



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 PM UTC

PDB ID : 4ZGZ / pdb_00004zgz
Title : STRUCTURE OF HUMAN ANTIZYME INHIBITOR IN COMPLEX WITH
A C-TERMINAL FRAGMENT OF ANTIZYME
Authors : Chen, S.F.; Wu, H.Y.; Chan, N.L.
Deposited on : 2015-04-24
Resolution : 5.81 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

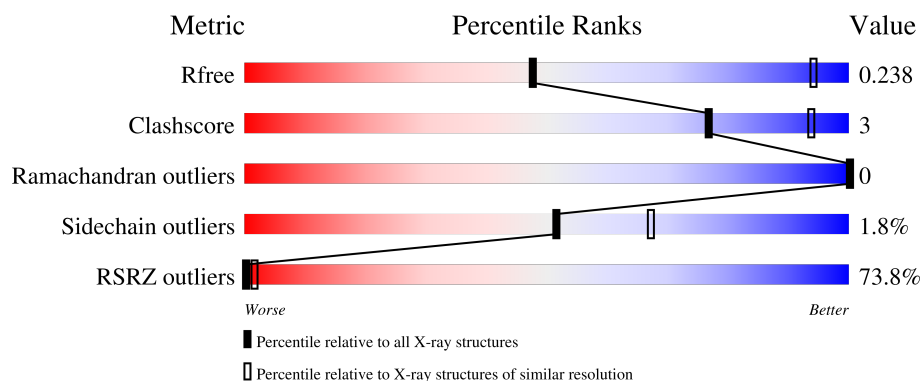
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.81 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}	180053	1126 (7.64-4.00)
Clashscore	190562	1191 (7.64-4.00)
Ramachandran outliers	187476	1019 (7.60-4.00)
Sidechain outliers	187428	1009 (7.60-3.98)
RSRZ outliers	180081	1119 (7.64-4.00)

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	438	63% 84% 11%
1	C	438	66% 85% 11%
2	B	128	55% 69% 5% 27%
2	D	128	59% 70% 5% 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7456 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 Antizyme inhibitor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	1726	0	0
			2973	1919	470	561	23			
1	C	389	Total	C	N	O	S	1750	0	0
			2990	1927	479	562	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O14977
A	1	GLY	-	expression tag	UNP O14977
A	20	ASP	ASN	engineered mutation	UNP O14977
C	0	MET	-	initiating methionine	UNP O14977
C	1	GLY	-	expression tag	UNP O14977
C	20	ASP	ASN	engineered mutation	UNP O14977

- Molecule 2 is a protein called Ornithine decarboxylase antizyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	S	434	0	0
			738	481	123	131	3			
2	D	95	Total	C	N	O	S	451	0	0
			755	490	130	132	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	109	MET	-	initiating methionine	UNP P54368
B	229	LEU	-	expression tag	UNP P54368
B	230	GLU	-	expression tag	UNP P54368
B	231	HIS	-	expression tag	UNP P54368
B	232	HIS	-	expression tag	UNP P54368
B	233	HIS	-	expression tag	UNP P54368

Continued on next page...

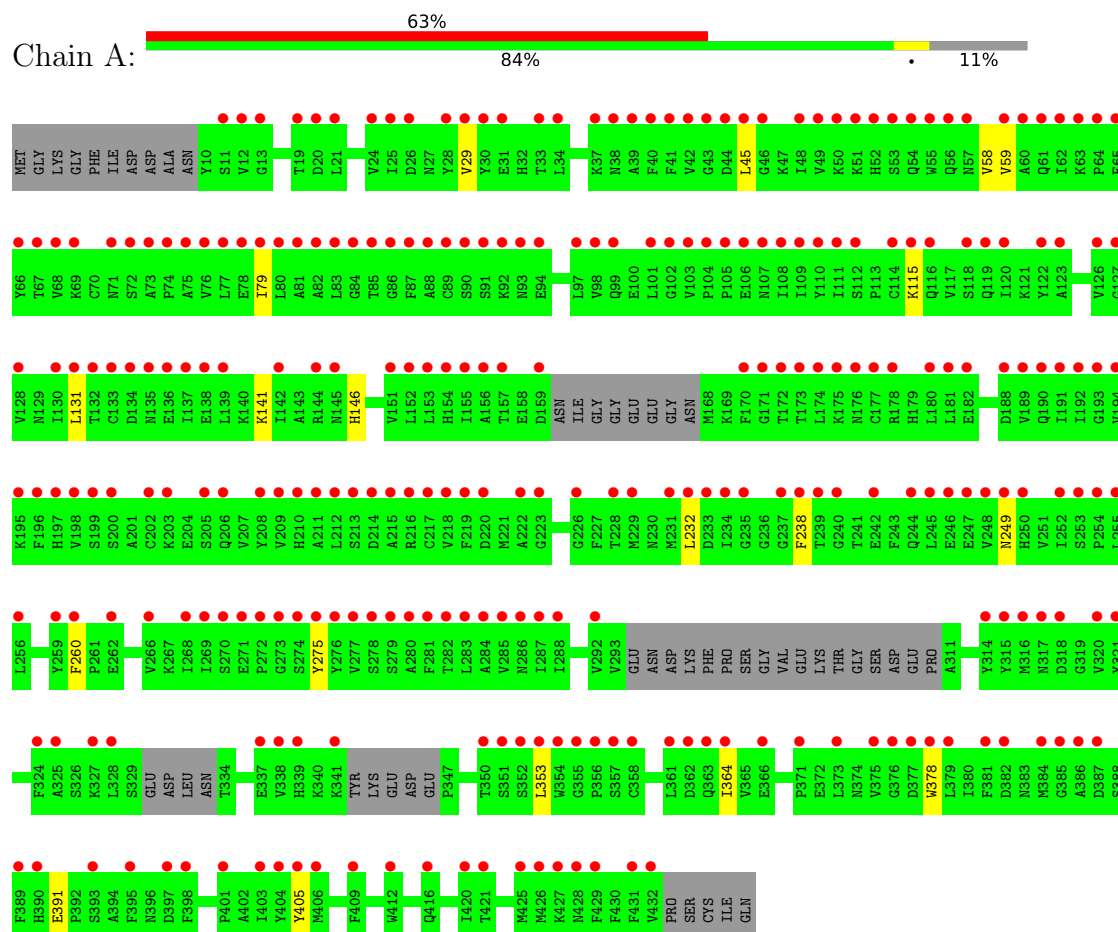
Continued from previous page...

