Full wwPDB X-ray Structure Validation Report ⓘ

Mar 28, 2023 – 10:19 AM EDT

PDB ID	:	8GAI
Title	:	Cavia porcellus (guinea pig) importin-alpha 1 in complex with Bimax2 peptide
Authors	:	Hawker, J.E.; Forwood, J.K.; Donnelly, C.M.; Stewart, M.
Deposited on	:	2023-02-22
Resolution	:	2.65 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	:	2.32.2
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)	:	2.32.2

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 2.65 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.
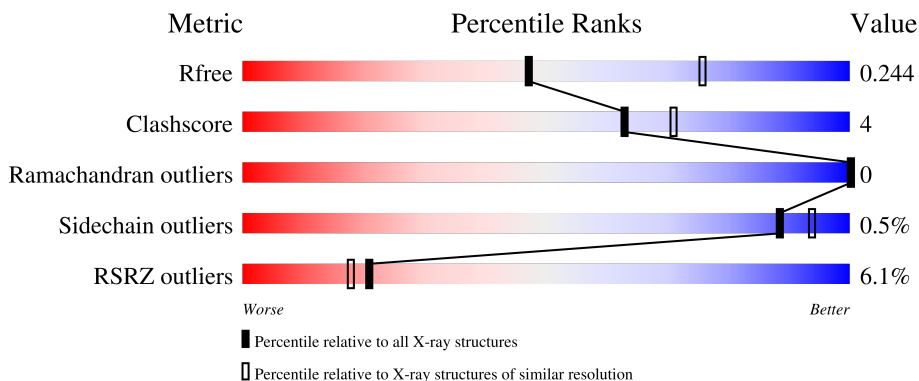
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	471	4% / 83% / 8% / 9%
1	C	471	4% / 82% / 10% / 8%
2	B	30	33% / 60% / 13% / 27%
2	D	30	20% / 87% / · / 10%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 14402 atoms, of which 7239 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 Importin subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total 6656	C 2095	H 3361	N 556	O 633	S 11	0	5	0
1	C	434	Total 6748	C 2124	H 3407	N 563	O 643	S 11	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLN	-	expression tag	UNP H0VVB1
A	60	SER	-	expression tag	UNP H0VVB1
C	59	GLN	-	expression tag	UNP H0VVB1
C	60	SER	-	expression tag	UNP H0VVB1

- Molecule 2 is a protein called Bimax2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	22	Total 414	C 122	H 207	N 48	O 37	0	0	0
2	D	27	Total 521	C 149	H 264	N 65	O 43	0	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total 21	O 21	0	0
3	B	3	Total 3	O 3	0	0
3	C	31	Total 31	O 31	0	0
3	D	8	Total 8	O 8	0	0

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.
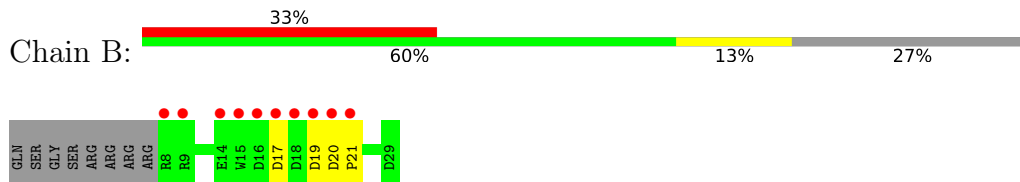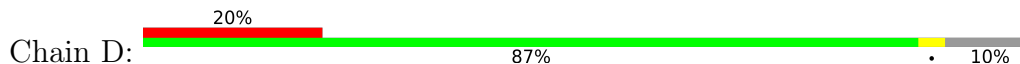
• Molecule 1: Importin subunit alpha
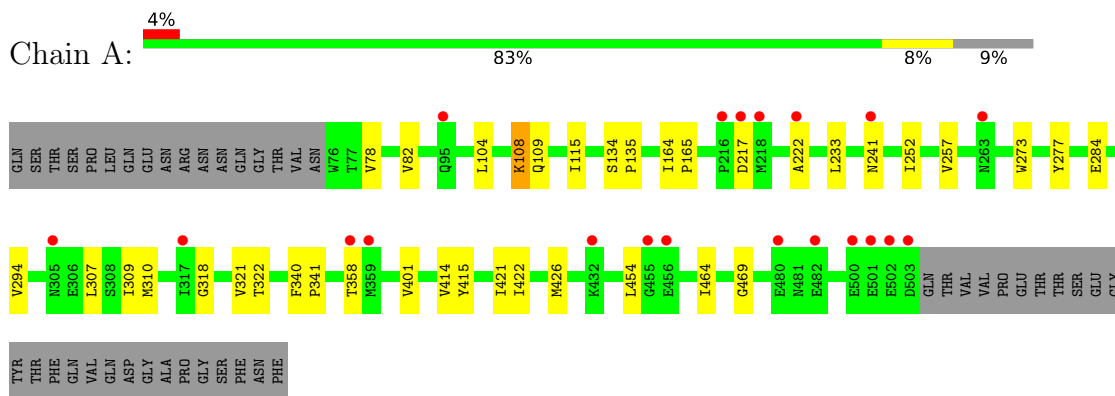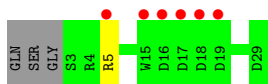

