



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 09:41 PM BST

PDB ID : 3V77  
Title : Crystal structure of a putative fumarylacetoacetate isomerase/hydrolase from *Oleispira antarctica*  
Authors : Stogios, P.J.; Kagan, O.; Di Leo, R.; Bochkarev, A.; Edwards, A.M.; Savchenko, A.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2011-12-20  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
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)	:	2.13.1

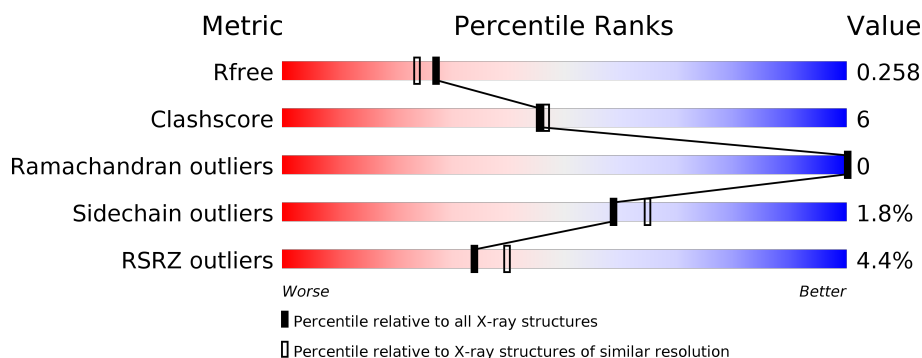
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	224	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>10%</div> </div> </div>
1	B	224	<div> <div>4%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	C	224	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	D	224	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>15%</div> </div> </div>
1	E	224	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	F	224	<div> <div>2%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>

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
3	TAR	D	302	-	-	X	-
4	ACT	A	304	-	-	X	-
4	ACT	C	304	-	-	X	-
4	ACT	D	304	-	-	X	-
4	ACT	E	303	-	-	X	-
4	ACT	F	303	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11452 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.

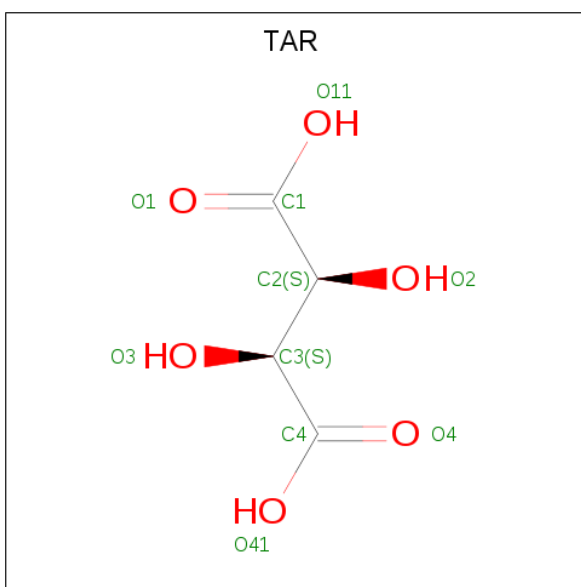
- Molecule 1 is a protein called Putative fumarylacetoacetate isomerase/hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	Se	0	2	0
			1697	1080	285	325	4	3			
1	B	224	Total	C	N	O	S	Se	0	1	0
			1691	1076	284	324	4	3			
1	C	224	Total	C	N	O	S	Se	0	1	0
			1694	1078	284	326	3	3			
1	D	224	Total	C	N	O	S	Se	0	0	0
			1688	1074	284	324	3	3			
1	E	224	Total	C	N	O	S	Se	0	0	0
			1688	1074	284	324	3	3			
1	F	224	Total	C	N	O	S	Se	0	0	0
			1688	1074	284	324	3	3			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

