\!6$	0.18	0
3	GOL	А	372	-	$5,\!5,\!5$	0.39	0	$5,\!5,\!5$	0.25	0
5	TAM	С	387	-	7,10,10	0.66	0	$9,\!12,\!12$	0.64	0
2	SO4	А	361	-	4,4,4	0.12	0	$6,\!6,\!6$	0.19	0
2	SO4	А	365	-	4,4,4	0.15	0	$6,\!6,\!6$	0.09	0
2	SO4	С	350	-	4,4,4	0.16	0	$6,\!6,\!6$	0.11	0
2	SO4	А	359	-	4,4,4	0.13	0	$6,\!6,\!6$	0.13	0
3	GOL	В	365	-	$5,\!5,\!5$	0.25	0	$5,\!5,\!5$	0.52	0
2	SO4	A	346	-	4,4,4	0.20	0	$6,\!6,\!6$	0.18	0
2	SO4	C	361	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	A	345	-	4,4,4	0.19	0	6,6,6	0.12	0
3	GOL	C	392	-	5,5,5	0.39	0	5,5,5	0.16	0
2	SO4	A	347	-	4,4,4	0.18	0	6,6,6	0.12	0
2	SO4	В	357	-	4,4,4	0.17	0	6,6,6	0.10	0
4	LDA	A	385	-	12,15,15	2.06	1 (8%)	14,17,17	0.49	0
2	SO4	В	360	-	4,4,4	0.17	0	$6,\!6,\!6$	0.09	0
6	FLC	С	388	-	12,12,12	1.79	4 (33%)	$17,\!17,\!17$	1.67	2 (11%)
3	GOL	В	373	-	$5,\!5,\!5$	0.40	0	$5,\!5,\!5$	0.18	0
3	GOL	B	366	-	5, 5, 5	0.49	0	$5,\!5,\!\overline{5}$	0.66	0
3	GOL	В	369	-	$5,\!5,\!5$	0.42	0	$5,\!5,\!5$	0.37	0
2	SO4	A	351		4,4,4	0.13	0	$6,\!6,\!6$	0.14	0



	T	<u> </u>	Ъ	τ・1	Bo	nd leng	ths	В	ond ang	les
IVIOI	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
2	SO4	А	369	-	4,4,4	0.25	0	$6,\!6,\!6$	0.09	0
3	GOL	А	377	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.37	0
3	GOL	С	390	-	$5,\!5,\!5$	0.36	0	$5,\!5,\!5$	0.31	0
4	LDA	В	376	-	$12,\!15,\!15$	2.05	1 (8%)	$14,\!17,\!17$	0.64	0
2	SO4	С	369	-	4,4,4	0.13	0	6,6,6	0.19	0
3	GOL	А	375	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.56	0
3	GOL	С	378	-	$5,\!5,\!5$	0.42	0	$5,\!5,\!5$	0.32	0
3	GOL	В	372	-	$5,\!5,\!5$	0.41	0	$5,\!5,\!5$	0.47	0
2	SO4	С	366	-	$4,\!4,\!4$	0.13	0	$6,\!6,\!6$	0.13	0
3	GOL	В	364	-	$5,\!5,\!5$	0.44	0	$5,\!5,\!5$	0.22	0
2	SO4	С	342	-	4,4,4	0.17	0	$6,\!6,\!6$	0.22	0
3	GOL	С	375	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	0.23	0
3	GOL	С	381	-	$5,\!5,\!5$	0.41	0	$5,\!5,\!5$	0.38	0
2	SO4	С	355	-	4,4,4	0.15	0	$6,\!6,\!6$	0.19	0
2	SO4	В	356	-	4,4,4	0.21	0	$6,\!6,\!6$	0.08	0
2	SO4	A	353	-	4,4,4	0.15	0	$6,\!6,\!6$	0.18	0
7	TLA	А	393	-	$9,\!9,\!9$	1.11	0	$12,\!12,\!12$	1.09	1 (8%)
2	SO4	А	362	-	4,4,4	0.13	0	$6,\!6,\!6$	0.18	0
2	SO4	В	355	-	$4,\!4,\!4$	0.16	0	$6,\!6,\!6$	0.12	0
2	SO4	С	348	-	4,4,4	0.19	0	$6,\!6,\!6$	0.18	0
2	SO4	С	372	-	4,4,4	0.20	0	$6,\!6,\!6$	0.12	0
2	SO4	С	345	-	4,4,4	0.14	0	$6,\!6,\!6$	0.19	0
3	GOL	С	1325	-	$5,\!5,\!5$	0.31	0	$5,\!5,\!5$	0.28	0
4	LDA	В	378	-	$12,\!15,\!15$	2.05	1 (8%)	$14,\!17,\!17$	0.51	0
2	SO4	А	364	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.08	0
2	SO4	В	351	-	$4,\!4,\!4$	0.38	0	$6,\!6,\!6$	0.37	0
2	SO4	В	342	-	4,4,4	0.11	0	$6,\!6,\!6$	0.15	0
3	GOL	А	379	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.26	0
2	SO4	С	353	-	4,4,4	0.11	0	$6,\!6,\!6$	0.13	0
2	SO4	A	363	-	4,4,4	0.17	0	$6,\!6,\!6$	0.12	0
3	GOL	A	383	-	$5,\!5,\!5$	0.40	0	$5,\!5,\!5$	0.36	0
2	SO4	A	342	-	4,4,4	0.16	0	$6,\!6,\!6$	0.11	0
2	SO4	B	352	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	В	361	-	4,4,4	0.11	0	$6,\!6,\!6$	0.14	0
4	LDA	А	386	-	$12,\!15,\!15$	1.98	1 (8%)	$14,\!17,\!17$	0.71	0
2	SO4	С	363	-	4,4,4	0.16	0	$6,\!6,\!6$	0.09	0
6	FLC	C	389	-	$12,\!12,\!12$	1.23	1 (8%)	$17,\!17,\!17$	5.33	7 (41%)
2	SO4	С	349	-	4,4,4	0.19	0	$6,\!6,\!6$	0.13	0
2	SO4	А	357	-	4,4,4	0.12	0	$6,\!6,\!6$	0.22	0
2	SO4	С	344	-	4,4,4	0.20	0	$6,\!6,\!6$	0.13	0
2	SO4	С	347	-	4,4,4	0.12	0	$6,\!6,\!6$	0.22	0
3	GOL	A	376	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.35	0



