



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:45 AM GMT

PDB ID : 2Y6Q  
Title : STRUCTURE OF THE TETX MONOOXYGENASE IN COMPLEX WITH  
THE SUBSTRATE 7-IODOTETRACYCLINE  
Authors : Volkers, G.; Palm, G.J.; Weiss, M.S.; Wright, G.D.; Hinrichs, W.  
Deposited on : 2011-01-25  
Resolution : 2.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

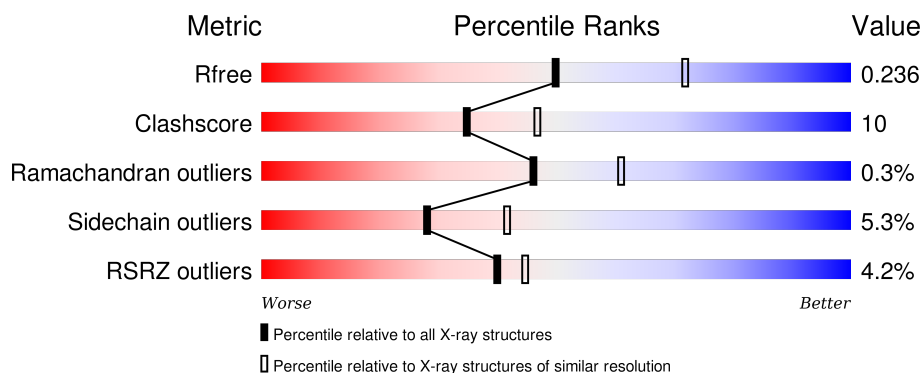
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	398	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>•• 8%</div> </div> </div>
1	B	398	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>• 8%</div> </div> </div>
1	C	398	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>• 8%</div> </div> </div>
1	D	398	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>•• 8%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11961 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TETX2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	2	0
			2865	1817	483	553	12			
1	B	368	Total	C	N	O	S	0	2	0
			2863	1816	482	553	12			
1	C	367	Total	C	N	O	S	0	0	0
			2828	1793	476	547	12			
1	D	365	Total	C	N	O	S	0	0	0
			2812	1782	473	545	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	EXPRESSION TAG	UNP Q93L51
A	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
A	-7	SER	-	EXPRESSION TAG	UNP Q93L51
A	-6	SER	-	EXPRESSION TAG	UNP Q93L51
A	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
A	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
A	0	HIS	-	EXPRESSION TAG	UNP Q93L51
A	1	SER	-	EXPRESSION TAG	UNP Q93L51
A	2	SER	-	EXPRESSION TAG	UNP Q93L51
A	3	GLY	-	EXPRESSION TAG	UNP Q93L51
A	4	LEU	-	EXPRESSION TAG	UNP Q93L51
A	5	VAL	-	EXPRESSION TAG	UNP Q93L51
A	6	PRO	-	EXPRESSION TAG	UNP Q93L51
A	7	ARG	-	EXPRESSION TAG	UNP Q93L51
A	8	GLY	-	EXPRESSION TAG	UNP Q93L51
A	9	SER	-	EXPRESSION TAG	UNP Q93L51
A	10	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-9	MET	-	EXPRESSION TAG	UNP Q93L51

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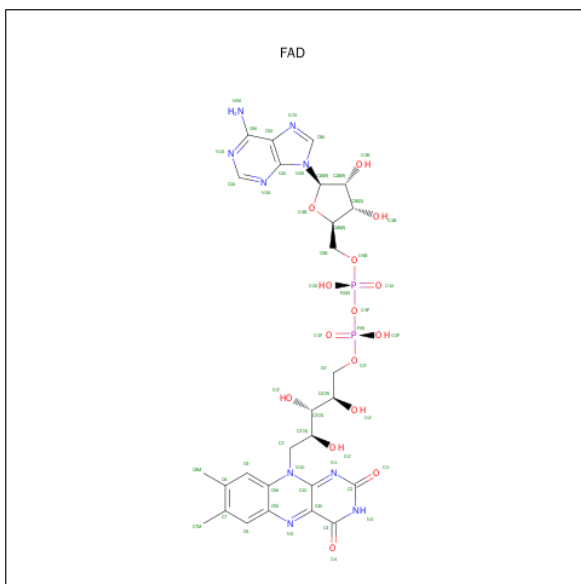
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
B	-7	SER	-	EXPRESSION TAG	UNP Q93L51
B	-6	SER	-	EXPRESSION TAG	UNP Q93L51
B	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
B	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
B	0	HIS	-	EXPRESSION TAG	UNP Q93L51
B	1	SER	-	EXPRESSION TAG	UNP Q93L51
B	2	SER	-	EXPRESSION TAG	UNP Q93L51
B	3	GLY	-	EXPRESSION TAG	UNP Q93L51
B	4	LEU	-	EXPRESSION TAG	UNP Q93L51
B	5	VAL	-	EXPRESSION TAG	UNP Q93L51
B	6	PRO	-	EXPRESSION TAG	UNP Q93L51
B	7	ARG	-	EXPRESSION TAG	UNP Q93L51
B	8	GLY	-	EXPRESSION TAG	UNP Q93L51
B	9	SER	-	EXPRESSION TAG	UNP Q93L51
B	10	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-9	MET	-	EXPRESSION TAG	UNP Q93L51
C	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
C	-7	SER	-	EXPRESSION TAG	UNP Q93L51
C	-6	SER	-	EXPRESSION TAG	UNP Q93L51
C	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
C	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
C	0	HIS	-	EXPRESSION TAG	UNP Q93L51
C	1	SER	-	EXPRESSION TAG	UNP Q93L51
C	2	SER	-	EXPRESSION TAG	UNP Q93L51
C	3	GLY	-	EXPRESSION TAG	UNP Q93L51
C	4	LEU	-	EXPRESSION TAG	UNP Q93L51
C	5	VAL	-	EXPRESSION TAG	UNP Q93L51
C	6	PRO	-	EXPRESSION TAG	UNP Q93L51
C	7	ARG	-	EXPRESSION TAG	UNP Q93L51
C	8	GLY	-	EXPRESSION TAG	UNP Q93L51
C	9	SER	-	EXPRESSION TAG	UNP Q93L51
C	10	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-9	MET	-	EXPRESSION TAG	UNP Q93L51
D	-8	GLY	-	EXPRESSION TAG	UNP Q93L51
D	-7	SER	-	EXPRESSION TAG	UNP Q93L51

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	SER	-	EXPRESSION TAG	UNP Q93L51
D	-5	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-4	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-3	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-2	HIS	-	EXPRESSION TAG	UNP Q93L51
D	-1	HIS	-	EXPRESSION TAG	UNP Q93L51
D	0	HIS	-	EXPRESSION TAG	UNP Q93L51
D	1	SER	-	EXPRESSION TAG	UNP Q93L51
D	2	SER	-	EXPRESSION TAG	UNP Q93L51
D	3	GLY	-	EXPRESSION TAG	UNP Q93L51
D	4	LEU	-	EXPRESSION TAG	UNP Q93L51
D	5	VAL	-	EXPRESSION TAG	UNP Q93L51
D	6	PRO	-	EXPRESSION TAG	UNP Q93L51
D	7	ARG	-	EXPRESSION TAG	UNP Q93L51
D	8	GLY	-	EXPRESSION TAG	UNP Q93L51
D	9	SER	-	EXPRESSION TAG	UNP Q93L51
D	10	HIS	-	EXPRESSION TAG	UNP Q93L51