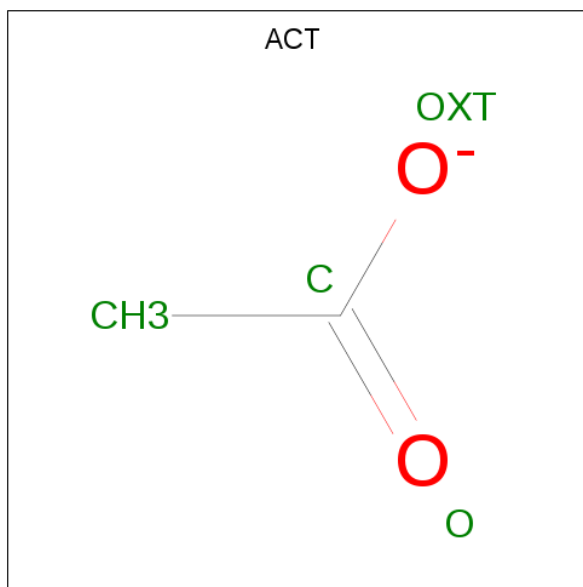
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	2	Total	Zn	0	0
			2	2		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	E	1	Total	C	O	0	0
			10	4	6		
3	F	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		

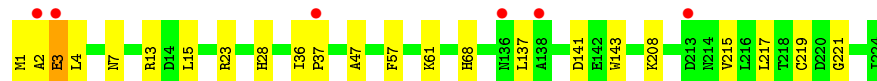
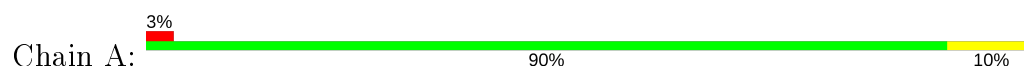
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	230	Total	O	0	3
			233	233		
5	B	180	Total	O	0	2
			182	182		
5	C	184	Total	O	0	0
			184	184		
5	D	168	Total	O	0	1
			169	169		
5	E	172	Total	O	0	2
			174	174		
5	F	241	Total	O	0	2
			243	243		

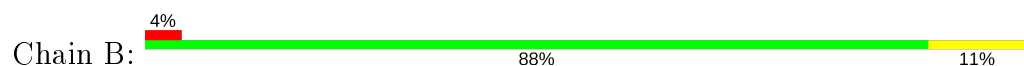
### 3 Residue-property plots [i](#)

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.

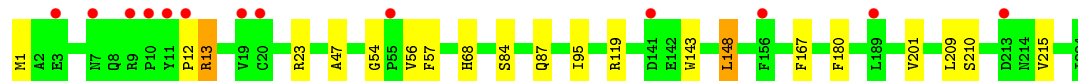
- Molecule 1: Putative fumarylacetoacetate isomerase/hydrolase



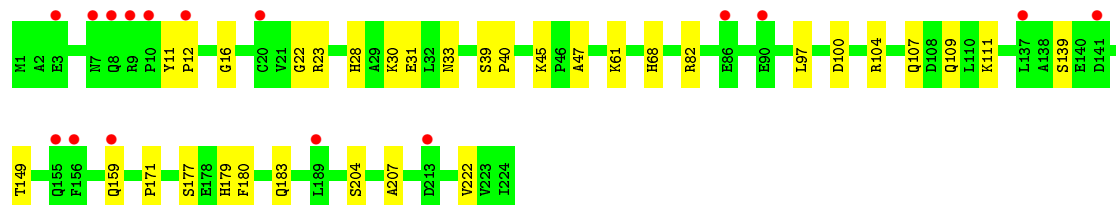
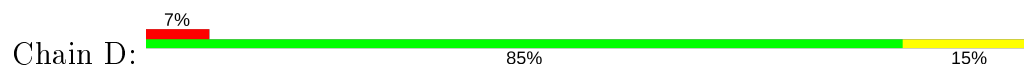
- Molecule 1: Putative fumarylacetoacetate isomerase/hydrolase



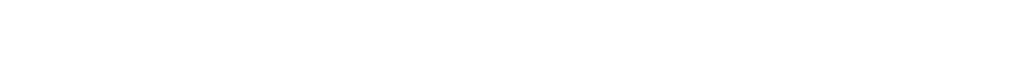
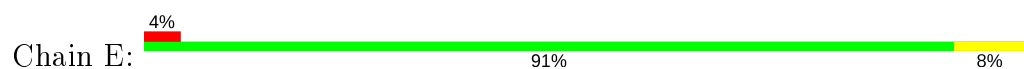
- Molecule 1: Putative fumarylacetoacetate isomerase/hydrolase