Mal	Turne	Chain	Dec	Timle	Bo	Bond lengths		Bond angles		
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	В	371	-	$5,\!5,\!5$	0.41	0	$5,\!5,\!5$	0.42	0
3	GOL	А	371	-	$5,\!5,\!5$	0.45	0	$5,\!5,\!5$	0.21	0
2	SO4	С	358	-	$4,\!4,\!4$	0.12	0	$6,\!6,\!6$	0.15	0
3	GOL	С	373	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.28	0
3	GOL	С	374	-	$5,\!5,\!5$	0.38	0	$5,\!5,\!5$	0.45	0
3	GOL	А	373	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.22	0
2	SO4	С	367	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.19	0
2	SO4	В	346	-	$4,\!4,\!4$	0.14	0	$6,\!6,\!6$	0.16	0
2	SO4	С	364	-	$4,\!4,\!4$	0.12	0	$6,\!6,\!6$	0.22	0
4	LDA	С	384	-	$12,\!15,\!15$	2.05	1 (8%)	$14,\!17,\!17$	0.67	0
2	SO4	В	362	-	4,4,4	0.14	0	$6,\!6,\!6$	0.11	0
4	LDA	В	379	-	12,15,15	2.04	1 (8%)	14,17,17	0.65	0
2	SO4	А	354	-	4,4,4	0.16	0	6,6,6	0.14	0
4	LDA	А	384	-	12,15,15	1.94	1 (8%)	14,17,17	0.73	0
3	GOL	С	379	_	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.23	0
2	SO4	С	359	_	4,4,4	0.17	0	6,6,6	0.05	0
3	GOL	В	370	-	5,5,5	0.35	0	5,5,5	0.30	0
3	GOL	А	380	-	$5,\!5,\!5$	0.39	0	5,5,5	0.41	0
3	GOL	А	381	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.32	0
2	SO4	А	350	-	4,4,4	0.18	0	6,6,6	0.16	0
3	GOL	А	382	-	$5,\!5,\!5$	0.35	0	$5,\!5,\!5$	0.18	0
4	LDA	В	380	-	12,15,15	2.04	1 (8%)	14,17,17	0.69	0
2	SO4	С	365	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	В	353	-	4,4,4	0.14	0	6,6,6	0.18	0
2	SO4	А	358	-	4,4,4	0.12	0	6,6,6	0.23	0
4	LDA	С	383	-	12,15,15	1.99	1 (8%)	14,17,17	0.73	0
2	SO4	A	355	-	4,4,4	0.19	0	6,6,6	0.25	0
5	TAM	А	391	-	7,10,10	0.55	0	9,12,12	0.53	0
2	SO4	С	346	-	4,4,4	0.16	0	6,6,6	0.12	0
6	FLC	А	392	-	12,12,12	1.76	2 (16%)	17,17,17	4.95	7 (41%)
2	SO4	А	366	-	4,4,4	0.19	0	6,6,6	0.09	0
2	SO4	С	360	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	В	349	-	4,4,4	0.12	0	6,6,6	0.16	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
5	TAM	С	386	-	-	10/12/12/12	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	А	371	-	-	3/4/4/4	-
3	GOL	С	380	-	-	4/4/4/4	-
3	GOL	А	370	-	-	2/4/4/4	-
3	GOL	А	375	-	-	3/4/4/4	-
4	LDA	А	387	-	-	10/13/13/13	-
4	LDA	В	375	_	-	7/13/13/13	-
3	GOL	С	378	-	-	0/4/4/4	_
3	GOL	С	373	-	-	0/4/4/4	-
3	GOL	В	372	-	-	1/4/4/4	-
3	GOL	С	374	-	-	0/4/4/4	-
3	GOL	С	377	-	-	2/4/4/4	-
3	GOL	С	394	-	-	2/4/4/4	-
4	LDA	А	388	-	-	7/13/13/13	-
4	LDA	А	389	-	-	7/13/13/13	-
5	TAM	В	382	-	-	8/12/12/12	_
3	GOL	В	364	-	-	0/4/4/4	-
3	GOL	С	376	-	-	1/4/4/4	-
3	GOL	А	373	-	-	4/4/4/4	-
3	GOL	С	375	-	-	2/4/4/4	-
3	GOL	С	381	-	-	4/4/4/4	-
4	LDA	С	382	-	-	10/13/13/13	-
5	TAM	А	390	-	-	7/12/12/12	-
3	GOL	А	372	-	-	2/4/4/4	-
3	GOL	А	378	-	-	2/4/4/4	-
7	TLA	А	393	-	-	2/12/12/12	-
5	TAM	С	387	-	-	6/12/12/12	-
4	LDA	С	384	-	-	10/13/13/13	-
4	LDA	В	379	-	-	8/13/13/13	_
3	GOL	С	1325	-	-	4/4/4/4	_
3	GOL	В	368	-	-	0/4/4/4	-
4	LDA	А	384	-	-	10/13/13/13	_
3	GOL	В	365	-	-	4/4/4/4	_
3	GOL	С	379	-	-	2/4/4/4	-
4	LDA	В	378	_	-	4/13/13/13	_
4	LDA	В	381	-	-	7/13/13/13	_