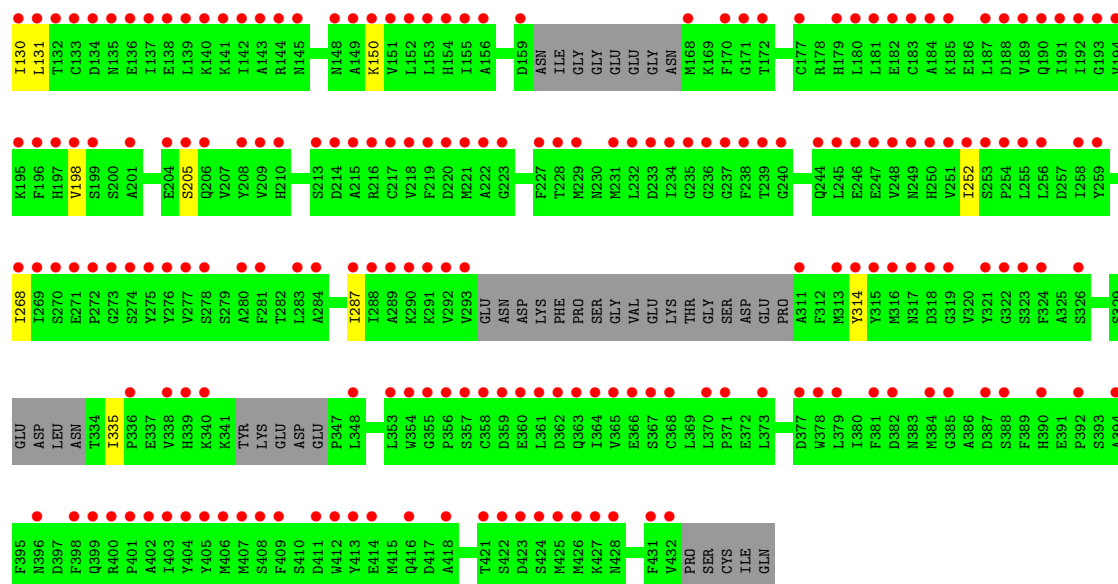
Chain	Residue	Modelled	Actual	Comment	Reference
B	234	HIS	-	expression tag	UNP P54368
B	235	HIS	-	expression tag	UNP P54368
B	236	HIS	-	expression tag	UNP P54368
D	109	MET	-	initiating methionine	UNP P54368
D	229	LEU	-	expression tag	UNP P54368
D	230	GLU	-	expression tag	UNP P54368
D	231	HIS	-	expression tag	UNP P54368
D	232	HIS	-	expression tag	UNP P54368
D	233	HIS	-	expression tag	UNP P54368
D	234	HIS	-	expression tag	UNP P54368
D	235	HIS	-	expression tag	UNP P54368
D	236	HIS	-	expression tag	UNP P54368

3 Residue-property plots

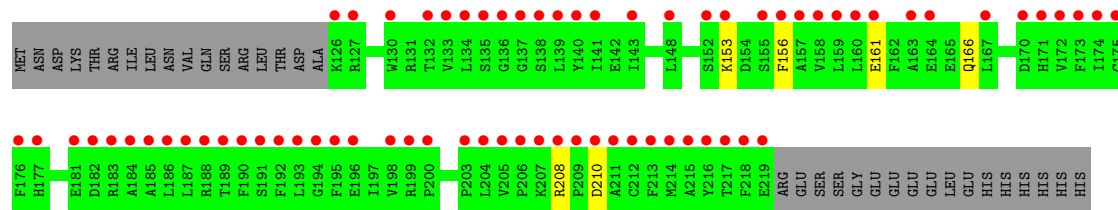
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Antizyme inhibitor 1

