Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:36 PM GMT

PDB ID	:	4PER
Title	:	Structure of Gallus gallus ribonuclease inhibitor complexed with Gallus gallus ribonuclease I
Authors	:	Bianchetti, C.M.; Lomax, J.E.; Raines, R.T.; Fox, B.G.
Deposited on	:	2014-04-24
Resolution	:	1.92 Å(reported)

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 (i)

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

The reported resolution of this entry is 1.92 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		1.8%
RSRZ outliers		52.2%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
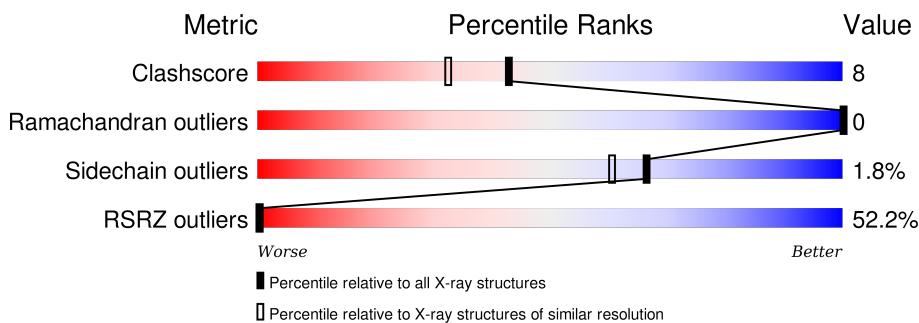
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	6540 (1.94-1.90)
Ramachandran outliers	100387	6464 (1.94-1.90)
Sidechain outliers	100360	6465 (1.94-1.90)
RSRZ outliers	91569	5846 (1.94-1.90)

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 <=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	460	46% / 84% 14% ·
2	B	113	73% / 75% 19% · ·
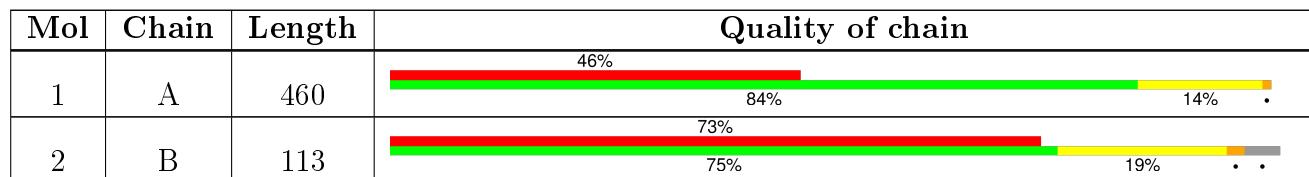
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4636 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 Ribonuclease Inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total 3533	C 2198	N 596	O 701	S 38	0	10	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	TYR	-	expression tag	UNP Q5ZIY8
A	-2	PHE	-	expression tag	UNP Q5ZIY8
A	-1	GLN	-	expression tag	UNP Q5ZIY8
A	0	GLY	-	expression tag	UNP Q5ZIY8
A	10	ILE	MET	conflict	UNP Q5ZIY8