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



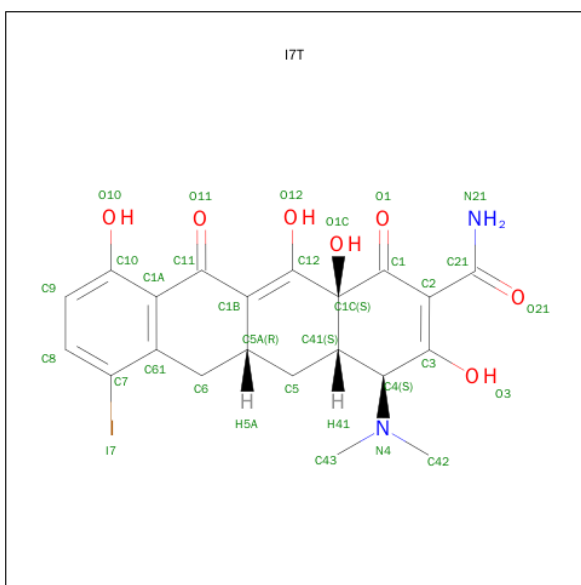
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 3 is 7-iodotetracycline (three-letter code: I7T) (formula:  $C_{21}H_{21}IN_2O_7$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 21	I 1	N 2	O 7	0	0
3	B	1	Total 31	C 21	I 1	N 2	O 7	0	0
3	C	1	Total 31	C 21	I 1	N 2	O 7	0	0
3	D	1	Total 31	C 21	I 1	N 2	O 7	0	0

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



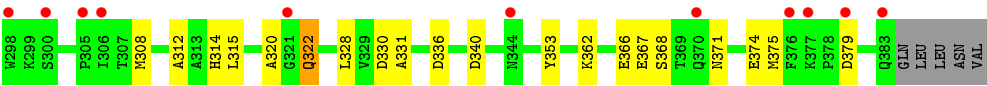
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

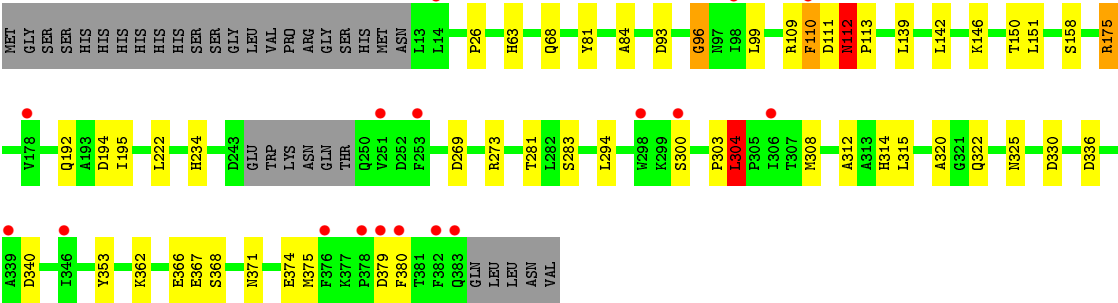
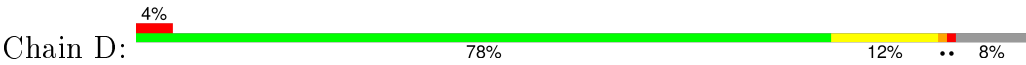
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total 61	O 61	0	0
5	B	55	Total 55	O 55	0	0
5	C	47	Total 47	O 47	0	0
5	D	34	Total 34	O 34	0	0







● Molecule 1: TETX2 PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.70 Å 79.96 Å 88.00 Å 111.10° 90.41° 92.96°	Depositor
Resolution (Å)	51.98 – 2.37 51.92 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.5 (51.98-2.37) 68.7 (51.92-2.37)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 2.37 Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, $R_{free}$	0.218 , 0.238 0.218 , 0.236	Depositor DCC
$R_{free}$ test set	2623 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52900 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I7T, SO4, FAD

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	1.06	4/2929 (0.1%)	0.92	3/3973 (0.1%)
1	B	1.02	3/2927 (0.1%)	0.89	5/3971 (0.1%)
1	C	0.87	3/2886 (0.1%)	0.85	5/3919 (0.1%)
1	D	0.85	1/2868 (0.0%)	0.84	3/3893 (0.1%)
All	All	0.96	11/11610 (0.1%)	0.88	16/15756 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	2
1	D	0	2
All	All	0	9

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	GLY	N-CA	5.69	1.54	1.46
1	B	322[A]	GLN	C-O	5.68	1.34	1.23
1	B	322[B]	GLN	C-O	5.68	1.34	1.23
1	A	363	GLU	CG-CD	5.61	1.60	1.51
1	D	96	GLY	N-CA	5.60	1.54	1.46
1	A	347	GLU	CG-CD	5.58	1.60	1.51
1	B	320	ALA	CA-CB	5.53	1.64	1.52
1	C	295	GLU	CB-CG	5.22	1.62	1.52
1	C	209	CYS	CB-SG	5.21	1.91	1.82
1	C	96	GLY	N-CA	5.11	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	ASN	CB-CG	5.06	1.62	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	D	304	LEU	CB-CG-CD1	7.27	123.36	111.00
1	D	175	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	175	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	B	121	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	C	175	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	D	175	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	104	VAL	CG1-CB-CG2	6.33	121.04	110.90
1	C	194	ASP	CB-CG-OD1	6.17	123.85	118.30
1	B	215	MET	CG-SD-CE	-6.11	90.42	100.20
1	C	175	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	99	LEU	CB-CG-CD2	5.66	120.63	111.00
1	B	175	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	175	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	121	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	C	215	MET	CG-SD-CE	-5.26	91.78	100.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ASN	Peptide
1	A	94	GLU	Peptide
1	B	109	ARG	Peptide
1	B	112	ASN	Peptide
1	B	94	GLU	Peptide
1	C	109	ARG	Peptide
1	C	112	ASN	Peptide
1	D	109	ARG	Peptide
1	D	112	ASN	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2865	0	2752	90	0
1	B	2863	0	2745	60	0
1	C	2828	0	2688	48	0
1	D	2812	0	2685	36	0
2	A	53	0	31	5	0
2	B	53	0	30	2	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	31	0	18	4	0
3	B	31	0	18	4	0
3	C	31	0	18	2	0
3	D	31	0	18	1	0
4	A	15	0	0	1	0
4	B	15	0	0	0	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
5	A	61	0	0	15	0
5	B	55	0	0	6	0
5	C	47	0	0	6	0
5	D	34	0	0	1	0
All	All	11961	0	11065	227	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 10.

