



## Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:41 pm BST

PDB ID : 3TFZ  
Title : Crystal structure of Zhui aromatase/cyclase from Streptomyces sp. R1128  
Authors : Ames, B.D.; Lee, M.Y.; Moody, C.; Zhang, W.; Tang, Y.; Wong, S.K.; Tsai, S.C.  
Deposited on : 2011-08-16  
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

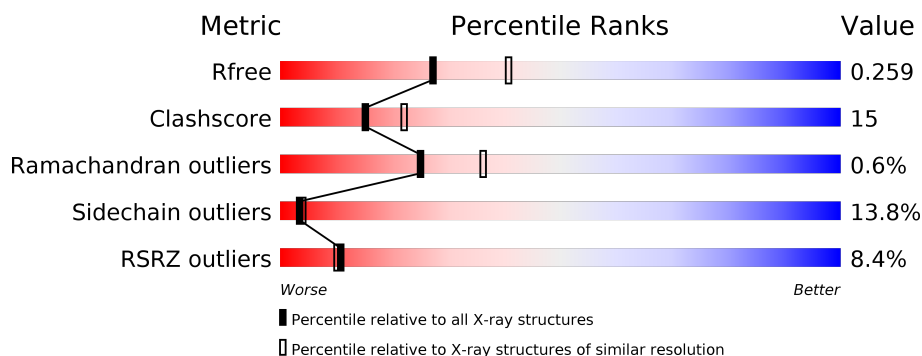
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	172	<div> <div>0%</div> <div> <div>69%</div> <div>22%</div> <div>5%</div> <div>• •</div> </div> </div>
1	B	172	<div> <div>5%</div> <div> <div>73%</div> <div>18%</div> <div>• • •</div> </div> </div>
1	C	172	<div> <div>19%</div> <div> <div>57%</div> <div>30%</div> <div>6%</div> <div>• 5%</div> </div> </div>
1	D	172	<div> <div>15%</div> <div> <div>51%</div> <div>30%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	E	172	<div> <div>6%</div> <div> <div>65%</div> <div>23%</div> <div>8%</div> <div>• •</div> </div> </div>
1	F	172	<div> <div>3%</div> <div> <div>66%</div> <div>19%</div> <div>6%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7945 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 Cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1300	811	237	249	3			
1	B	165	Total	C	N	O	S	0	0	0
			1282	800	234	245	3			
1	C	164	Total	C	N	O	S	0	0	0
			1275	795	233	244	3			
1	D	164	Total	C	N	O	S	0	0	0
			1275	795	233	244	3			
1	E	165	Total	C	N	O	S	0	0	0
			1281	798	234	246	3			
1	F	161	Total	C	N	O	S	0	0	0
			1262	788	230	241	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q9F6D3
A	-1	SER	-	EXPRESSION TAG	UNP Q9F6D3
A	0	HIS	-	EXPRESSION TAG	UNP Q9F6D3
B	-2	GLY	-	EXPRESSION TAG	UNP Q9F6D3
B	-1	SER	-	EXPRESSION TAG	UNP Q9F6D3
B	0	HIS	-	EXPRESSION TAG	UNP Q9F6D3
C	-2	GLY	-	EXPRESSION TAG	UNP Q9F6D3
C	-1	SER	-	EXPRESSION TAG	UNP Q9F6D3
C	0	HIS	-	EXPRESSION TAG	UNP Q9F6D3
D	-2	GLY	-	EXPRESSION TAG	UNP Q9F6D3
D	-1	SER	-	EXPRESSION TAG	UNP Q9F6D3
D	0	HIS	-	EXPRESSION TAG	UNP Q9F6D3
E	-2	GLY	-	EXPRESSION TAG	UNP Q9F6D3
E	-1	SER	-	EXPRESSION TAG	UNP Q9F6D3
E	0	HIS	-	EXPRESSION TAG	UNP Q9F6D3
F	-2	GLY	-	EXPRESSION TAG	UNP Q9F6D3
F	-1	SER	-	EXPRESSION TAG	UNP Q9F6D3

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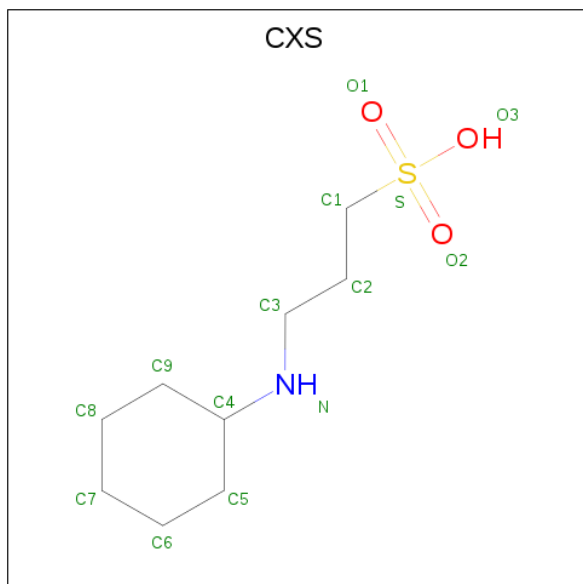
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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	EXPRESSION TAG	UNP Q9F6D3

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total K 1 1	0	0
2	A	1	Total K 1 1	0	0
2	F	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0

- Molecule 3 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula: C<sub>9</sub>H<sub>19</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 14 9 1 3 1	0	0
3	B	1	Total C N O S 14 9 1 3 1	0	0
3	C	1	Total C N O S 14 9 1 3 1	0	0
3	D	1	Total C N O S 14 9 1 3 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	E	1	Total	C	N	O	S	0	0
			14	9	1	3	1		
3	F	1	Total	C	N	O	S	0	0
			14	9	1	3	1		

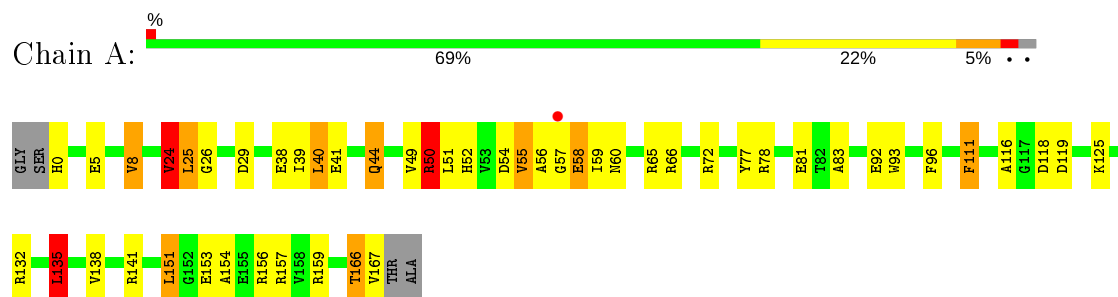
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	36	Total	O	0	0
			36	36		
4	C	17	Total	O	0	0
			17	17		
4	D	17	Total	O	0	0
			17	17		
4	E	21	Total	O	0	0
			21	21		
4	F	13	Total	O	0	0
			13	13		