- Molecule 2 is a protein called Angiogenin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	109	Total 870	C 538	N 171	O 154	S 7	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	195	Total 195	O 195	0	0
3	B	38	Total 38	O 38	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: Ribonuclease Inhibitor
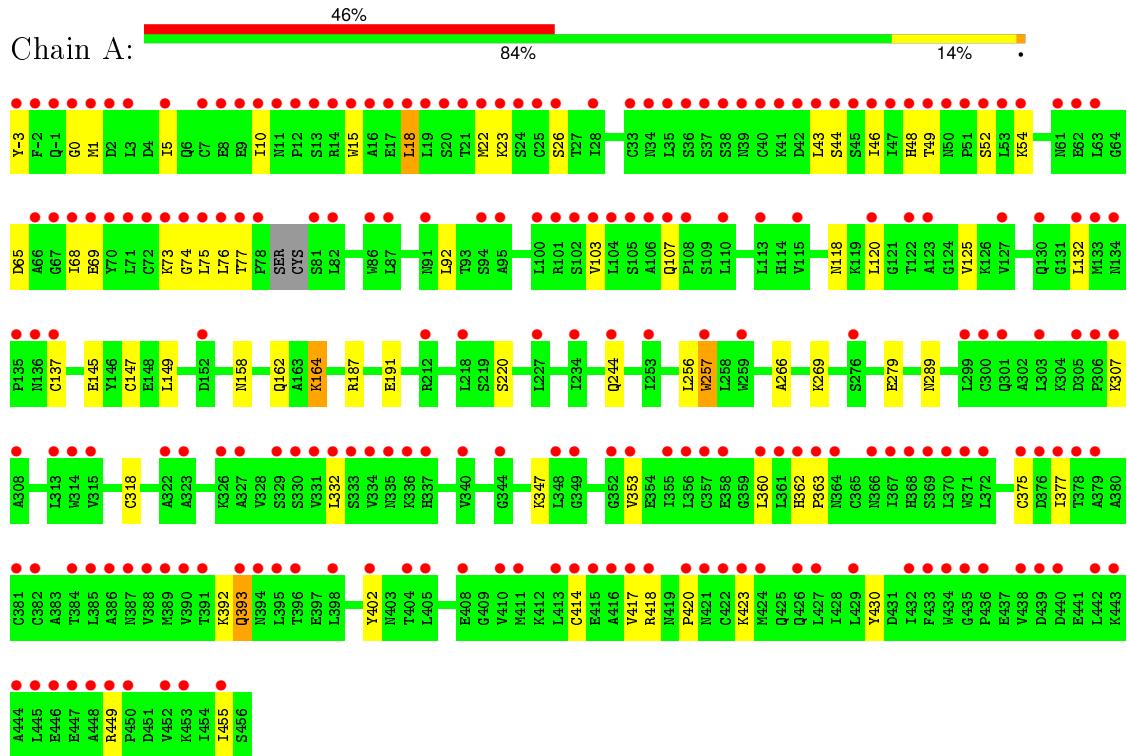
- Molecule 2: Angiogenin
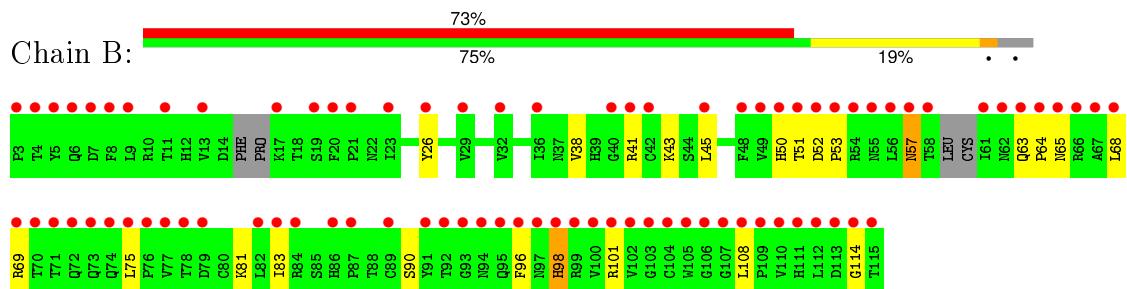
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	52.66Å　　84.54Å　　121.66Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	39.81　–　1.92 41.96　–　1.77	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.81-1.92) 91.3 (41.96-1.77)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.43 (at 1.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.202　,　　　0.254 0.197　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	1.8	Xtriage
Anisotropy	2.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 60.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	0 of 50821 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4636	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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	0.45	0/3607	0.58	2/4886 (0.0%)
2	B	0.39	0/889	0.61	0/1205
All	All	0.44	0/4496	0.59	2/6091 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	TRP	CA-CB-CG	-5.68	102.91	113.70
1	A	393	GLN	CA-CB-CG	5.42	125.31	113.40

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	3533	0	3583	57	0
2	B	870	0	851	24	0
3	A	195	0	0	3	0
3	B	38	0	0	0	0
All	All	4636	0	4434	72	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 8.

