



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 11:19 PM EDT

PDB ID : 4ILI
Title : Crystal structure of an Aar2p S253E phosphomimetic mutant protein
Authors : Weber, G.; Heroven, C.; Santos, K.F.; Wahl, M.C.
Deposited on : 2012-12-31
Resolution : 3.20 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

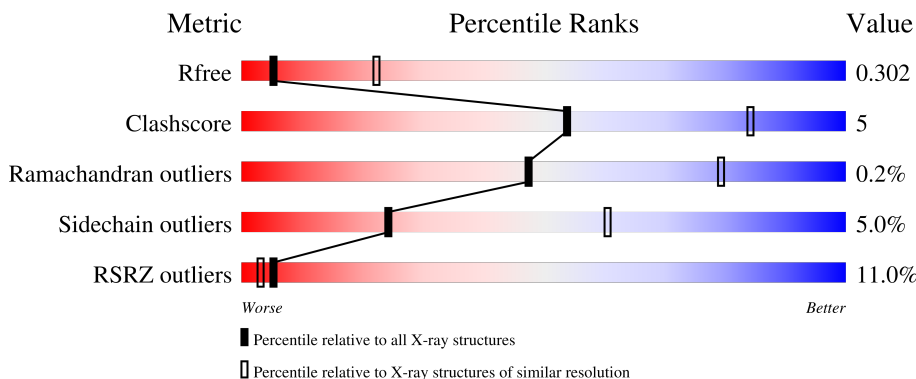
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 $\leq 5\%$. 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	313	 10% 76% 16% • 7%
1	B	313	 11% 78% 13% • 7%

2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 4831 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 A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	290	2403	1539	390	458	16	0	0	0
1	B	292	2428	1556	391	463	18	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	SER	LEU	engineered mutation	UNP P32357
A	154	SER	LYS	engineered mutation	UNP P32357
A	?	-	LEU	deletion	UNP P32357
A	?	-	GLN	deletion	UNP P32357
A	?	-	LYS	deletion	UNP P32357
A	?	-	ALA	deletion	UNP P32357
A	?	-	GLY	deletion	UNP P32357
A	?	-	LYS	deletion	UNP P32357
A	?	-	MET	deletion	UNP P32357
A	?	-	GLU	deletion	UNP P32357
A	?	-	ALA	deletion	UNP P32357
A	?	-	LYS	deletion	UNP P32357
A	?	-	ASN	deletion	UNP P32357
A	?	-	GLU	deletion	UNP P32357
A	?	-	ASP	deletion	UNP P32357
A	253	GLU	SER	engineered mutation	UNP P32357
A	319	LEU	-	expression tag	UNP P32357
A	320	GLU	-	expression tag	UNP P32357
A	321	HIS	-	expression tag	UNP P32357
A	322	HIS	-	expression tag	UNP P32357
A	323	HIS	-	expression tag	UNP P32357
A	324	HIS	-	expression tag	UNP P32357
A	325	HIS	-	expression tag	UNP P32357
A	326	HIS	-	expression tag	UNP P32357
B	153	SER	LEU	engineered mutation	UNP P32357

Continued on next page...