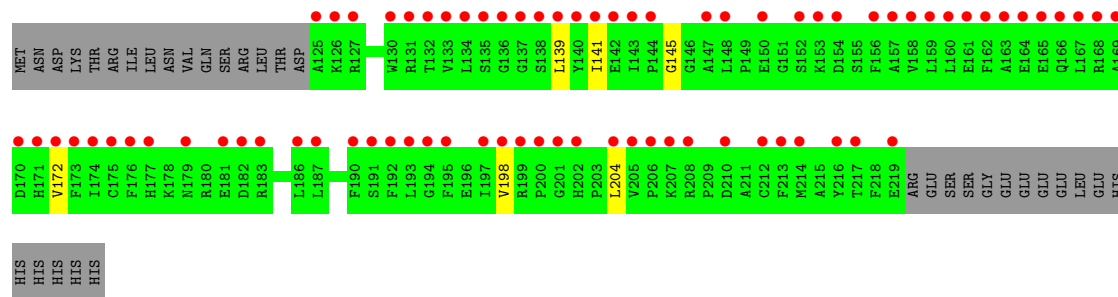




• Molecule 2: Ornithine decarboxylase antizyme 1



• Molecule 2: Ornithine decarboxylase antizyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	166.56Å 166.56Å 144.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.92 – 5.81 25.92 – 5.81	Depositor EDS
% Data completeness (in resolution range)	98.2 (25.92-5.81) 91.9 (25.92-5.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 5.64Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE:1.7.3_928)	Depositor
R, R_{free}	0.188 , 0.240 0.190 , 0.238	Depositor DCC
R_{free} test set	594 reflections (2.43%)	wwPDB-VP
Wilson B-factor (Å ²)	330.6	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	2.04 , 373.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l 0.054 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	7456	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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

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	0.30	0/3039	0.79	6/4120 (0.1%)
1	C	0.31	0/3056	0.78	3/4140 (0.1%)
2	B	0.29	0/759	0.82	0/1028
2	D	0.31	0/776	0.84	1/1049 (0.1%)
All	All	0.30	0/7630	0.80	10/10337 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	SER	CA-C-N	7.11	126.74	119.56
1	C	112	SER	C-N-CA	7.11	126.74	119.56
1	A	391	GLU	CA-C-N	5.74	125.93	119.90
1	A	391	GLU	C-N-CA	5.74	125.93	119.90
1	C	205	SER	N-CA-C	5.69	117.17	110.97
1	A	260	PHE	CA-C-N	5.35	125.55	120.31
1	A	260	PHE	C-N-CA	5.35	125.55	120.31
1	A	146	HIS	CA-C-N	5.33	124.94	119.56
1	A	146	HIS	C-N-CA	5.33	124.94	119.56
2	D	145	GLY	N-CA-C	5.01	117.84	112.33

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	2973	0	2882	9	0
1	C	2990	0	2913	4	0
2	B	738	0	714	2	0
2	D	755	0	741	2	0
All	All	7456	0	7250	17	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 3.

All (17) 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:238:PHE:HB2	1:A:275:TYR:HB2	1.77	0.67
1:C:110:TYR:HB3	1:C:131:LEU:HD13	1.82	0.61
1:A:45:LEU:HD11	1:A:405:TYR:HB3	1.83	0.60
1:A:115:LYS:O	1:A:141:LYS:NZ	2.38	0.55
2:D:139:LEU:HG	2:D:172:VAL:HG12	1.91	0.52
2:B:153:LYS:HA	2:B:156:PHE:CE2	2.45	0.52
1:C:68:VAL:HG21	1:C:94:GLU:CD	2.35	0.51
1:A:58:VAL:HG12	1:A:59:VAL:HG23	1.96	0.47
1:A:232:LEU:HD23	1:A:232:LEU:HA	1.88	0.44
1:A:353:LEU:HG	1:A:364:ILE:HD12	1.99	0.44
1:A:58:VAL:HG13	1:A:249:ASN:HD22	1.83	0.42
1:C:287:ILE:HD11	1:C:314:TYR:HB2	2.00	0.42
1:A:29:VAL:HG22	1:A:378:TRP:CE3	2.55	0.42
2:B:208:ARG:HG2	2:B:210:ASP:OD1	2.20	0.42
2:D:141:ILE:O	2:D:141:ILE:HG13	2.19	0.42
1:A:45:LEU:HD12	1:A:45:LEU:H	1.85	0.41
1:C:130:ILE:HA	1:C:150:LYS:HB2	2.03	0.40

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	379/438 (86%)	367 (97%)	12 (3%)	0	100	100
1	C	379/438 (86%)	367 (97%)	12 (3%)	0	100	100
2	B	92/128 (72%)	90 (98%)	2 (2%)	0	100	100
2	D	93/128 (73%)	91 (98%)	2 (2%)	0	100	100
All	All	943/1132 (83%)	915 (97%)	28 (3%)	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	321/376 (85%)	319 (99%)	2 (1%)	78	82
1	C	324/376 (86%)	316 (98%)	8 (2%)	42	62
2	B	76/111 (68%)	74 (97%)	2 (3%)	40	61
2	D	78/111 (70%)	76 (97%)	2 (3%)	40	61
All	All	799/974 (82%)	785 (98%)	14 (2%)	51	67

