



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:23 PM GMT

PDB ID : 4C65
Title : Crystal structure of A. niger ochratoxinase
Authors : Dobritsch, D.; Wang, H.; Schneider, G.; Yu, S.
Deposited on : 2013-09-17
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

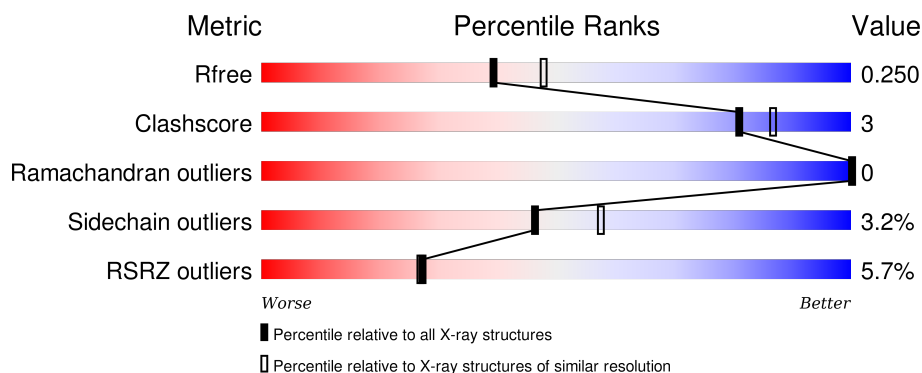
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	438	<div> <div>5%</div> <div>89%</div> <div>11%</div> </div>
1	B	438	<div> <div>4%</div> <div>89%</div> <div>8%</div> </div>
1	C	438	<div> <div>5%</div> <div>89%</div> <div>9%</div> </div>
1	D	438	<div> <div>5%</div> <div>90%</div> <div>10%</div> </div>
1	E	438	<div> <div>4%</div> <div>89%</div> <div>10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	438	<div><div></div><div>4%</div><div>91%</div><div>8%</div><div></div></div>
1	G	438	<div><div></div><div>9%</div><div>88%</div><div>9%</div><div></div></div>
1	H	438	<div><div></div><div>9%</div><div>88%</div><div>10%</div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27300 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 OCHRATOXINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	2	0
			3281	2078	569	621	13			
1	B	430	Total	C	N	O	S	0	4	0
			3250	2060	565	612	13			
1	C	433	Total	C	N	O	S	0	5	0
			3274	2075	568	618	13			
1	D	435	Total	C	N	O	S	0	1	0
			3264	2067	567	617	13			
1	E	435	Total	C	N	O	S	0	1	0
			3267	2069	567	618	13			
1	F	434	Total	C	N	O	S	0	1	0
			3260	2065	569	613	13			
1	G	431	Total	C	N	O	S	0	0	0
			3236	2050	563	610	13			
1	H	429	Total	C	N	O	S	0	1	0
			3228	2045	564	606	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	223	Total	O	0	2
			225	225		
2	B	175	Total	O	0	0
			175	175		
2	C	138	Total	O	0	0
			138	138		
2	D	128	Total	O	0	1
			129	129		
2	E	187	Total	O	0	0
			187	187		
2	F	154	Total	O	0	0
			154	154		

Continued on next page...

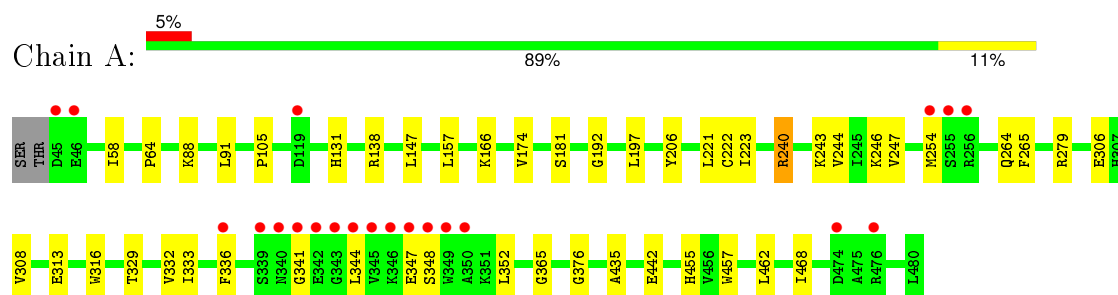
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	137	Total 137	O 137	0	0
2	H	95	Total 95	O 95	0	0