• Molecule 1: Importin subunit alpha
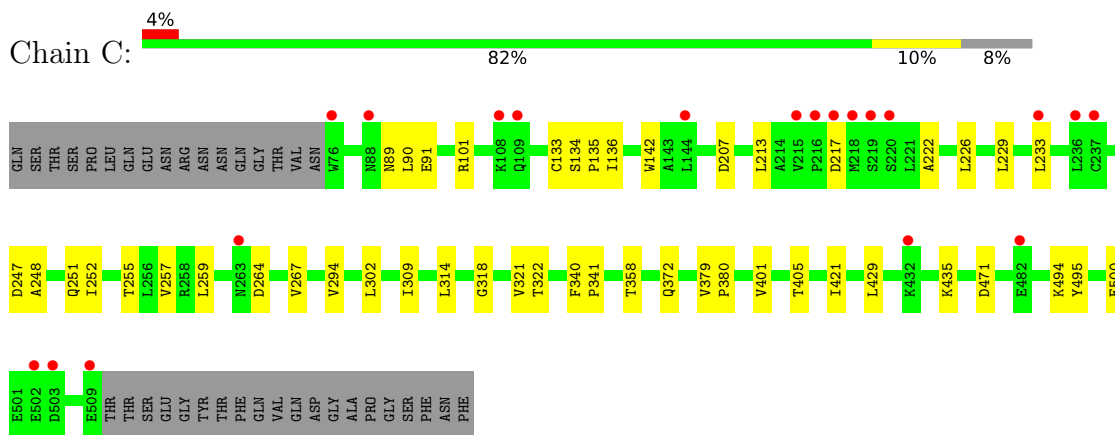
• Molecule 2: Bimax2

• Molecule 2: Bimax2

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.01Å 99.27Å 123.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.65 19.95 – 2.65	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.95-2.65) 93.7 (19.95-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.67Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.202 , 0.241 0.204 , 0.244	Depositor DCC
R_{free} test set	1334 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 44.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14402	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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 20.44 % 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 8.6805e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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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 (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	0.26	0/3368	0.47	0/4591
1	C	0.27	0/3415	0.47	0/4657
2	B	0.26	0/210	0.75	0/275
2	D	0.26	0/260	0.80	0/339
All	All	0.26	0/7253	0.50	0/9862

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 (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	3295	3361	3343	27	0
1	C	3341	3407	3389	33	0
2	B	207	207	207	4	0
2	D	257	264	264	0	0
3	A	21	0	0	1	0
3	B	3	0	0	1	0
3	C	31	0	0	1	0
3	D	8	0	0	0	1
All	All	7163	7239	7203	62	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 4.