- Molecule 1: Putative fumarylacetoacetate isomerase/hydrolase

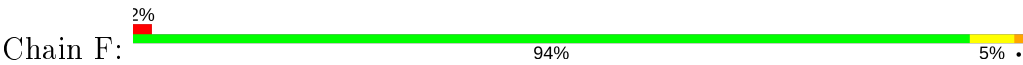


- Molecule 1: Putative fumarylacetoacetate isomerase/hydrolase





● Molecule 1: Putative fumarylacetoacetate isomerase/hydrolase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.26Å 161.39Å 114.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.51 – 2.10 27.51 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.51-2.10) 99.6 (27.51-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.199 , 0.256 0.202 , 0.258	Depositor DCC
$R_{free}$ test set	4262 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.7	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.008 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2 *h-1/2*k 0.004 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/ 2*h+1/2*k 0.003 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2 *h-1/2*k 0.001 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1 /2*h+1/2*k 0.008 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, TAR, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.53	0/1736	0.63	0/2356
1	B	0.51	0/1727	0.61	0/2344
1	C	0.48	0/1730	0.60	1/2348 (0.0%)
1	D	0.50	0/1721	0.60	0/2336
1	E	0.51	0/1721	0.63	0/2336
1	F	0.55	0/1721	0.63	0/2336
All	All	0.51	0/10356	0.62	1/14056 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	LEU	CA-CB-CG	5.82	128.69	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1697	0	1714	27	0
1	B	1691	0	1706	19	1
1	C	1694	0	1707	16	0
1	D	1688	0	1701	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1688	0	1701	20	0
1	F	1688	0	1701	17	1
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	20	0	8	1	0
3	B	10	0	4	1	0
3	C	20	0	8	2	0
3	D	20	0	8	5	0
3	E	10	0	4	0	0
3	F	10	0	4	1	0
4	A	4	0	3	3	0
4	B	4	0	3	1	0
4	C	4	0	3	3	0
4	D	4	0	3	8	0
4	E	4	0	3	7	0
4	F	4	0	3	4	0
5	A	233	0	0	5	0
5	B	182	0	0	3	0
5	C	184	0	0	3	0
5	D	169	0	0	6	0
5	E	174	0	0	2	0
5	F	243	0	0	5	0
All	All	11452	0	10284	131	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (131) 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:23:ARG:HE	4:A:304:ACT:H1	1.14	1.08
1:A:2:ALA:CB	1:A:3:GLU:HA	1.84	1.07
1:A:2:ALA:HB1	1:A:3:GLU:HA	1.04	1.01
1:E:111:LYS:NZ	4:E:303:ACT:H3	1.76	1.00
1:C:23:ARG:HE	4:C:304:ACT:H1	1.25	0.98
1:A:2:ALA:HB1	1:A:3:GLU:CA	1.96	0.95
1:E:23:ARG:HH21	4:E:303:ACT:H1	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ARG:HH21	4:D:304:ACT:H1	1.33	0.92
1:E:111:LYS:HZ1	4:E:303:ACT:H3	1.35	0.87
4:C:304:ACT:H2	5:C:536:HOH:O	1.75	0.86
1:D:111:LYS:NZ	4:D:304:ACT:H3	1.91	0.84