All (227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ILE:CG1	1:A:309:ILE:CD1	1.75	1.57
1:A:98:ILE:CG2	1:B:359:ILE:HG23	1.62	1.29
1:A:383:GLN:CB	1:B:359:ILE:HD12	1.67	1.24
1:A:383:GLN:CB	1:B:359:ILE:CD1	2.16	1.22
1:B:96:GLY:HA2	5:B:2014:HOH:O	1.38	1.21
1:A:96:GLY:HA2	5:A:2008:HOH:O	1.45	1.16
1:C:96:GLY:HA2	5:C:2008:HOH:O	1.52	1.10
1:A:322[A]:GLN:HA	5:A:2049:HOH:O	1.49	1.10
1:A:98:ILE:HG21	1:B:359:ILE:CG2	1.85	1.06
1:A:375:MET:SD	3:A:1385:I7T:I7	2.83	1.06
1:A:104:VAL:HG22	1:A:106:PRO:HD2	1.36	1.06
1:A:175:ARG:HD3	1:A:308:MET:HE1	1.28	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ILE:HG21	1:B:359:ILE:HG23	1.04	1.04
1:C:175:ARG:HD3	1:C:308:MET:HE1	1.35	1.02
1:A:322[B]:GLN:OE1	1:A:323:GLY:N	1.92	1.01
1:D:175:ARG:HD3	1:D:308:MET:HE1	1.40	0.99
1:A:379:ASP:HB2	1:B:65:GLY:HA3	1.46	0.96
1:B:175:ARG:HD3	1:B:308:MET:HE1	1.48	0.95
1:C:255:ASN:HD21	1:C:257:ASN:HB2	1.31	0.95
1:A:383:GLN:CB	1:B:359:ILE:HD13	1.97	0.90
1:A:107:GLU:CB	5:A:2013:HOH:O	2.22	0.87
1:A:107:GLU:HB3	5:A:2013:HOH:O	1.76	0.84
1:A:98:ILE:HG22	1:B:359:ILE:HG23	1.61	0.82
1:D:325:ASN:HB2	5:D:2030:HOH:O	1.79	0.81
1:C:96:GLY:HA3	5:C:2009:HOH:O	1.80	0.79
1:A:104:VAL:HG22	1:A:106:PRO:CD	2.11	0.79
1:A:99:LEU:HD13	1:B:359:ILE:HD11	1.66	0.78
1:A:137:ARG:NH1	4:A:1386:SO4:O2	2.14	0.78
1:A:98:ILE:CG2	1:B:359:ILE:CG2	2.50	0.78
1:A:175:ARG:HD3	1:A:308:MET:CE	2.12	0.77
1:A:151:LEU:HD12	1:A:151:LEU:N	2.01	0.76
1:A:322[B]:GLN:HA	5:A:2049:HOH:O	1.86	0.75
1:C:215:MET:HE1	5:C:2033:HOH:O	1.86	0.74
1:C:269:ASP:HB2	5:C:2036:HOH:O	1.87	0.74
1:A:95:LYS:O	5:A:2008:HOH:O	2.08	0.72
1:A:104:VAL:HG13	1:A:107:GLU:OE1	1.90	0.71
1:C:99:LEU:HD13	1:C:100:SER:N	2.06	0.71
1:C:93:ASP:OD1	1:C:96:GLY:N	2.23	0.70
1:B:146:LYS:HD2	5:B:2025:HOH:O	1.91	0.70
2:A:1384:FAD:H6	3:A:1385:I7T:H433	1.71	0.70
1:D:93:ASP:OD1	1:D:96:GLY:N	2.24	0.70
1:D:151:LEU:HD12	1:D:151:LEU:N	2.07	0.70
1:C:255:ASN:ND2	1:C:257:ASN:HB2	2.06	0.69
2:B:1384:FAD:H6	3:B:1385:I7T:H433	1.76	0.68
1:C:308:MET:CE	1:C:312:ALA:HB1	2.26	0.66
1:A:99:LEU:HB2	1:B:359:ILE:HG12	1.78	0.66
1:C:192:GLN:HE21	1:C:234:HIS:CE1	2.14	0.65
1:A:321:GLY:O	5:A:2049:HOH:O	2.15	0.65
1:B:175:ARG:HD3	1:B:308:MET:CE	2.25	0.65
1:B:151:LEU:HD12	1:B:151:LEU:N	2.11	0.65
1:A:98:ILE:HG23	1:B:359:ILE:HA	1.80	0.63
1:C:112:ASN:H	1:C:113:PRO:HD3	1.64	0.63
1:A:96:GLY:CA	5:A:2008:HOH:O	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322[B]:GLN:HG3	1:A:364:ALA:HB1	1.82	0.62
1:D:194:ASP:OD1	1:D:234:HIS:HD2	1.82	0.62
3:C:1385:I7T:O3	3:C:1385:I7T:H422	1.99	0.62
2:A:1384:FAD:H6	3:A:1385:I7T:C43	2.29	0.62
1:A:377:LYS:CB	5:A:2055:HOH:O	2.48	0.62
1:D:112:ASN:H	1:D:113:PRO:HD3	1.66	0.61
1:D:192:GLN:HE21	1:D:234:HIS:CE1	2.19	0.61
1:A:379:ASP:CB	1:B:65:GLY:HA3	2.25	0.61
1:D:308:MET:CE	1:D:312:ALA:HB1	2.31	0.61
1:C:192:GLN:HE21	1:C:234:HIS:HE1	1.49	0.60
1:B:308:MET:CE	1:B:312:ALA:HB1	2.31	0.60
1:D:139:LEU:HD21	1:D:142:LEU:HD13	1.83	0.60
1:D:175:ARG:CD	1:D:308:MET:HE1	2.26	0.60
1:A:112:ASN:H	1:A:113:PRO:HD3	1.67	0.60
1:A:175:ARG:CD	1:A:308:MET:HE1	2.18	0.59
1:B:375:MET:SD	3:B:1385:I7T:I7	3.31	0.59
1:C:222:LEU:CD2	1:C:375:MET:HE2	2.32	0.59
1:B:112:ASN:H	1:B:113:PRO:HD3	1.68	0.59
1:B:192:GLN:HE21	1:B:234:HIS:CE1	2.21	0.58
1:A:84:ALA:HB1	1:A:113:PRO:HB2	1.86	0.58
1:A:98:ILE:CG2	1:B:359:ILE:HA	2.33	0.58
1:A:98:ILE:HD11	1:B:363:GLU:HG3	1.86	0.57
1:D:222:LEU:CD2	1:D:375:MET:HE3	2.34	0.57
1:B:322[B]:GLN:HG3	1:B:364:ALA:HB1	1.86	0.57
1:A:93:ASP:OD1	1:A:96:GLY:N	2.38	0.56
1:A:104:VAL:CG1	1:A:107:GLU:OE1	2.52	0.56
