

wwPDB X-ray Structure Validation Summary Report (i)

Mar 10, 2021 - 02:05 am GMT

PDB ID : 6ZNR

Title: MaeB PTA domain R535A mutant Authors: Lovering, A.L.; Harding, C.J.

Deposited on : 2020-07-06

Resolution : 2.22 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

EDS : 2.17.1

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)

al geometry (DNA, RNA) : Parkinson et al. (1996)

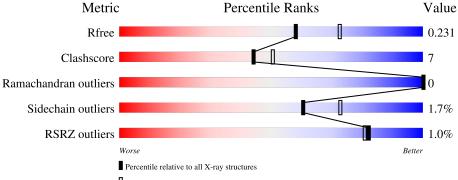
Ideal geometry (DNA, RNA) : Parkin Validation Pipeline (wwPDB-VP) : 2.17.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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.



Percentile relative to X-ray structures of similar resolution

Metric	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	362	79%	13%	• 7%
1	В	362	78%	14%	• 7%
1	С	362	83%	9%	• 6%
1	D	362	76%	15%	•• 6%
1	Е	362	81%	11%	• 7%



Continued from previous page...

Mol	Chain	Length	Quality of chain		
1	F	362	% 	12%	• 7%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16005 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	С	N	О	S	0	0	0
1	A	330	2592	1655	441	485	11	0	0	
1	В	338	Total	С	N	О	S	0	0	0
1	Б	330	2592	1655	441	485	11	0	0	
1	D	340	Total	С	N	О	S	0	0	
1	ש	340	2608	1664	445	488	11		0	
1	F	338	Total	С	N	О	S	0	0	0
1	L'	330	2592	1655	441	485	11	0	0	
1	Е	338	Total	С	N	О	S	0	0	0
1	1 E	330	2592	1655	441	485	11	0	0	
1	C	220	Total	С	N	О	S	0	0	0
1	1 C	339	2597	1658	442	486	11		0	

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	initiating methionine	UNP Q6MM15
A	420	GLY	-	expression tag	UNP Q6MM15
A	421	SER	-	expression tag	UNP Q6MM15
A	422	SER	-	expression tag	UNP Q6MM15
A	423	HIS	_	expression tag	UNP Q6MM15
A	424	HIS	-	expression tag	UNP Q6MM15
A	425	HIS	_	expression tag	UNP Q6MM15
A	426	HIS	_	expression tag	UNP Q6MM15
A	427	HIS	_	expression tag	UNP Q6MM15
A	428	HIS	_	expression tag	UNP Q6MM15
A	429	SER	-	expression tag	UNP Q6MM15
A	430	SER	_	expression tag	UNP Q6MM15
A	431	GLY	-	expression tag	UNP Q6MM15
A	432	LEU	-	expression tag	UNP Q6MM15
A	433	VAL	-	expression tag	UNP Q6MM15
A	434	PRO	-	expression tag	UNP Q6MM15
A	435	ALA	-	expression tag	UNP Q6MM15



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	GLY	_	expression tag	UNP Q6MM15
A	437	SER	-	expression tag	UNP Q6MM15
A	438	HIS	-	expression tag	UNP Q6MM15
A	535	ALA	ARG	engineered mutation	UNP Q6MM15
В	419	MET	_	initiating methionine	UNP Q6MM15
В	420	GLY	_	expression tag	UNP Q6MM15
В	421	SER	_	expression tag	UNP Q6MM15
В	422	SER	_	expression tag	UNP Q6MM15
В	423	HIS	_	expression tag	UNP Q6MM15
В	424	HIS	-	expression tag	UNP Q6MM15
В	425	HIS	_	expression tag	UNP Q6MM15
В	426	HIS	_	expression tag	UNP Q6MM15
В	427	HIS	_	expression tag	UNP Q6MM15
В	428	HIS	_	expression tag	UNP Q6MM15
В	429	SER	_	expression tag	UNP Q6MM15
В	430	SER	_	expression tag	UNP Q6MM15
В	431	GLY	_	expression tag	UNP Q6MM15
В	432	LEU	_	expression tag	UNP Q6MM15
В	433	VAL	_	expression tag	UNP Q6MM15
В	434	PRO	-	expression tag	UNP Q6MM15
В	435	ALA	-	expression tag	UNP Q6MM15
В	436	GLY	-	expression tag	UNP Q6MM15
В	437	SER	-	expression tag	UNP Q6MM15
В	438	HIS	-	expression tag	UNP Q6MM15
В	535	ALA	ARG	engineered mutation	UNP Q6MM15
D	419	MET	-	initiating methionine	UNP Q6MM15
D	420	GLY	_	expression tag	UNP Q6MM15
D	421	SER	_	expression tag	UNP Q6MM15
D	422	SER	_	expression tag	UNP Q6MM15
D	423	HIS	_	expression tag	UNP Q6MM15
D	424	HIS	_	expression tag	UNP Q6MM15
D	425	HIS	_	expression tag	UNP Q6MM15
D	426	HIS	-	expression tag	UNP Q6MM15
D	427	HIS	_	expression tag	UNP Q6MM15
D	428	HIS	_	expression tag	UNP Q6MM15
D	429	SER	-	expression tag	UNP Q6MM15
D	430	SER		expression tag	UNP Q6MM15
D	431	GLY	-	expression tag	UNP Q6MM15
D	432	LEU		expression tag	UNP Q6MM15
D	433	VAL	-	expression tag	UNP Q6MM15
D	434	PRO	-	expression tag	UNP Q6MM15
D	435	ALA	-	expression tag	UNP Q6MM15