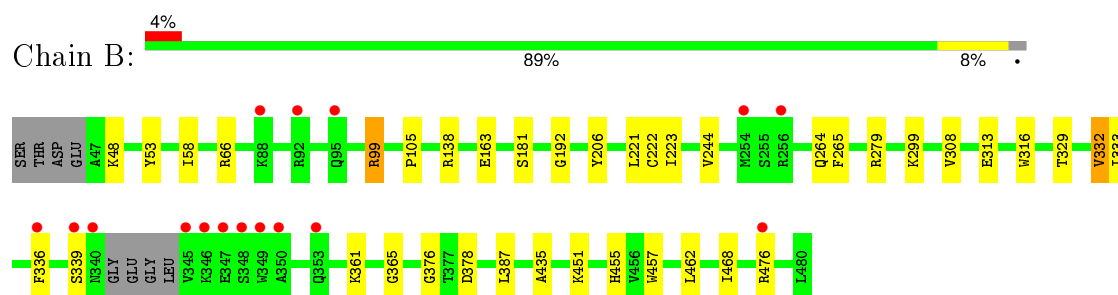
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

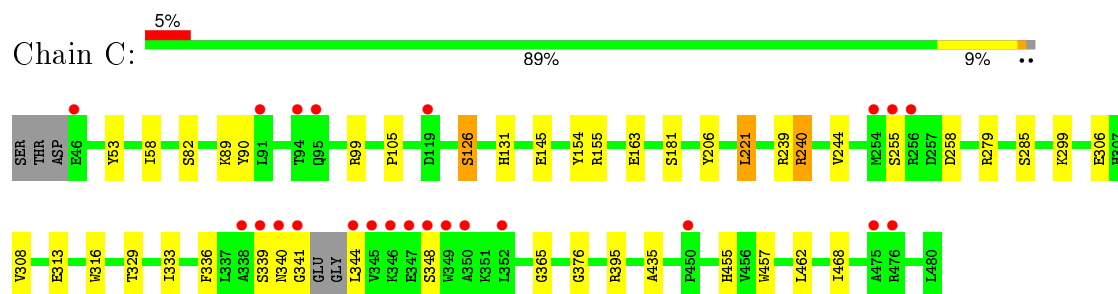
• Molecule 1: OCHRATOXINASE



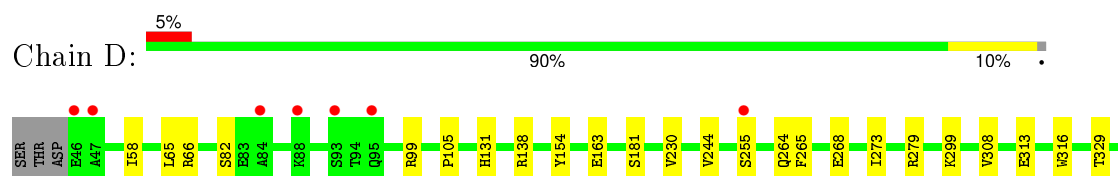
• Molecule 1: OCHRATOXINASE

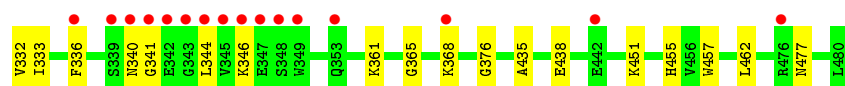


• Molecule 1: OCHRATOXINASE

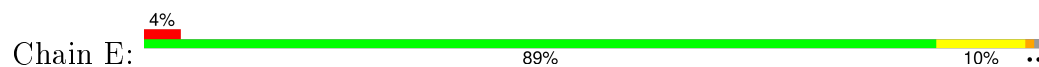


• Molecule 1: OCHRATOXINASE

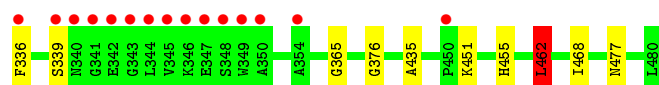
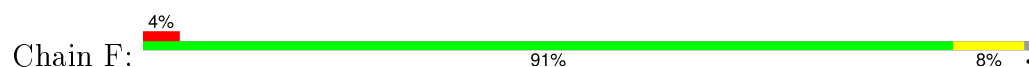