1:C:68:GLN:NE2	1:C:81:TYR:OH	2.38	0.56
1:A:192:GLN:HE21	1:A:234:HIS:CE1	2.24	0.56
1:C:151:LEU:N	1:C:151:LEU:HD12	2.20	0.56
1:A:192:GLN:HE21	1:A:234:HIS:HE1	1.54	0.56
1:D:68:GLN:NE2	1:D:81:TYR:OH	2.39	0.56
1:A:314:HIS:NE2	1:A:330:ASP:OD2	2.37	0.55
1:B:146:LYS:CE	5:B:2025:HOH:O	2.55	0.55
1:A:229:ASN:ND2	5:A:2039:HOH:O	2.40	0.55
1:C:175:ARG:HD3	1:C:308:MET:CE	2.25	0.55
1:D:294:LEU:HD11	1:D:314:HIS:HB3	1.88	0.55
1:A:95:LYS:CB	5:A:2009:HOH:O	2.54	0.54
1:A:176:LYS:O	1:A:299:LYS:NZ	2.37	0.54
1:D:84:ALA:HB1	1:D:113:PRO:HB2	1.88	0.54
1:D:314:HIS:O	1:D:315:LEU:C	2.46	0.54
1:B:13:LEU:N	1:B:15:SER:HG	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:LEU:HD11	1:C:314:HIS:HB3	1.89	0.54
1:B:95:LYS:CB	5:B:2015:HOH:O	2.55	0.54
1:A:101:THR:O	1:A:101:THR:HG22	2.08	0.54
1:A:309:ILE:CB	1:A:309:ILE:CD1	2.77	0.53
1:B:314:HIS:NE2	1:B:330:ASP:OD2	2.38	0.53
1:C:328:LEU:O	1:C:331:ALA:HB3	2.08	0.53
1:C:112:ASN:H	1:C:113:PRO:CD	2.22	0.53
1:A:383:GLN:CB	1:B:359:ILE:HB	2.39	0.53
1:B:112:ASN:H	1:B:113:PRO:CD	2.22	0.53
1:A:320:ALA:C	1:A:322[B]:GLN:H	2.13	0.52
1:C:84:ALA:HB1	1:C:113:PRO:HB2	1.90	0.52
1:A:194:ASP:OD1	1:A:234:HIS:HD2	1.93	0.52
1:D:112:ASN:H	1:D:113:PRO:CD	2.23	0.52
1:D:192:GLN:HE21	1:D:234:HIS:HE1	1.55	0.52
1:D:308:MET:HE2	1:D:312:ALA:HB1	1.92	0.52
1:A:112:ASN:H	1:A:113:PRO:CD	2.22	0.52
1:B:101:THR:HG22	1:B:101:THR:O	2.10	0.52
1:B:93:ASP:OD1	1:B:96:GLY:N	2.43	0.51
1:B:192:GLN:HE21	1:B:234:HIS:HE1	1.56	0.51
2:C:1384:FAD:N1	2:C:1384:FAD:H2'	2.25	0.51
1:A:175:ARG:HG2	1:A:308:MET:HE3	1.91	0.51
1:A:22:ILE:HD13	1:A:22:ILE:N	2.25	0.51
1:B:195:ILE:HD11	1:B:281:THR:OG1	2.11	0.51
1:A:175:ARG:HG2	1:A:308:MET:CE	2.41	0.51
1:A:308:MET:CE	1:A:312:ALA:HB1	2.41	0.51
1:A:195:ILE:HD11	1:A:281:THR:OG1	2.10	0.51
1:C:194:ASP:OD1	1:C:234:HIS:HD2	1.95	0.50
3:D:1385:I7T:O3	3:D:1385:I7T:H422	2.12	0.50
2:A:1384:FAD:HM82	5:A:2016:HOH:O	2.11	0.49
1:C:175:ARG:CD	1:C:308:MET:HE1	2.25	0.49
1:A:322[B]:GLN:CA	5:A:2049:HOH:O	2.54	0.49
1:D:222:LEU:HD22	1:D:375:MET:HE3	1.93	0.49
1:A:320:ALA:C	1:A:322[A]:GLN:H	2.16	0.49
1:B:375:MET:HG2	1:B:380:PHE:CE2	2.47	0.49
1:D:314:HIS:NE2	1:D:330:ASP:OD2	2.37	0.49
1:A:96:GLY:HA3	5:A:2010:HOH:O	2.12	0.49
1:D:151:LEU:CD1	1:D:151:LEU:N	2.75	0.49
1:C:362:LYS:O	1:C:366:GLU:HG2	2.12	0.49
1:A:98:ILE:HG22	1:B:359:ILE:HG12	1.95	0.48
1:C:255:ASN:HD22	1:C:258:SER:H	1.60	0.48
1:C:108:ASN:ND2	5:C:2011:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:GLU:O	1:A:376:PHE:HD2	1.96	0.48
1:D:362:LYS:O	1:D:366:GLU:HG2	2.13	0.48
1:A:151:LEU:N	1:A:151:LEU:CD1	2.74	0.48
1:B:84:ALA:HB1	1:B:113:PRO:HB2	1.96	0.48
1:C:314:HIS:NE2	1:C:330:ASP:OD2	2.44	0.48
1:C:308:MET:HE3	1:C:312:ALA:HB1	1.96	0.48
1:D:320:ALA:C	1:D:322:GLN:H	2.18	0.47
1:A:308:MET:HE2	1:A:312:ALA:HB1	1.96	0.47
1:A:99:LEU:HB2	1:B:359:ILE:CG1	2.44	0.47
1:B:308:MET:HE2	1:B:312:ALA:HB1	1.95	0.47
1:A:13:LEU:N	1:A:15:SER:HG	2.13	0.46
1:B:146:LYS:CD	5:B:2025:HOH:O	2.56	0.46
1:C:314:HIS:O	1:C:315:LEU:C	2.53	0.46
1:A:98:ILE:CG2	1:B:359:ILE:CA	2.93	0.46
1:A:139:LEU:HD21	1:A:142:LEU:HD13	1.98	0.46
1:C:375:MET:HB3	1:C:375:MET:HE2	1.78	0.46
1:D:320:ALA:HB2	1:D:368:SER:HA	1.98	0.46
1:B:308:MET:HB3	1:B:308:MET:HE2	1.65	0.46
1:B:110:PHE:O	1:B:110:PHE:CD1	2.69	0.46
1:C:110:PHE:HB2	5:C:2012:HOH:O	2.15	0.46
1:C:226:ASN:OD1	1:C:226:ASN:C	2.55	0.46
3:B:1385:I7T:H432	3:B:1385:I7T:H41	1.63	0.45
1:A:110:PHE:O	1:A:110:PHE:CD1	2.69	0.45
1:C:222:LEU:HD22	1:C:375:MET:HE2	1.98	0.45
1:A:21:ILE:C	1:A:22:ILE:HD13	2.37	0.45