Continued from previous page...

Chain	Residue	Modelled Modelled	Actual	Comment	Reference
D	436	GLY	-	expression tag	UNP Q6MM15
D	437	SER	_	expression tag	UNP Q6MM15
D	438	HIS	_	expression tag	UNP Q6MM15
D	535	ALA	ARG	engineered mutation	UNP Q6MM15
F	419	MET	_	initiating methionine	UNP Q6MM15
F	420	GLY	_	expression tag	UNP Q6MM15
F	421	SER	-	expression tag	UNP Q6MM15
F	422	SER	_	expression tag	UNP Q6MM15
F	423	HIS	_	expression tag	UNP Q6MM15
F	424	HIS	_	expression tag	UNP Q6MM15
F	425	HIS	-	expression tag	UNP Q6MM15
F	426	HIS	_	expression tag	UNP Q6MM15
F	427	HIS	_	expression tag	UNP Q6MM15
F	428	HIS	-	expression tag	UNP Q6MM15
F	429	SER	-	expression tag	UNP Q6MM15
F	430	SER	_	expression tag	UNP Q6MM15
F	431	GLY	-	expression tag	UNP Q6MM15
F	432	LEU	_	expression tag	UNP Q6MM15
F	433	VAL	-	expression tag	UNP Q6MM15
F	434	PRO	_	expression tag	UNP Q6MM15
F	435	ALA	_	expression tag	UNP Q6MM15
F	436	GLY	-	expression tag	UNP Q6MM15
F	437	SER	-	expression tag	UNP Q6MM15
F	438	HIS	-	expression tag	UNP Q6MM15
F	535	ALA	ARG	engineered mutation	UNP Q6MM15
Е	419	MET	_	initiating methionine	UNP Q6MM15
Е	420	GLY	_	expression tag	UNP Q6MM15
Е	421	SER	_	expression tag	UNP Q6MM15
Е	422	SER	_	expression tag	UNP Q6MM15
Е	423	HIS	_	expression tag	UNP Q6MM15
Е	424	HIS	_	expression tag	UNP Q6MM15
Е	425	HIS	_	expression tag	UNP Q6MM15
Е	426	HIS	_	expression tag	UNP Q6MM15
Е	427	HIS	_	expression tag	UNP Q6MM15
Е	428	HIS	_	expression tag	UNP Q6MM15
Е	429	SER		expression tag	UNP Q6MM15
Е	430	SER		expression tag	UNP Q6MM15
Е	431	GLY		expression tag	UNP Q6MM15
Е	432	LEU	-	expression tag	UNP Q6MM15
Е	433	VAL	-	expression tag	UNP Q6MM15
Е	434	PRO	-	expression tag	UNP Q6MM15
Е	435	ALA	-	expression tag	UNP Q6MM15



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Е	436	GLY	-	expression tag	UNP Q6MM15
Е	437	SER	-	expression tag	UNP Q6MM15
Е	438	HIS	-	expression tag	UNP Q6MM15
Е	535	ALA	ARG	engineered mutation	UNP Q6MM15
С	419	MET	-	initiating methionine	UNP Q6MM15
С	420	GLY	-	expression tag	UNP Q6MM15
С	421	SER	-	expression tag	UNP Q6MM15
С	422	SER	-	expression tag	UNP Q6MM15
С	423	HIS	-	expression tag	UNP Q6MM15
С	424	HIS	-	expression tag	UNP Q6MM15
С	425	HIS	-	expression tag	UNP Q6MM15
С	426	HIS	-	expression tag	UNP Q6MM15
С	427	HIS	-	expression tag	UNP Q6MM15
С	428	HIS	-	expression tag	UNP Q6MM15
С	429	SER	-	expression tag	UNP Q6MM15
С	430	SER	-	expression tag	UNP Q6MM15
С	431	GLY	-	expression tag	UNP Q6MM15
С	432	LEU	-	expression tag	UNP Q6MM15
С	433	VAL	-	expression tag	UNP Q6MM15
С	434	PRO	=	expression tag	UNP Q6MM15
С	435	ALA	-	expression tag	UNP Q6MM15
С	436	GLY	-	expression tag	UNP Q6MM15
С	437	SER	-	expression tag	UNP Q6MM15
С	438	HIS	-	expression tag	UNP Q6MM15
С	535	ALA	ARG	engineered mutation	UNP Q6MM15

• Molecule 2 is water.