All (72) close contacts within the same asymmetric unit are listed below, sorted by their clash

Full wwPDB X-ray Structure Validation Report

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:PRO:O	2:B:57:ASN:ND2	2.06	0.87
2:B:57:ASN:H	2:B:57:ASN:HD22	1.27	0.82
1:A:455:ILE:HD12	2:B:41:ARG:HH11	1.46	0.79
1:A:75:LEU:HD12	1:A:103:VAL:HG22	1.67	0.77
2:B:57:ASN:N	2:B:57:ASN:HD22	1.82	0.76
2:B:38:VAL:HG23	2:B:41:ARG:HH21	1.53	0.74
1:A:23:LYS:NZ	1:A:49:THR:OG1	2.26	0.68
1:A:257:TRP:CZ3	2:B:83:ILE:O	2.49	0.66
1:A:5:ILE:HD11	1:A:18:LEU:HD21	1.79	0.65
1:A:75:LEU:HD11	1:A:103:VAL:HG13	1.78	0.65
1:A:402:TYR:OH	2:B:45:LEU:O	2.15	0.64
2:B:101:ARG:HB3	2:B:114:GLY:HA3	1.81	0.62
1:A:10:ILE:HG21	1:A:15:TRP:HE3	1.64	0.62
2:B:96:PHE:HB3	2:B:98:HIS:ND1	2.15	0.61
1:A:48:HIS:CD2	1:A:77:THR:HG22	2.35	0.61
1:A:402:TYR:OH	2:B:43:LYS:HE2	2.02	0.58
1:A:75:LEU:HD13	1:A:75:LEU:O	2.03	0.58
1:A:257:TRP:HZ3	2:B:83:ILE:O	1.89	0.55
1:A:256:LEU:C	1:A:257:TRP:HD1	2.10	0.54
1:A:65:ASP:O	1:A:69:GLU:HG3	2.07	0.54
1:A:455:ILE:HD12	2:B:41:ARG:NH1	2.20	0.54
1:A:393:GLN:HE22	1:A:423:LYS:HE2	1.73	0.53
1:A:393:GLN:NE2	1:A:423:LYS:HG2	2.24	0.53
1:A:455:ILE:HG23	2:B:41:ARG:HH11	1.74	0.52
1:A:43:LEU:HA	1:A:46:ILE:HD12	1.92	0.52
1:A:75:LEU:O	1:A:107:GLN:NE2	2.44	0.51
1:A:393:GLN:NE2	1:A:423:LYS:HE2	2.27	0.50
1:A:158:ASN:O	1:A:162:GLN:HG2	2.11	0.50
1:A:75:LEU:CD1	1:A:103:VAL:HG13	2.41	0.50
1:A:417:VAL:O	1:A:449:ARG:HD3	2.12	0.50
1:A:18:LEU:O	1:A:22:MET:HG3	2.11	0.49
1:A:0:GLY:HA3	1:A:26:SER:HB2	1.94	0.49
1:A:244:GLN:OE1	3:A:593:HOH:O	2.20	0.48
2:B:63:GLN:HG2	2:B:69:ARG:HD2	1.95	0.48
2:B:26:TYR:OH	2:B:50:HIS:HE1	1.97	0.48
1:A:347:LYS:HE2	1:A:347:LYS:HB3	1.56	0.47
2:B:83:ILE:HG12	2:B:90:SER:O	2.14	0.47
1:A:332:LEU:HD13	1:A:360:LEU:HD23	1.96	0.47
1:A:257:TRP:CD1	1:A:257:TRP:N	2.80	0.47
1:A:187:ARG:NH1	1:A:191:GLU:OE2	2.47	0.47
1:A:73:LYS:O	1:A:76:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:VAL:HG21	1:A:377:ILE:HG21	1.97	0.46
1:A:10:ILE:HG21	1:A:15:TRP:CE3	2.47	0.46
2:B:57:ASN:ND2	2:B:57:ASN:N	2.57	0.46
1:A:187:ARG:NH2	3:A:501:HOH:O	2.21	0.46
1:A:125:VAL:HG21	1:A:149:LEU:HD21	1.98	0.46
1:A:455:ILE:HG23	2:B:41:ARG:NH1	2.31	0.45
2:B:51:THR:HG21	2:B:75:LEU:HD13	1.98	0.45
1:A:266:ALA:O	1:A:269:LYS:HG3	2.17	0.45
1:A:256:LEU:C	1:A:257:TRP:CD1	2.90	0.44
1:A:137:CYS:SG	1:A:164:LYS:HE3	2.57	0.44
1:A:44:SER:O	1:A:74:GLY:HA3	2.17	0.43
1:A:132:LEU:O	1:A:164:LYS:HE2	2.18	0.43
1:A:414:CYS:O	1:A:418:ARG:HG3	2.18	0.43
1:A:392:LYS:HA	1:A:392:LYS:HD2	1.78	0.43
1:A:420:PRO:O	1:A:423:LYS:NZ	2.50	0.43
1:A:68:ILE:HD13	1:A:92:LEU:HD21	2.01	0.43
2:B:45:LEU:HD22	2:B:81:LYS:HE2	2.00	0.43
1:A:120:LEU:HD23	1:A:147:CYS:SG	2.59	0.42
1:A:-3:TYR:N	3:A:507:HOH:O	2.52	0.42
2:B:63:GLN:HB3	2:B:64:PRO:HD2	2.01	0.42
1:A:362:HIS:O	1:A:392:LYS:NZ	2.52	0.42
2:B:108:LEU:HA	2:B:108:LEU:HD23	1.71	0.41
1:A:362:HIS:HA	1:A:363:PRO:HD3	1.90	0.41
1:A:430:TYR:CG	2:B:43:LYS:HE3	2.55	0.41
1:A:289:ASN:O	1:A:318:CYS:HA	2.20	0.41
1:A:375[B]:CYS:SG	1:A:377:ILE:HG23	2.60	0.41
1:A:52:SER:O	1:A:54:LYS:HG3	2.21	0.41
2:B:68:LEU:HD13	2:B:101:ARG:HH21	1.86	0.41
1:A:118:ASN:O	1:A:120:LEU:HD22	2.21	0.41
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.66	0.40
1:A:279:GLU:HG3	1:A:307:LYS:HG2	2.02	0.40