1:B:68:GLN:NE2	1:B:81:TYR:OH	2.50	0.45
1:B:263:LEU:HB3	1:B:278:ILE:HD13	1.98	0.45
1:A:150:THR:C	1:A:151:LEU:HD12	2.37	0.45
1:A:222:LEU:HD22	1:A:375:MET:HE2	1.99	0.45
2:B:1384:FAD:H6	3:B:1385:I7T:C43	2.46	0.45
1:D:84:ALA:CB	1:D:113:PRO:HB2	2.47	0.45
1:C:320:ALA:C	1:C:322:GLN:H	2.20	0.45
1:C:149:TRP:O	1:C:160:THR:HA	2.17	0.45
1:D:195:ILE:HD11	1:D:281:THR:OG1	2.17	0.45
1:A:84:ALA:CB	1:A:113:PRO:HB2	2.47	0.45
1:A:78:GLN:HG2	1:C:64:LYS:HB3	1.98	0.45
1:D:375:MET:HG2	1:D:380:PHE:CE2	2.52	0.45
1:C:263:LEU:HB3	1:C:278:ILE:HD13	1.98	0.44
1:D:110:PHE:O	1:D:112:ASN:N	2.49	0.44
1:D:194:ASP:OD1	1:D:234:HIS:CD2	2.66	0.44
1:B:194:ASP:OD1	1:B:234:HIS:HD2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:TRP:O	1:B:160:THR:HA	2.18	0.44
1:B:362:LYS:O	1:B:366:GLU:HG2	2.17	0.44
1:B:151:LEU:CD1	1:B:151:LEU:N	2.78	0.44
1:B:245:TRP:HA	1:B:250:GLN:HE21	1.82	0.44
1:A:287:LEU:HD21	2:A:1384:FAD:HM83	1.98	0.44
2:D:1384:FAD:H2'	2:D:1384:FAD:N1	2.33	0.44
1:C:320:ALA:HB2	1:C:368:SER:HA	2.00	0.44
1:B:139:LEU:HD21	1:B:142:LEU:HD13	2.00	0.44
1:A:375:MET:HG2	1:A:380:PHE:CE2	2.53	0.43
1:D:375:MET:HB3	1:D:375:MET:HE3	1.80	0.43
1:A:308:MET:HE2	1:A:308:MET:HB3	1.76	0.43
1:B:146:LYS:HE2	5:B:2025:HOH:O	2.18	0.43
1:A:351:LYS:HZ2	1:A:355:GLN:HE21	1.65	0.43
1:A:306:ILE:HG23	1:A:306:ILE:O	2.17	0.43
1:A:294:LEU:HD11	1:A:314:HIS:HB3	1.99	0.43
1:B:320:ALA:HB2	1:B:368:SER:HA	2.00	0.43
1:C:222:LEU:CD2	1:C:375:MET:CE	2.97	0.43
1:A:308:MET:HE1	1:A:312:ALA:O	2.19	0.43
1:C:139:LEU:HD21	1:C:142:LEU:HD13	2.00	0.43
1:C:195:ILE:HD11	1:C:281:THR:OG1	2.19	0.43
1:A:320:ALA:HB2	1:A:368:SER:HA	2.01	0.43
1:A:149:TRP:O	1:A:160:THR:HA	2.19	0.43
1:A:375:MET:HB3	1:A:375:MET:HE2	1.72	0.42
1:C:84:ALA:CB	1:C:113:PRO:HB2	2.49	0.42
1:D:308:MET:HB3	1:D:308:MET:HE2	1.85	0.42
1:C:139:LEU:HD23	1:C:174:VAL:HG11	2.00	0.42
1:A:351:LYS:NZ	1:A:355:GLN:HE21	2.16	0.42
1:B:84:ALA:CB	1:B:113:PRO:HB2	2.49	0.42
1:C:110:PHE:O	1:C:112:ASN:N	2.52	0.42
1:A:239:PHE:HA	1:A:376:PHE:HE1	1.84	0.42
2:A:1384:FAD:C6	3:A:1385:I7T:C43	2.95	0.41
1:C:221:ASN:HD22	1:C:239:PHE:HB3	1.86	0.41
1:D:303:PRO:O	1:D:304:LEU:HD13	2.20	0.41
1:D:110:PHE:O	1:D:111:ASP:C	2.58	0.41
1:A:249:THR:CB	1:A:250:GLN:HE21	2.33	0.41
1:B:175:ARG:HG2	1:B:308:MET:CE	2.51	0.41
1:C:110:PHE:O	1:C:111:ASP:C	2.58	0.41
1:D:110:PHE:O	1:D:112:ASN:HB2	2.21	0.41
1:B:308:MET:HE1	1:B:312:ALA:O	2.21	0.41
1:B:146:LYS:HE2	1:B:146:LYS:H	1.85	0.41
3:C:1385:I7T:C42	3:C:1385:I7T:O3	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PHE:O	1:B:111:ASP:C	2.59	0.41
1:A:175:ARG:CD	1:A:308:MET:CE	2.90	0.40
1:D:150:THR:C	1:D:151:LEU:HD12	2.41	0.40
1:A:139:LEU:HD23	1:A:174:VAL:HG11	2.03	0.40
1:C:263:LEU:HA	1:C:263:LEU:HD23	1.94	0.40
1:C:308:MET:HE2	1:C:312:ALA:HB1	1.99	0.40
1:D:63:HIS:HA	1:D:111:ASP:HA	2.03	0.40
1:B:328:LEU:O	1:B:331:ALA:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/398 (92%)	345 (94%)	19 (5%)	2 (0%)	34	46
1	B	366/398 (92%)	347 (95%)	18 (5%)	1 (0%)	46	61
1	C	363/398 (91%)	343 (94%)	19 (5%)	1 (0%)	46	61
1	D	361/398 (91%)	344 (95%)	16 (4%)	1 (0%)	46	61
All	All	1456/1592 (92%)	1379 (95%)	72 (5%)	5 (0%)	46	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
1	B	112	ASN
1	C	112	ASN
1	D	112	ASN
1	A	321	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	304/345 (88%)	288 (95%)	16 (5%)	28	42
1	B	303/345 (88%)	288 (95%)	15 (5%)	30	45
1	C	296/345 (86%)	281 (95%)	15 (5%)	29	44
1	D	296/345 (86%)	279 (94%)	17 (6%)	25	37
All	All	1199/1380 (87%)	1136 (95%)	63 (5%)	28	42