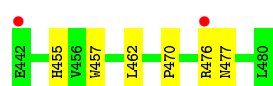
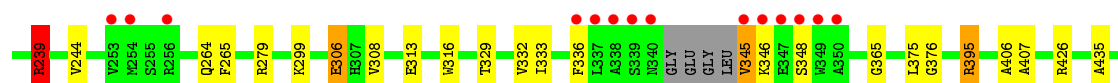
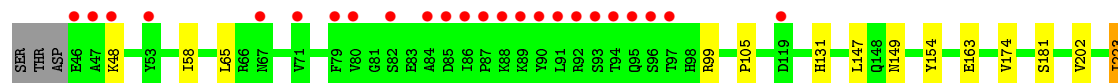
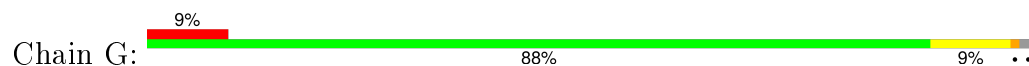
● Molecule 1: OCHRATOXINASE



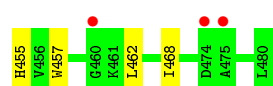
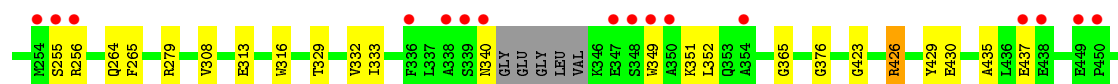
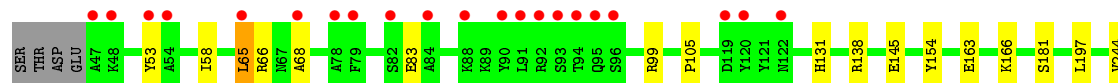
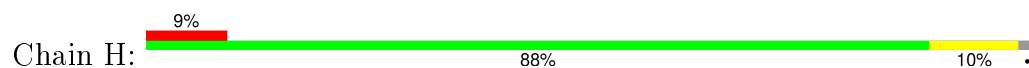
● Molecule 1: OCHRATOXINASE



● Molecule 1: OCHRATOXINASE



● Molecule 1: OCHRATOXINASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.85Å 78.92Å 217.00Å 90.00° 105.05° 90.00°	Depositor
Resolution (Å)	37.79 – 2.20 37.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.6 (37.79-2.20) 87.6 (37.76-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.213 , 0.245 0.217 , 0.250	Depositor DCC
R_{free} test set	7696 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.5	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	7 of 153341 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27300	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.80 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.4166e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [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	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.56	0/3359	0.75	6/4557 (0.1%)
1	B	0.54	0/3333	0.78	8/4521 (0.2%)
1	C	0.55	0/3360	0.75	8/4557 (0.2%)
1	D	0.55	0/3339	0.75	8/4531 (0.2%)
1	E	0.56	0/3342	0.74	5/4536 (0.1%)
1	F	0.55	0/3335	0.81	12/4525 (0.3%)
1	G	0.54	1/3307 (0.0%)	0.77	11/4487 (0.2%)
1	H	0.54	0/3302	0.84	12/4479 (0.3%)
All	All	0.55	1/26677 (0.0%)	0.77	70/36193 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	306	GLU	CD-OE1	5.46	1.31	1.25

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	138	ARG	NE-CZ-NH2	-14.20	113.20	120.30
1	H	138[A]	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	H	138[B]	ARG	NE-CZ-NH2	-13.90	113.35	120.30
1	F	138	ARG	NE-CZ-NH1	13.75	127.18	120.30
1	H	138[A]	ARG	NE-CZ-NH1	12.84	126.72	120.30

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	3281	0	3261	29	1
1	B	3250	0	3238	22	0
1	C	3274	0	3263	23	1
1	D	3264	0	3243	19	0
1	E	3267	0	3244	27	1
1	F	3260	0	3245	24	1
1	G	3236	0	3214	20	1
1	H	3228	0	3212	22	1
2	A	225	0	0	2	0
2	B	175	0	0	1	0
2	C	138	0	0	2	0
2	D	129	0	0	1	0
2	E	187	0	0	3	0
2	F	154	0	0	3	0
2	G	137	0	0	1	0
2	H	95	0	0	2	0
All	All	27300	0	25920	172	3

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 3.