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All (62) 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:C:213:LEU:HD21	1:C:259:LEU:HD11	1.36	1.06
1:C:207:ASP:OD1	1:C:251:GLN:NE2	2.18	0.76
1:A:415:TYR:OH	3:A:601:HOH:O	2.05	0.75
2:B:19:ASP:OD2	3:B:101:HOH:O	2.07	0.72
1:C:213:LEU:HD23	1:C:255:THR:CG2	2.20	0.70
1:A:217:ASP:HB3	1:A:222:ALA:HB1	1.76	0.68
1:A:284:GLU:OE1	1:A:284:GLU:N	2.24	0.67
1:C:257:VAL:HG22	1:C:294:VAL:CG1	2.26	0.65
1:A:257:VAL:HG22	1:A:294:VAL:CG1	2.29	0.63
1:C:213:LEU:HD23	1:C:255:THR:HG21	1.80	0.62
1:C:247:ASP:OD1	1:C:248:ALA:N	2.34	0.60
1:A:318:GLY:O	1:A:322:THR:HG23	2.03	0.58
1:C:233:LEU:HD11	1:C:252:ILE:HD12	1.85	0.57
1:A:241:ASN:O	1:A:241:ASN:ND2	2.37	0.57
1:C:213:LEU:HD13	1:C:229:LEU:HB3	1.89	0.54
1:C:318:GLY:O	1:C:322:THR:HG23	2.08	0.53
1:A:233:LEU:HD11	1:A:252:ILE:HD12	1.91	0.52
1:A:414:VAL:HG21	1:A:454:LEU:HD11	1.93	0.51
1:A:307:LEU:HD12	1:A:310:MET:HE3	1.92	0.50
1:A:426:MET:HG2	1:A:469:GLY:HA2	1.93	0.49
1:C:321:VAL:HG21	1:C:358:THR:HG23	1.93	0.49
1:C:372:GLN:NE2	3:C:602:HOH:O	2.45	0.48
1:A:401:VAL:HG21	1:A:421:ILE:HD11	1.96	0.48
1:A:321:VAL:HG21	1:A:358:THR:HG23	1.95	0.47
1:C:217:ASP:CB	1:C:222:ALA:HB1	2.45	0.46
1:A:78:VAL:O	1:A:82:VAL:HG23	2.15	0.46
1:C:340:PHE:N	1:C:341:PRO:CD	2.78	0.46
1:C:401:VAL:HG21	1:C:421:ILE:HD11	1.98	0.45
1:C:302:LEU:HD11	1:C:314:LEU:HD13	1.98	0.45
1:A:340:PHE:N	1:A:341:PRO:CD	2.79	0.45
1:A:104:LEU:HD21	1:A:115:ILE:HD12	1.99	0.45
1:A:134:SER:N	1:A:135:PRO:CD	2.79	0.45
1:C:217:ASP:HB3	1:C:222:ALA:HB1	1.98	0.45
1:A:217:ASP:CB	1:A:222:ALA:HB1	2.45	0.44
1:C:401:VAL:O	1:C:405:THR:HG23	2.17	0.44
2:B:17:ASP:OD1	2:B:20:ASP:N	2.51	0.44
1:C:101:ARG:HD3	1:C:142:TRP:CD2	2.53	0.43
1:C:217:ASP:HB3	1:C:222:ALA:CB	2.49	0.43
1:C:134:SER:N	1:C:135:PRO:CD	2.81	0.43
1:A:273:TRP:CD2	2:B:21:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:LEU:HD11	1:C:252:ILE:CD1	2.46	0.43
1:C:257:VAL:HG22	1:C:294:VAL:HG11	1.98	0.43
1:C:213:LEU:HD12	1:C:226:LEU:HD12	2.01	0.43
1:C:133:CYS:O	1:C:136:ILE:HG22	2.19	0.42
1:A:108:LYS:HD3	1:A:109:GLN:H	1.83	0.42
1:C:435:LYS:O	1:C:435:LYS:HD3	2.19	0.42
1:A:426:MET:HE1	1:A:464:ILE:HG12	2.01	0.42
1:C:379:VAL:HB	1:C:380:PRO:HD3	2.01	0.42
1:C:309:ILE:N	1:C:309:ILE:HD12	2.35	0.41
1:A:277:TYR:OH	2:B:21:PRO:HD2	2.21	0.41
1:A:422:ILE:HG23	1:A:426:MET:HE2	2.03	0.41
1:A:309:ILE:HD12	1:A:309:ILE:N	2.35	0.41
1:C:101:ARG:HD2	1:C:101:ARG:C	2.41	0.41
1:A:164:ILE:HB	1:A:165:PRO:HD3	2.02	0.41
1:A:257:VAL:HG22	1:A:294:VAL:HG11	2.00	0.41
1:A:426:MET:HG2	1:A:469:GLY:CA	2.50	0.41
1:C:89:ASN:OD1	1:C:91:GLU:N	2.53	0.41
1:C:90:LEU:HD21	1:C:133:CYS:HB2	2.02	0.41
1:C:264:ASP:HB3	1:C:267:VAL:HB	2.03	0.41
1:C:494:LYS:HD2	1:C:495:TYR:CE2	2.55	0.41
1:A:233:LEU:HD11	1:A:252:ILE:CD1	2.51	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:HOH:O	3:D:105:HOH:O[4_445]	2.01	0.19