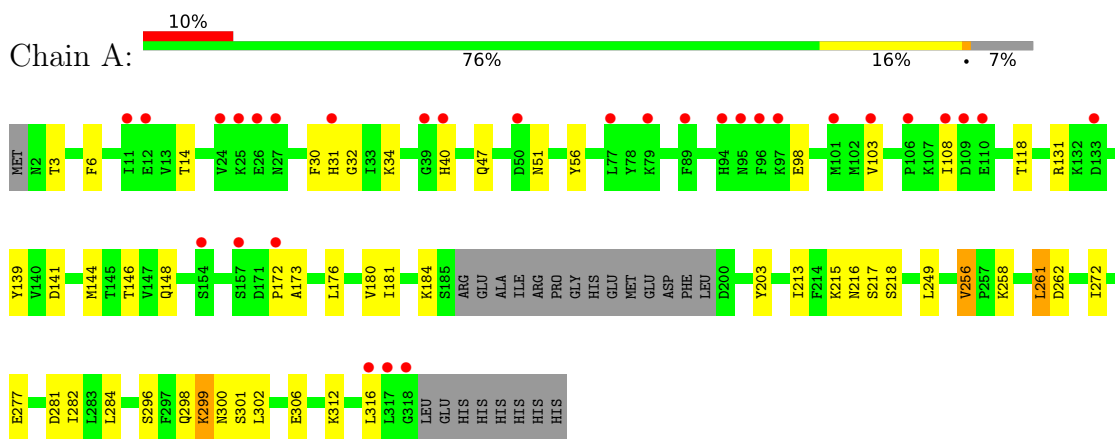
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	154	SER	LYS	engineered mutation	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	GLY	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	MET	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ASN	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	?	-	ASP	deletion	UNP P32357
B	253	GLU	SER	engineered mutation	UNP P32357
B	319	LEU	-	expression tag	UNP P32357
B	320	GLU	-	expression tag	UNP P32357
B	321	HIS	-	expression tag	UNP P32357
B	322	HIS	-	expression tag	UNP P32357
B	323	HIS	-	expression tag	UNP P32357
B	324	HIS	-	expression tag	UNP P32357
B	325	HIS	-	expression tag	UNP P32357
B	326	HIS	-	expression tag	UNP P32357

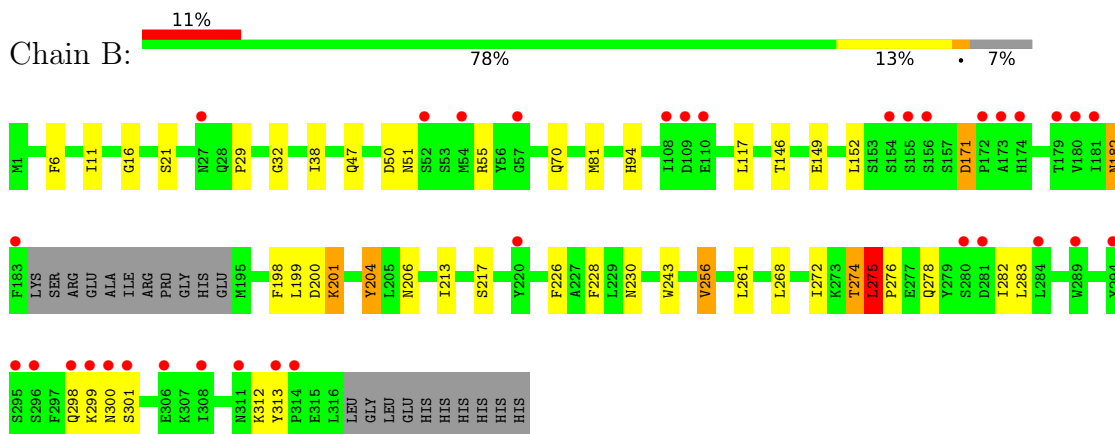
3 Residue-property plots [i](#)

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: A1 cistron-splicing factor AAR2



- Molecule 1: A1 cistron-splicing factor AAR2



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	62.82Å 62.82Å 326.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.26 – 3.20 45.26 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.26-3.20) 99.6 (45.26-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.19Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.260 , 0.305 0.261 , 0.302	Depositor DCC
R_{free} test set	663 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtrriage
Anisotropy	0.316	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 94.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.085 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4831	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.23	0/2466	0.37	0/3332
1	B	0.23	0/2492	0.39	1/3367 (0.0%)
All	All	0.23	0/4958	0.38	1/6699 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	LEU	CA-CB-CG	5.57	128.12	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2403	0	2286	26	0
1	B	2428	0	2305	27	0
All	All	4831	0	4591	50	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 5.