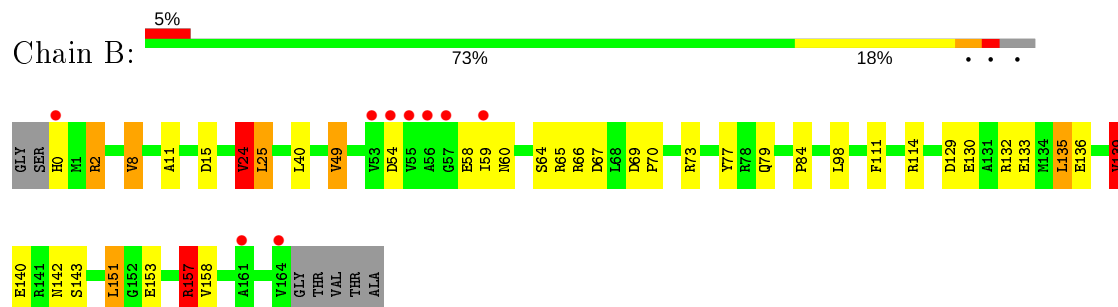
### 3 Residue-property plots [i](#)

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

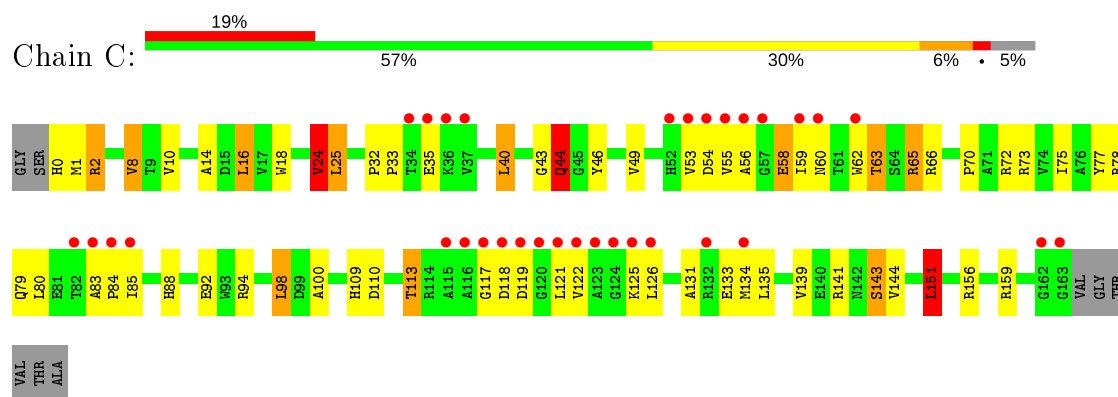
#### • Molecule 1: Cyclase



#### • Molecule 1: Cyclase

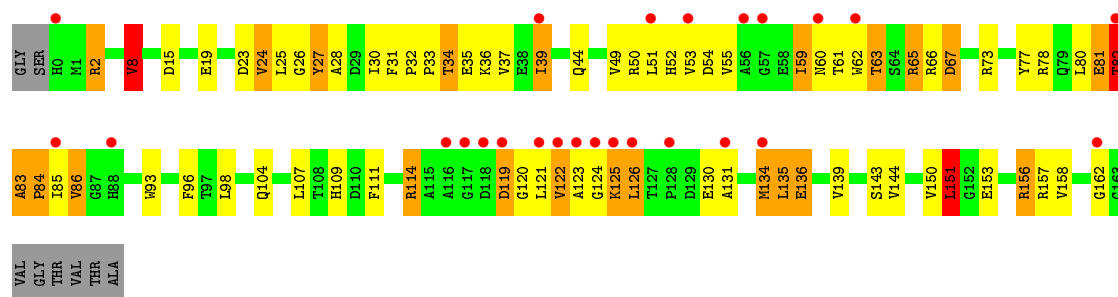


#### • Molecule 1: Cyclase

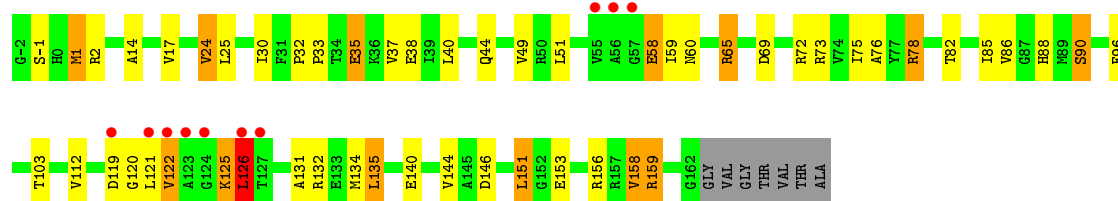


#### • Molecule 1: Cyclase

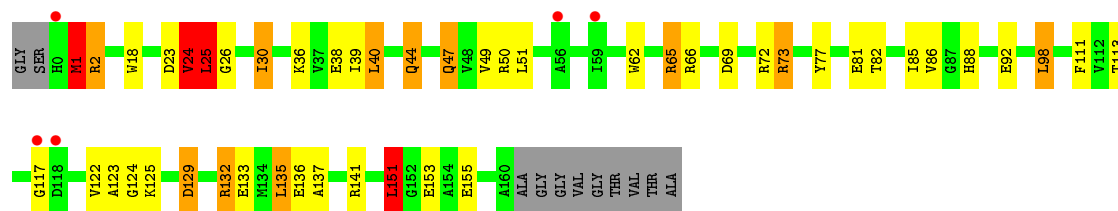




• Molecule 1: Cyclase



• Molecule 1: Cyclase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.02Å 135.73Å 175.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 43.45 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.39) 99.2 (43.45-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.52 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.193 , 0.261 0.192 , 0.259	Depositor DCC
$R_{free}$ test set	2430 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7945	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, CXS

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	1.51	13/1323 (1.0%)	1.56	22/1803 (1.2%)
1	B	1.40	4/1305 (0.3%)	1.30	9/1778 (0.5%)
1	C	1.20	2/1298 (0.2%)	1.21	12/1768 (0.7%)
1	D	1.23	6/1298 (0.5%)	1.23	15/1768 (0.8%)
1	E	1.30	4/1304 (0.3%)	1.51	23/1776 (1.3%)
1	F	1.23	5/1285 (0.4%)	1.25	16/1751 (0.9%)
All	All	1.32	34/7813 (0.4%)	1.35	97/10644 (0.9%)