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	431/471 (92%)	426 (99%)	5 (1%)	0	100	100
1	C	437/471 (93%)	430 (98%)	7 (2%)	0	100	100
2	B	20/30 (67%)	19 (95%)	1 (5%)	0	100	100
2	D	25/30 (83%)	22 (88%)	3 (12%)	0	100	100
All	All	913/1002 (91%)	897 (98%)	16 (2%)	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	366/401 (91%)	365 (100%)	1 (0%)	92	96
1	C	372/401 (93%)	370 (100%)	2 (0%)	88	94
2	B	22/29 (76%)	22 (100%)	0	100	100
2	D	27/29 (93%)	26 (96%)	1 (4%)	34	50
All	All	787/860 (92%)	783 (100%)	4 (0%)	88	94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	C	471	ASP
1	C	500	GLU
2	D	5	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	428/471 (90%)	0.25	20 (4%)	31	28	28, 43, 73, 120	0
1	C	434/471 (92%)	0.24	20 (4%)	32	29	28, 44, 76, 125	0
2	B	22/30 (73%)	2.01	10 (45%)	0	0	32, 64, 114, 145	0
2	D	27/30 (90%)	1.20	6 (22%)	0	0	34, 47, 119, 150	0
All	All	911/1002 (90%)	0.32	56 (6%)	21	18	28, 43, 80, 150	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	15	TRP	8.2
1	A	503	ASP	7.1
2	D	17	ASP	6.1
2	D	15	TRP	6.1
2	B	8	ARG	5.7
2	B	17	ASP	5.1
1	A	217	ASP	5.0
1	A	218	MET	5.0
1	C	503	ASP	4.9
1	C	218	MET	4.9
1	C	216	PRO	4.6
1	A	501	GLU	4.5
1	C	88	ASN	4.5
2	B	18	ASP	4.3
2	B	16	ASP	4.1
2	B	9	ARG	4.0
2	D	5	ARG	4.0
1	A	502	GLU	4.0
1	A	216	PRO	3.8
2	B	14	GLU	3.8
1	C	217	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	215	VAL	3.7
2	D	19	ASP	3.6
1	A	500	GLU	3.4
1	A	263	ASN	3.1
1	A	241	ASN	3.0
2	D	18	ASP	3.0
2	B	21	PRO	2.7
1	A	432	LYS	2.7
2	B	20	ASP	2.7
1	C	502	GLU	2.7
2	B	19	ASP	2.6
1	C	432	LYS	2.6
1	A	480	GLU	2.5
1	C	219	SER	2.5
1	C	76	TRP	2.4
2	D	16	ASP	2.4
1	A	317	ILE	2.3
1	C	220	SER	2.3
1	A	482	GLU	2.3
1	A	222	ALA	2.3
1	A	305	ASN	2.2
1	C	233	LEU	2.2
1	A	455	GLY	2.2
1	A	358	THR	2.2
1	C	263	ASN	2.2
1	C	144	LEU	2.1
1	C	237	CYS	2.1
1	C	509	GLU	2.1
1	A	359	MET	2.1
1	C	108	LYS	2.1
1	A	456	GLU	2.1
1	C	236	LEU	2.1
1	A	95	GLN	2.0
1	C	109	GLN	2.0
1	C	482	GLU	2.0

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.