1:D:171:PRO:HB2	3:D:303:TAR:H3	1.60	0.83
1:B:23:ARG:HE	4:B:303:ACT:H1	1.43	0.81
4:A:304:ACT:H2	5:A:489:HOH:O	1.80	0.81
1:F:104:ARG:HH11	1:F:107:GLN:HE22	1.29	0.79
1:D:28:HIS:HE1	3:D:302:TAR:O3	1.66	0.79
1:C:84:SER:H	1:C:87:GLN:HE21	1.30	0.79
1:E:104:ARG:HH11	1:E:107:GLN:HE22	1.34	0.74
1:D:104:ARG:HH11	1:D:107:GLN:HE22	1.35	0.74
1:D:111:LYS:HZ3	4:D:304:ACT:H3	1.49	0.74
1:F:212:GLU:O	1:F:213:ASP:HB2	1.86	0.72
1:C:95:ILE:HG22	1:C:209:LEU:HD21	1.72	0.70
1:E:111:LYS:HZ2	4:E:303:ACT:H3	1.57	0.70
1:A:1:MSE:HG2	1:A:47:ALA:HB1	1.73	0.70
1:E:111:LYS:NZ	4:E:303:ACT:CH3	2.52	0.70
1:C:95:ILE:CG2	1:C:209:LEU:HD21	2.21	0.69
1:C:167:PHE:HD2	3:C:303:TAR:H2	1.57	0.69
4:F:303:ACT:H2	5:F:595:HOH:O	1.91	0.69
1:A:1:MSE:HE1	1:D:183:GLN:HG2	1.76	0.68
1:A:208:LYS:HD3	1:A:215:VAL:HG22	1.76	0.68
1:C:95:ILE:HD11	1:C:143:TRP:HZ3	1.59	0.67
1:D:23:ARG:HH21	4:D:304:ACT:CH3	2.05	0.67
1:A:1:MSE:HG2	1:A:47:ALA:CB	2.26	0.66
1:B:152:LYS:CB	1:B:157:GLN:HG3	2.26	0.66
1:D:28:HIS:CE1	3:D:302:TAR:O3	2.52	0.63
1:F:1:MSE:HA	1:F:1:MSE:HE3	1.79	0.62
1:B:45:LYS:CE	1:B:100:ASP:OD1	2.48	0.62
1:D:28:HIS:HD2	1:D:31:GLU:OE2	1.82	0.61
1:E:200:GLU:HG3	5:E:536:HOH:O	1.98	0.61
1:B:1:MSE:HE1	1:B:47:ALA:HB1	1.83	0.61
1:F:104:ARG:HH11	1:F:107:GLN:NE2	1.97	0.60
1:D:61:LYS:O	5:D:542:HOH:O	2.16	0.60
1:A:2:ALA:CB	1:A:3:GLU:CA	2.69	0.60
1:D:33:ASN:HB2	5:D:508:HOH:O	2.01	0.60
1:A:28:HIS:NE2	3:A:303:TAR:O2	2.28	0.59
1:E:115:HIS:HB3	1:E:116:PRO:HD2	1.85	0.58
1:B:170:LEU:HB2	1:B:171:PRO:HD3	1.84	0.58
1:A:13:ARG:HD2	5:A:578:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:LYS:HZ2	4:E:303:ACT:CH3	2.15	0.57
1:B:152:LYS:HB3	1:B:157:GLN:HG3	1.85	0.57
1:B:152:LYS:HB2	1:B:157:GLN:HG3	1.86	0.57
1:D:149:THR:HG22	1:D:159:GLN:HG3	1.85	0.57
1:E:7:ASN:ND2	1:E:7:ASN:H	2.02	0.56
1:D:204:SER:HB3	1:D:222:VAL:HG12	1.89	0.55
1:E:78:LYS:NZ	1:E:90:GLU:HG3	2.22	0.54
1:D:111:LYS:NZ	4:D:304:ACT:CH3	2.69	0.54
1:B:68:HIS:HE1	5:B:539:HOH:O	1.92	0.53
1:E:137:LEU:HD22	1:E:142:GLU:HG2	1.89	0.53
1:D:22:GLY:O	3:D:302:TAR:O2	2.24	0.53
1:E:104:ARG:HH11	1:E:107:GLN:NE2	2.04	0.53
1:F:104:ARG:NH1	1:F:107:GLN:HE22	2.02	0.52
1:D:68:HIS:HE1	5:D:505:HOH:O	1.92	0.52
1:F:68:HIS:HE1	5:F:599:HOH:O	1.92	0.52
1:C:68:HIS:HE1	5:C:538:HOH:O	1.92	0.52
1:F:23:ARG:HE	4:F:303:ACT:H3	1.74	0.52
1:F:23:ARG:HE	4:F:303:ACT:CH3	2.23	0.51
1:C:1:MSE:HE1	1:C:47:ALA:HB1	1.92	0.51
5:A:571:HOH:O	1:D:179:HIS:HD2	1.92	0.51
1:F:1:MSE:HA	1:F:1:MSE:CE	2.40	0.50
1:C:12:PRO:HB2	1:C:13:ARG:HH11	1.76	0.50
1:D:23:ARG:NH2	4:D:304:ACT:H1	2.14	0.50
1:E:23:ARG:HH21	4:E:303:ACT:CH3	2.13	0.50