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	99	LEU
1	A	104	VAL
1	A	110	PHE
1	A	146	LYS
1	A	158	SER
1	A	269	ASP
1	A	273	ARG
1	A	283	SER
1	A	336	ASP
1	A	340	ASP
1	A	353	TYR
1	A	367	GLU
1	A	371	ASN
1	A	374	GLU
1	A	379	ASP
1	B	13	LEU
1	B	99	LEU
1	B	110	PHE
1	B	146	LYS
1	B	158	SER
1	B	183	VAL
1	B	269	ASP
1	B	273	ARG

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Mol	Chain	Res	Type
1	B	283	SER
1	B	336	ASP
1	B	353	TYR
1	B	367	GLU
1	B	371	ASN
1	B	374	GLU
1	B	379	ASP
1	C	110	PHE
1	C	146	LYS
1	C	158	SER
1	C	255	ASN
1	C	269	ASP
1	C	273	ARG
1	C	283	SER
1	C	322	GLN
1	C	336	ASP
1	C	340	ASP
1	C	353	TYR
1	C	367	GLU
1	C	371	ASN
1	C	374	GLU
1	C	379	ASP
1	D	26	PRO
1	D	99	LEU
1	D	110	PHE
1	D	146	LYS
1	D	158	SER
1	D	269	ASP
1	D	273	ARG
1	D	283	SER
1	D	300	SER
1	D	304	LEU
1	D	336	ASP
1	D	340	ASP
1	D	353	TYR
1	D	367	GLU
1	D	371	ASN
1	D	374	GLU
1	D	379	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	190	ASN
1	A	201	ASN
1	A	221	ASN
1	A	234	HIS
1	A	250	GLN
1	A	355	GLN
1	A	370	GLN
1	B	38	ASN
1	B	68	GLN
1	B	190	ASN
1	B	201	ASN
1	B	221	ASN
1	B	234	HIS
1	B	250	GLN
1	B	370	GLN
1	B	371	ASN
1	C	68	GLN
1	C	190	ASN
1	C	201	ASN
1	C	221	ASN
1	C	234	HIS
1	C	255	ASN
1	C	370	GLN
1	C	371	ASN
1	D	68	GLN
1	D	190	ASN
1	D	201	ASN
1	D	207	GLN
1	D	221	ASN
1	D	234	HIS
1	D	370	GLN
1	D	371	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

