



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:34 PM GMT

PDB ID : 4CMR
Title : The crystal structure of novel exo-type maltose-forming amylase(Py04_0872)
from Pyrococcus sp. ST04
Authors : Park, K.-H.; Jung, J.-H.; Park, C.-S.; Woo, E.-J.
Deposited on : 2014-01-17
Resolution : 1.80 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
<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

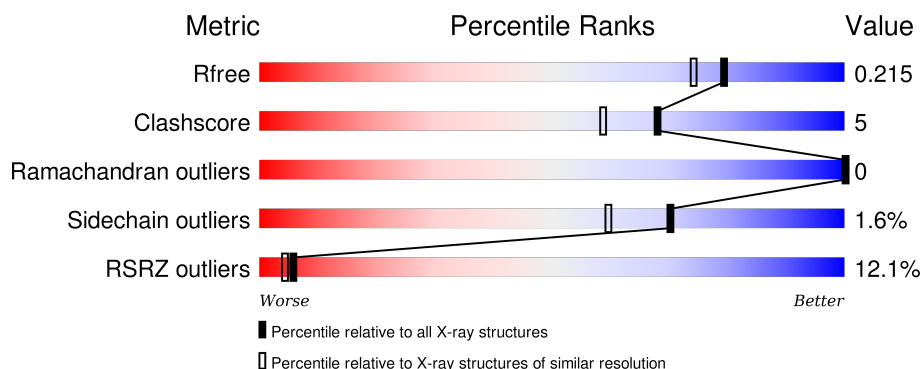
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	597	<div> <div>3%</div> <div>92%</div> <div>8%</div> </div>
1	B	597	<div> <div>21%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10845 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 GLYCOSYL HYDROLASE/DEACETYLASE FAMILY PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	Se	0	0	0
			4958	3212	815	908	6	17			
1	B	595	Total	C	N	O	S	Se	0	0	0
			4941	3202	812	904	6	17			

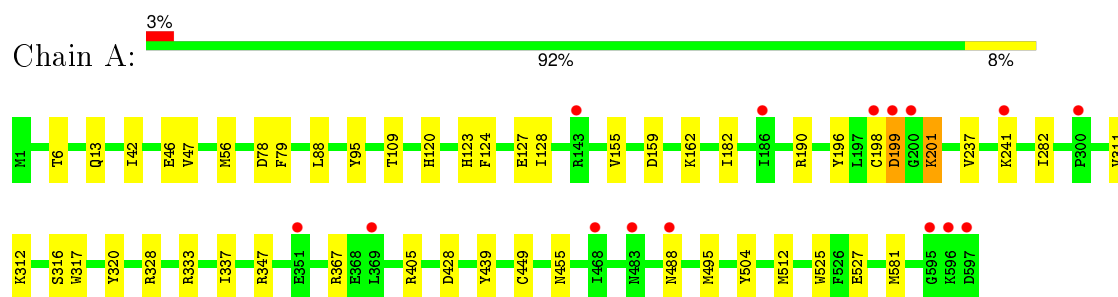
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	774	Total	O	0	0
			774	774		
2	B	172	Total	O	0	0
			172	172		

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: GLYCOSYL HYDROLASE/DEACETYLASE FAMILY PROTEIN



• Molecule 1: GLYCOSYL HYDROLASE/DEACETYLASE FAMILY PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.64Å 370.79Å 82.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.13 – 1.80 33.13 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.1 (33.13-1.80) 94.7 (33.13-1.77)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.15 (at 1.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.198 , 0.225 0.188 , 0.215	Depositor DCC
R_{free} test set	1817 reflections (1.15%)	DCC
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 172314 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10845	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.50	1/5076 (0.0%)	0.62	3/6842 (0.0%)
1	B	0.29	0/5059	0.54	3/6820 (0.0%)
All	All	0.41	1/10135 (0.0%)	0.58	6/13662 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	449	CYS	CB-SG	-7.35	1.69	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	GLU	CB-CA-C	-18.30	73.81	110.40
1	A	198	CYS	CB-CA-C	-8.50	93.41	110.40
1	A	198	CYS	N-CA-C	-7.79	89.98	111.00
1	A	199	ASP	N-CA-C	-6.62	93.12	111.00
1	B	45	GLU	CB-CA-C	-6.49	97.43	110.40
1	B	43	ARG	N-CA-C	-5.68	95.65	111.00

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	4958	0	4856	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4941	0	4839	61	0
2	A	774	0	0	9	4
2	B	172	0	0	4	0
All	All	10845	0	9695	92	4