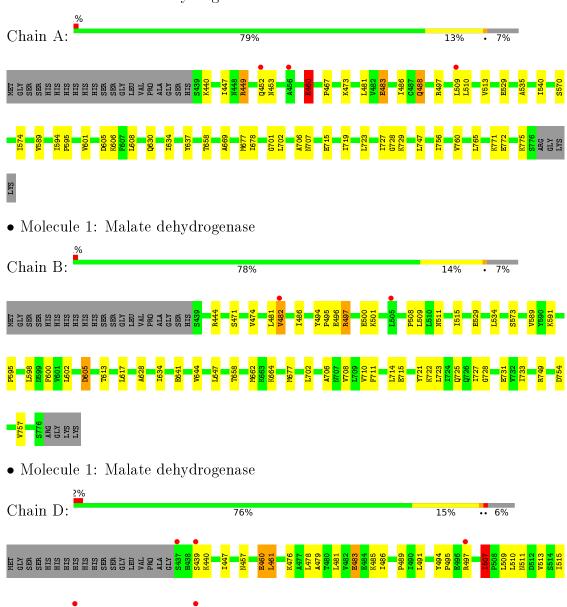
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	62	Total O 62 62	0	0
2	В	97	Total O 97 97	0	0
2	D	54	Total O 54 54	0	0
2	F	58	Total O 58 58	0	0
2	E	69	Total O 69 69	0	0
2	С	92	Total O 92 92	0	0



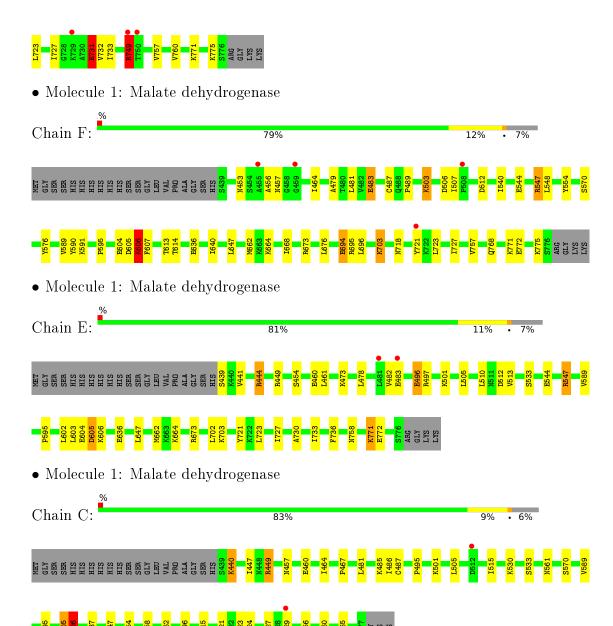
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Malate dehydrogenase









4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	129.24Å 183.12Å 119.53Å	Depositor
a, b, c, α , β , γ	90.00° 117.08° 90.00°	Depositor
Resolution (Å)	69.41 - 2.22	Depositor
Resolution (A)	69.41 - 2.22	EDS
% Data completeness	97.8 (69.41-2.22)	Depositor
(in resolution range)	98.1 (69.41-2.22)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.21 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
P. P.	0.189 , 0.231	Depositor
R, R_{free}	0.190 , 0.231	DCC
R_{free} test set	6035 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 45.1	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16005	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	Bo	nd lengths	Bond angles		
		RMSZ	# Z >5	RMSZ	# Z >5	
1	A	0.51	0/2636	0.73	7/3569 (0.2%)	
1	В	0.50	0/2636	0.75	$6/3569 \ (0.2\%)$	
1	С	0.49	$1/2641 \ (0.0\%)$	0.78	8/3576 (0.2%)	
1	D	0.62	$6/2653 \; (0.2\%)$	0.80	4/3592 (0.1%)	
1	E	0.52	1/2636~(0.0%)	0.85	$14/3569 \ (0.4\%)$	
1	F	0.49	$1/2636 \ (0.0\%)$	0.77	9/3569 (0.3%)	
All	All	0.52	$9/15838 \; (0.1\%)$	0.78	48/21444 (0.2%)	