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	В	377	-	-	10/13/13/13	-
3	GOL	В	367	-	-	2/4/4/4	_
3	GOL	В	370	-	-	2/4/4/4	-
3	GOL	А	380	-	-	$\frac{4}{4/4}$	-
5	TAM	С	393	-	-	6/12/12/12	-
3	GOL	С	390	-	_	0/4/4/4	_
3	GOL	С	392	-	-	0/4/4/4	-
3	GOL	А	381	-	-	1/4/4/4	-
4	LDA	А	385	-	-	6/13/13/13	-
3	GOL	А	379	-	-	2/4/4/4	-
3	GOL	А	382	-	-	2/4/4/4	_
3	GOL	В	373	-	-	0/4/4/4	-
3	GOL	В	374	-	-	2/4/4/4	-
4	LDA	В	380	-	-	7/13/13/13	-
4	LDA	С	385	-	-	8/13/13/13	-
6	FLC	С	388	-	-	6/16/16/16	-
3	GOL	А	383	-	-	2/4/4/4	-
6	FLC	С	391	-	-	4/16/16/16	-
3	GOL	В	366	-	_	1/4/4/4	-
3	GOL	В	369	-	-	1/4/4/4	-
4	LDA	А	386	-	-	9/13/13/13	-
4	LDA	С	383	-	-	4/13/13/13	-
3	GOL	А	374	_	_	0/4/4/4	_
6	FLC	С	389	-	-	8/16/16/16	-
5	TAM	А	391	-	-	8/12/12/12	-
6	FLC	А	392	-	-	10/16/16/16	-
3	GOL	А	377	-	-	4/4/4/4	-
3	GOL	А	376	-	-	3/4/4/4	-
7	TLA	В	383	-	-	4/12/12/12	-
3	GOL	В	371	-	-	0/4/4/4	-
4	LDA	В	376	-	-	8/13/13/13	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	Ideal(Å)
4	В	375	LDA	O1-N1	-7.36	1.24	1.42
4	С	384	LDA	O1-N1	-7.05	1.25	1.42



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	В	376	LDA	O1-N1	-7.04	1.25	1.42
4	В	378	LDA	O1-N1	-7.00	1.25	1.42
4	В	380	LDA	O1-N1	-6.98	1.25	1.42
4	А	385	LDA	O1-N1	-6.96	1.25	1.42
4	В	379	LDA	O1-N1	-6.90	1.26	1.42
4	С	385	LDA	O1-N1	-6.86	1.26	1.42
4	А	388	LDA	O1-N1	-6.85	1.26	1.42
4	С	383	LDA	O1-N1	-6.84	1.26	1.42
4	С	382	LDA	O1-N1	-6.83	1.26	1.42
4	А	387	LDA	O1-N1	-6.80	1.26	1.42
4	А	386	LDA	O1-N1	-6.80	1.26	1.42
4	А	384	LDA	O1-N1	-6.67	1.26	1.42
4	А	389	LDA	O1-N1	-6.64	1.26	1.42
4	В	377	LDA	O1-N1	-6.38	1.27	1.42
4	В	381	LDA	O1-N1	-6.32	1.27	1.42
6	А	392	FLC	CG-CB	4.22	1.59	1.53
6	С	388	FLC	CB-CBC	3.26	1.56	1.53
6	С	388	FLC	OHB-CB	2.35	1.47	1.43
6	С	388	FLC	CG-CB	2.25	1.56	1.53
6	С	389	FLC	CB-CBC	2.15	1.55	1.53
6	А	392	FLC	OG1-CGC	2.13	1.29	1.22
6	С	388	FLC	OG1-CGC	2.05	1.28	1.22

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	С	391	FLC	OHB-CB-CBC	-14.50	88.51	108.86
6	С	389	FLC	OHB-CB-CBC	-12.95	90.69	108.86
6	А	392	FLC	OHB-CB-CBC	-12.61	91.16	108.86
6	С	389	FLC	OHB-CB-CA	-10.96	83.75	109.40
6	С	389	FLC	OHB-CB-CG	-10.69	84.38	109.40
6	А	392	FLC	OHB-CB-CA	-10.53	84.75	109.40
6	С	391	FLC	OHB-CB-CA	-10.43	85.00	109.40
6	С	391	FLC	OHB-CB-CG	-8.94	88.49	109.40
6	А	392	FLC	OHB-CB-CG	-7.46	91.95	109.40
6	А	392	FLC	CG-CB-CBC	6.06	123.14	110.11
6	С	389	FLC	CA-CB-CBC	5.83	122.64	110.11
6	С	391	FLC	CG-CB-CA	5.57	123.68	109.16
6	С	389	FLC	CG-CB-CA	4.44	120.74	109.16
6	С	388	FLC	OB2-CBC-CB	4.29	120.50	113.05
6	А	392	FLC	CA-CB-CBC	4.05	118.81	110.11
6	С	391	FLC	CG-CB-CBC	3.97	118.63	110.11



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	С	391	FLC	CB-CA-CAC	3.47	122.22	113.81
6	А	392	FLC	CG-CB-CA	3.40	118.02	109.16
6	А	392	FLC	OB2-CBC-CB	3.33	118.84	113.05
6	С	389	FLC	OB2-CBC-CB	3.23	118.66	113.05
6	С	391	FLC	CA-CB-CBC	3.22	117.03	110.11
6	С	388	FLC	OB1-CBC-CB	-3.04	117.95	122.25
4	В	375	LDA	CM2-N1-C1	2.73	115.98	110.23
6	С	389	FLC	CG-CB-CBC	2.44	115.34	110.11
7	А	393	TLA	O41-C4-C3	2.42	119.82	113.27
6	С	391	FLC	OB2-CBC-CB	2.36	117.15	113.05
4	А	387	LDA	CM2-N1-C1	2.25	114.96	110.23

There are no chirality outliers.

All (279) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	370	GOL	C1-C2-C3-O3
3	А	371	GOL	O1-C1-C2-C3
3	А	372	GOL	C1-C2-C3-O3
3	А	373	GOL	C1-C2-C3-O3
3	А	376	GOL	O1-C1-C2-O2
3	А	376	GOL	O1-C1-C2-C3
3	А	377	GOL	O1-C1-C2-O2
3	А	377	GOL	O1-C1-C2-C3
3	А	378	GOL	C1-C2-C3-O3
3	А	379	GOL	C1-C2-C3-O3
3	А	379	GOL	O2-C2-C3-O3
3	В	365	GOL	O1-C1-C2-O2
3	В	365	GOL	O1-C1-C2-C3
3	В	365	GOL	C1-C2-C3-O3
3	В	367	GOL	O1-C1-C2-C3
3	В	374	GOL	O1-C1-C2-O2
3	В	374	GOL	O1-C1-C2-C3
3	С	377	GOL	C1-C2-C3-O3
3	С	377	GOL	O2-C2-C3-O3
3	С	379	GOL	O1-C1-C2-O2
3	С	379	GOL	O1-C1-C2-C3
3	С	380	GOL	C1-C2-C3-O3
3	С	1325	GOL	C1-C2-C3-O3
4	A	384	LDA	C2-C1-N1-O1
4	A	384	LDA	C2-C1-N1-CM1
4	A	387	LDA	C2-C1-N1-O1