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	D	0	2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	76	ALA	CA-CB	8.00	1.69	1.52
1	F	38	GLU	CD-OE1	7.48	1.33	1.25
1	A	38	GLU	CD-OE2	7.46	1.33	1.25
1	D	27	TYR	CE2-CZ	7.19	1.47	1.38
1	D	86	VAL	C-O	7.04	1.36	1.23
1	B	49	VAL	CB-CG2	-6.84	1.38	1.52
1	A	41	GLU	CG-CD	6.76	1.62	1.51
1	E	90	SER	CB-OG	-6.56	1.33	1.42
1	A	26	GLY	C-O	-6.42	1.13	1.23
1	F	92	GLU	CB-CG	6.22	1.64	1.52
1	A	81	GLU	CB-CG	6.06	1.63	1.52
1	C	72	ARG	CZ-NH1	6.00	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	36	LYS	CD-CE	5.81	1.65	1.51
1	A	93	TRP	CE3-CZ3	5.77	1.48	1.38
1	D	27	TYR	CD1-CE1	5.73	1.48	1.39
1	F	24	VAL	CB-CG1	-5.69	1.41	1.52
1	A	92	GLU	CB-CG	-5.67	1.41	1.52
1	B	158	VAL	CB-CG1	5.67	1.64	1.52
1	C	14	ALA	CA-CB	5.63	1.64	1.52
1	E	17	VAL	CB-CG2	5.54	1.64	1.52
1	D	150	VAL	CB-CG1	5.35	1.64	1.52
1	E	140	GLU	CD-OE1	5.32	1.31	1.25
1	A	111	PHE	CD2-CE2	5.30	1.49	1.39
1	A	77	TYR	CD2-CE2	-5.29	1.31	1.39
1	F	18	TRP	CE3-CZ3	5.28	1.47	1.38
1	A	96	PHE	CD2-CE2	-5.22	1.28	1.39
1	A	116	ALA	CA-CB	5.19	1.63	1.52
1	D	86	VAL	C-N	5.18	1.42	1.33
1	B	11	ALA	CA-CB	5.17	1.63	1.52
1	A	156	ARG	CB-CG	-5.16	1.38	1.52
1	B	140	GLU	CD-OE1	5.16	1.31	1.25
1	A	5	GLU	CB-CG	-5.12	1.42	1.52
1	A	154	ALA	CA-CB	5.11	1.63	1.52
1	D	136	GLU	CG-CD	5.02	1.59	1.51

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	NE-CZ-NH2	-19.95	110.32	120.30
1	A	72	ARG	NE-CZ-NH1	18.60	129.60	120.30
1	E	78	ARG	NE-CZ-NH2	-17.10	111.75	120.30
1	E	65	ARG	NE-CZ-NH2	-14.02	113.29	120.30
1	E	65	ARG	NE-CZ-NH1	13.45	127.03	120.30
1	A	132	ARG	NE-CZ-NH2	-13.38	113.61	120.30
1	E	78	ARG	NE-CZ-NH1	12.34	126.47	120.30
1	E	151	LEU	CA-CB-CG	9.28	136.65	115.30
1	C	65	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	B	151	LEU	CA-CB-CG	8.86	135.68	115.30
1	C	72	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	E	73	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	151	LEU	CA-CB-CG	8.54	134.94	115.30
1	F	73	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	B	98	LEU	CB-CG-CD2	-8.28	96.93	111.00
1	A	8	VAL	CG1-CB-CG2	8.18	123.99	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	73	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	D	151	LEU	CA-CB-CG	8.07	133.87	115.30
1	F	65	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	A	132	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	72	ARG	CD-NE-CZ	7.71	134.39	123.60
1	D	125	LYS	CB-CA-C	-7.67	95.06	110.40
1	C	151	LEU	CA-CB-CG	7.63	132.86	115.30
1	D	78	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	D	73	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	2	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	40	LEU	CA-CB-CG	7.40	132.33	115.30
1	E	1	MET	CG-SD-CE	7.30	111.88	100.20
1	D	126	LEU	N-CA-CB	7.20	124.81	110.40
1	F	25	LEU	CA-CB-CG	7.18	131.81	115.30
1	F	98	LEU	CA-CB-CG	7.12	131.68	115.30
1	F	98	LEU	CB-CG-CD2	-7.12	98.89	111.00
1	A	151	LEU	CB-CG-CD1	7.09	123.05	111.00
1	A	159	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	151	LEU	CB-CG-CD1	7.00	122.91	111.00
1	A	78	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	E	24	VAL	CG1-CB-CG2	6.95	122.01	110.90
1	E	132	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	D	98	LEU	CB-CG-CD1	6.90	122.72	111.00
1	F	23	ASP	CB-CG-OD1	6.62	124.26	118.30
1	B	139	VAL	CG1-CB-CG2	6.62	121.49	110.90
1	D	65	ARG	NE-CZ-NH2	6.59	123.59	120.30
1	A	25	LEU	CA-CB-CG	6.56	130.40	115.30
1	B	24	VAL	CB-CA-C	-6.52	99.01	111.40
1	D	157	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	118	ASP	CB-CG-OD1	6.50	124.15	118.30
1	E	132	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	F	151	LEU	CA-CB-CG	6.42	130.07	115.30
1	C	24	VAL	CG1-CB-CG2	6.41	121.15	110.90
1	E	78	ARG	CD-NE-CZ	6.28	132.39	123.60
1	C	24	VAL	CB-CA-C	-6.16	99.70	111.40
1	E	69	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	F	65	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	E	146	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	125	LYS	N-CA-C	6.07	127.38	111.00
1	A	50	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	A	141	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	B	8	VAL	CG1-CB-CG2	6.01	120.52	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ARG	CB-CA-C	6.01	122.42	110.40
1	F	24	VAL	CB-CA-C	-5.99	100.03	111.40
1	E	24	VAL	CA-CB-CG2	5.96	119.84	110.90
1	E	151	LEU	CB-CG-CD1	5.94	121.09	111.00
1	D	67	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	25	LEU	CA-CB-CG	5.91	128.88	115.30
1	B	157	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	E	24	VAL	CB-CA-C	-5.85	100.29	111.40
1	A	8	VAL	CA-CB-CG1	5.79	119.59	110.90
1	C	65	ARG	CG-CD-NE	-5.79	99.65	111.80
1	F	24	VAL	CG1-CB-CG2	5.75	120.09	110.90
1	A	132	ARG	CG-CD-NE	-5.74	99.75	111.80
1	C	72	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	E	134	MET	CG-SD-CE	5.65	109.23	100.20
1	D	67	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	F	117	GLY	N-CA-C	5.55	126.97	113.10
1	F	151	LEU	CB-CG-CD1	5.54	120.41	111.00
1	C	98	LEU	CB-CG-CD2	-5.48	101.69	111.00
1	F	40	LEU	CB-CG-CD1	5.44	120.25	111.00
1	C	44	GLN	C-N-CA	-5.39	110.98	122.30
1	E	135	LEU	CB-CG-CD2	5.38	120.14	111.00
1	E	146	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	D	151	LEU	CB-CG-CD1	5.28	119.98	111.00
1	C	94	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	E	144	VAL	CB-CA-C	5.28	121.42	111.40
1	A	38	GLU	OE1-CD-OE2	5.27	129.62	123.30
1	F	47	GLN	CB-CA-C	5.25	120.91	110.40
1	A	24	VAL	CG1-CB-CG2	5.24	119.29	110.90
1	A	119	ASP	CB-CG-OD1	5.24	123.01	118.30
1	C	16	LEU	CB-CG-CD2	5.17	119.80	111.00
1	D	124	GLY	N-CA-C	-5.17	100.17	113.10
1	D	157	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	E	126	LEU	CA-CB-CG	5.11	127.04	115.30
1	F	1	MET	N-CA-C	-5.10	97.23	111.00
1	B	98	LEU	CA-CB-CG	5.09	127.01	115.30
1	D	8	VAL	CG1-CB-CG2	5.08	119.03	110.90
1	E	78	ARG	CG-CD-NE	-5.07	101.15	111.80
1	F	40	LEU	CA-CB-CG	5.05	126.93	115.30
1	A	135	LEU	CB-CG-CD2	5.00	119.50	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	123	ALA	Peptide
1	D	34	THR	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	1300	0	1282	29	0
1	B	1282	0	1263	15	0
1	C	1275	0	1254	48	0
1	D	1275	0	1254	87	0
1	E	1281	0	1259	36	0
1	F	1262	0	1243	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	14	0	19	1	0
3	B	14	0	19	1	0
3	C	14	0	19	2	0
3	D	28	0	38	2	0
3	E	14	0	19	1	0
3	F	14	0	18	2	0
4	A	64	0	0	2	0
4	B	36	0	0	1	0
4	C	17	0	0	0	0
4	D	17	0	0	0	0
4	E	21	0	0	0	0
4	F	13	0	0	3	0
All	All	7945	0	7687	232	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 15.