20 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	FAD	A	1384	-	48,58,58	1.39	5 (10%)	54,89,89	2.55	14 (25%)
3	I7T	A	1385	-	33,34,34	1.67	2 (6%)	38,55,55	2.03	12 (31%)
4	SO4	A	1386	-	4,4,4	0.43	0	6,6,6	0.53	0
4	SO4	A	1387	-	4,4,4	0.16	0	6,6,6	0.47	0
4	SO4	A	1388	-	4,4,4	0.19	0	6,6,6	0.27	0
2	FAD	B	1384	-	48,58,58	1.59	12 (25%)	54,89,89	2.45	12 (22%)
3	I7T	B	1385	-	33,34,34	1.68	3 (9%)	38,55,55	1.55	7 (18%)
4	SO4	B	1386	-	4,4,4	0.16	0	6,6,6	0.41	0
4	SO4	B	1387	-	4,4,4	0.13	0	6,6,6	0.23	0
4	SO4	B	1388	-	4,4,4	0.06	0	6,6,6	0.29	0
2	FAD	C	1384	-	48,58,58	1.47	7 (14%)	54,89,89	2.43	16 (29%)
3	I7T	C	1385	-	33,34,34	1.61	4 (12%)	38,55,55	1.90	11 (28%)
4	SO4	C	1386	-	4,4,4	0.21	0	6,6,6	0.27	0
4	SO4	C	1387	-	4,4,4	0.20	0	6,6,6	0.38	0
4	SO4	C	1388	-	4,4,4	0.15	0	6,6,6	0.40	0
2	FAD	D	1384	-	48,58,58	1.58	10 (20%)	54,89,89	2.56	14 (25%)
3	I7T	D	1385	-	33,34,34	1.51	3 (9%)	38,55,55	1.93	12 (31%)
4	SO4	D	1386	-	4,4,4	0.29	0	6,6,6	0.26	0
4	SO4	D	1387	-	4,4,4	0.10	0	6,6,6	0.33	0
4	SO4	D	1388	-	4,4,4	0.17	0	6,6,6	0.50	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	FAD	A	1384	-	-	0/30/50/50	0/6/6/6
3	I7T	A	1385	-	-	0/8/66/66	0/4/4/4
4	SO4	A	1386	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1387	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1388	-	-	0/0/0/0	0/0/0/0
2	FAD	B	1384	-	-	0/30/50/50	0/6/6/6
3	I7T	B	1385	-	-	0/8/66/66	0/4/4/4
4	SO4	B	1386	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1387	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1388	-	-	0/0/0/0	0/0/0/0
2	FAD	C	1384	-	-	0/30/50/50	0/6/6/6
3	I7T	C	1385	-	-	0/8/66/66	0/4/4/4
4	SO4	C	1386	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1387	-	-	0/0/0/0	0/0/0/0
4	SO4	C	1388	-	-	0/0/0/0	0/0/0/0
2	FAD	D	1384	-	-	0/30/50/50	0/6/6/6
3	I7T	D	1385	-	-	0/8/66/66	0/4/4/4
4	SO4	D	1386	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1387	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1388	-	-	0/0/0/0	0/0/0/0

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1385	I7T	C7-I7	-7.79	1.89	2.10
3	A	1385	I7T	C7-I7	-7.27	1.91	2.10
3	C	1385	I7T	C7-I7	-6.72	1.92	2.10
3	D	1385	I7T	C7-I7	-6.47	1.93	2.10
3	A	1385	I7T	C5A-C1B	-2.79	1.48	1.51
2	B	1384	FAD	O2B-C2B	-2.62	1.36	1.43
2	D	1384	FAD	O5'-C5'	-2.53	1.34	1.44
2	C	1384	FAD	O5'-C5'	-2.45	1.34	1.44
2	D	1384	FAD	O2B-C2B	-2.32	1.37	1.43
2	B	1384	FAD	O5'-C5'	-2.31	1.35	1.44
2	D	1384	FAD	C10-N10	-2.23	1.36	1.39
3	C	1385	I7T	C1C-C1	-2.15	1.51	1.55
2	B	1384	FAD	O4B-C4B	-2.15	1.40	1.45
2	A	1384	FAD	C5A-C4A	-2.14	1.35	1.40
2	A	1384	FAD	O4B-C4B	-2.12	1.40	1.45
2	B	1384	FAD	C4-C4X	-2.05	1.37	1.41
2	D	1384	FAD	C1'-N10	2.02	1.50	1.48
2	B	1384	FAD	C1'-N10	2.05	1.50	1.48
2	B	1384	FAD	C10-N1	2.07	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1384	FAD	C8A-N7A	2.07	1.38	1.34
3	C	1385	I7T	C61-C7	2.28	1.44	1.40
2	B	1384	FAD	C2A-N1A	2.29	1.38	1.33
3	C	1385	I7T	C4-N4	2.29	1.52	1.47
2	D	1384	FAD	C2A-N1A	2.31	1.38	1.33
3	D	1385	I7T	C61-C7	2.37	1.44	1.40
3	D	1385	I7T	C1A-C11	2.42	1.52	1.46
3	B	1385	I7T	C1A-C11	2.44	1.52	1.46
3	B	1385	I7T	C6-C61	2.49	1.55	1.51
2	B	1384	FAD	C4-N3	2.51	1.37	1.33
2	C	1384	FAD	C2A-N3A	2.63	1.36	1.32
2	B	1384	FAD	C2A-N3A	2.74	1.37	1.32
2	D	1384	FAD	C5X-N5	2.78	1.39	1.35
2	B	1384	FAD	C5X-N5	2.83	1.39	1.35
2	C	1384	FAD	C8A-N7A	2.95	1.40	1.34
2	A	1384	FAD	C4-N3	3.07	1.38	1.33
2	C	1384	FAD	C1'-N10	3.12	1.51	1.48
2	C	1384	FAD	C5X-N5	3.32	1.40	1.35
2	A	1384	FAD	C5X-N5	3.36	1.40	1.35
2	D	1384	FAD	C2A-N3A	3.48	1.38	1.32
2	B	1384	FAD	C5'-C4'	3.71	1.57	1.51
2	C	1384	FAD	C4X-N5	4.28	1.40	1.33
2	C	1384	FAD	C4-N3	4.35	1.41	1.33
2	D	1384	FAD	C4X-N5	4.40	1.40	1.33
2	B	1384	FAD	C4X-N5	4.82	1.40	1.33
2	D	1384	FAD	C4-N3	4.82	1.42	1.33
2	A	1384	FAD	C4X-N5	5.26	1.41	1.33