1:A:137:LEU:HD12	1:A:143:TRP:CE2	2.47	0.49
1:B:28:HIS:NE2	3:B:302:TAR:O2	2.29	0.49
1:D:45:LYS:CE	1:D:100:ASP:OD1	2.61	0.49
1:E:78:LYS:HZ2	1:E:90:GLU:HG3	1.76	0.49
1:C:95:ILE:HD11	1:C:143:TRP:CZ3	2.44	0.48
1:F:212:GLU:O	1:F:213:ASP:CB	2.60	0.48
4:F:303:ACT:H3	5:F:472:HOH:O	2.12	0.48
1:C:119:ARG:HH22	1:F:175:HIS:HE1	1.61	0.48
1:A:1:MSE:HG3	1:A:47:ALA:O	2.13	0.48
1:C:210:SER:HB3	1:C:215:VAL:HA	1.96	0.48
1:C:23:ARG:NE	4:C:304:ACT:H1	2.10	0.48
1:F:143:TRP:CD1	1:F:170:LEU:HD11	2.49	0.47
1:D:179:HIS:HE1	5:D:526:HOH:O	1.97	0.47
1:B:45:LYS:HE3	1:B:100:ASP:OD1	2.14	0.47
1:E:104:ARG:NH1	1:E:107:GLN:HE22	2.10	0.47
1:A:57:PHE:CE2	1:A:221:GLY:HA3	2.50	0.47
1:C:54:GLY:HA2	1:C:56:VAL:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:LYS:HG3	5:D:509:HOH:O	2.15	0.47
1:F:157:GLN:NE2	5:F:543:HOH:O	2.47	0.47
1:F:175:HIS:HB2	5:F:598:HOH:O	2.14	0.47
1:A:137:LEU:HD12	1:A:143:TRP:CD2	2.50	0.46
1:A:217:LEU:HD13	1:A:219[A]:CYS:SG	2.56	0.46
1:B:105:ASP:O	1:B:109:GLN:HG3	2.14	0.46
1:A:37:PRO:HB3	5:D:539:HOH:O	2.16	0.46
1:B:104:ARG:HH11	1:B:107:GLN:HE22	1.63	0.45
1:B:57:PHE:HZ	1:B:205:LEU:HD12	1.82	0.45
1:B:45:LYS:HE2	1:B:100:ASP:OD1	2.16	0.45
1:D:45:LYS:HE3	1:D:100:ASP:OD1	2.17	0.45
1:D:11:TYR:CD1	1:D:12:PRO:HD2	2.52	0.45
1:A:1:MSE:CG	1:A:47:ALA:HB1	2.44	0.45
1:B:107:GLN:O	1:B:111:LYS:HG3	2.17	0.45
1:D:16:GLY:O	1:D:47:ALA:HB2	2.16	0.45
1:E:66:VAL:HG22	1:E:103:LEU:HD23	2.00	0.44
1:C:167:PHE:CD2	3:C:303:TAR:H2	2.46	0.44
1:A:4:LEU:HD21	1:A:15:LEU:HD13	1.99	0.43
1:D:22:GLY:O	3:D:302:TAR:C2	2.66	0.43
1:E:155:GLN:HG2	5:E:521:HOH:O	2.18	0.43
1:B:3:GLU:HB2	5:B:416:HOH:O	2.19	0.42
1:E:137:LEU:HD21	1:E:211:LEU:HD11	2.01	0.42
1:A:1:MSE:HG3	1:A:47:ALA:C	2.39	0.42
1:B:155:GLN:HB3	5:B:538:HOH:O	2.19	0.42
1:C:201:VAL:HG23	5:C:456:HOH:O	2.19	0.42
1:F:22:GLY:HA2	3:F:302:TAR:H3	2.00	0.42
1:A:36:ILE:HA	1:A:37:PRO:HD3	1.89	0.42
1:D:111:LYS:HZ1	4:D:304:ACT:H3	1.78	0.42
1:A:7:ASN:OD1	5:A:603:HOH:O	2.22	0.42
1:B:67:HIS:HA	1:B:197:GLY:O	2.20	0.42
1:F:137:LEU:HD12	1:F:143:TRP:CE2	2.55	0.41
1:D:39:SER:HA	1:D:40:PRO:HD3	1.89	0.41
1:B:60:PRO:HD2	1:B:66:VAL:HG21	2.02	0.41
1:F:1:MSE:CA	1:F:1:MSE:HE3	2.48	0.41
1:D:97:LEU:HD13	1:D:207:ALA:HB1	2.03	0.41
1:A:68:HIS:CD2	1:A:68:HIS:O	2.75	0.40
1:A:61:LYS:HD3	1:A:61:LYS:HA	1.87	0.40
1:A:23:ARG:NE	4:A:304:ACT:H1	2.00	0.40
1:A:3:GLU:H	1:A:3:GLU:HG2	1.49	0.40
1:A:68:HIS:HE1	5:A:574:HOH:O	2.04	0.40
1:D:111:LYS:HZ1	4:D:304:ACT:CH3	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:SER:O	1:E:88:VAL:HG23	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLU:O	1:F:9:ARG:NH1[3_555]	2.19	0.01