All (232) 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:D:81:GLU:CA	1:D:82:THR:HG23	1.36	1.48
1:D:55:VAL:CG2	1:D:60:ASN:HB2	1.65	1.25
1:D:81:GLU:N	1:D:82:THR:HG23	1.53	1.22
1:D:81:GLU:HA	1:D:82:THR:CG2	1.76	1.15
1:D:55:VAL:HG21	1:D:60:ASN:HB2	1.26	1.14
1:D:81:GLU:HG2	1:D:81:GLU:O	1.49	1.10
1:E:159:ARG:HG2	1:E:159:ARG:HH11	1.16	1.08
1:D:81:GLU:CA	1:D:82:THR:CG2	2.29	1.07
1:D:84:PRO:HG3	1:D:114:ARG:CB	1.89	1.01
1:A:166:THR:HG22	1:A:167:VAL:H	1.26	1.01
1:C:63:THR:HG22	1:C:80:LEU:HB2	1.41	0.99
1:E:159:ARG:HG2	1:E:159:ARG:NH1	1.70	0.97
1:D:81:GLU:HA	1:D:82:THR:HG23	1.00	0.96
1:D:65:ARG:NH1	1:D:67:ASP:OD2	2.00	0.95
1:E:159:ARG:CG	1:E:159:ARG:HH11	1.79	0.95
1:D:81:GLU:N	1:D:82:THR:CG2	2.30	0.94
1:D:84:PRO:HA	1:D:86:VAL:N	1.84	0.93
1:D:55:VAL:CG2	1:D:60:ASN:CB	2.47	0.91
1:C:1:MET:CE	1:C:88:HIS:CD2	2.54	0.91
1:F:85:ILE:HD12	1:F:122:VAL:HG12	1.51	0.90
1:D:84:PRO:HG3	1:D:114:ARG:HB2	1.52	0.90
1:C:1:MET:HE1	1:C:88:HIS:CD2	2.07	0.88
1:E:119:ASP:N	1:E:120:GLY:HA2	1.90	0.86
1:D:84:PRO:HA	1:D:86:VAL:H	1.38	0.86
1:C:83:ALA:HB1	1:C:84:PRO:CD	2.13	0.78
1:D:53:VAL:HG12	1:D:54:ASP:H	1.47	0.78
1:D:55:VAL:HG21	1:D:60:ASN:CB	2.11	0.77
1:D:84:PRO:HD3	1:D:114:ARG:HG3	1.66	0.77
1:D:81:GLU:O	1:D:81:GLU:CG	2.30	0.76
1:C:10:VAL:HG22	1:C:151:LEU:HB2	1.67	0.75
1:C:83:ALA:HB1	1:C:84:PRO:HD3	1.68	0.74
1:D:80:LEU:C	1:D:82:THR:CG2	2.57	0.74
1:A:50:ARG:HH11	1:A:50:ARG:HG2	1.53	0.73
1:D:28:ALA:HB2	1:D:37:VAL:HG23	1.69	0.73
1:D:63:THR:HG22	1:D:80:LEU:HB2	1.71	0.73
1:D:80:LEU:C	1:D:82:THR:HG23	2.09	0.73
1:D:34:THR:HG21	1:D:51:LEU:HD23	1.71	0.72
1:C:1:MET:HE3	1:C:88:HIS:CD2	2.22	0.72
1:E:88:HIS:NE2	1:E:90:SER:HB2	2.04	0.72
1:D:2:ARG:HB3	1:D:2:ARG:NH1	2.04	0.70
1:D:2:ARG:HH11	1:D:2:ARG:HB3	1.56	0.70
1:F:85:ILE:CD1	1:F:122:VAL:HG12	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:ASP:N	1:D:120:GLY:HA2	2.05	0.70
1:D:36:LYS:HB3	1:D:52:HIS:CD2	2.27	0.69
1:D:81:GLU:HA	1:D:82:THR:CB	2.22	0.69
1:F:137:ALA:O	1:F:141:ARG:HG3	1.94	0.68
1:F:26:GLY:O	1:F:30:ILE:HG23	1.94	0.67
1:D:84:PRO:HG3	1:D:114:ARG:CG	2.25	0.66
1:D:139:VAL:O	1:D:143:SER:HB2	1.95	0.66
1:D:55:VAL:HG23	1:D:60:ASN:HB2	1.73	0.66
1:A:50:ARG:HG2	1:A:50:ARG:NH1	2.09	0.65
1:D:84:PRO:CD	1:D:114:ARG:HG3	2.25	0.65
1:D:82:THR:OG1	1:D:83:ALA:N	2.30	0.64
1:D:49:VAL:HG13	1:D:51:LEU:HD12	1.80	0.64
1:D:122:VAL:HG11	1:D:131:ALA:HB2	1.78	0.64
1:C:24:VAL:HG13	1:C:66:ARG:CZ	2.28	0.63
1:D:24:VAL:O	1:D:27:TYR:HB2	1.98	0.63
1:D:34:THR:CG2	1:D:51:LEU:HD23	2.28	0.63
1:B:111:PHE:CD2	1:B:135:LEU:HD13	2.34	0.62
1:A:153:GLU:OE2	1:E:78:ARG:NH2	2.33	0.62
1:C:63:THR:CG2	1:C:80:LEU:HB2	2.24	0.62
1:D:125:LYS:O	1:D:126:LEU:HD23	2.00	0.62
1:E:119:ASP:H	1:E:120:GLY:HA2	1.65	0.61
1:A:44:GLN:CD	1:A:44:GLN:H	2.02	0.61
1:E:126:LEU:HD23	1:E:131:ALA:HA	1.82	0.61
1:F:123:ALA:O	1:F:125:LYS:HG2	2.01	0.61
1:B:111:PHE:HD2	1:B:135:LEU:HD13	1.66	0.61
1:C:55:VAL:O	1:C:58:GLU:HG2	2.01	0.60
1:C:98:LEU:HD13	1:D:96:PHE:HZ	1.65	0.60
1:D:30:ILE:O	1:D:32:PRO:HD3	2.01	0.60
1:E:58:GLU:HG2	1:E:60:ASN:HD21	1.66	0.60
1:C:139:VAL:O	1:C:143:SER:HB2	2.02	0.60
1:B:64:SER:HB3	1:B:79:GLN:HA	1.84	0.59
1:E:30:ILE:O	1:E:32:PRO:HD3	2.03	0.59
1:A:50:ARG:HH11	1:A:50:ARG:CG	2.14	0.59
1:E:159:ARG:CG	1:E:159:ARG:NH1	2.44	0.59
1:F:129:ASP:HB2	4:F:185:HOH:O	2.03	0.59
1:D:84:PRO:CG	1:D:114:ARG:HG3	2.33	0.58
1:E:85:ILE:HG22	1:E:122:VAL:HG22	1.86	0.58
1:F:141:ARG:NH2	4:F:175:HOH:O	2.36	0.58