Mol	Chain	Res	Type	Atoms
4	А	387	LDA	C2-C1-N1-CM2
4	A	387	LDA	N1-C1-C2-C3
4	А	389	LDA	C2-C1-N1-CM1
4	А	389	LDA	C2-C1-N1-CM2
4	В	376	LDA	C2-C1-N1-CM2
4	В	377	LDA	C2-C1-N1-CM1
4	В	377	LDA	C2-C1-N1-CM2
4	В	381	LDA	C2-C1-N1-CM1
4	В	381	LDA	C2-C1-N1-CM2
4	С	382	LDA	C2-C1-N1-O1
4	С	382	LDA	C2-C1-N1-CM1
4	С	382	LDA	C2-C1-N1-CM2
4	С	384	LDA	C2-C1-N1-CM2
4	С	384	LDA	N1-C1-C2-C3
4	С	385	LDA	C2-C1-N1-CM1
4	С	385	LDA	N1-C1-C2-C3
5	А	390	TAM	C2-C-C1-C4
5	А	390	TAM	C3-C-C1-C4
5	А	390	TAM	N-C-C1-C4
5	А	390	TAM	C1-C-C3-C6
5	А	390	TAM	C2-C-C3-C6
5	А	390	TAM	N-C-C3-C6
5	А	391	TAM	C2-C-C1-C4
5	А	391	TAM	C3-C-C1-C4
5	А	391	TAM	N-C-C1-C4
5	А	391	TAM	C1-C-C2-C5
5	А	391	TAM	C3-C-C2-C5
5	А	391	TAM	N-C-C2-C5
5	А	391	TAM	C-C3-C6-O6
5	В	382	TAM	C2-C-C1-C4
5	В	382	TAM	C3-C-C1-C4
5	В	382	TAM	N-C-C1-C4
5	В	382	TAM	C1-C-C3-C6
5	B	382	TAM	$C2-\overline{C-C3-C6}$
5	B	382	TAM	N-C-C3-C6
5	В	382	TAM	C-C1-C4-O4
5	В	382	TAM	C-C2-C5-O5
5	C	386	TAM	C2-C-C1-C4
5	C	386	TAM	C3-C-C1-C4
5	C	386	TAM	N-C-C1-C4
5	C	386	TAM	C1-C-C2-C5
$\overline{5}$	С	386	TAM	C3-C-C2-C5