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ILE
1	A	131	LEU
2	B	161	GLU
2	B	166	GLN
1	C	31	GLU
1	C	37	LYS
1	C	59	VAL
1	C	79	ILE
1	C	198	VAL
1	C	252	ILE
1	C	268	ILE
1	C	335	ILE
2	D	198	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	204	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	135	ASN
1	A	244	GLN
1	A	390	HIS
1	C	52	HIS
1	C	129	ASN
1	C	210	HIS
1	C	390	HIS

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 oligosaccharides 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	388/438 (88%)	4.27	277 (71%) 0 2	1, 13, 23, 35	388 (100%)
1	C	389/438 (88%)	4.23	288 (74%) 0 2	1, 12, 29, 42	389 (100%)
2	B	94/128 (73%)	4.96	71 (75%) 0 1	4, 20, 37, 57	94 (100%)
2	D	94/128 (73%)	5.15	76 (80%) 0 1	4, 19, 34, 48	94 (100%)
All	All	965/1132 (85%)	4.41	712 (73%) 0 2	1, 13, 30, 57	965 (100%)

All (712) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	289	ALA	39.8
2	D	175	CYS	21.7
1	C	288	ILE	21.1
2	B	204	LEU	20.9
1	A	355	GLY	19.2
1	A	122	TYR	17.1
1	C	424	SER	16.6
2	B	140	TYR	16.0
1	A	82	ALA	15.8
1	C	427	LYS	15.3
1	C	43	GLY	15.2
1	A	157	THR	15.1
1	A	85	THR	15.1
1	C	422	SER	14.7
1	C	270	SER	14.1
1	C	119	GLN	13.7
1	A	214	ASP	13.3
1	A	79	ILE	13.3
1	A	84	GLY	13.3
1	C	114	CYS	12.6
2	B	173	PHE	12.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	125	ALA	12.5
1	C	102	GLY	12.4
2	D	219	GLU	12.2
1	C	64	PRO	12.2
2	B	172	VAL	11.9
1	A	339	HIS	11.9
1	A	81	ALA	11.9
1	A	139	LEU	11.8
1	A	226	GLY	11.8
1	A	386	ALA	11.8
2	B	170	ASP	11.6
1	C	232	LEU	11.5
1	A	285	VAL	11.4
1	A	112	SER	11.3
1	A	280	ALA	11.3
1	A	108	ILE	11.2
1	A	116	GLN	11.2
1	A	156	ALA	11.2
2	B	219	GLU	11.1
1	C	46	GLY	11.0
2	D	173	PHE	11.0
1	C	236	GLY	10.9
1	C	315	TYR	10.9
2	B	199	ARG	10.8
1	A	76	VAL	10.7
1	A	103	VAL	10.7
1	C	63	LYS	10.6
1	A	198	VAL	10.5
1	A	135	ASN	10.4
2	D	154	ASP	10.4
2	D	144	PRO	10.3
2	B	139	LEU	10.2
2	D	204	LEU	10.2
1	A	357	SER	10.2
1	A	428	ASN	10.2
1	A	403	ILE	10.2
1	A	99	GLN	10.1
1	C	113	PRO	10.1
1	C	250	HIS	10.0
1	C	38	ASN	9.9
1	A	362	ASP	9.9
1	A	110	TYR	9.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	235	GLY	9.9
1	C	321	TYR	9.9
1	C	355	GLY	9.9
1	A	136	GLU	9.8
1	C	126	VAL	9.8
2	D	157	ALA	9.8
2	D	213	PHE	9.8
2	B	200	PRO	9.8
2	D	199	ARG	9.7
1	C	89	CYS	9.7
2	B	192	PHE	9.6
2	D	174	ILE	9.6
1	A	387	ASP	9.6
1	A	133	CYS	9.6
1	A	237	GLY	9.5
2	D	176	PHE	9.4
1	C	128	VAL	9.4
1	A	48	ILE	9.4
1	A	80	LEU	9.3
1	A	78	GLU	9.2
1	C	404	TYR	9.2
1	C	105	PRO	9.1
1	A	238	PHE	9.1
2	D	133	VAL	9.1
1	A	66	TYR	9.1
2	D	216	TYR	9.1
1	C	117	VAL	9.1
1	C	33	THR	9.1
1	C	271	GLU	9.0
2	B	176	PHE	9.0
2	B	133	VAL	8.9
2	B	132	THR	8.9
1	C	425	MET	8.9
1	C	272	PRO	8.9
1	C	403	ILE	8.9
1	A	87	PHE	8.8
1	C	387	ASP	8.8