1:B:15:ASP:OD1	1:B:73:ARG:NH1	2.36	0.58
1:D:84:PRO:HG3	1:D:114:ARG:HG3	1.85	0.58
1:D:130:GLU:O	1:D:134:MET:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:TRP:HB2	1:C:79:GLN:OE1	2.04	0.57
1:A:166:THR:HG22	1:A:167:VAL:N	2.08	0.57
1:E:153:GLU:OE2	1:E:156:ARG:NH1	2.37	0.57
1:E:72:ARG:NH1	1:F:98:LEU:O	2.38	0.56
1:C:8:VAL:HG13	1:C:151:LEU:HD23	1.87	0.56
1:D:59:ILE:HG12	1:D:59:ILE:O	2.05	0.56
1:F:24:VAL:HG13	1:F:66:ARG:CZ	2.35	0.56
1:D:55:VAL:HG22	1:D:60:ASN:CB	2.34	0.56
1:A:50:ARG:HD2	1:A:51:LEU:N	2.20	0.56
1:C:0:HIS:HB3	1:E:119:ASP:O	2.06	0.55
1:D:125:LYS:CG	1:D:125:LYS:O	2.54	0.55
1:D:85:ILE:HG22	1:D:85:ILE:O	2.07	0.55
1:F:85:ILE:HD12	1:F:122:VAL:CG1	2.32	0.55
1:C:54:ASP:O	1:C:141:ARG:NH2	2.40	0.55
1:D:51:LEU:O	1:D:61:THR:HA	2.07	0.55
1:B:65:ARG:NH1	1:B:67:ASP:OD1	2.39	0.55
1:A:44:GLN:H	1:A:44:GLN:NE2	2.05	0.54
1:A:153:GLU:CD	1:E:78:ARG:HH22	2.12	0.53
1:E:35:GLU:OE1	1:E:59:ILE:HD11	2.08	0.53
1:D:84:PRO:HA	1:D:85:ILE:C	2.27	0.53
1:A:50:ARG:NH1	4:A:215:HOH:O	2.39	0.53
1:C:32:PRO:HD2	1:C:33:PRO:HD2	1.90	0.53
1:E:125:LYS:HD3	1:E:126:LEU:HD13	1.91	0.53
1:B:135:LEU:O	1:B:139:VAL:HG13	2.10	0.52
1:D:122:VAL:HG13	1:D:126:LEU:HB2	1.91	0.52
1:D:85:ILE:O	1:D:85:ILE:CG2	2.57	0.52
1:D:55:VAL:HG21	1:D:60:ASN:HD22	1.73	0.52
1:B:129:ASP:O	1:B:133:GLU:HG2	2.10	0.51
1:C:63:THR:HG23	1:C:80:LEU:HD12	1.93	0.51
1:D:84:PRO:CA	1:D:86:VAL:H	2.17	0.51
1:C:53:VAL:HB	1:C:62:TRP:CH2	2.46	0.50
1:C:98:LEU:HD13	1:D:96:PHE:CZ	2.46	0.50
1:E:85:ILE:HG22	1:E:122:VAL:CG2	2.41	0.50
1:D:158:VAL:O	1:D:162:GLY:N	2.45	0.50
1:A:52:HIS:HB3	1:A:59:ILE:HD11	1.92	0.50
1:C:59:ILE:O	1:C:59:ILE:HG13	2.11	0.50
1:D:82:THR:O	1:D:83:ALA:O	2.30	0.50
1:F:111:PHE:HD2	1:F:135:LEU:HD13	1.76	0.50
1:C:156:ARG:HG2	1:C:159:ARG:HH22	1.77	0.50
1:C:43:GLY:HA3	1:C:46:TYR:CE1	2.47	0.50
1:D:50:ARG:HA	1:D:62:TRP:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASP:HB3	1:E:78:ARG:HD2	1.93	0.49
1:B:25:LEU:HB2	4:B:203:HOH:O	2.12	0.49
1:C:32:PRO:CD	1:C:33:PRO:HD2	2.42	0.49
1:C:109:HIS:NE2	3:C:170:CXS:H4	2.28	0.49
1:B:24:VAL:HG13	1:B:66:ARG:CZ	2.42	0.49
1:F:1:MET:SD	1:F:88:HIS:HD2	2.35	0.49
1:C:40:LEU:N	1:C:40:LEU:CD1	2.76	0.49
1:C:18:TRP:CE2	1:C:70:PRO:HB3	2.48	0.49
1:F:113:THR:HG21	1:F:132:ARG:HA	1.93	0.48
1:A:111:PHE:HD2	1:A:135:LEU:HD13	1.78	0.48
1:C:65:ARG:O	1:C:77:TYR:HA	2.13	0.48
1:D:34:THR:HG21	1:D:51:LEU:CD2	2.42	0.48
1:D:34:THR:HG22	1:D:35:GLU:H	1.79	0.48
1:A:153:GLU:O	1:A:157:ARG:HG3	2.13	0.48
1:B:132:ARG:O	1:B:136:GLU:HG3	2.13	0.48
1:F:151:LEU:HD13	1:F:155:GLU:CD	2.33	0.48
1:D:122:VAL:HG11	1:D:131:ALA:CB	2.43	0.48
1:E:82:THR:HB	1:E:86:VAL:HB	1.96	0.48
1:A:111:PHE:CD2	1:A:135:LEU:HD13	2.49	0.48
1:A:65:ARG:NH1	1:C:78:ARG:NH2	2.62	0.48
1:D:119:ASP:HB2	1:D:121:LEU:H	1.79	0.48
1:F:132:ARG:O	1:F:136:GLU:HG3	2.13	0.48
1:F:62:TRP:HB2	1:F:81:GLU:O	2.14	0.48
1:D:8:VAL:HG13	1:D:151:LEU:HD23	1.96	0.47
1:D:27:TYR:O	1:D:31:PHE:HB2	2.14	0.47
1:C:56:ALA:HB3	1:C:134:MET:CE	2.44	0.47
1:C:156:ARG:O	1:C:156:ARG:HD2	2.15	0.47
1:D:125:LYS:O	1:D:125:LYS:HG2	2.15	0.47
1:F:44:GLN:HE21	1:F:44:GLN:HA	1.79	0.47
1:F:85:ILE:CD1	1:F:122:VAL:CG1	2.92	0.47
1:C:83:ALA:CB	1:C:84:PRO:CD	2.85	0.47
1:D:63:THR:CG2	1:D:80:LEU:HB2	2.42	0.47
1:E:119:ASP:N	1:E:120:GLY:CA	2.72	0.47
1:F:73:ARG:HD3	4:F:174:HOH:O	2.14	0.47
1:F:82:THR:HB	1:F:86:VAL:HB	1.97	0.47
1:C:0:HIS:CB	1:E:119:ASP:O	2.62	0.47
1:A:60:ASN:OD1	1:A:83:ALA:HB1	2.14	0.47