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Mol	Chain	Res	Type	Atoms
5	С	386	TAM	N-C-C2-C5
5	С	386	TAM	C1-C-C3-C6
5	С	386	TAM	C2-C-C3-C6
5	С	386	TAM	N-C-C3-C6
5	С	386	TAM	C-C1-C4-O4
5	С	387	TAM	C2-C-C1-C4
5	С	387	TAM	C3-C-C1-C4
5	С	387	TAM	N-C-C1-C4
5	С	387	TAM	C-C3-C6-O6
5	С	393	TAM	C2-C-C1-C4
5	С	393	TAM	C3-C-C1-C4
5	С	393	TAM	N-C-C1-C4
5	С	393	TAM	C-C2-C5-O5
6	А	392	FLC	CAC-CA-CB-CG
6	А	392	FLC	CA-CB-CBC-OB1
6	А	392	FLC	CA-CB-CBC-OB2
6	А	392	FLC	CG-CB-CBC-OB1
6	А	392	FLC	CG-CB-CBC-OB2
6	А	392	FLC	OHB-CB-CBC-OB1
6	А	392	FLC	OHB-CB-CBC-OB2
6	А	392	FLC	CA-CB-CG-CGC
6	С	388	FLC	CA-CB-CBC-OB1
6	С	388	FLC	CA-CB-CBC-OB2
6	С	388	FLC	OHB-CB-CBC-OB1
6	С	388	FLC	OHB-CB-CBC-OB2
6	С	389	FLC	CAC-CA-CB-CBC
6	С	389	FLC	OHB-CB-CBC-OB2
6	С	389	FLC	OHB-CB-CG-CGC
6	С	391	FLC	CAC-CA-CB-CBC
6	С	391	FLC	CAC-CA-CB-CG
6	С	391	FLC	CA-CB-CG-CGC
7	А	393	TLA	O1-C1-C2-O2
7	A	393	TLA	O11-C1-C2-O2
7	B	383	TLA	O11-C1-C2-O2
6	A	392	FLC	CAC-CA-CB-OHB
7	В	383	TLA	O1-C1-C2-O2
3	А	382	GOL	O2-C2-C3-O3
3	С	380	GOL	O1-C1-C2-O2
4	A	386	LDA	C2-C3-C4-C5
4	B	377	LDA	C3-C4-C5-C6
6	С	389	FLC	CA-CB-CG-CGC
4	А	384	LDA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	А	387	LDA	C2-C3-C4-C5
4	В	379	LDA	C5-C6-C7-C8
4	В	380	LDA	C3-C4-C5-C6
4	С	385	LDA	C7-C8-C9-C10
4	В	380	LDA	C11-C10-C9-C8
3	А	373	GOL	O1-C1-C2-C3
3	А	375	GOL	O1-C1-C2-C3
3	А	375	GOL	C1-C2-C3-O3
3	А	380	GOL	C1-C2-C3-O3
3	А	382	GOL	C1-C2-C3-O3
3	В	369	GOL	C1-C2-C3-O3
3	В	370	GOL	C1-C2-C3-O3
3	С	375	GOL	C1-C2-C3-O3
3	С	380	GOL	O1-C1-C2-C3
3	С	381	GOL	O1-C1-C2-C3
3	С	381	GOL	C1-C2-C3-O3
3	С	394	GOL	C1-C2-C3-O3
4	А	385	LDA	C7-C8-C9-C10
4	В	380	LDA	C6-C7-C8-C9
4	С	385	LDA	C11-C10-C9-C8
4	А	386	LDA	C5-C6-C7-C8
4	С	382	LDA	C3-C4-C5-C6
4	А	389	LDA	C2-C3-C4-C5
4	В	381	LDA	C6-C7-C8-C9
4	А	386	LDA	C3-C4-C5-C6
4	А	388	LDA	C7-C8-C9-C10
4	A	386	LDA	C6-C7-C8-C9
4	В	377	LDA	C7-C8-C9-C10
4	A	386	LDA	C11-C10-C9-C8
4	А	389	LDA	C3-C4-C5-C6
4	В	380	LDA	C7-C8-C9-C10
4	В	381	LDA	C7-C8-C9-C10
4	С	382	LDA	C7-C8-C9-C10
4	С	382	LDA	C6-C7-C8-C9
4	В	379	LDA	C11-C10-C9-C8
3	A	370	GOL	O2-C2-C3-O3
3	A	371	GOL	O1-C1-C2-O2
3	A	372	GOL	O2-C2-C3-O3
3	A	373	GOL	O1-C1-C2-O2
3	A	375	GOL	O2-C2-C3-O3
3	A	378	GOL	O2-C2-C3-O3
3	С	380	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	С	381	GOL	O1-C1-C2-O2
3	С	394	GOL	O2-C2-C3-O3
4	В	375	LDA	C11-C10-C9-C8
4	С	385	LDA	C2-C3-C4-C5
4	А	387	LDA	C5-C6-C7-C8
4	С	383	LDA	C7-C8-C9-C10
4	А	384	LDA	C6-C7-C8-C9
4	С	384	LDA	C2-C3-C4-C5
4	А	387	LDA	C1-C2-C3-C4
4	В	375	LDA	C1-C2-C3-C4
4	С	382	LDA	C1-C2-C3-C4
4	В	377	LDA	C4-C5-C6-C7
4	С	385	LDA	C6-C7-C8-C9
4	А	386	LDA	C7-C8-C9-C10
4	А	387	LDA	C7-C8-C9-C10
4	А	388	LDA	C4-C5-C6-C7
4	В	380	LDA	C4-C5-C6-C7
4	А	385	LDA	C6-C7-C8-C9
4	В	376	LDA	C6-C7-C8-C9
4	С	382	LDA	C2-C3-C4-C5
4	А	388	LDA	C1-C2-C3-C4
4	А	386	LDA	C9-C10-C11-C12
5	А	390	TAM	C-C2-C5-O5
3	А	380	GOL	O2-C2-C3-O3
3	В	367	GOL	O1-C1-C2-O2
3	В	370	GOL	O2-C2-C3-O3
3	С	375	GOL	O2-C2-C3-O3
3	С	381	GOL	O2-C2-C3-O3
4	А	388	LDA	C9-C10-C11-C12
7	В	383	TLA	C2-C3-C4-O4
4	В	376	LDA	C1-C2-C3-C4
4	С	383	LDA	C6-C7-C8-C9
4	A	388	LDA	C6-C7-C8-C9
4	A	384	LDA	C1-C2-C3-C4
4	В	379	LDA	C1-C2-C3-C4
4	A	384	LDA	N1-C1-C2-C3
4	A	385	LDA	N1-C1-C2-C3
4	A	386	LDA	N1-C1-C2-C3
4	A	388	LDA	N1-C1-C2-C3
4	B	375	LDA	N1-C1-C2-C3
4	В	380	LDA	N1-C1-C2-C3
4	C	383	LDA	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	А	384	LDA	C7-C8-C9-C10
4	С	382	LDA	C11-C10-C9-C8
6	С	389	FLC	OHB-CB-CBC-OB1
6	С	389	FLC	CA-CB-CBC-OB1
6	С	389	FLC	CA-CB-CBC-OB2
7	В	383	TLA	C2-C3-C4-O41
3	А	383	GOL	O2-C2-C3-O3
3	В	365	GOL	O2-C2-C3-O3
4	А	384	LDA	C3-C4-C5-C6
6	С	391	FLC	OHB-CB-CG-CGC
4	А	386	LDA	C4-C5-C6-C7
4	А	384	LDA	C9-C10-C11-C12
4	С	384	LDA	C3-C4-C5-C6
4	В	379	LDA	C6-C7-C8-C9
4	В	375	LDA	C9-C10-C11-C12
4	С	383	LDA	C9-C10-C11-C12
6	С	388	FLC	OHB-CB-CG-CGC
4	А	388	LDA	C5-C6-C7-C8
4	А	384	LDA	C2-C1-N1-CM2
4	А	387	LDA	C2-C1-N1-CM1
4	В	376	LDA	C2-C1-N1-CM1
4	С	384	LDA	C2-C1-N1-CM1
4	С	385	LDA	C2-C1-N1-CM2
3	А	373	GOL	O2-C2-C3-O3
3	В	366	GOL	O1-C1-C2-O2
3	С	1325	GOL	O2-C2-C3-O3
4	А	387	LDA	C9-C10-C11-C12
3	А	377	GOL	C1-C2-C3-O3
3	С	376	GOL	O1-C1-C2-C3
3	С	1325	GOL	O1-C1-C2-C3
4	С	384	LDA	C1-C2-C3-C4
4	В	376	LDA	C5-C6-C7-C8
4	В	381	LDA	C11-C10-C9-C8
4	В	379	LDA	C2-C3-C4-C5
4	В	377	LDA	C2-C3-C4-C5
4	А	389	LDA	C2-C1-N1-O1
4	В	376	LDA	C2-C1-N1-O1
4	В	381	LDA	C2-C1-N1-O1
4	С	384	LDA	C2-C1-N1-O1
4	В	379	LDA	C4-C5-C6-C7
6	А	392	FLC	OHB-CB-CG-CGC
4	С	382	LDA	C9-C10-C11-C12



