WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2021 – 10:02 am BST

PDB ID	:	7AI2
Title	:	Crystal structure of Se-Met labelled MCE domain of Mce4A from Mycobacterium tuberculosis H37Rv
Authors	:	Asthana, P.; Venkatesan, R.
Deposited on	:	2020-09-25
Resolution	:	3.61 Å(reported)

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

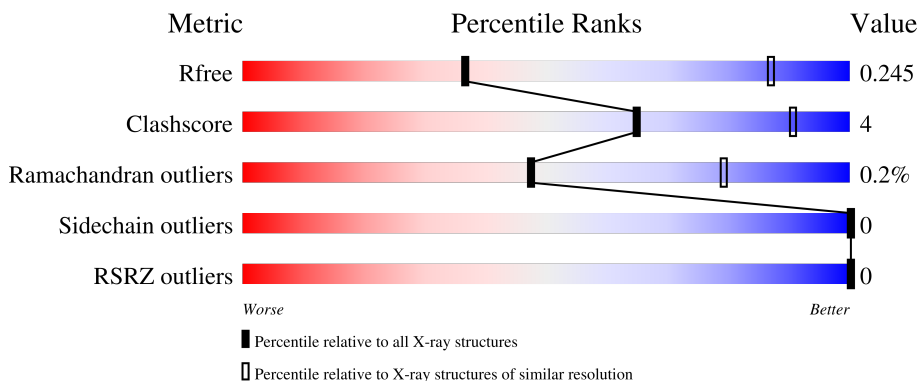|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.61 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		0
RSRZ outliers		0

Worse ← → *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1290 (3.74-3.50)
Clashscore	141614	1387 (3.74-3.50)
Ramachandran outliers	138981	1339 (3.74-3.50)
Sidechain outliers	138945	1339 (3.74-3.50)
RSRZ outliers	127900	1191 (3.74-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	138	65%　　12%　　22%
1	B	138	66%　　16%　　18%
1	C	138	78%　　·　　18%
1	D	138	75%　　·　　22%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 3271 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 Mce-family protein Mce4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	Se	0	0	0
			797	501	143	151	2			
1	B	113	Total	C	N	O	Se	0	0	0
			841	531	148	159	3			
1	C	113	Total	C	N	O	Se	0	0	0
			841	531	148	159	3			
1	D	107	Total	C	N	O	Se	0	0	0
			792	498	141	151	2			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MSE	-	initiating methionine	UNP I6YC99
A	12	LYS	-	expression tag	UNP I6YC99
A	13	HIS	-	expression tag	UNP I6YC99
A	14	HIS	-	expression tag	UNP I6YC99
A	15	HIS	-	expression tag	UNP I6YC99
A	16	HIS	-	expression tag	UNP I6YC99
A	17	HIS	-	expression tag	UNP I6YC99
A	18	HIS	-	expression tag	UNP I6YC99
A	19	PRO	-	expression tag	UNP I6YC99
A	20	MSE	-	expression tag	UNP I6YC99
A	21	SER	-	expression tag	UNP I6YC99
A	22	ASP	-	expression tag	UNP I6YC99
A	23	TYR	-	expression tag	UNP I6YC99
A	24	ASP	-	expression tag	UNP I6YC99
A	25	ILE	-	expression tag	UNP I6YC99
A	26	PRO	-	expression tag	UNP I6YC99
A	27	THR	-	expression tag	UNP I6YC99
A	28	THR	-	expression tag	UNP I6YC99
A	29	GLU	-	expression tag	UNP I6YC99
A	30	ASN	-	expression tag	UNP I6YC99
A	31	LEU	-	expression tag	UNP I6YC99