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	В	0	1
1	С	0	1
All	All	0	2

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	${f Res}$	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(\mathbf{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	D	461	LEU	C-N	8.22	1.49	1.34
1	D	507	ILE	C-N	8.04	1.49	1.34
1	D	604	GLU	CD-OE1	6.67	1.32	1.25
1	F	694	GLU	CD-OE1	-6.43	1.18	1.25
1	D	591	LYS	CD-CE	6.13	1.66	1.51

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	С	606	LYS	CA-CB-CG	12.62	141.16	113.40
1	E	444	ARG	CA-CB-CG	-9.30	92.94	113.40
1	E	444	ARG	NE-CZ-NH1	-9.18	115.71	120.30



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	С	449	ARG	NE-CZ-NH2	8.95	124.77	120.30
1	E	605	ASP	CB-CG-OD2	-8.90	110.29	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	В	605	ASP	Peptide
1	С	605	ASP	Peptide

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	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	A	2592	0	2665	44	0
1	В	2592	0	2667	35	0
1	С	2597	0	2669	29	0
1	D	2608	0	2677	50	1
1	E	2592	0	2667	27	0
1	F	2592	0	2667	34	0
2	A	62	0	0	0	0
2	В	97	0	0	6	0
2	С	92	0	0	3	0
2	D	54	0	0	0	0
2	Ε	69	0	0	2	0
2	F	58	0	0	1	0
All	All	16005	0	16012	209	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 7.

The worst 5 of 209 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:D:479:ALA:O	1:D:483:GLU:OE2	1.52	1.24



Continued from previous page...

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:F:694:GLU:OE1	1:F:703:LYS:HE2	1.58	1.03
1:C:457:ASN:O	1:C:460:GLU:OE1	1.75	1.01
1:C:605:ASP:OD1	1:C:606:LYS:HB3	1.59	1.00
1:F:456:ALA:C	1:F:457:ASN:HD22	1.63	1.00

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	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)
1:D:775:LYS:NZ	1:D:775:LYS:NZ[2_556]	1.99	0.21

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	${f Analy sed}$	Favoured	Allowed	Outliers	Perce	ntiles
1	A	$336/362 \; (93\%)$	332 (99%)	4 (1%)	0	100	100
1	В	$336/362 \ (93\%)$	334 (99%)	2 (1%)	0	100	100
1	$^{\mathrm{C}}$	337/362~(93%)	333 (99%)	4 (1%)	0	100	100
1	D	$338/362 \ (93\%)$	333 (98%)	5 (2%)	0	100	100
1	E	$336/362 \; (93\%)$	332 (99%)	4 (1%)	0	100	100
1	F	$336/362 \; (93\%)$	330 (98%)	6 (2%)	0	100	100
All	All	$2019/2172 \; (93\%)$	1994 (99%)	25 (1%)	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	${\rm sidechain}$	conformation	was
analysed, and the total number of	f residues	•						

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	281/300 (94%)	278 (99%)	3 (1%)	73 84
1	В	281/300 (94%)	278 (99%)	3 (1%)	73 84
1	$^{\mathrm{C}}$	281/300 (94%)	277 (99%)	4 (1%)	67 78
1	D	283/300 (94%)	275 (97%)	8 (3%)	43 54
1	E	281/300 (94%)	274 (98%)	7 (2%)	47 58
1	F	281/300 (94%)	277 (99%)	4 (1%)	67 78
All	All	1688/1800 (94%)	1659 (98%)	29 (2%)	60 73

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	${f Res}$	Type
1	F	503	LYS
1	С	606	LYS
1	F	606	LYS
1	Е	721	TYR
1	F	605	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	D	562	GLN
1	F	457	ASN
1	С	561	ASN
1	F	768	GLN
1	В	511	ASN

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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9	
1	A	$338/362 \ (93\%)$	-0.10	3 (0%) 8	84	83	32, 51, 94, 121	0
1	В	$338/362 \ (93\%)$	-0.21	2 (0%) 8	89	88	28, 47, 90, 117	0
1	С	$339/362 \ (93\%)$	-0.17	2 (0%) 8	89	88	26, 47, 81, 101	0
1	D	340/362 (93%)	0.02	8 (2%)	59	57	29, 57, 104, 144	0
1	E	338/362 (93%)	-0.11	2 (0%) 8	89	88	30, 51, 94, 108	0
1	F	338/362 (93%)	-0.03	4 (1%)	79	77	34, 59, 104, 125	0
All	All	2031/2172 (93%)	-0.10	21 (1%)	82	81	26, 52, 96, 144	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	456	ALA	5.8
1	D	439	SER	4.3
1	С	729	LYS	4.2
1	D	437	SER	3.5
1	F	455	ALA	3.3

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)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