1	C	101	LEU	8.7
1	C	76	VAL	8.7
1	C	116	GLN	8.7
1	C	170	PHE	8.6
1	A	268	ILE	8.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	198	VAL	8.6
1	C	406	MET	8.4
2	D	200	PRO	8.4
2	D	139	LEU	8.4
1	C	268	ILE	8.3
1	A	175	LYS	8.3
2	B	215	ALA	8.3
1	C	85	THR	8.3
1	C	104	PRO	8.2
2	D	169	ALA	8.2
1	C	54	GLN	8.2
2	D	141	ILE	8.2
1	A	217	CYS	8.2
1	A	213	SER	8.1
2	D	132	THR	8.1
2	D	130	TRP	8.1
1	C	45	LEU	8.0
1	A	126	VAL	8.0
1	C	109	ILE	7.9
1	A	177	CYS	7.9
1	C	48	ILE	7.9
1	C	190	GLN	7.9
1	A	119	GLN	7.9
1	C	82	ALA	7.9
1	C	217	CYS	7.9
1	A	71	ASN	7.8
2	B	181	GLU	7.8
2	B	212	CYS	7.8
2	D	160	LEU	7.8
2	D	127	ARG	7.8
2	D	140	TYR	7.7
1	C	52	HIS	7.7
1	C	152	LEU	7.7
1	A	240	GLY	7.7
1	C	136	GLU	7.6
1	A	354	TRP	7.6
1	A	270	SER	7.6
1	C	135	ASN	7.6
2	D	206	PRO	7.6
1	C	134	ASP	7.6
1	C	120	ILE	7.6
2	D	143	ILE	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	381	PHE	7.5
1	A	321	TYR	7.5
1	C	405	TYR	7.5
2	D	135	SER	7.4
1	C	83	LEU	7.4
1	C	283	LEU	7.4
1	A	211	ALA	7.4
1	C	418	ALA	7.4
1	A	327	LYS	7.4
2	D	193	LEU	7.4
1	A	191	ILE	7.4
1	A	89	CYS	7.3
1	C	280	ALA	7.3
2	B	174	ILE	7.3
1	C	130	ILE	7.3
1	C	291	LYS	7.3
2	D	136	GLY	7.3
1	A	114	CYS	7.3
1	A	377	ASP	7.2
1	C	151	VAL	7.2
1	A	11	SER	7.2
1	A	151	VAL	7.2
1	A	194	VAL	7.2
1	C	204	GLU	7.2
2	B	210	ASP	7.2
1	C	233	ASP	7.1
2	B	160	LEU	7.1
1	A	64	PRO	7.1
1	A	52	HIS	7.1
1	A	281	PHE	7.1
1	C	112	SER	7.1
1	A	55	TRP	7.1
2	B	130	TRP	7.1
1	C	110	TYR	7.1
2	D	187	LEU	7.1
1	C	238	PHE	7.1
2	D	171	HIS	7.0
1	C	290	LYS	7.0
2	B	158	VAL	7.0
2	B	195	PHE	7.0
1	C	208	TYR	6.9
1	C	65	PHE	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	126	LYS	6.9
1	C	62	ILE	6.9
1	A	218	VAL	6.9
2	B	216	TYR	6.9
1	A	196	PHE	6.9
1	A	276	TYR	6.8
1	C	231	MET	6.8
1	A	364	ILE	6.7
1	A	356	PRO	6.7
1	C	205	SER	6.7
2	D	191	SER	6.7
1	A	287	ILE	6.7
1	C	155	ILE	6.7
1	A	283	LEU	6.7
2	B	175	CYS	6.6
2	D	212	CYS	6.6
2	B	134	LEU	6.6
1	C	392	PRO	6.6
2	B	194	GLY	6.6
1	C	323	SER	6.6
1	A	134	ASP	6.6
1	A	67	THR	6.6
1	A	275	TYR	6.6
1	C	314	TYR	6.6
1	A	86	GLY	6.6
1	A	65	PHE	6.6
1	C	99	GLN	6.6
1	A	274	SER	6.6
2	D	214	MET	6.5
2	B	156	PHE	6.5
1	A	138	GLU	6.5
1	A	98	VAL	6.5
1	C	340	LYS	6.5
1	A	277	VAL	6.5
1	C	251	VAL	6.4
1	A	132	THR	6.4
1	A	144	ARG	6.4
1	A	115	LYS	6.4
1	C	234	ILE	6.4
2	B	214	MET	6.4
1	C	42	VAL	6.4
1	A	101	LEU	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	128	VAL	6.3
1	C	98	VAL	6.3
1	C	273	GLY	6.3
1	C	57	ASN	6.3
1	C	58	VAL	6.3
1	C	373	LEU	6.2
2	B	209	PRO	6.2
1	A	215	ALA	6.2
1	C	168	MET	6.2
1	A	155	ILE	6.2
1	A	88	ALA	6.2
1	A	384	MET	6.2
1	C	215	ALA	6.2
2	B	141	ILE	6.2
1	A	208	TYR	6.2
1	C	196	PHE	6.2
1	C	213	SER	6.2
1	C	194	VAL	6.2
1	C	364	ILE	6.1
2	B	208	ARG	6.1
1	C	139	LEU	6.1
1	C	228	THR	6.0
1	C	275	TYR	6.0