Mol	Chain	Res	Type	Atoms
4	В	379	LDA	C7-C8-C9-C10
5	С	387	TAM	C-C2-C5-O5
4	А	385	LDA	C2-C3-C4-C5
6	С	388	FLC	CAC-CA-CB-CG
6	С	389	FLC	CBC-CB-CG-CGC
4	В	377	LDA	C11-C10-C9-C8
4	А	387	LDA	C3-C4-C5-C6
3	А	371	GOL	C1-C2-C3-O3
3	А	377	GOL	O2-C2-C3-O3
3	А	380	GOL	O1-C1-C2-O2
3	В	372	GOL	O2-C2-C3-O3
4	В	375	LDA	C7-C8-C9-C10
4	В	376	LDA	C4-C5-C6-C7
4	В	378	LDA	C3-C4-C5-C6
4	В	379	LDA	C9-C10-C11-C12
4	A	389	LDA	C1-C2-C3-C4
4	С	384	LDA	C9-C10-C11-C12
4	A	389	LDA	C9-C10-C11-C12
4	В	380	LDA	C5-C6-C7-C8
5	С	387	TAM	N-C-C2-C5
5	C	393	TAM	N-C-C2-C5
4	B	377	LDA	C6-C7-C8-C9
5	С	393	TAM	C3-C-C2-C5
4	С	384	LDA	C11-C10-C9-C8
3	С	1325	GOL	O1-C1-C2-O2
4	В	378	LDA	C11-C10-C9-C8
4	В	378	LDA	C1-C2-C3-C4
4	A	385	LDA	C3-C4-C5-C6
4	В	375	LDA	C3-C4-C5-C6
4	В	381	LDA	C4-C5-C6-C7
4	В	378	LDA	C4-C5-C6-C7
4	А	385	LDA	C5-C6-C7-C8
3	A	380	GOL	O1-C1-C2-C3
3	A	381	GOL	O1-C1-C2-C3
3	A	383	GOL	C1-C2-C3-O3
4	С	384	LDA	C6-C7-C8-C9
4	В	377	LDA	C5-C6-C7-C8
4	В	377	LDA	C2-C1-N1-O1
4	С	385	LDA	C2-C1-N1-O1
3	A	376	GOL	O2-C2-C3-O3
5	A	391	TAM	C1-C-C3-C6
4	В	375	LDA	C5-C6-C7-C8

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Mol	Chain	$\mathbf{Res}$	Type	Atoms
4	В	376	LDA	C2-C3-C4-C5

There are no ring outliers.

42 monomers are involved in 87 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	394	GOL	1	0
2	С	343	SO4	1	0
5	А	390	TAM	10	0
2	В	354	SO4	1	0
2	В	345	SO4	2	0
3	В	368	GOL	1	0
4	В	381	LDA	1	0
2	В	348	SO4	1	0
4	В	377	LDA	2	0
5	С	393	TAM	3	0
4	С	385	LDA	4	0
6	С	391	FLC	1	0
7	В	383	TLA	1	0
5	С	386	TAM	4	0
3	А	370	GOL	2	0
4	В	375	LDA	3	0
4	А	388	LDA	1	0
2	С	370	SO4	2	0
4	С	382	LDA	4	0
5	С	387	TAM	5	0
2	А	361	SO4	3	0
3	В	365	GOL	4	0
3	С	392	GOL	1	0
6	С	388	FLC	5	0
4	В	376	LDA	1	0
3	А	375	GOL	1	0
3	В	364	GOL	1	0
3	С	375	GOL	6	0
2	С	348	SO4	1	0
2	А	363	SO4	1	0
4	А	386	LDA	1	0
2	С	364	SO4	1	0
4	С	384	LDA	4	0
4	В	379	LDA	2	0
4	А	384	LDA	4	0
3	А	380	GOL	1	0



	0	-	1 0		
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	350	SO4	1	0
4	В	380	LDA	3	0
2	С	365	SO4	1	0
2	А	358	SO4	1	0
4	С	383	LDA	4	0
5	А	391	TAM	1	0

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#### 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,  $95^{th}$  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	$OWAB(Å^2)$	Q<0.9
1	А	334/341~(97%)	0.17	15 (4%) 33 23	34, 57, 80, 91	0
1	В	334/341~(97%)	0.13	8 (2%) 59 49	34, 56, 68, 88	0
1	С	334/341~(97%)	0.20	9 (2%) 54 44	34, 58, 81, 92	0
All	All	1002/1023~(97%)	0.17	32 (3%) 47 37	34, 57, 79, 92	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	289	ASP	5.8
1	А	320	ASN	5.4
1	А	288	ALA	4.6
1	В	7	ASP	4.5
1	В	4	TYR	3.5
1	А	321	ASP	3.3
1	В	6	LYS	3.3
1	А	6	LYS	3.0
1	С	290	LEU	2.9
1	А	241	THR	2.9
1	С	181	PHE	2.8
1	В	8	GLY	2.7
1	С	166	ASN	2.7
1	А	319	GLU	2.7
1	С	280	GLN	2.6
1	А	229	TYR	2.6
1	А	318	ASP	2.5
1	С	279	LYS	2.5
1	С	289	ASP	2.5
1	А	13	LEU	2.5
1	В	202	ARG	2.2
1	A	3	ILE	2.2
1	В	27	GLY	2.1



Mol	Chain	Res	Type	RSRZ
1	С	168	GLN	2.1
1	В	328	GLY	2.1
1	А	239	GLU	2.1
1	А	209	ALA	2.1
1	В	318	ASP	2.1
1	С	4	TYR	2.0
1	С	320	ASN	2.0
1	А	317	LEU	2.0
1	А	290	LEU	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 monosaccharides 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. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	GOL	С	376	6/6	0.31	0.47	134,135,135,135	0
2	SO4	А	369	5/5	0.34	0.69	164,164,164,164	0
3	GOL	С	379	6/6	0.41	0.88	122,123,124,124	0
3	GOL	А	378	6/6	0.47	0.89	118,119,119,119	0
2	SO4	С	360	5/5	0.47	0.36	170,170,170,170	0
3	GOL	А	377	6/6	0.47	0.33	82,83,84,84	0
4	LDA	В	381	16/16	0.56	0.47	83,90,105,105	0
4	LDA	А	385	16/16	0.57	0.74	106,112,117,117	0
3	GOL	С	394	6/6	0.58	0.25	67,69,70,70	0
3	GOL	В	373	6/6	0.64	0.70	107,108,109,109	0
2	SO4	В	343	5/5	0.67	0.45	151,151,151,151	0
3	GOL	А	372	6/6	0.67	0.34	86,88,88,88	0
3	GOL	В	367	6/6	0.67	0.31	85,85,86,86	0
2	SO4	В	351	5/5	0.68	0.61	174,174,175,175	0