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	464/460 (101%)	452 (97%)	12 (3%)	0	100	100
2	B	103/113 (91%)	97 (94%)	6 (6%)	0	100	100
All	All	567/573 (99%)	549 (97%)	18 (3%)	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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/407 (102%)	409 (99%)	6 (1%)	74	70
2	B	99/103 (96%)	95 (96%)	4 (4%)	38	25
All	All	514/510 (101%)	504 (98%)	10 (2%)	66	58

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	18	LEU
1	A	145	GLU
1	A	164	LYS
1	A	220[A]	SER
1	A	220[B]	SER
2	B	52	ASP
2	B	57	ASN
2	B	65	ASN
2	B	98	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	393	GLN
2	B	57	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 carbohydrates 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, 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	458/460 (99%)	2.41	213 (46%)	0	0	5, 27, 50, 64	0
2	B	109/113 (96%)	3.74	83 (76%)	0	0	20, 36, 69, 76	0
All	All	567/573 (98%)	2.66	296 (52%)	0	0	5, 29, 58, 76	0

All (296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	ILE	13.0
2	B	67	ALA	12.1
2	B	58	THR	11.9
1	A	18	LEU	11.2
1	A	78	PRO	10.0
1	A	77	THR	9.6
1	A	-1	GLN	9.3
1	A	76	LEU	9.1
1	A	-3	TYR	8.8
2	B	68	LEU	8.7
2	B	54	ARG	8.5
1	A	15	TRP	8.4
1	A	10	ILE	8.3
1	A	13	SER	8.2
2	B	108	LEU	7.9
2	B	4	THR	7.9
1	A	402	TYR	7.7
2	B	65	ASN	7.6
2	B	62	ASN	7.5
2	B	55	ASN	7.5
1	A	19	LEU	7.2
1	A	11	ASN	7.2
2	B	114	GLY	7.0
2	B	69	ARG	6.8