1	C	86	GLY	6.0
1	A	324	PHE	6.0
1	A	317	ASN	6.0
1	A	316	MET	6.0
1	C	339	HIS	6.0
2	D	190	PHE	5.9
1	A	390	HIS	5.9
2	D	156	PHE	5.9
2	D	168	ARG	5.9
1	C	118	SER	5.9
1	C	412	TRP	5.9
1	A	338	VAL	5.9
1	C	255	LEU	5.9
2	B	218	PHE	5.9
1	C	50	LYS	5.8
1	A	233	ASP	5.8
1	A	63	LYS	5.8
2	D	159	LEU	5.8
1	C	138	GLU	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	322	GLY	5.8
1	A	315	TYR	5.8
1	A	352	SER	5.8
2	D	158	VAL	5.8
1	A	153	LEU	5.7
2	D	142	GLU	5.7
2	D	186	LEU	5.7
1	C	277	VAL	5.7
1	C	356	PRO	5.7
1	C	75	ALA	5.7
1	A	83	LEU	5.6
1	C	188	ASP	5.6
1	C	367	SER	5.6
1	A	216	ARG	5.6
1	C	90	SER	5.6
1	A	137	ILE	5.6
1	C	111	ILE	5.6
1	A	223	GLY	5.6
1	C	133	CYS	5.6
1	A	174	LEU	5.6
1	C	72	SER	5.5
1	C	235	GLY	5.5
2	B	196	GLU	5.5
1	A	123	ALA	5.5
1	A	72	SER	5.5
1	C	122	TYR	5.5
1	A	39	ALA	5.5
1	A	272	PRO	5.5
1	C	362	ASP	5.5
1	C	189	VAL	5.5
1	C	287	ILE	5.5
1	A	130	ILE	5.4
1	A	61	GLN	5.4
2	D	172	VAL	5.4
1	A	197	HIS	5.4
1	A	232	LEU	5.4
2	D	138	SER	5.4
1	A	228	THR	5.4
1	C	39	ALA	5.4
1	C	401	PRO	5.3
1	A	202	CYS	5.3
2	B	155	SER	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	207	LYS	5.3
1	C	318	ASP	5.2
2	B	159	LEU	5.2
1	A	195	LYS	5.2
1	A	190	GLN	5.2
1	A	397	ASP	5.2
1	C	388	SER	5.2
1	A	245	LEU	5.2
1	A	152	LEU	5.2
1	A	13	GLY	5.2
1	A	379	LEU	5.2
1	A	189	VAL	5.1
1	A	43	GLY	5.1
1	C	229	MET	5.1
1	C	431	PHE	5.1
2	D	137	GLY	5.1
1	C	253	SER	5.1
1	C	150	LYS	5.1
1	A	351	SER	5.1
1	C	93	ASN	5.1
1	C	184	ALA	5.1
1	A	220	ASP	5.1
1	C	123	ALA	5.0
1	A	320	VAL	5.0
1	C	55	TRP	5.0
1	C	181	LEU	5.0
1	C	214	ASP	5.0
1	A	29	VAL	5.0
1	C	269	ILE	5.0
2	B	137	GLY	5.0
2	B	206	PRO	5.0
2	D	164	GLU	5.0
2	B	193	LEU	4.9
1	A	30	TYR	4.9
1	C	180	LEU	4.9
2	D	163	ALA	4.9
2	B	136	GLY	4.9
1	A	54	GLN	4.9
1	A	44	ASP	4.9
1	C	348	LEU	4.9
2	D	134	LEU	4.9
1	A	41	PHE	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	191	SER	4.8
1	A	404	TYR	4.8
1	A	68	VAL	4.8
1	C	292	VAL	4.8
1	A	421	THR	4.8
1	A	259	TYR	4.8
2	B	152	SER	4.8
1	C	68	VAL	4.8
1	A	286	ASN	4.8
2	B	161	GLU	4.8
2	B	164	GLU	4.8
1	C	317	ASN	4.8
1	C	41	PHE	4.7
2	B	190	PHE	4.7
1	A	389	PHE	4.7
1	A	170	PHE	4.7
1	A	337	GLU	4.7
1	C	338	VAL	4.7
1	A	206	GLN	4.7
1	A	26	ASP	4.7
1	A	192	ILE	4.6
1	C	88	ALA	4.6
1	C	407	MET	4.6
1	C	61	GLN	4.6
1	A	50	LYS	4.6
1	A	358	CYS	4.6
2	B	167	LEU	4.6
2	B	184	ALA	4.6
2	D	210	ASP	4.6
1	A	363	GLN	4.6
1	C	400	ARG	4.5
1	C	121	LYS	4.5
2	B	217	THR	4.5
1	C	252	ILE	4.5
1	C	408	SER	4.5
1	A	188	ASP	4.5
1	A	431	PHE	4.5
1	A	104	PRO	4.4
1	C	358	CYS	4.4
1	A	212	LEU	4.4
1	C	66	TYR	4.4
1	C	276	TYR	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	350	THR	4.4
1	C	366	GLU	4.4
1	A	173	THR	4.4
1	A	38	ASN	4.4
1	A	378	TRP	4.4
1	A	252	ILE	4.3
1	A	229	MET	4.3
1	C	353	LEU	4.3