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1384	FAD	N3A-C2A-N1A	-14.43	117.85	128.89
2	A	1384	FAD	N3A-C2A-N1A	-13.14	118.84	128.89
2	C	1384	FAD	N3A-C2A-N1A	-11.55	120.05	128.89
2	B	1384	FAD	N3A-C2A-N1A	-9.74	121.43	128.89
3	A	1385	I7T	O12-C12-C1B	-6.30	117.81	123.84
2	B	1384	FAD	C4-C4X-C10	-5.99	116.11	119.94
2	C	1384	FAD	C1B-N9A-C4A	-5.17	119.14	126.94
2	A	1384	FAD	C1B-N9A-C4A	-4.84	119.64	126.94
3	D	1385	I7T	O12-C12-C1B	-3.97	120.04	123.84
3	D	1385	I7T	O1-C1-C2	-3.93	115.54	123.59
3	C	1385	I7T	O1C-C1C-C12	-3.90	102.85	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1384	FAD	O5'-P-O1P	-3.65	95.44	109.62
2	B	1384	FAD	P-O3P-PA	-3.60	122.61	132.73
2	D	1384	FAD	C1B-N9A-C4A	-3.57	121.55	126.94
3	A	1385	I7T	C41-C1C-C1	-3.57	107.10	111.17
2	C	1384	FAD	C4A-C5A-N7A	-3.39	106.36	109.48
2	A	1384	FAD	O3'-C3'-C2'	-3.37	100.25	108.75
2	B	1384	FAD	O3P-PA-O5B	-3.30	94.19	102.94
2	A	1384	FAD	P-O3P-PA	-3.26	123.57	132.73
3	B	1385	I7T	C21-C2-C1	-3.25	117.05	120.87
3	A	1385	I7T	C21-C2-C1	-3.21	117.09	120.87
2	C	1384	FAD	P-O3P-PA	-3.05	124.18	132.73
3	C	1385	I7T	O11-C11-C1A	-3.03	116.32	122.01
3	D	1385	I7T	O1C-C1C-C41	-2.93	106.48	110.17
3	B	1385	I7T	C41-C1C-C1	-2.92	107.83	111.17
3	C	1385	I7T	O12-C12-C1B	-2.85	121.11	123.84
2	C	1384	FAD	O5'-P-O1P	-2.82	98.66	109.62
3	A	1385	I7T	O1-C1-C2	-2.69	118.07	123.59
2	D	1384	FAD	O3'-C3'-C4'	-2.67	102.03	108.75
3	A	1385	I7T	O11-C11-C1A	-2.66	117.01	122.01
3	B	1385	I7T	O21-C21-N21	-2.66	116.14	122.76
2	A	1384	FAD	C4X-C4-N3	-2.47	120.21	123.59
2	A	1384	FAD	C4-C4X-C10	-2.41	118.40	119.94
3	B	1385	I7T	O1C-C1C-C12	-2.39	105.57	109.85
2	D	1384	FAD	C4-C4X-C10	-2.35	118.44	119.94
3	C	1385	I7T	O1C-C1C-C41	-2.35	107.22	110.17
3	A	1385	I7T	C8-C9-C10	-2.33	118.10	120.49
3	B	1385	I7T	O1-C1-C2	-2.33	118.81	123.59
3	D	1385	I7T	C41-C1C-C1	-2.31	108.54	111.17
2	B	1384	FAD	C1B-N9A-C4A	-2.28	123.50	126.94
3	C	1385	I7T	O21-C21-N21	-2.28	117.11	122.76
2	C	1384	FAD	N6A-C6A-N1A	-2.25	114.37	119.20
2	B	1384	FAD	O3B-C3B-C2B	-2.23	104.57	111.83
3	D	1385	I7T	O11-C11-C1A	-2.20	117.88	122.01
2	D	1384	FAD	C4X-C4-N3	-2.20	120.58	123.59
2	D	1384	FAD	P-O3P-PA	-2.16	126.67	132.73
3	D	1385	I7T	O1C-C1C-C12	-2.12	106.05	109.85
3	B	1385	I7T	C43-N4-C4	-2.07	109.01	114.07
2	C	1384	FAD	C4X-C4-N3	-2.05	120.78	123.59
3	A	1385	I7T	O1C-C1C-C12	-2.04	106.18	109.85
2	A	1384	FAD	O3B-C3B-C4B	-2.04	104.92	111.05
2	A	1384	FAD	O4'-C4'-C3'	2.02	114.09	109.02
2	D	1384	FAD	C4-C4X-N5	2.03	121.19	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1385	I7T	C2-C21-N21	2.04	123.19	119.27
2	D	1384	FAD	O2'-C2'-C1'	2.04	114.96	109.94
3	C	1385	I7T	C5-C5A-C1B	2.06	113.22	109.56
2	B	1384	FAD	C4-C4X-N5	2.09	121.25	118.72
2	C	1384	FAD	O2'-C2'-C1'	2.16	115.25	109.94
3	A	1385	I7T	O1-C1-C1C	2.17	123.26	118.72
3	C	1385	I7T	C1C-C1-C2	2.18	119.61	116.13
3	D	1385	I7T	C1C-C41-C4	2.21	114.70	111.73
2	C	1384	FAD	O2P-P-O3P	2.25	115.30	105.09
2	D	1384	FAD	O5B-PA-O1A	2.35	118.72	109.62
2	A	1384	FAD	C4X-N5-C5X	2.37	119.49	116.76
2	A	1384	FAD	O3P-P-O5'	2.45	109.43	102.94
3	D	1385	I7T	C5-C5A-C1B	2.46	113.94	109.56
2	D	1384	FAD	O4B-C1B-N9A	2.47	113.26	108.10
3	A	1385	I7T	C1C-C12-C1B	2.48	125.93	122.95
3	A	1385	I7T	O1C-C1C-C41	2.49	113.31	110.17
3	C	1385	I7T	C61-C7-I7	2.53	124.70	121.33
2	C	1384	FAD	C4X-N5-C5X	2.53	119.67	116.76
2	C	1384	FAD	C4-N3-C2	2.55	117.45	115.25
3	C	1385	I7T	C5A-C5-C41	2.55	115.62	110.71
2	A	1384	FAD	C4-C4X-N5	2.55	121.82	118.72
2	B	1384	FAD	O4'-C4'-C5'	2.57	115.78	110.19
2	D	1384	FAD	O4'-C4'-C3'	2.59	115.52	109.02
3	A	1385	I7T	C1C-C41-C4	2.84	115.54	111.73
3	B	1385	I7T	C11-C1B-C12	2.88	121.38	118.93
3	D	1385	I7T	O1-C1-C1C	3.07	125.14	118.72
2	C	1384	FAD	C4-C4X-N5	3.08	122.45	118.72
3	D	1385	I7T	C61-C7-I7	3.09	125.44	121.33
2	B	1384	FAD	O2A-PA-O3P	3.17	119.46	105.09
2	D	1384	FAD	C4-N3-C2	3.41	118.19	115.25
3	C	1385	I7T	C1C-C41-C4	3.46	116.37	111.73
2	D	1384	FAD	C5X-C9A-N10	3.54	120.31	117.62
2	C	1384	FAD	C4X-C10-N10	3.79	122.75	120.52
2	C	1384	FAD	O3P-P-O5'	3.84	113.12	102.94
2	A	1384	FAD	C1'-N10-C9A	3.89	123.23	118.86
2	C	1384	FAD	C1'-N10-C9A	3.92	123.26	118.86
2	B	1384	FAD	C5X-C9A-N10	4.00	120.66	117.62
2	C	1384	FAD	O4'-C4'-C3'	4.01	119.11	109.02
3	D	1385	I7T	C11-C1B-C12	4.44	122.70	118.93
3	A	1385	I7T	C11-C1B-C12	4.78	123.00	118.93
2	A	1384	FAD	C4-N3-C2	5.61	120.09	115.25
2	D	1384	FAD	C1'-N10-C9A	5.64	125.19	118.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1385	I7T	C11-C1B-C12	5.70	123.78	118.93
2	B	1384	FAD	C1'-N10-C9A	5.90	125.48	118.86
2	B	1384	FAD	C4-N3-C2	6.76	121.09	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1384	FAD	5	0
3	A	1385	I7T	4	0
4	A	1386	SO4	1	0
2	B	1384	FAD	2	0
3	B	1385	I7T	4	0
2	C	1384	FAD	1	0
3	C	1385	I7T	2	0
2	D	1384	FAD	1	0
3	D	1385	I7T	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	368/398 (92%)	0.24	11 (2%) 54 57	23, 43, 75, 101	0
1	B	368/398 (92%)	0.27	10 (2%) 58 61	24, 45, 80, 105	0
1	C	367/398 (92%)	0.50	23 (6%) 23 27	31, 57, 95, 133	0
1	D	365/398 (91%)	0.42	17 (4%) 35 40	32, 58, 97, 126	0
All	All	1468/1592 (92%)	0.36	61 (4%) 40 45	23, 51, 89, 133	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	PRO	9.9
1	B	378	PRO	5.6
1	C	379	ASP	5.1
1	C	321	GLY	5.0
1	A	379	ASP	4.5
1	D	379	ASP	4.4
1	B	380	PHE	4.2
1	C	250	GLN	3.8
1	D	380	PHE	3.8
1	D	376	PHE	3.8
1	C	245	TRP	3.6
1	C	15	SER	3.6
1	B	382	PHE	3.5
1	D	382	PHE	3.4
1	C	251	VAL	3.2
1	D	346	ILE	3.2
1	A	380	PHE	3.1
1	A	382	PHE	3.0
1	C	14	LEU	2.9
1	C	383	GLN	2.9
1	D	298	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	220	GLY	2.8
1	A	110	PHE	2.8
1	C	17	LYS	2.7
1	C	370	GLN	2.7
1	C	110	PHE	2.7
1	A	111	ASP	2.7
1	B	379	ASP	2.6
1	D	178	VAL	2.6
1	B	381	THR	2.6
1	A	376	PHE	2.6
1	A	13	LEU	2.6
1	B	242	PRO	2.5
1	B	383	GLN	2.5
1	C	344	ASN	2.4
1	A	249	THR	2.4
1	C	376	PHE	2.4
1	C	287	LEU	2.4
1	A	14	LEU	2.4
1	B	99	LEU	2.3
1	D	378	PRO	2.3
1	C	298	TRP	2.3
1	D	306	ILE	2.3
1	C	65	GLY	2.3
1	C	377	LYS	2.3
1	C	305	PRO	2.2
1	D	251	VAL	2.2
1	B	243	ASP	2.2
1	D	383	GLN	2.2
1	D	300	SER	2.2
1	D	98	ILE	2.1
1	C	98	ILE	2.1
1	A	104	VAL	2.1
1	D	253	PHE	2.1
1	D	339	ALA	2.1
1	D	110	PHE	2.1
1	C	231	GLY	2.1
1	C	300	SER	2.1
1	C	306	ILE	2.0
1	B	249	THR	2.0
1	D	14	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	I7T	B	1385	31/31	0.94	0.16	0.26	37,56,75,91	0
3	I7T	D	1385	31/31	0.94	0.15	0.08	64,72,85,101	0
2	FAD	B	1384	53/53	0.98	0.14	-0.27	19,33,50,53	0
2	FAD	A	1384	53/53	0.98	0.14	-0.32	20,31,55,58	0
2	FAD	D	1384	53/53	0.97	0.14	-0.42	27,39,58,63	0
2	FAD	C	1384	53/53	0.97	0.13	-0.53	26,36,57,61	0
3	I7T	A	1385	31/31	0.97	0.14	-0.58	32,49,64,76	0
3	I7T	C	1385	31/31	0.94	0.12	-0.69	57,71,86,99	0
4	SO4	C	1387	5/5	0.84	0.16	-	120,121,121,121	0
4	SO4	C	1388	5/5	0.95	0.08	-	75,77,79,81	0
4	SO4	A	1387	5/5	0.90	0.17	-	100,100,102,102	0
4	SO4	B	1387	5/5	0.89	0.11	-	106,106,107,107	0
4	SO4	B	1386	5/5	0.95	0.14	-	76,80,80,80	0
4	SO4	D	1388	5/5	0.96	0.15	-	77,78,79,81	0
4	SO4	A	1388	5/5	0.96	0.13	-	97,97,98,98	0
4	SO4	D	1386	5/5	0.96	0.11	-	76,76,77,77	0
4	SO4	B	1388	5/5	0.90	0.12	-	92,92,93,93	0
4	SO4	A	1386	5/5	0.96	0.11	-	79,80,82,84	0
4	SO4	D	1387	5/5	0.91	0.20	-	109,109,110,111	0
4	SO4	C	1386	5/5	0.98	0.07	-	73,74,77,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.