All (50) 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:141:ASP:HB3	1:A:144:MET:HG3	1.76	0.67
1:B:226:PHE:O	1:B:230:ASN:ND2	2.31	0.63
1:A:47:GLN:NE2	1:A:51:ASN:O	2.32	0.62
1:A:299:LYS:H	1:A:300:ASN:HA	1.64	0.61
1:A:131:ARG:HH11	1:A:172:PRO:HB2	1.67	0.60
1:B:275:LEU:HD11	1:B:313:TYR:HE2	1.67	0.59
1:B:47:GLN:OE1	1:B:55:ARG:NH1	2.36	0.59
1:A:272:ILE:O	1:A:312:LYS:NZ	2.34	0.58
1:A:261:LEU:HG	1:A:301:SER:HB3	1.85	0.58
1:B:201:LYS:HE2	1:B:204:TYR:CE2	2.38	0.58
1:A:216:ASN:HD22	1:B:94:HIS:HB2	1.69	0.57
1:B:70:GLN:NE2	1:B:81:MET:SD	2.78	0.57
1:B:171:ASP:OD1	1:B:171:ASP:N	2.40	0.55
1:B:282:ILE:HG12	1:B:283:LEU:H	1.71	0.55
1:B:6:PHE:HD2	1:B:32:GLY:HA2	1.73	0.54
1:A:131:ARG:HB3	1:A:173:ALA:HA	1.90	0.53
1:A:14:THR:HB	1:A:47:GLN:HB3	1.90	0.52
1:A:40:HIS:NE2	1:A:118:THR:O	2.34	0.52
1:A:216:ASN:ND2	1:B:94:HIS:HB2	2.24	0.51
1:A:146:THR:HG22	1:A:176:LEU:HB2	1.92	0.51
1:A:218:SER:OG	1:B:94:HIS:ND1	2.38	0.51
1:B:299:LYS:H	1:B:300:ASN:HA	1.76	0.51
1:A:299:LYS:N	1:A:300:ASN:HA	2.26	0.50
1:B:275:LEU:HD11	1:B:313:TYR:CE2	2.47	0.50
1:A:213:ILE:O	1:A:217:SER:HB3	2.12	0.50
1:B:298:GLN:NE2	1:B:301:SER:OG	2.42	0.50
1:B:146:THR:HG23	1:B:149:GLU:H	1.76	0.49
1:B:6:PHE:CD2	1:B:32:GLY:HA2	2.47	0.49
1:B:256:VAL:HG23	1:B:261:LEU:HD11	1.95	0.48
1:A:6:PHE:CD2	1:A:32:GLY:HA2	2.49	0.47
1:A:256:VAL:HG13	1:A:261:LEU:HD21	1.95	0.47
1:A:296:SER:HB2	1:A:302:LEU:H	1.81	0.46
1:B:117:LEU:HD21	1:B:274:THR:HG21	1.96	0.46
1:A:258:LYS:NZ	1:A:262:ASP:OD2	2.49	0.46
1:A:148:GLN:HB2	1:A:180:VAL:HG22	1.98	0.45
1:B:299:LYS:N	1:B:300:ASN:HA	2.32	0.45
1:B:268:LEU:O	1:B:272:ILE:HG12	2.17	0.45
1:B:50:ASP:OD1	1:B:51:ASN:N	2.50	0.44
1:A:31:HIS:CE1	1:A:98:GLU:HG3	2.53	0.44
1:B:182:ASN:ND2	1:B:206:ASN:OD1	2.51	0.43
1:B:213:ILE:O	1:B:217:SER:HB3	2.18	0.43
1:A:56:TYR:HB2	1:A:139:TYR:CE1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:SER:OG	1:A:306:GLU:OE2	2.37	0.43
1:A:30:PHE:HE1	1:A:103:VAL:HG23	1.84	0.43
1:A:3:THR:HG23	1:A:34:LYS:HA	2.02	0.42
1:B:11:ILE:H	1:B:11:ILE:HG13	1.76	0.41
1:B:228:PHE:HB2	1:B:243:TRP:CD1	2.56	0.41
1:B:16:GLY:HA2	1:B:21:SER:HA	2.03	0.41
1:A:181:ILE:HD13	1:A:249:LEU:HD22	2.02	0.41
1:B:276:PRO:O	1:B:313:TYR:OH	2.32	0.41