1	A	382	ASP	4.3
1	A	406	MET	4.3
1	A	271	GLU	4.3
1	C	245	LEU	4.3
2	D	208	ARG	4.3
1	A	102	GLY	4.3
1	A	209	VAL	4.3
1	A	371	PRO	4.2
1	A	73	ALA	4.2
1	C	193	GLY	4.2
1	A	45	LEU	4.2
1	A	90	SER	4.2
1	C	360	GLU	4.2
1	A	46	GLY	4.2
1	A	234	ILE	4.2
1	A	34	LEU	4.2
1	C	361	LEU	4.2
2	B	186	LEU	4.2
1	C	149	ALA	4.2
2	B	163	ALA	4.1
2	D	167	LEU	4.1
1	A	427	LYS	4.1
1	A	279	SER	4.1
1	C	199	SER	4.1
1	C	69	LYS	4.1
1	C	197	HIS	4.1
1	A	91	SER	4.1
1	A	253	SER	4.1
2	D	197	ILE	4.1
1	A	314	TYR	4.1
1	A	210	HIS	4.0
1	C	218	VAL	4.0
1	A	181	LEU	4.0
1	A	395	PHE	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	53	SER	4.0
1	A	353	LEU	4.0
1	C	398	PHE	4.0
1	C	409	PHE	3.9
2	B	213	PHE	3.9
1	C	156	ALA	3.9
1	A	21	LEU	3.9
1	A	109	ILE	3.9
1	A	97	LEU	3.9
1	A	385	GLY	3.9
2	B	182	ASP	3.9
1	C	79	ILE	3.9
1	A	248	VAL	3.9
1	C	246	GLU	3.9
1	A	105	PRO	3.8
1	C	336	PRO	3.8
1	A	25	ILE	3.8
1	C	316	MET	3.8
2	D	153	LYS	3.8
2	D	131	ARG	3.8
1	A	75	ALA	3.8
1	A	278	SER	3.8
1	C	363	GLN	3.8
1	C	177	CYS	3.8
2	B	171	HIS	3.8
1	A	193	GLY	3.8
1	A	219	PHE	3.8
2	D	170	ASP	3.8
2	D	161	GLU	3.8
1	C	132	THR	3.7
2	D	152	SER	3.7
1	C	18	GLY	3.7
1	C	249	ASN	3.7
1	C	378	TRP	3.7
2	D	166	GLN	3.7
2	B	187	LEU	3.7
1	C	206	GLN	3.7
1	A	120	ILE	3.7
1	A	244	GLN	3.7
1	A	412	TRP	3.7
1	A	53	SER	3.7
2	B	207	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	159	ASP	3.7
1	C	414	GLU	3.7
1	A	318	ASP	3.6
2	D	205	VAL	3.6
1	A	269	ILE	3.6
1	A	405	TYR	3.6
1	C	284	ALA	3.6
1	A	255	LEU	3.6
2	B	203	PRO	3.6
1	A	131	LEU	3.6
1	C	411	ASP	3.6
1	C	319	GLY	3.6
1	A	398	PHE	3.6
1	C	281	PHE	3.6
1	A	92	LYS	3.6
1	A	199	SER	3.6
2	D	162	PHE	3.6
1	A	31	GLU	3.6
1	A	256	LEU	3.5
2	D	194	GLY	3.5
1	C	354	TRP	3.5
1	C	248	VAL	3.5
1	A	142	ILE	3.5
1	A	107	ASN	3.5
1	A	180	LEU	3.5
1	C	259	TYR	3.5
1	A	145	ASN	3.5
1	C	153	LEU	3.5
1	C	237	GLY	3.5
1	A	94	GLU	3.5
1	C	40	PHE	3.4
1	C	222	ALA	3.4
1	C	390	HIS	3.4
1	A	401	PRO	3.4
1	C	209	VAL	3.4
1	C	97	LEU	3.4
1	A	292	VAL	3.4
1	A	154	HIS	3.4
1	C	247	GLU	3.4
1	A	42	VAL	3.4
1	C	220	ASP	3.4
1	C	240	GLY	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	3.4
1	C	201	ALA	3.3
1	A	118	SER	3.3
1	C	59	VAL	3.3
1	C	221	MET	3.3
1	C	239	THR	3.3
2	D	126	LYS	3.3
1	A	20	ASP	3.2
1	A	62	ILE	3.2
1	A	429	PHE	3.2
1	C	326	SER	3.2
2	D	195	PHE	3.2
1	A	416	GLN	3.2
1	C	34	LEU	3.2
1	C	187	LEU	3.2
1	C	219	PHE	3.2
1	A	33	THR	3.2
1	C	108	ILE	3.2
2	B	148	LEU	3.2
1	A	172	THR	3.2
1	C	172	THR	3.2
1	A	56	GLN	3.2
1	C	191	ILE	3.2
1	C	80	LEU	3.1
1	C	365	VAL	3.1
1	A	19	THR	3.1
2	D	192	PHE	3.1
1	A	49	VAL	3.1
1	C	25	ILE	3.1
1	A	373	LEU	3.1
2	D	198	VAL	3.1
1	A	127	GLY	3.1
2	B	189	THR	3.1
1	A	74	PRO	3.1
1	C	44	ASP	3.0
1	C	311	ALA	3.0
2	B	157	ALA	3.0
2	D	182	ASP	3.0
1	C	140	LYS	3.0
1	C	357	SER	3.0