	Type	Chain	ls page.	 Atoms	BSCC	RSR	<b>B</b> -factors $(Å^2)$	0<0.9
5	ТАМ	Cliain	303	11/11	0.68	0.20	60.61.61.61	<b>Q</b> <0.3
3	COL		378	6/6	0.00	0.20	83 85 85 86	0
3 3	COL		376	6/6	0.70	0.30	101 102 102 102	0
$\frac{1}{2}$	SO4		366	5/5	0.70	0.20	101,102,102,102 $1/8,1/8,1/8,1/8$	0
5	TAM		301	$\frac{5}{5}$	0.70	0.00	62 63 63 64	11
			380	11/11 16/16	0.71	0.31	75.03.105.106	0
6	EDA FLC		302	10/10 12/12	$\begin{array}{c} 0.71 \\ 0.71 \end{array}$	0.40	120, 120, 120, 121, 121	0
0	FLC SO4		392	5/5	$\begin{array}{c} 0.71 \\ 0.72 \end{array}$	0.44	120,120,121,121 142,144,144,144	0
5	TAM	A C	386		0.72	0.70	143,144,144,144 50 51 51 52	11
<u> </u>		B	377	11/11 16/16	0.72 0.72	0.28 0.34	87 101 108 108	0
4		B	360	6/6	0.72	0.34 0.27	80.82.84.85	0
		D C	385	16/16	$\begin{array}{c} 0.12 \\ \hline 0.73 \end{array}$	0.21	01.07.103.103	0
-4 5	TAM		200	$\frac{10}{11}$	$\begin{array}{r} 0.73 \\ 0.73 \end{array}$	$\begin{array}{c} 0.41 \\ 0.70 \end{array}$		11
5	TAM	A P	200		0.73	0.19	19,21,22,22 52,54,55,55	11
<u> </u>			387	11/11 16/16	0.74	0.18	65 82 05 06	0
$\frac{4}{2}$	SO4	R R	361	5/5	0.75	0.39	00,82,90,90	0
3	COL	C	375	6/6	0.70	$\begin{array}{c} 0.22 \\ 0.22 \end{array}$	143,143,144,144 117 110 110 120	0
3	COL	B	371	6/6	0.70	0.22	88 80 80 80	0
3 3	GOL		371	6/6	0.70	0.45	85 85 86 86	0
3	GOL		377	6/6	0.77	0.00	07 07 00 00	0
$\frac{1}{2}$	SO4		366	5/5	0.77	0.25 0.35	167 167 167 167	0
3	GOL		381	6/6	0.77	0.35	95 96 96 97	0
3	GOL	C	1325	6/6	0.77	0.50	113 114 115 115	0
$\frac{0}{2}$	SO4	B	344	5/5	$\frac{0.11}{0.77}$	0.01	134 134 134 134 134	0
$\frac{2}{2}$	SO4	B	355	5/5	0.78	0.42	142 142 142 142	0
2	SO4	A	365	5/5	0.78	0.30	131 131 132 132	0
3	GOL	C	392	6/6	0.78	0.36	101,101,102,102 104,105,105,105	0
3	GOL	B	374	6/6	0.78	0.68	84.85.86.87	0
2	SO4	B	362	5/5	0.78	0.54	148.148.148.149	0
3	GOL	A	383	6/6	0.78	0.30	90.91.91.92	0
2	SO4	C	353	$\frac{5}{5}$	0.78	0.31	128.128.128.128	0
2	SO4	C	359	5/5	0.78	0.58	143.144.144.144	0
3	GOL	C	390	6/6	0.79	0.26	94,96,97,97	0
2	SO4	A	359	5/5	0.79	0.35	136,136,136,136	0
3	GOL	А	382	6/6	0.79	0.25	82,84,84,86	0
7	TLA	А	393	10/10	0.79	0.32	125,126,126,127	0
4	LDA	В	379	16/16	0.80	0.23	73,87,96,96	0
2	SO4	В	345	5/5	0.80	0.35	106,106,107,107	0
2	SO4	С	369	5/5	0.80	0.34	114,114,114,114	0
3	GOL	В	368	6/6	0.80	0.33	87,88,88,89	0
6	FLC	С	389	13/13	0.80	0.33	95,97,98,99	0
2	SO4	А	363	5/5	0.80	0.18	138,138,138,139	0