## 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	224/224 (100%)	220 (98%)	4 (2%)	0	100	100
1	B	223/224 (100%)	213 (96%)	10 (4%)	0	100	100
1	C	223/224 (100%)	215 (96%)	8 (4%)	0	100	100
1	D	222/224 (99%)	212 (96%)	10 (4%)	0	100	100
1	E	222/224 (99%)	217 (98%)	5 (2%)	0	100	100
1	F	222/224 (99%)	217 (98%)	5 (2%)	0	100	100
All	All	1336/1344 (99%)	1294 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	187/182 (103%)	185 (99%)	2 (1%)	73	79
1	B	186/182 (102%)	183 (98%)	3 (2%)	62	69
1	C	186/182 (102%)	182 (98%)	4 (2%)	52	57
1	D	185/182 (102%)	180 (97%)	5 (3%)	44	48
1	E	185/182 (102%)	181 (98%)	4 (2%)	52	57
1	F	185/182 (102%)	183 (99%)	2 (1%)	73	79
All	All	1114/1092 (102%)	1094 (98%)	20 (2%)	59	65

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	141	ASP
1	B	34	ASN
1	B	155	GLN
1	B	156	PHE
1	C	13	ARG
1	C	57	PHE
1	C	148	LEU
1	C	180	PHE
1	D	82	ARG
1	D	109	GLN
1	D	139	SER
1	D	177	SER
1	D	180	PHE
1	E	7	ASN
1	E	39	SER
1	E	85	THR
1	E	211	LEU
1	F	1	MSE
1	F	213	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	157	GLN
1	B	68	HIS
1	B	107	GLN
1	B	144	GLN

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Mol	Chain	Res	Type
1	B	157	GLN
1	C	87	GLN
1	D	28	HIS
1	D	34	ASN
1	D	107	GLN
1	D	157	GLN
1	D	179	HIS
1	E	7	ASN
1	E	33	ASN
1	E	107	GLN
1	E	179	HIS
1	F	68	HIS
1	F	107	GLN
1	F	157	GLN
1	F	175	HIS