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Mol	Chain	Res	Type	RSRZ
2	B	102	VAL	6.7
2	B	106	GLY	6.5
1	A	433	PHE	6.4
1	A	-2	PHE	6.4
1	A	41	LYS	6.3
2	B	99	ARG	6.2
1	A	75	LEU	6.1
1	A	106	ALA	6.1
1	A	390	VAL	6.0
1	A	47	ILE	6.0
1	A	404	THR	5.9
2	B	64	PRO	5.8
2	B	77	VAL	5.8
2	B	115	THR	5.8
2	B	63	GLN	5.7
1	A	394	ASN	5.7
1	A	40	CYS	5.6
1	A	43	LEU	5.5
1	A	38	SER	5.5
1	A	9	GLU	5.4
1	A	20	SER	5.4
2	B	52	ASP	5.4
2	B	98	HIS	5.4
2	B	105	TRP	5.4
1	A	418	ARG	5.3
1	A	33	CYS	5.3
2	B	50	HIS	5.3
1	A	16	ALA	5.3
1	A	448	ALA	5.3
1	A	48	HIS	5.2
1	A	36	SER	5.2
2	B	72	GLN	5.2
1	A	257	TRP	5.2
1	A	2	ASP	5.2
2	B	107	GLY	5.1
2	B	57	ASN	5.1
2	B	76	PRO	5.0
1	A	21	THR	5.0
2	B	3	PRO	5.0
1	A	70	TYR	5.0
2	B	13	VAL	4.8
1	A	450	PRO	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	56	LEU	4.7
1	A	364	ASN	4.7
1	A	73	LYS	4.7
1	A	71	LEU	4.7
1	A	417	VAL	4.7
1	A	63	LEU	4.6
1	A	445	LEU	4.6
1	A	135	PRO	4.6
2	B	96	PHE	4.5
2	B	112	LEU	4.5
1	A	340	VAL	4.5
1	A	23	LYS	4.5
1	A	363	PRO	4.4
1	A	361	LEU	4.4
1	A	0	GLY	4.4
2	B	71	THR	4.3
1	A	360	LEU	4.3
2	B	104	CYS	4.3
1	A	393	GLN	4.3
1	A	449	ARG	4.3
1	A	443	LYS	4.2
1	A	334	VAL	4.2
1	A	51	PRO	4.2
1	A	410	VAL	4.2
1	A	17	GLU	4.2
1	A	415	GLU	4.2
1	A	67	GLY	4.2
1	A	388	VAL	4.2
1	A	35	LEU	4.2
1	A	336	LYS	4.1
2	B	97	ASN	4.1
2	B	74	GLN	4.1
1	A	44	SER	4.1
2	B	51	THR	4.1
1	A	452	VAL	4.1
2	B	53	PRO	4.0
1	A	49	THR	4.0
1	A	438	VAL	3.9
1	A	420	PRO	3.9
1	A	24	SER	3.9
1	A	52	SER	3.9
2	B	9	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	26	SER	3.8
1	A	1	MET	3.8
1	A	314	TRP	3.8
1	A	68	ILE	3.8
1	A	103	VAL	3.8
1	A	3	LEU	3.8
1	A	371	TRP	3.8
2	B	100	VAL	3.8
1	A	333	SER	3.7
2	B	7	ASP	3.7
1	A	12	PRO	3.7
2	B	78	THR	3.7
1	A	136	ASN	3.7
1	A	307	LYS	3.7
2	B	103	GLY	3.7
1	A	34[A]	ASN	3.6
1	A	442	LEU	3.6
1	A	434	TRP	3.6
1	A	446	GLU	3.6
1	A	335	ASN	3.6
1	A	323	ALA	3.6
2	B	19	SER	3.6
1	A	444	ALA	3.6
2	B	66	ARG	3.6
1	A	368[A]	HIS	3.5
2	B	86	HIS	3.5
1	A	53	LEU	3.5
2	B	109	PRO	3.5
1	A	72	CYS	3.5
1	A	46	ILE	3.5
1	A	22	MET	3.5
1	A	37	SER	3.5
1	A	432	ILE	3.5
1	A	369	SER	3.5
2	B	48	PHE	3.4
1	A	306	PRO	3.4
1	A	382	CYS	3.4
2	B	5	TYR	3.4
1	A	322	ALA	3.4
1	A	391	THR	3.4
1	A	331	VAL	3.4
1	A	421	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	120	LEU	3.4
2	B	73	GLN	3.3
2	B	83	ILE	3.3
1	A	385	LEU	3.3
1	A	329	SER	3.3
1	A	332	LEU	3.3
2	B	75	LEU	3.3
1	A	100	LEU	3.2
1	A	389	MET	3.2
2	B	45	LEU	3.2
1	A	14	ARG	3.2
1	A	61	ASN	3.2