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	286/313 (91%)	278 (97%)	8 (3%)	0	100	100
1	B	288/313 (92%)	268 (93%)	19 (7%)	1 (0%)	41	74
All	All	574/626 (92%)	546 (95%)	27 (5%)	1 (0%)	47	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/291 (93%)	257 (95%)	13 (5%)	25	61
1	B	273/291 (94%)	259 (95%)	14 (5%)	24	60
All	All	543/582 (93%)	516 (95%)	27 (5%)	24	60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ILE
1	A	184	LYS
1	A	203	TYR
1	A	215	LYS
1	A	256	VAL
1	A	261	LEU
1	A	277	GLU
1	A	281	ASP
1	A	282	ILE
1	A	284	LEU
1	A	298	GLN
1	A	299	LYS
1	A	316	LEU
1	B	38	ILE
1	B	152	LEU
1	B	171	ASP
1	B	182	ASN
1	B	198	PHE
1	B	199	LEU
1	B	200	ASP
1	B	201	LYS
1	B	204	TYR
1	B	256	VAL
1	B	274	THR
1	B	275	LEU
1	B	278	GLN
1	B	312	LYS

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

Mol	Chain	Res	Type
1	A	216	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

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	290/313 (92%)	0.46	30 (10%) 6 4	66, 111, 211, 330	0
1	B	292/313 (93%)	0.74	34 (11%) 4 3	97, 153, 257, 374	0
All	All	582/626 (92%)	0.60	64 (10%) 5 3	66, 136, 242, 374	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	SER	7.3
1	A	27	ASN	6.5
1	A	318	GLY	5.7
1	A	109	ASP	5.5
1	B	109	ASP	5.2
1	B	289	TRP	5.0
1	A	24	VAL	5.0
1	B	174	HIS	4.9
1	A	101	MET	4.7
1	A	110	GLU	4.6
1	B	27	ASN	4.5
1	A	12	GLU	4.4
1	A	108	ILE	4.2
1	A	172	PRO	4.1
1	B	314	PRO	4.1
1	B	108	ILE	4.0
1	B	301	SER	4.0
1	A	154	SER	3.8
1	B	295	SER	3.8
1	A	26	GLU	3.7
1	B	281	ASP	3.6
1	A	96	PHE	3.5
1	B	296	SER	3.4
1	B	155	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	110	GLU	3.3
1	A	39	GLY	3.3
1	A	89	PHE	3.2
1	A	317	LEU	3.2
1	B	299	LYS	3.1
1	B	294	TYR	3.1
1	A	157	SER	3.1
1	A	25	LYS	3.0
1	B	306	GLU	2.9
1	B	183	PHE	2.9
1	A	94	HIS	2.9
1	B	280	SER	2.9
1	B	300	ASN	2.7
1	B	181	ILE	2.7
1	B	298	GLN	2.7
1	B	172	PRO	2.7
1	A	50	ASP	2.6
1	B	313	TYR	2.6
1	A	31	HIS	2.6
1	A	11	ILE	2.6
1	B	54	MET	2.5
1	B	173	ALA	2.5
1	A	77	LEU	2.4
1	B	284	LEU	2.4
1	A	316	LEU	2.4
1	B	180	VAL	2.4
1	A	40	HIS	2.4
1	A	133	ASP	2.3
1	A	103	VAL	2.3
1	B	154	SER	2.3
1	A	79	LYS	2.3
1	B	179	THR	2.2
1	B	220	TYR	2.2
1	A	106	PRO	2.2
1	A	95	ASN	2.2
1	B	52	SER	2.2
1	B	57	GLY	2.1
1	B	308	ILE	2.1
1	A	97	LYS	2.0
1	B	311	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.