### 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](#)

Of 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TAR	B	302	2	3,9,9	1.41	1 (33%)	6,12,12	3.30	2 (33%)
3	TAR	C	302	2	3,9,9	1.47	1 (33%)	6,12,12	4.27	4 (66%)
3	TAR	A	305	2	3,9,9	0.60	0	6,12,12	0.90	0
3	TAR	D	303	-	3,9,9	0.93	0	6,12,12	1.00	0
4	ACT	D	304	-	1,3,3	0.19	0	0,3,3	0.00	-
3	TAR	D	302	2	3,9,9	1.12	0	6,12,12	3.66	3 (50%)
4	ACT	F	303	-	1,3,3	0.06	0	0,3,3	0.00	-
4	ACT	A	304	-	1,3,3	0.49	0	0,3,3	0.00	-
4	ACT	B	303	-	1,3,3	0.77	0	0,3,3	0.00	-
4	ACT	C	304	-	1,3,3	0.02	0	0,3,3	0.00	-
3	TAR	A	303	2	3,9,9	1.85	1 (33%)	6,12,12	4.70	4 (66%)
3	TAR	C	303	-	3,9,9	0.52	0	6,12,12	1.06	0
4	ACT	E	303	-	1,3,3	0.15	0	0,3,3	0.00	-
3	TAR	F	302	2	3,9,9	1.98	1 (33%)	6,12,12	5.08	4 (66%)
3	TAR	E	302	2	3,9,9	1.78	1 (33%)	6,12,12	4.93	4 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TAR	B	302	2	-	4/4/12/12	-
3	TAR	C	302	2	-	4/4/12/12	-
3	TAR	A	305	2	-	4/4/12/12	-
3	TAR	D	303	-	-	1/4/12/12	-
3	TAR	D	302	2	-	4/4/12/12	-
3	TAR	A	303	2	-	4/4/12/12	-
3	TAR	C	303	-	-	0/4/12/12	-
3	TAR	F	302	2	-	4/4/12/12	-
3	TAR	E	302	2	-	4/4/12/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	302	TAR	O3-C3	3.17	1.48	1.42
3	A	303	TAR	O3-C3	2.86	1.48	1.42
3	E	302	TAR	O2-C2	2.72	1.48	1.42
3	B	302	TAR	O2-C2	-2.28	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	TAR	O2-C2	2.13	1.46	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	TAR	C4-C3-C2	-9.02	93.69	113.11
3	C	302	TAR	C1-C2-C3	-8.89	93.97	113.11
3	E	302	TAR	C1-C2-C3	-8.80	94.16	113.11
3	F	302	TAR	C4-C3-C2	-8.74	94.30	113.11
3	B	302	TAR	C4-C3-C2	-6.83	98.41	113.11
3	F	302	TAR	O3-C3-C4	-6.80	94.73	111.10
3	D	302	TAR	C1-C2-C3	-6.27	99.61	113.11
3	E	302	TAR	O2-C2-C1	-6.14	96.32	111.10
3	D	302	TAR	O2-C2-C1	-5.28	98.40	111.10
3	A	303	TAR	O3-C3-C4	-5.06	98.93	111.10
3	F	302	TAR	C1-C2-C3	4.12	121.97	113.11
3	E	302	TAR	O2-C2-C3	3.95	122.10	108.90
3	B	302	TAR	O3-C3-C4	-3.79	101.97	111.10
3	A	303	TAR	O3-C3-C2	3.72	121.33	108.90
3	F	302	TAR	O3-C3-C2	3.55	120.74	108.90
3	C	302	TAR	O2-C2-C1	-3.53	102.61	111.10
3	E	302	TAR	C4-C3-C2	3.40	120.43	113.11
3	C	302	TAR	O2-C2-C3	3.28	119.85	108.90
3	D	302	TAR	C4-C3-C2	2.78	119.09	113.11
3	A	303	TAR	C1-C2-C3	2.76	119.05	113.11
3	C	302	TAR	O3-C3-C2	2.06	115.79	108.90