1	C	56	GLN	3.0
1	C	60	ALA	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	24	VAL	3.0
1	C	278	SER	3.0
2	B	205	VAL	3.0
2	B	135	SER	3.0
1	A	203	LYS	3.0
1	C	377	ASP	2.9
2	B	211	ALA	2.9
1	C	384	MET	2.9
1	A	28	TYR	2.9
1	A	250	HIS	2.9
2	D	202	HIS	2.9
1	A	12	VAL	2.9
1	A	249	ASN	2.9
1	C	385	GLY	2.9
1	A	111	ILE	2.9
1	A	222	ALA	2.9
1	C	394	ALA	2.9
1	A	231	MET	2.9
1	C	256	LEU	2.9
1	C	26	ASP	2.9
2	B	143	ILE	2.8
1	C	47	LYS	2.8
2	B	177	HIS	2.8
1	A	247	GLU	2.8
2	D	183	ARG	2.8
1	C	254	PRO	2.8
1	C	141	LYS	2.8
1	C	103	VAL	2.8
1	C	71	ASN	2.8
1	C	129	ASN	2.8
1	C	142	ILE	2.8
2	D	201	GLY	2.8
1	A	51	LYS	2.8
1	A	106	GLU	2.8
1	A	57	ASN	2.7
1	C	183	CYS	2.7
1	A	288	ILE	2.7
1	C	144	ARG	2.7
2	B	138	SER	2.7
1	C	137	ILE	2.7
1	C	423	ASP	2.7
1	A	200	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	127	GLY	2.7
1	C	148	ASN	2.7
1	C	244	GLN	2.7
1	C	399	GLN	2.7
1	C	413	TYR	2.6
1	C	293	VAL	2.6
1	A	176	ASN	2.6
1	C	49	VAL	2.6
1	C	428	ASN	2.6
1	A	37	LYS	2.6
1	C	195	LYS	2.6
1	C	91	SER	2.6
1	C	185	LYS	2.6
2	B	183	ARG	2.6
1	C	154	HIS	2.5
1	A	171	GLY	2.5
1	A	376	GLY	2.5
2	D	150	GLU	2.5
2	D	148	LEU	2.5
1	A	260	PHE	2.5
1	C	32	HIS	2.5
1	C	143	ALA	2.5
1	A	361	LEU	2.5
1	C	421	THR	2.5
1	C	124	ALA	2.5
1	C	28	TYR	2.5
1	A	273	GLY	2.5
1	C	359	ASP	2.5
1	C	192	ILE	2.5
1	C	216	ARG	2.5
1	C	274	SER	2.4
1	A	178	ARG	2.4
1	C	171	GLY	2.4
1	C	115	LYS	2.4
1	C	370	LEU	2.4
2	D	179	ASN	2.4
1	A	420	ILE	2.4
1	A	425	MET	2.4
1	C	371	PRO	2.4
1	A	69	LYS	2.4
1	C	87	PHE	2.4
1	C	145	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	37	LYS	2.4
2	D	165	GLU	2.4
1	A	205	SER	2.4
1	C	368	CYS	2.4
1	C	432	VAL	2.4
1	A	341	LYS	2.4
1	C	396	ASN	2.4
1	A	59	VAL	2.3
1	C	313	MET	2.3
1	C	402	ALA	2.3
2	D	181	GLU	2.3
1	A	254	PRO	2.3
1	C	227	PHE	2.3
1	A	284	ALA	2.3
1	A	239	THR	2.3
2	B	153	LYS	2.3
1	A	282	THR	2.3
1	C	379	LEU	2.3
1	A	426	MET	2.3
1	A	77	LEU	2.3
1	C	29	VAL	2.3
1	A	159	ASP	2.2
1	A	242	GLU	2.2
1	C	182	GLU	2.2
1	C	15	LEU	2.2
1	A	432	VAL	2.2
1	C	81	ALA	2.2
1	C	11	SER	2.2
2	B	188	ARG	2.2
1	C	179	HIS	2.2
2	B	127	ARG	2.2
2	D	147	ALA	2.2
1	A	93	ASN	2.2
1	A	246	GLU	2.2
1	A	366	GLU	2.2
1	A	262	GLU	2.2
1	C	198	VAL	2.2
1	C	24	VAL	2.1
1	A	182	GLU	2.1
1	A	375	VAL	2.1
1	C	223	GLY	2.1
1	C	381	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	382	ASP	2.1
1	C	426	MET	2.1
1	C	67	THR	2.1
2	D	217	THR	2.1
1	A	393	SER	2.1
1	A	325	ALA	2.1
1	C	131	LEU	2.1
1	A	409	PHE	2.1
1	C	77	LEU	2.1
2	D	177	HIS	2.1
1	A	266	VAL	2.1
1	A	40	PHE	2.0
1	C	210	HIS	2.0
2	B	185	ALA	2.0
1	C	416	GLN	2.0
1	C	258	ILE	2.0
1	C	107	ASN	2.0
1	A	60	ALA	2.0
1	C	324	PHE	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 oligosaccharides 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.