The worst 5 of 172 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:H:65:LEU:HG	1:H:68:ALA:HB2	1.55	0.88
1:C:341:GLY:HA2	1:C:344:LEU:HD12	1.60	0.82
1:A:166:LYS:HE2	2:A:2077:HOH:O	1.81	0.79
1:H:462:LEU:HD23	1:H:468:ILE:HD11	1.69	0.75
1:A:206:TYR:CD2	1:A:221:LEU:HD23	2.21	0.75

All (3) 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:F:239[A]:ARG:NH2	1:H:197:LEU:O[2_554]	1.77	0.43
1:A:197:LEU:O	1:C:239[A]:ARG:NH2[2_555]	1.83	0.37
1:E:197:LEU:O	1:G:239:ARG:NH2[2_554]	2.02	0.18

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	436/438 (100%)	421 (97%)	15 (3%)	0	100	100
1	B	430/438 (98%)	415 (96%)	15 (4%)	0	100	100
1	C	434/438 (99%)	419 (96%)	15 (4%)	0	100	100
1	D	434/438 (99%)	419 (96%)	15 (4%)	0	100	100
1	E	434/438 (99%)	416 (96%)	18 (4%)	0	100	100
1	F	433/438 (99%)	414 (96%)	19 (4%)	0	100	100
1	G	427/438 (98%)	412 (96%)	15 (4%)	0	100	100
1	H	426/438 (97%)	411 (96%)	15 (4%)	0	100	100
All	All	3454/3504 (99%)	3327 (96%)	127 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	333/333 (100%)	325 (98%)	8 (2%)	57	69
1	B	331/333 (99%)	324 (98%)	7 (2%)	61	74
1	C	334/333 (100%)	323 (97%)	11 (3%)	45	56
1	D	331/333 (99%)	320 (97%)	11 (3%)	45	56
1	E	331/333 (99%)	317 (96%)	14 (4%)	36	44
1	F	330/333 (99%)	320 (97%)	10 (3%)	48	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	328/333 (98%)	312 (95%)	16 (5%)	31	36
1	H	327/333 (98%)	317 (97%)	10 (3%)	47	59
All	All	2645/2664 (99%)	2558 (97%)	87 (3%)	46	56

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	154	TYR
1	E	346	LYS
1	H	154	TYR
1	E	221	LEU
1	E	336	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	HIS
1	B	169	ASN
1	E	148	GLN
1	F	280	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

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	436/438 (99%)	0.07	21 (4%) 34 34	12, 20, 48, 86	0
1	B	430/438 (98%)	0.04	16 (3%) 45 44	13, 23, 48, 80	0
1	C	433/438 (98%)	0.10	23 (5%) 30 29	10, 22, 50, 82	0
1	D	435/438 (99%)	0.22	23 (5%) 30 29	12, 25, 49, 97	0
1	E	435/438 (99%)	0.06	18 (4%) 41 39	13, 21, 49, 92	0
1	F	434/438 (99%)	0.09	18 (4%) 41 39	10, 24, 51, 98	0
1	G	431/438 (98%)	0.32	40 (9%) 11 10	14, 28, 59, 89	0
1	H	429/438 (97%)	0.34	40 (9%) 11 10	13, 30, 62, 80	0
All	All	3463/3504 (98%)	0.16	199 (5%) 27 27	10, 24, 56, 98	0

The worst 5 of 199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	343	GLY	9.3
1	E	344	LEU	8.6
1	A	343	GLY	8.5
1	F	343	GLY	7.6
1	D	341	GLY	7.1

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 carbohydrates 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.