1:B:153:GLU:O	1:B:157:ARG:HG2	2.14	0.47
1:F:25:LEU:CD2	1:F:39:ILE:HD12	2.45	0.46
1:D:23:ASP:O	1:D:25:LEU:O	2.33	0.46
1:B:84:PRO:O	1:B:114:ARG:NE	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ALA:HA	1:E:103:THR:OG1	2.15	0.46
1:F:69:ASP:OD1	1:F:72:ARG:HG3	2.15	0.46
1:F:2:ARG:HD3	1:F:136:GLU:OE2	2.15	0.46
1:A:65:ARG:NH1	1:C:78:ARG:HH22	2.13	0.45
1:A:65:ARG:HH12	1:C:78:ARG:NH2	2.14	0.45
1:D:153:GLU:OE2	1:D:156:ARG:NH1	2.49	0.45
1:D:2:ARG:HH11	1:D:2:ARG:CB	2.28	0.45
1:F:1:MET:SD	1:F:88:HIS:CD2	3.09	0.45
1:C:125:LYS:HG3	1:C:126:LEU:H	1.82	0.45
1:C:1:MET:HE3	1:C:88:HIS:HD2	1.77	0.45
1:E:35:GLU:HG3	1:E:59:ILE:HD13	1.98	0.45
1:C:75:ILE:O	1:C:92:GLU:HA	2.16	0.45
1:D:25:LEU:HD11	1:D:39:ILE:HG13	1.98	0.45
1:C:8:VAL:CG1	1:C:151:LEU:HD23	2.46	0.44
1:D:49:VAL:HG13	1:D:51:LEU:CD1	2.46	0.44
1:D:84:PRO:HG3	1:D:114:ARG:HB3	1.87	0.44
1:D:84:PRO:HB3	1:D:85:ILE:HA	1.99	0.44
1:D:122:VAL:CG1	1:D:126:LEU:HB2	2.46	0.44
1:D:53:VAL:HG12	1:D:54:ASP:N	2.26	0.44
1:E:125:LYS:HB2	1:E:126:LEU:HD13	2.00	0.44
1:D:15:ASP:O	1:D:19:GLU:HG2	2.17	0.44
1:E:37:VAL:HG22	1:E:51:LEU:HD23	1.99	0.44
1:E:58:GLU:CG	1:E:60:ASN:HD21	2.29	0.44
1:E:88:HIS:HB3	1:E:112:VAL:HG12	1.99	0.44
1:F:113:THR:HG22	1:F:135:LEU:HD12	1.99	0.44
1:A:39:ILE:CG2	1:E:-1:SER:HB3	2.48	0.43
1:D:93:TRP:CD2	1:D:107:LEU:HD13	2.53	0.43
1:D:139:VAL:O	1:D:143:SER:CB	2.64	0.43
1:D:62:TRP:HE1	3:D:170:CXS:H31	1.82	0.43
1:B:69:ASP:HA	1:B:70:PRO:HD2	1.77	0.43
1:C:2:ARG:O	1:C:110:ASP:HA	2.18	0.43
1:A:59:ILE:HG23	1:A:59:ILE:O	2.19	0.43
1:D:26:GLY:O	1:D:30:ILE:HG12	2.18	0.43
1:D:33:PRO:HB2	1:D:53:VAL:CG1	2.48	0.43
1:D:111:PHE:HD2	1:D:135:LEU:HD13	1.83	0.43
1:D:65:ARG:O	1:D:77:TYR:HA	2.19	0.43
1:A:56:ALA:O	1:A:57:GLY:C	2.56	0.43
1:C:56:ALA:HB3	1:C:134:MET:HE2	2.00	0.43
1:A:39:ILE:HG21	1:E:-1:SER:HB3	2.01	0.43
1:C:113:THR:HG21	1:C:131:ALA:HB1	2.00	0.43
1:D:85:ILE:HD13	1:D:126:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:VAL:HG13	1:A:66:ARG:CZ	2.49	0.42
1:C:43:GLY:O	1:C:44:GLN:C	2.58	0.42
1:C:119:ASP:HB3	1:C:121:LEU:HG	2.02	0.42
1:D:24:VAL:HG13	1:D:66:ARG:CZ	2.50	0.42
1:C:119:ASP:CB	1:C:121:LEU:HG	2.49	0.42
1:E:32:PRO:HB2	1:E:33:PRO:HD3	2.01	0.42
1:F:77:TYR:CZ	3:F:171:CXS:H21	2.55	0.42
1:F:111:PHE:CD2	1:F:135:LEU:HD13	2.55	0.42
1:B:129:ASP:OD1	1:B:132:ARG:NH1	2.53	0.42
1:F:153:GLU:OE1	1:F:153:GLU:HA	2.20	0.41
1:B:77:TYR:HB2	3:B:171:CXS:O1	2.21	0.41
3:F:171:CXS:H91	3:F:171:CXS:H31	1.78	0.41
1:A:0:HIS:HB3	4:A:222:HOH:O	2.21	0.41
1:C:40:LEU:HD12	1:C:40:LEU:N	2.35	0.41
1:A:65:ARG:HH12	1:C:78:ARG:HH22	1.68	0.41
1:E:51:LEU:HD13	3:E:171:CXS:O3	2.20	0.41
1:D:109:HIS:NE2	3:D:170:CXS:H51	2.36	0.41
1:E:158:VAL:HG12	1:E:159:ARG:N	2.35	0.41
1:E:75:ILE:HD13	1:E:75:ILE:HG21	1.77	0.41
1:F:25:LEU:HD22	1:F:39:ILE:CD1	2.51	0.40
3:A:171:CXS:H31	3:A:171:CXS:H52	1.97	0.40
1:A:50:ARG:HD2	1:A:51:LEU:H	1.85	0.40
1:A:55:VAL:N	1:A:58:GLU:O	2.50	0.40
1:E:96:PHE:HZ	1:F:98:LEU:HD13	1.85	0.40
1:D:96:PHE:HB2	1:D:104:GLN:HB3	2.04	0.40
1:C:66:ARG:NH1	3:C:170:CXS:O1	2.53	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	166/172 (96%)	159 (96%)	7 (4%)	0	100	100
1	B	163/172 (95%)	157 (96%)	6 (4%)	0	100	100
1	C	162/172 (94%)	148 (91%)	12 (7%)	2 (1%)	13	19
1	D	162/172 (94%)	139 (86%)	20 (12%)	3 (2%)	8	10
1	E	163/172 (95%)	153 (94%)	10 (6%)	0	100	100
1	F	159/172 (92%)	154 (97%)	4 (2%)	1 (1%)	25	36
All	All	975/1032 (94%)	910 (93%)	59 (6%)	6 (1%)	25	36