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Chain	Residue	Modelled	Actual	Comment	Reference
A	32	TYR	-	expression tag	UNP I6YC99
A	33	PHE	-	expression tag	UNP I6YC99
A	34	GLN	-	expression tag	UNP I6YC99
A	35	GLY	-	expression tag	UNP I6YC99
A	36	ALA	-	expression tag	UNP I6YC99
A	37	MSE	-	expression tag	UNP I6YC99
A	38	ALA	-	expression tag	UNP I6YC99
A	141	LEU	-	expression tag	UNP I6YC99
A	142	GLU	-	expression tag	UNP I6YC99
A	143	HIS	-	expression tag	UNP I6YC99
A	144	HIS	-	expression tag	UNP I6YC99
A	145	HIS	-	expression tag	UNP I6YC99
A	146	HIS	-	expression tag	UNP I6YC99
A	147	HIS	-	expression tag	UNP I6YC99
A	148	HIS	-	expression tag	UNP I6YC99
B	11	MSE	-	initiating methionine	UNP I6YC99
B	12	LYS	-	expression tag	UNP I6YC99
B	13	HIS	-	expression tag	UNP I6YC99
B	14	HIS	-	expression tag	UNP I6YC99
B	15	HIS	-	expression tag	UNP I6YC99
B	16	HIS	-	expression tag	UNP I6YC99
B	17	HIS	-	expression tag	UNP I6YC99
B	18	HIS	-	expression tag	UNP I6YC99
B	19	PRO	-	expression tag	UNP I6YC99
B	20	MSE	-	expression tag	UNP I6YC99
B	21	SER	-	expression tag	UNP I6YC99
B	22	ASP	-	expression tag	UNP I6YC99
B	23	TYR	-	expression tag	UNP I6YC99
B	24	ASP	-	expression tag	UNP I6YC99
B	25	ILE	-	expression tag	UNP I6YC99
B	26	PRO	-	expression tag	UNP I6YC99
B	27	THR	-	expression tag	UNP I6YC99
B	28	THR	-	expression tag	UNP I6YC99
B	29	GLU	-	expression tag	UNP I6YC99
B	30	ASN	-	expression tag	UNP I6YC99
B	31	LEU	-	expression tag	UNP I6YC99
B	32	TYR	-	expression tag	UNP I6YC99
B	33	PHE	-	expression tag	UNP I6YC99
B	34	GLN	-	expression tag	UNP I6YC99
B	35	GLY	-	expression tag	UNP I6YC99
B	36	ALA	-	expression tag	UNP I6YC99
B	37	MSE	-	expression tag	UNP I6YC99

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Chain	Residue	Modelled	Actual	Comment	Reference
B	38	ALA	-	expression tag	UNP I6YC99
B	141	LEU	-	expression tag	UNP I6YC99
B	142	GLU	-	expression tag	UNP I6YC99
B	143	HIS	-	expression tag	UNP I6YC99
B	144	HIS	-	expression tag	UNP I6YC99
B	145	HIS	-	expression tag	UNP I6YC99
B	146	HIS	-	expression tag	UNP I6YC99
B	147	HIS	-	expression tag	UNP I6YC99
B	148	HIS	-	expression tag	UNP I6YC99
C	11	MSE	-	initiating methionine	UNP I6YC99
C	12	LYS	-	expression tag	UNP I6YC99
C	13	HIS	-	expression tag	UNP I6YC99
C	14	HIS	-	expression tag	UNP I6YC99
C	15	HIS	-	expression tag	UNP I6YC99
C	16	HIS	-	expression tag	UNP I6YC99
C	17	HIS	-	expression tag	UNP I6YC99
C	18	HIS	-	expression tag	UNP I6YC99
C	19	PRO	-	expression tag	UNP I6YC99
C	20	MSE	-	expression tag	UNP I6YC99
C	21	SER	-	expression tag	UNP I6YC99
C	22	ASP	-	expression tag	UNP I6YC99
C	23	TYR	-	expression tag	UNP I6YC99
C	24	ASP	-	expression tag	UNP I6YC99
C	25	ILE	-	expression tag	UNP I6YC99
C	26	PRO	-	expression tag	UNP I6YC99
C	27	THR	-	expression tag	UNP I6YC99
C	28	THR	-	expression tag	UNP I6YC99
C	29	GLU	-	expression tag	UNP I6YC99
C	30	ASN	-	expression tag	UNP I6YC99
C	31	LEU	-	expression tag	UNP I6YC99
C	32	TYR	-	expression tag	UNP I6YC99
C	33	PHE	-	expression tag	UNP I6YC99
C	34	GLN	-	expression tag	UNP I6YC99
C	35	GLY	-	expression tag	UNP I6YC99
C	36	ALA	-	expression tag	UNP I6YC99
C	37	MSE	-	expression tag	UNP I6YC99
C	38	ALA	-	expression tag	UNP I6YC99
C	141	LEU	-	expression tag	UNP I6YC99
C	142	GLU	-	expression tag	UNP I6YC99
C	143	HIS	-	expression tag	UNP I6YC99
C	144	HIS	-	expression tag	UNP I6YC99
C	145	HIS	-	expression tag	UNP I6YC99