2	B	36	ILE	3.2
1	A	439	ASP	3.2
2	B	8	PHE	3.2
1	A	423	LYS	3.2
1	A	424	MET	3.1
1	A	413	LEU	3.1
2	B	49	VAL	3.1
2	B	29	VAL	3.1
1	A	39	ASN	3.1
1	A	25	CYS	3.1
1	A	447	GLU	3.1
1	A	326	LYS	3.0
1	A	66	ALA	3.0
1	A	426	GLN	3.0
1	A	411	MET	3.0
1	A	62	GLU	3.0
2	B	21	PRO	3.0
1	A	8	GLU	2.9
1	A	69	GLU	2.9
1	A	42	ASP	2.9
1	A	104	LEU	2.9
1	A	440	ASP	2.9
1	A	315	VAL	2.9
2	B	20	PHE	2.9
2	B	113	ASP	2.9
1	A	102	SER	2.9
1	A	74	GLY	2.9
1	A	398	LEU	2.8
2	B	93	GLY	2.8
2	B	6	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	81	SER	2.8
1	A	5	ILE	2.8
1	A	386	ALA	2.8
2	B	23	ILE	2.8
1	A	130	GLN	2.8
1	A	91[A]	ASN	2.8
1	A	435	GLY	2.8
1	A	110	LEU	2.8
1	A	416	ALA	2.8
1	A	54	LYS	2.8
1	A	387	ASN	2.7
1	A	45	SER	2.7
2	B	32	VAL	2.7
2	B	95	GLN	2.7
1	A	101	ARG	2.7
1	A	366	ASN	2.7
1	A	105	SER	2.7
2	B	82	LEU	2.7
1	A	375[A]	CYS	2.6
1	A	384	THR	2.6
1	A	370	LEU	2.6
1	A	7	CYS	2.6
2	B	87	PRO	2.6
1	A	427	LEU	2.6
2	B	70	THR	2.6
1	A	305	ASP	2.6
1	A	107	GLN	2.6
2	B	110	VAL	2.6
1	A	376	ASP	2.6
2	B	89	CYS	2.5
1	A	301	GLN	2.5
2	B	17	LYS	2.5
1	A	414	CYS	2.5
1	A	436	PRO	2.5
1	A	86	TRP	2.4
1	A	127	VAL	2.4
1	A	379	ALA	2.4
2	B	26	TYR	2.4
1	A	396	THR	2.4
1	A	405	LEU	2.4
1	A	429	LEU	2.4
1	A	353	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	234	ILE	2.4
1	A	300	CYS	2.4
2	B	41	ARG	2.4
2	B	101	ARG	2.4
1	A	94	SER	2.4
2	B	92	THR	2.4
1	A	378	THR	2.3
2	B	11	THR	2.3
2	B	42	CYS	2.3
1	A	115	VAL	2.3
1	A	372	LEU	2.3
1	A	28	ILE	2.3
1	A	381	CYS	2.3
2	B	111	HIS	2.3
1	A	344	GLY	2.3
1	A	377	ILE	2.3
1	A	455	ILE	2.3
1	A	134	ASN	2.2
1	A	137	CYS	2.2
1	A	330	SER	2.2
1	A	356	LEU	2.2
1	A	357	CYS	2.2
1	A	212	ARG	2.2
1	A	253	ILE	2.2
1	A	355	ILE	2.2
1	A	303	LEU	2.2
1	A	348	LEU	2.2
1	A	349	GLY	2.2
2	B	79	ASP	2.2
1	A	395	LEU	2.2
1	A	133	MET	2.2
1	A	422	CYS	2.2
1	A	358	GLU	2.2
1	A	362	HIS	2.2
1	A	113	LEU	2.2
1	A	218	LEU	2.2
1	A	299	LEU	2.2
1	A	276[A]	SER	2.2
1	A	50	ASN	2.1
1	A	95	ALA	2.1
1	A	152	ASP	2.1
1	A	244	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	91	TYR	2.1
1	A	132	LEU	2.1
2	B	94	ASN	2.1
2	B	40	GLY	2.1
1	A	367	ILE	2.1
1	A	313	LEU	2.1
1	A	108	PRO	2.1
1	A	337	HIS	2.1
1	A	259	TRP	2.1
1	A	453	LYS	2.1
1	A	408	GLU	2.1
1	A	308	ALA	2.1
1	A	352	GLY	2.1
1	A	87	LEU	2.1
1	A	123	ALA	2.0
1	A	227	LEU	2.0
1	A	82	LEU	2.0
1	A	122	THR	2.0
2	B	84	ARG	2.0
1	A	327	ALA	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 carbohydrates 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.