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Mol	Type	Chain	$\operatorname{Res}$	Atoms	RSCC	RSR	$B$ -factors $(A^2)$	Q < 0.9
2	SO4	С	363	5/5	0.81	0.23	144,144,145,145	0
3	GOL	В	372	6/6	0.81	0.43	74,75,76,76	0
2	SO4	С	364	5/5	0.81	0.59	$143,\!143,\!144,\!144$	0
3	GOL	В	364	6/6	0.81	0.30	99,100,101,101	0
2	SO4	С	354	5/5	0.81	0.60	$152,\!152,\!152,\!153$	0
2	SO4	В	350	5/5	0.81	0.27	$159,\!159,\!159,\!159,\!159$	0
6	FLC	С	391	13/13	0.81	0.15	85,87,87,88	0
2	SO4	А	364	5/5	0.81	0.24	$145,\!145,\!145,\!145$	0
3	GOL	В	366	6/6	0.82	0.40	56,60,61,63	0
6	FLC	С	388	13/13	0.82	0.44	42,44,46,46	0
4	LDA	А	388	16/16	0.82	0.33	101,107,115,115	0
2	SO4	С	372	5/5	0.82	0.28	$134,\!134,\!134,\!135$	0
3	GOL	А	379	6/6	0.82	0.17	82,84,85,85	0
2	SO4	А	358	5/5	0.83	0.32	126,126,126,126	0
2	SO4	С	352	5/5	0.84	0.14	112,112,112,112	0
2	SO4	С	370	5/5	0.85	0.21	139,139,139,139	0
2	SO4	С	371	5/5	0.85	0.17	137,137,137,137	0
2	SO4	С	348	5/5	0.85	0.27	98,98,99,99	0
2	SO4	С	361	5/5	0.85	0.24	122,123,123,123	0
2	SO4	С	347	5/5	0.86	0.30	119,119,119,119	0
3	GOL	А	375	6/6	0.86	0.35	81,81,82,82	0
2	SO4	В	357	5/5	0.86	0.31	113,113,113,114	0
2	SO4	В	353	5/5	0.86	0.33	121,121,121,121	0
3	GOL	А	370	6/6	0.86	0.31	82,83,84,84	0
3	GOL	С	380	6/6	0.86	0.22	96,96,97,97	0
4	LDA	В	378	16/16	0.86	0.34	73,84,95,95	0
2	SO4	А	354	5/5	0.86	0.25	122,122,123,123	0
3	GOL	С	373	6/6	0.86	0.33	70,72,72,73	0
3	GOL	С	374	6/6	0.86	0.17	91,91,92,92	0
2	SO4	А	351	5/5	0.87	0.45	128,128,128,128	0
2	SO4	В	358	5/5	0.87	0.45	110,110,110,110	0
2	SO4	А	345	5/5	0.87	0.19	112,112,112,112	0
2	SO4	С	356	5/5	0.87	0.41	113,113,114,114	0
2	SO4	С	357	5/5	0.87	0.19	119,120,120,120	0
2	SO4	С	351	5/5	0.87	0.30	105,106,107,107	0
7	TLA	В	383	10/10	0.87	0.23	76,79,80,80	0
3	GOL	А	373	6/6	0.88	0.24	89,90,90,90	0
2	SO4	В	356	5/5	0.88	0.33	139,139,139,139	0
2	SO4	С	368	5/5	0.88	0.45	114,114,114,114	0
5	TAM	С	387	11/11	0.88	0.23	21,23,24,26	11
2	SO4	А	343	$\frac{1}{5/5}$	0.88	0.24	142,142,142,142	0
2	SO4	С	350	5/5	0.88	0.25	146,146,147,147	0

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Mol	Type	Chain	$\mathbf{Res}$	Atoms	RSCC	RSR	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9
2	SO4	А	362	5/5	0.88	0.24	$133,\!134,\!134,\!134$	0
2	SO4	В	346	5/5	0.88	0.19	144,144,144,144	0
2	SO4	С	362	5/5	0.88	0.36	148,149,149,149	0
2	SO4	В	347	5/5	0.88	0.22	98,99,99,100	0
2	SO4	С	346	5/5	0.88	0.44	124,125,125,125	0
2	SO4	С	345	5/5	0.89	0.18	113,113,113,114	0
2	SO4	А	367	5/5	0.89	0.25	114,114,115,115	0
2	SO4	А	347	5/5	0.89	0.31	103,104,104,104	0
4	LDA	В	380	16/16	0.89	0.22	80,84,86,86	0
3	GOL	В	370	6/6	0.89	0.31	85,85,86,86	0
3	GOL	А	374	6/6	0.89	0.40	81,83,83,84	0
2	SO4	В	354	5/5	0.89	0.27	$153,\!153,\!153,\!153$	0
2	SO4	В	363	5/5	0.89	0.28	123,123,123,123	0
2	SO4	С	343	5/5	0.89	0.33	126,126,127,127	0
4	LDA	С	383	16/16	0.90	0.24	$35,\!48,\!68,\!69$	0
2	SO4	В	349	5/5	0.90	0.31	104,105,105,105	0
2	SO4	А	356	5/5	0.90	0.28	104,104,104,104	0
2	SO4	А	348	5/5	0.90	0.16	141,141,141,141	0
2	SO4	А	342	5/5	0.90	0.29	132,132,132,132	0
2	SO4	А	360	5/5	0.90	0.22	120,120,121,121	0
4	LDA	С	382	16/16	0.90	0.34	43,56,67,67	0
4	LDA	В	376	16/16	0.91	0.37	72,76,81,81	0
3	GOL	В	365	6/6	0.91	0.17	78,78,79,80	0
2	SO4	А	344	5/5	0.91	0.26	105,105,106,106	0
2	SO4	С	349	5/5	0.92	0.29	96,97,97,97	0
2	SO4	В	360	5/5	0.92	0.15	113,113,113,113	0
3	GOL	А	380	6/6	0.92	0.19	76,77,77,77	0
2	SO4	А	346	5/5	0.92	0.15	105,105,105,106	0
4	LDA	А	384	16/16	0.92	0.42	51,59,71,71	0
2	SO4	А	349	5/5	0.92	0.19	113,113,113,114	0
2	SO4	В	348	5/5	0.93	0.21	107,107,107,108	0
2	SO4	А	352	5/5	0.93	0.44	113,113,113,114	0
2	SO4	А	355	5/5	0.93	0.17	133,133,133,133	0
2	SO4	С	358	5/5	0.93	0.13	120,120,120,120	0
2	SO4	А	353	5/5	0.93	0.32	129,130,130,130	0
4	LDA	А	386	16/16	0.93	0.28	46,49,61,62	0
2	SO4	В	342	5/5	0.94	0.36	101,101,101,101	0
3	GOL	С	381	6/6	0.94	0.31	77,78,78,79	0
2	SO4	А	361	5/5	0.94	0.30	126,127,127,127	0
2	SO4	С	355	5/5	0.94	0.19	109,110,110,110	0
2	SO4	С	342	5/5	0.94	0.23	83,83,84,86	0
2	SO4	А	357	5/5	0.94	0.25	106,106,107,107	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	LDA	В	375	16/16	0.94	0.31	57,60,62,62	0
2	SO4	С	365	5/5	0.96	0.35	100,100,101,101	0
4	LDA	С	384	16/16	0.96	0.18	41,45,58,58	0
2	SO4	В	352	5/5	0.96	0.18	102,102,102,102	0
2	SO4	С	367	5/5	0.96	0.39	99,100,100,100	0
2	SO4	В	359	5/5	0.96	0.29	108,108,108,108	0
2	SO4	С	344	5/5	0.97	0.10	82,82,83,84	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