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| Chain	Residue	Modelled	Actual	Comment	Reference
C	146	HIS	-	expression tag	UNP I6YC99
C	147	HIS	-	expression tag	UNP I6YC99
C	148	HIS	-	expression tag	UNP I6YC99
D	11	MSE	-	initiating methionine	UNP I6YC99
D	12	LYS	-	expression tag	UNP I6YC99
D	13	HIS	-	expression tag	UNP I6YC99
D	14	HIS	-	expression tag	UNP I6YC99
D	15	HIS	-	expression tag	UNP I6YC99
D	16	HIS	-	expression tag	UNP I6YC99
D	17	HIS	-	expression tag	UNP I6YC99
D	18	HIS	-	expression tag	UNP I6YC99
D	19	PRO	-	expression tag	UNP I6YC99
D	20	MSE	-	expression tag	UNP I6YC99
D	21	SER	-	expression tag	UNP I6YC99
D	22	ASP	-	expression tag	UNP I6YC99
D	23	TYR	-	expression tag	UNP I6YC99
D	24	ASP	-	expression tag	UNP I6YC99
D	25	ILE	-	expression tag	UNP I6YC99
D	26	PRO	-	expression tag	UNP I6YC99
D	27	THR	-	expression tag	UNP I6YC99
D	28	THR	-	expression tag	UNP I6YC99
D	29	GLU	-	expression tag	UNP I6YC99
D	30	ASN	-	expression tag	UNP I6YC99
D	31	LEU	-	expression tag	UNP I6YC99
D	32	TYR	-	expression tag	UNP I6YC99
D	33	PHE	-	expression tag	UNP I6YC99
D	34	GLN	-	expression tag	UNP I6YC99
D	35	GLY	-	expression tag	UNP I6YC99
D	36	ALA	-	expression tag	UNP I6YC99
D	37	MSE	-	expression tag	UNP I6YC99
D	38	ALA	-	expression tag	UNP I6YC99
D	141	LEU	-	expression tag	UNP I6YC99
D	142	GLU	-	expression tag	UNP I6YC99
D	143	HIS	-	expression tag	UNP I6YC99
D	144	HIS	-	expression tag	UNP I6YC99
D	145	HIS	-	expression tag	UNP I6YC99
D	146	HIS	-	expression tag	UNP I6YC99
D	147	HIS	-	expression tag	UNP I6YC99
D	148	HIS	-	expression tag	UNP I6YC99

3 Residue-property plots ⓘ

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.
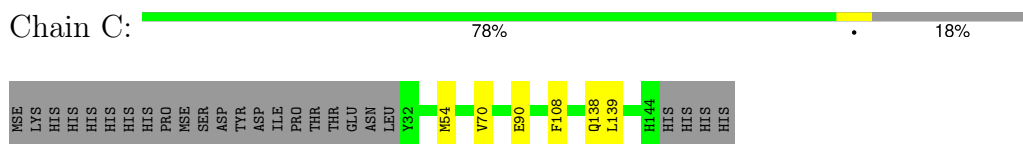
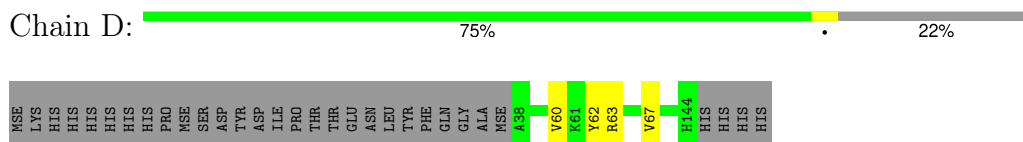- Molecule 1: Mce-family protein Mce4A
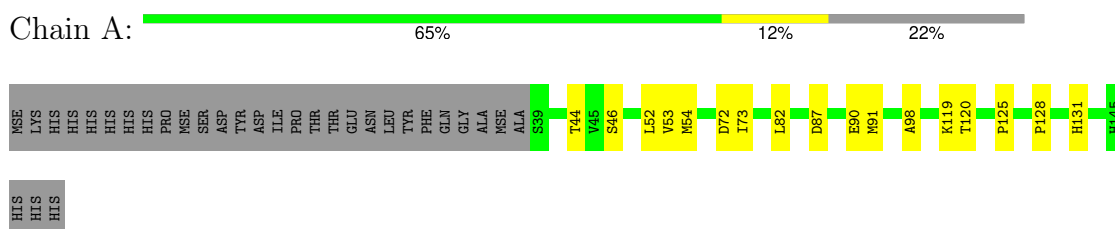
Chain A:

- Molecule 1: Mce-family protein Mce4A

Chain B:

- Molecule 1: Mce-family protein Mce4A

Chain C:

- Molecule 1: Mce-family protein Mce4A

Chain D:
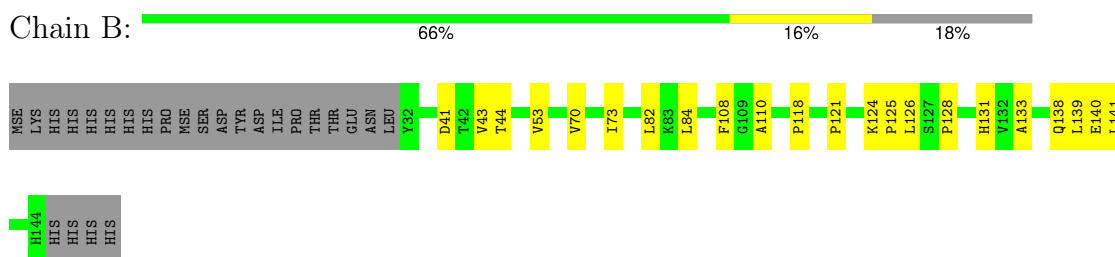
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	134.02Å 134.02Å 105.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.87 – 3.61	Depositor
	48.04 – 3.61	EDS
% Data completeness (in resolution range)	99.9 (43.87-3.61)	Depositor
	99.9 (48.04-3.61)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.216 , 0.247	Depositor
	0.216 , 0.245	DCC
R_{free} test set	655 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å^2)	133.0	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< |L| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.116 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3271	wwPDB-VP
Average B, all atoms (Å^2)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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	0.24	0/811	0.45	0/1096
1	B	0.25	0/855	0.47	0/1153
1	C	0.24	0/855	0.46	0/1153
1	D	0.24	0/805	0.45	0/1088
All	All	0.24	0/3326	0.46	0/4490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	797	0	814	13	0
1	B	841	0	855	18	0
1	C	841	0	855	4	0
1	D	792	0	812	2	0
All	All	3271	0	3336	27	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 4.

The worst 5 of 27 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:52:LEU:HD11	1:B:110:ALA:HB2	1.79	0.65
1:A:98:ALA:HA	1:B:118:PRO:HD3	1.83	0.61
1:B:43:VAL:O	1:B:84:LEU:HB2	2.06	0.55
1:A:54:MSE:HE3	1:B:110:ALA:HB1	1.87	0.54
1:D:62:TYR:CE2	1:D:63:ARG:HG3	2.42	0.54

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/138 (76%)	98 (93%)	6 (6%)	1 (1%)	15	54
1	B	111/138 (80%)	103 (93%)	8 (7%)	0	100	100
1	C	111/138 (80%)	104 (94%)	7 (6%)	0	100	100
1	D	105/138 (76%)	100 (95%)	5 (5%)	0	100	100
All	All	432/552 (78%)	405 (94%)	26 (6%)	1 (0%)	47	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	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	88/111 (79%)	88 (100%)	0	100	100
1	B	91/111 (82%)	91 (100%)	0	100	100
1	C	91/111 (82%)	91 (100%)	0	100	100
1	D	87/111 (78%)	87 (100%)	0	100	100
All	All	357/444 (80%)	357 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	138	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	105/138 (76%)	-0.09	0	100	100	105, 150, 207, 244	0
1	B	110/138 (79%)	-0.19	0	100	100	95, 151, 214, 259	0
1	C	110/138 (79%)	-0.19	0	100	100	96, 156, 226, 251	0
1	D	105/138 (76%)	-0.19	0	100	100	97, 147, 232, 293	0
All	All	430/552 (77%)	-0.17	0	100	100	95, 151, 226, 293	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.