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100	ALA
1	D	82	THR
1	F	124	GLY
1	D	83	ALA
1	C	117	GLY
1	D	84	PRO

### 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	134/136 (98%)	119 (89%)	15 (11%)	6	8
1	B	132/136 (97%)	114 (86%)	18 (14%)	3	4
1	C	131/136 (96%)	109 (83%)	22 (17%)	2	2
1	D	131/136 (96%)	113 (86%)	18 (14%)	3	4
1	E	132/136 (97%)	113 (86%)	19 (14%)	3	3
1	F	131/136 (96%)	114 (87%)	17 (13%)	4	4
All	All	791/816 (97%)	682 (86%)	109 (14%)	3	4

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	24	VAL
1	A	25	LEU
1	A	40	LEU
1	A	44	GLN
1	A	49	VAL
1	A	50	ARG
1	A	54	ASP
1	A	55	VAL
1	A	58	GLU
1	A	125	LYS
1	A	135	LEU
1	A	138	VAL
1	A	151	LEU
1	A	166	THR
1	B	0	HIS
1	B	2	ARG
1	B	8	VAL
1	B	24	VAL
1	B	25	LEU
1	B	40	LEU
1	B	49	VAL
1	B	54	ASP
1	B	58	GLU
1	B	59	ILE
1	B	60	ASN
1	B	130	GLU
1	B	135	LEU
1	B	139	VAL
1	B	142	ASN
1	B	143	SER
1	B	151	LEU
1	B	157	ARG
1	C	2	ARG
1	C	8	VAL
1	C	16	LEU
1	C	24	VAL
1	C	25	LEU
1	C	35	GLU
1	C	40	LEU
1	C	44	GLN
1	C	49	VAL
1	C	58	GLU

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Mol	Chain	Res	Type
1	C	60	ASN
1	C	63	THR
1	C	73	ARG
1	C	85	ILE
1	C	113	THR
1	C	118	ASP
1	C	122	VAL
1	C	133	GLU
1	C	135	LEU
1	C	143	SER
1	C	144	VAL
1	C	151	LEU
1	D	2	ARG
1	D	8	VAL
1	D	24	VAL
1	D	39	ILE
1	D	44	GLN
1	D	59	ILE
1	D	63	THR
1	D	81	GLU
1	D	82	THR
1	D	114	ARG
1	D	119	ASP
1	D	122	VAL
1	D	134	MET
1	D	135	LEU
1	D	136	GLU
1	D	144	VAL
1	D	151	LEU
1	D	156	ARG
1	E	1	MET
1	E	2	ARG
1	E	24	VAL
1	E	25	LEU
1	E	35	GLU
1	E	38	GLU
1	E	40	LEU
1	E	44	GLN
1	E	49	VAL
1	E	58	GLU
1	E	65	ARG
1	E	121	LEU

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Mol	Chain	Res	Type
1	E	122	VAL
1	E	125	LYS
1	E	126	LEU
1	E	135	LEU
1	E	151	LEU
1	E	158	VAL
1	E	159	ARG
1	F	1	MET
1	F	2	ARG
1	F	24	VAL
1	F	25	LEU
1	F	30	ILE
1	F	40	LEU
1	F	44	GLN
1	F	47	GLN
1	F	49	VAL
1	F	50	ARG
1	F	51	LEU
1	F	65	ARG
1	F	129	ASP
1	F	132	ARG
1	F	133	GLU
1	F	135	LEU
1	F	151	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	44	GLN
1	B	142	ASN
1	C	44	GLN
1	D	6	HIS
1	E	52	HIS
1	E	60	ASN
1	F	44	GLN
1	F	60	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	CXS	E	171	-	14,14,14	1.56	2 (14%)	18,18,18	2.52	6 (33%)
3	CXS	A	171	-	14,14,14	1.64	1 (7%)	18,18,18	2.87	6 (33%)
3	CXS	D	170	-	14,14,14	1.65	1 (7%)	18,18,18	2.09	6 (33%)
3	CXS	C	170	-	14,14,14	1.87	1 (7%)	18,18,18	2.09	5 (27%)
3	CXS	F	171	-	14,14,14	1.76	1 (7%)	18,18,18	3.13	5 (27%)
3	CXS	B	171	-	14,14,14	1.48	2 (14%)	18,18,18	2.49	7 (38%)
3	CXS	D	171	-	14,14,14	1.55	2 (14%)	18,18,18	2.86	5 (27%)

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	CXS	E	171	-	-	4/8/16/16	0/1/1/1
3	CXS	A	171	-	-	4/8/16/16	0/1/1/1
3	CXS	D	170	-	-	4/8/16/16	0/1/1/1
3	CXS	C	170	-	-	3/8/16/16	0/1/1/1
3	CXS	F	171	-	-	6/8/16/16	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CXS	B	171	-	-	4/8/16/16	0/1/1/1
3	CXS	D	171	-	-	5/8/16/16	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	170	CXS	C1-S	-6.19	1.68	1.77
3	F	171	CXS	C1-S	-5.84	1.69	1.77
3	A	171	CXS	C1-S	-5.44	1.69	1.77
3	D	170	CXS	C1-S	-5.06	1.70	1.77
3	E	171	CXS	C1-S	-4.05	1.71	1.77
3	D	171	CXS	C1-S	-3.91	1.72	1.77
3	B	171	CXS	C1-S	-3.91	1.72	1.77
3	E	171	CXS	O2-S	2.93	1.53	1.45
3	D	171	CXS	C5-C4	2.52	1.57	1.52
3	B	171	CXS	O1-S	2.43	1.52	1.45

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	171	CXS	O2-S-C1	10.33	119.35	106.92
3	A	171	CXS	O1-S-C1	9.02	117.77	106.92
3	D	171	CXS	O1-S-C1	7.36	115.78	106.92
3	E	171	CXS	O1-S-C1	6.88	115.19	106.92
3	F	171	CXS	C2-C1-S	6.27	122.86	113.25
3	B	171	CXS	O1-S-C1	5.85	113.96	106.92
3	D	171	CXS	C3-N-C4	5.63	125.19	114.14
3	D	170	CXS	C3-N-C4	5.50	124.93	114.14
3	C	170	CXS	C3-N-C4	5.39	124.72	114.14
3	E	171	CXS	C3-N-C4	5.01	123.98	114.14
3	B	171	CXS	O3-S-C1	4.63	113.25	105.77
3	B	171	CXS	O2-S-C1	-4.44	101.56	106.92
3	D	171	CXS	O3-S-O1	-4.43	100.44	111.27
3	A	171	CXS	C9-C4-C5	-4.40	103.19	110.82
3	D	171	CXS	C8-C9-C4	4.12	118.86	111.11
3	A	171	CXS	C3-N-C4	3.96	121.92	114.14
3	E	171	CXS	C9-C4-C5	-3.77	104.28	110.82
3	D	171	CXS	C7-C8-C9	3.59	118.73	111.42
3	C	170	CXS	O3-S-C1	3.41	111.29	105.77
3	D	170	CXS	C8-C9-C4	3.26	117.24	111.11
3	B	171	CXS	O2-S-O1	-3.21	102.84	113.95
3	F	171	CXS	O2-S-O1	-3.11	103.18	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	170	CXS	O1-S-C1	2.84	110.33	106.92
3	A	171	CXS	C8-C7-C6	-2.77	102.64	111.18
3	B	171	CXS	C3-N-C4	2.74	119.53	114.14
3	A	171	CXS	O3-S-O1	-2.62	104.86	111.27
3	D	170	CXS	O1-S-C1	2.62	110.07	106.92
3	F	171	CXS	C8-C9-C4	2.60	116.01	111.11
3	E	171	CXS	O3-S-O1	-2.60	104.93	111.27
3	C	170	CXS	O2-S-C1	2.59	110.04	106.92
3	D	170	CXS	O3-S-C1	2.56	109.92	105.77
3	E	171	CXS	C8-C9-C4	2.51	115.83	111.11
3	D	170	CXS	C2-C1-S	2.38	116.89	113.25
3	E	171	CXS	C7-C8-C9	2.37	116.24	111.42
3	C	170	CXS	O3-S-O2	-2.18	105.96	111.27
3	F	171	CXS	C7-C8-C9	-2.14	107.05	111.42
3	B	171	CXS	C7-C6-C5	2.14	115.78	111.42
3	A	171	CXS	C7-C6-C5	2.11	115.72	111.42
3	B	171	CXS	C9-C4-C5	-2.10	107.18	110.82
3	D	170	CXS	O2-S-O1	-2.01	106.99	113.95