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	302	TAR	C1-C2-C3-C4
3	F	302	TAR	O2-C2-C3-O3
3	F	302	TAR	O2-C2-C3-C4
3	B	302	TAR	C1-C2-C3-C4
3	B	302	TAR	O2-C2-C3-C4
3	C	302	TAR	C1-C2-C3-O3
3	C	302	TAR	C1-C2-C3-C4
3	C	302	TAR	O2-C2-C3-O3
3	A	305	TAR	C1-C2-C3-O3
3	A	305	TAR	C1-C2-C3-C4
3	A	305	TAR	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	D	302	TAR	C1-C2-C3-O3
3	D	302	TAR	C1-C2-C3-C4
3	D	302	TAR	O2-C2-C3-O3
3	A	303	TAR	C1-C2-C3-C4
3	A	303	TAR	O2-C2-C3-O3
3	A	303	TAR	O2-C2-C3-C4
3	E	302	TAR	C1-C2-C3-O3
3	E	302	TAR	C1-C2-C3-C4
3	E	302	TAR	O2-C2-C3-O3
3	D	302	TAR	O2-C2-C3-C4
3	E	302	TAR	O2-C2-C3-C4
3	B	302	TAR	O2-C2-C3-O3
3	A	305	TAR	O2-C2-C3-O3
3	D	303	TAR	C1-C2-C3-C4
3	A	303	TAR	C1-C2-C3-O3
3	C	302	TAR	O2-C2-C3-C4
3	F	302	TAR	C1-C2-C3-O3
3	B	302	TAR	C1-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	TAR	1	0
3	D	303	TAR	1	0
4	D	304	ACT	8	0
3	D	302	TAR	4	0
4	F	303	ACT	4	0
4	A	304	ACT	3	0
4	B	303	ACT	1	0
4	C	304	ACT	3	0
3	A	303	TAR	1	0
3	C	303	TAR	2	0
4	E	303	ACT	7	0
3	F	302	TAR	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	221/224 (98%)	-0.13	6 (2%) 54 60	18, 27, 43, 49	0
1	B	221/224 (98%)	0.31	8 (3%) 42 49	22, 35, 50, 55	0
1	C	221/224 (98%)	0.30	13 (5%) 22 27	22, 35, 55, 62	0
1	D	221/224 (98%)	0.47	16 (7%) 15 19	23, 36, 57, 67	0
1	E	221/224 (98%)	0.17	10 (4%) 33 38	22, 32, 50, 61	0
1	F	221/224 (98%)	-0.08	5 (2%) 60 65	20, 29, 44, 58	0
All	All	1326/1344 (98%)	0.17	58 (4%) 34 40	18, 32, 53, 67	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	138	ALA	7.1
1	A	2	ALA	5.9
1	D	156	PHE	5.5
1	C	10	PRO	4.8
1	D	8	GLN	4.6
1	F	137	LEU	4.5
1	F	138	ALA	4.3
1	B	33	ASN	4.2
1	E	10	PRO	3.9
1	D	10	PRO	3.9
1	D	9	ARG	3.9
1	C	156	PHE	3.8
1	D	12	PRO	3.6
1	C	9	ARG	3.6
1	E	9	ARG	3.6
1	C	12	PRO	3.6
1	A	138	ALA	3.3
1	B	38	SER	3.3
1	C	7	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	189	LEU	3.2
1	A	37	PRO	3.1
1	B	36	ILE	3.1
1	F	136	ASN	3.0
1	C	213	ASP	2.9
1	F	86	GLU	2.9
1	C	11	TYR	2.8
1	E	139	SER	2.7
1	C	55	PRO	2.7
1	B	166	LEU	2.7
1	E	189	LEU	2.6
1	D	189	LEU	2.6
1	E	137	LEU	2.6
1	D	141	ASP	2.5
1	B	62	ASP	2.5
1	F	82	ARG	2.5
1	E	141	ASP	2.5
1	D	155	GLN	2.4
1	B	213	ASP	2.4
1	B	82	ARG	2.4
1	C	141	ASP	2.4
1	D	213	ASP	2.4
1	D	137	LEU	2.4
1	C	19	VAL	2.4
1	D	90	GLU	2.3
1	A	213	ASP	2.3
1	D	159	GLN	2.3
1	B	37	PRO	2.2
1	E	13	ARG	2.2
1	D	7	ASN	2.2
1	E	82	ARG	2.2
1	C	3	GLU	2.1
1	A	3	GLU	2.1
1	E	136	ASN	2.1
1	D	20	CYS	2.1
1	D	3	GLU	2.0
1	A	136	ASN	2.0
1	C	20	CYS	2.0
1	D	86	GLU	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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	TAR	D	303	10/10	0.48	0.34	76,77,78,78	0
3	TAR	C	303	10/10	0.53	0.28	59,62,63,64	0
4	ACT	B	303	4/4	0.74	0.21	48,48,49,49	0
3	TAR	A	305	10/10	0.78	0.18	59,62,63,64	0
4	ACT	C	304	4/4	0.81	0.23	35,36,36,37	0
4	ACT	F	303	4/4	0.82	0.17	36,37,37,38	0
3	TAR	B	302	10/10	0.86	0.15	30,34,34,36	0
4	ACT	E	303	4/4	0.86	0.16	33,34,35,35	0
3	TAR	D	302	10/10	0.88	0.16	27,32,35,37	0
3	TAR	F	302	10/10	0.88	0.15	23,27,31,32	0
3	TAR	E	302	10/10	0.88	0.16	27,29,32,33	0
3	TAR	A	303	10/10	0.90	0.15	22,29,32,32	0
4	ACT	A	304	4/4	0.91	0.10	38,39,39,39	0
3	TAR	C	302	10/10	0.92	0.16	29,32,34,34	0
4	ACT	D	304	4/4	0.93	0.15	34,34,34,35	0
2	ZN	B	301	1/1	0.97	0.03	32,32,32,32	0
2	ZN	A	302	1/1	0.98	0.02	39,39,39,39	0
2	ZN	A	301	1/1	0.99	0.05	25,25,25,25	0
2	ZN	C	301	1/1	0.99	0.05	29,29,29,29	0
2	ZN	D	301	1/1	0.99	0.04	31,31,31,31	0
2	ZN	E	301	1/1	0.99	0.04	26,26,26,26	0
2	ZN	F	301	1/1	1.00	0.04	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.