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	171	CXS	S-C1-C2-C3
3	A	171	CXS	C5-C4-N-C3
3	F	171	CXS	C1-C2-C3-N
3	F	171	CXS	C9-C4-N-C3
3	B	171	CXS	C2-C1-S-O2
3	B	171	CXS	C2-C1-S-O3
3	D	171	CXS	C1-C2-C3-N
3	D	171	CXS	C9-C4-N-C3
3	D	170	CXS	C2-C1-S-O3
3	F	171	CXS	C2-C1-S-O3
3	C	170	CXS	C1-C2-C3-N
3	E	171	CXS	S-C1-C2-C3
3	E	171	CXS	C2-C3-N-C4
3	B	171	CXS	C2-C3-N-C4
3	D	170	CXS	C2-C1-S-O1
3	D	170	CXS	C2-C1-S-O2
3	F	171	CXS	C2-C1-S-O1
3	F	171	CXS	C2-C1-S-O2
3	B	171	CXS	C2-C1-S-O1

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Mol	Chain	Res	Type	Atoms
3	D	171	CXS	C2-C1-S-O2
3	C	170	CXS	S-C1-C2-C3
3	A	171	CXS	C2-C3-N-C4
3	D	170	CXS	C2-C3-N-C4
3	C	170	CXS	C2-C3-N-C4
3	F	171	CXS	C5-C4-N-C3
3	E	171	CXS	C2-C1-S-O2
3	E	171	CXS	C1-C2-C3-N
3	A	171	CXS	C9-C4-N-C3
3	D	171	CXS	C5-C4-N-C3
3	D	171	CXS	C2-C1-S-O3

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	171	CXS	1	0
3	A	171	CXS	1	0
3	D	170	CXS	2	0
3	C	170	CXS	2	0
3	F	171	CXS	2	0
3	B	171	CXS	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	168/172 (97%)	0.05	1 (0%) 89 88	12, 24, 46, 69	0
1	B	165/172 (95%)	0.14	9 (5%) 25 24	13, 28, 63, 88	0
1	C	164/172 (95%)	0.77	33 (20%) 1 0	22, 48, 100, 131	0
1	D	164/172 (95%)	0.72	25 (15%) 2 1	19, 54, 123, 156	0
1	E	165/172 (95%)	0.07	10 (6%) 21 20	17, 34, 82, 118	0
1	F	161/172 (93%)	0.09	5 (3%) 49 47	19, 41, 93, 128	0
All	All	987/1032 (95%)	0.30	83 (8%) 11 10	12, 36, 97, 156	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	163	GLY	9.3
1	B	164	VAL	7.9
1	B	161	ALA	7.8
1	D	57	GLY	6.7
1	C	162	GLY	6.4
1	C	56	ALA	6.3
1	C	117	GLY	6.1
1	F	117	GLY	6.1
1	C	59	ILE	5.9
1	D	62	TRP	5.7
1	D	117	GLY	5.5
1	F	56	ALA	5.5
1	D	116	ALA	5.4
1	D	125	LYS	5.4
1	B	56	ALA	5.3
1	E	56	ALA	5.3
1	D	56	ALA	5.1
1	C	124	GLY	5.0
1	C	115	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	119	ASP	4.8
1	C	116	ALA	4.7
1	C	35	GLU	4.5
1	D	121	LEU	4.5
1	E	124	GLY	4.5
1	D	126	LEU	4.4
1	D	122	VAL	4.3
1	C	120	GLY	4.3
1	C	62	TRP	4.3
1	C	121	LEU	4.2
1	F	0	HIS	4.0
1	D	134	MET	4.0
1	C	52	HIS	4.0
1	D	85	ILE	3.9
1	C	118	ASP	3.8
1	C	57	GLY	3.7
1	C	134	MET	3.7
1	E	119	ASP	3.5
1	B	59	ILE	3.5
1	C	34	THR	3.5
1	E	126	LEU	3.1
1	B	55	VAL	3.1
1	C	53	VAL	3.0
1	B	54	ASP	3.0
1	F	118	ASP	3.0
1	D	39	ILE	3.0
1	D	51	LEU	3.0
1	D	118	ASP	3.0
1	C	37	VAL	2.9
1	D	82	THR	2.9
1	C	125	LYS	2.8
1	D	88	HIS	2.8
1	B	53	VAL	2.7
1	C	84	PRO	2.7
1	C	122	VAL	2.7
1	E	123	ALA	2.7
1	C	60	ASN	2.6
1	B	0	HIS	2.6
1	E	122	VAL	2.6
1	D	0	HIS	2.6
1	C	85	ILE	2.6
1	D	124	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	123	ALA	2.5
1	D	53	VAL	2.5
1	E	121	LEU	2.4
1	D	60	ASN	2.4
1	D	119	ASP	2.4
1	C	126	LEU	2.4
1	D	123	ALA	2.4
1	D	162	GLY	2.3
1	E	57	GLY	2.3
1	E	55	VAL	2.3
1	C	54	ASP	2.3
1	C	36	LYS	2.2
1	D	128	PRO	2.2
1	C	132	ARG	2.2
1	C	55	VAL	2.1
1	C	83	ALA	2.1
1	C	82	THR	2.1
1	B	57	GLY	2.1
1	D	131	ALA	2.1
1	A	57	GLY	2.1
1	E	127	THR	2.0
1	F	59	ILE	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. 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(Å <sup>2</sup> )	Q<0.9
3	CXS	B	171	14/14	0.76	0.21	57,60,80,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CXS	D	170	14/14	0.88	0.19	76,81,85,85	0
3	CXS	E	171	14/14	0.90	0.18	39,45,51,57	0
2	K	F	170	1/1	0.95	0.05	53,53,53,53	0
3	CXS	D	171	14/14	0.95	0.14	38,41,49,49	0
3	CXS	C	170	14/14	0.96	0.18	55,57,61,62	0
3	CXS	F	171	14/14	0.97	0.13	44,47,51,52	0
3	CXS	A	171	14/14	0.98	0.17	27,36,41,41	0
2	K	B	170	1/1	0.98	0.06	56,56,56,56	0
2	K	E	170	1/1	0.98	0.03	36,36,36,36	0
2	K	A	170	1/1	0.99	0.10	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.