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 (92) 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:B:141:ILE:O	1:B:170:LYS:NZ	2.10	0.84
1:B:349:TYR:OH	1:B:532:GLU:OE2	2.01	0.78
1:B:211:TYR:OH	2:B:2102:HOH:O	2.08	0.71
1:A:527:GLU:OE1	2:A:2692:HOH:O	2.08	0.71
1:B:35:LEU:HD23	1:B:594:LYS:HB2	1.74	0.69
1:B:82:PHE:CE2	1:B:86:MSE:HE3	2.27	0.69
1:B:449:CYS:SG	2:B:2155:HOH:O	2.52	0.67
1:A:196:TYR:CE1	1:A:311:VAL:HG12	2.31	0.66
1:A:123:HIS:NE2	1:A:159:ASP:OD2	2.29	0.65
1:B:537:LYS:NZ	1:B:569:GLU:OE1	2.31	0.63
1:B:280:GLU:OE2	1:B:296:TYR:OH	2.17	0.63
1:B:581:MSE:HE2	1:B:581:MSE:HA	1.83	0.60
1:A:182:ILE:HG22	1:A:328:ARG:NE	2.16	0.60
1:B:31:TYR:OH	1:B:89:LYS:NZ	2.30	0.59
1:A:455:ASN:HB2	2:A:2633:HOH:O	2.02	0.59
1:B:345:ILE:HG22	1:B:515:LEU:HD12	1.84	0.58
1:B:197:LEU:HG	1:B:199:ASP:H	1.67	0.58
1:A:127:GLU:HG3	2:A:2266:HOH:O	2.08	0.54
1:B:273:GLY:O	1:B:277:ARG:HD3	2.08	0.54
1:B:51:ASN:OD1	1:B:54:ARG:HG3	2.09	0.53
1:B:437:ARG:NH1	1:B:474:GLU:OE2	2.42	0.52
1:B:123:HIS:ND1	1:B:163:ILE:HD11	2.24	0.52
1:B:78:ASP:HB3	1:B:109:THR:HB	1.92	0.51
1:B:146:ILE:O	1:B:289:ARG:NH2	2.36	0.51
1:A:237:VAL:O	1:A:241:LYS:HG2	2.11	0.51
1:B:120:HIS:O	1:B:367:ARG:HD3	2.10	0.50
1:B:527:GLU:OE2	1:B:530:ARG:NH2	2.45	0.50
1:A:312:LYS:HE2	2:A:2486:HOH:O	2.12	0.50
1:A:13:GLN:NE2	1:A:56:MSE:HG2	2.27	0.49
1:B:13:GLN:NE2	1:B:56:MSE:HG2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ILE:HG13	1:B:567:LEU:HD21	1.94	0.49
1:B:484:GLU:HG3	1:B:486:ARG:H	1.77	0.49
1:B:88:LEU:HB2	1:B:95:TYR:CD2	2.47	0.48
1:A:504:TYR:HB2	1:A:525:TRP:CE2	2.49	0.48
1:B:337:ILE:HD11	1:B:512:MSE:HE1	1.94	0.48
1:B:226:LEU:HB3	1:B:270:TRP:CE2	2.49	0.48
1:A:42:ILE:HD12	1:A:47:VAL:HG21	1.96	0.48
1:B:127:GLU:OE2	1:B:131:LYS:NZ	2.37	0.47
1:A:120:HIS:O	1:A:367:ARG:HD3	2.14	0.47
1:B:4:LYS:HE3	1:B:296:TYR:CZ	2.50	0.47
1:A:581:MSE:HA	1:A:581:MSE:HE2	1.95	0.47
1:B:338:ARG:HD2	1:B:341:ASP:OD1	2.14	0.47
1:B:320:TYR:CZ	1:B:333:ARG:HG3	2.50	0.46
1:B:561:ILE:O	1:B:565:TYR:HB2	2.16	0.46
1:B:516:GLU:HB3	1:B:518:TRP:CD1	2.51	0.46
1:B:155:VAL:HG22	1:B:316:SER:HB3	1.98	0.46
1:B:556:ASP:OD1	1:B:556:ASP:N	2.39	0.46
1:B:523:LYS:O	1:B:527:GLU:HG3	2.16	0.45
1:B:45:GLU:HG3	1:B:46:GLU:N	2.26	0.45
1:B:403:PHE:O	2:B:2027:HOH:O	2.21	0.45
1:A:46:GLU:HG3	2:A:2115:HOH:O	2.17	0.45
1:A:6:THR:HB	1:A:282:ILE:O	2.16	0.45
1:B:559:SER:O	1:B:563:THR:HG23	2.17	0.45
1:A:88:LEU:HB2	1:A:95:TYR:CD2	2.52	0.44
1:B:564:LEU:HA	1:B:564:LEU:HD23	1.77	0.44
1:A:78:ASP:HB3	1:A:109:THR:HB	1.99	0.44
1:A:199:ASP:O	1:A:201:LYS:N	2.51	0.44
1:A:162:LYS:HD2	1:A:199:ASP:OD2	2.18	0.44
1:A:190:ARG:HA	2:A:2379:HOH:O	2.18	0.44
1:B:320:TYR:CE2	1:B:347:ARG:HD2	2.53	0.43
1:B:332:MSE:HG3	1:B:345:ILE:HD13	1.99	0.43
1:B:320:TYR:CZ	1:B:347:ARG:HD2	2.54	0.43
1:A:337:ILE:HD11	1:A:512:MSE:HE1	1.99	0.43
1:B:216:PHE:CZ	1:B:267:PHE:HB2	2.54	0.43
1:B:513:LYS:HE2	1:B:513:LYS:HA	2.00	0.43
1:A:320:TYR:CE2	1:A:347:ARG:HD2	2.53	0.43
1:A:320:TYR:CZ	1:A:333:ARG:HG3	2.54	0.43
1:A:128:ILE:HD12	1:A:439:TYR:OH	2.18	0.43
1:A:237:VAL:HG13	1:A:241:LYS:HE2	2.01	0.42
1:B:557:MSE:HB3	1:B:557:MSE:HE2	1.79	0.42
1:B:508:ASP:HA	1:B:510:PHE:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:PHE:CE2	1:B:572:PRO:HA	2.54	0.42
1:B:537:LYS:HG2	1:B:569:GLU:OE1	2.20	0.42
1:B:208:ARG:HA	1:B:249:PHE:O	2.20	0.42
1:B:453:TRP:CE2	1:B:577:ILE:HG23	2.55	0.42
1:B:523:LYS:HE2	1:B:523:LYS:HB3	1.79	0.41
1:A:201:LYS:HB3	2:A:2397:HOH:O	2.20	0.41
1:B:215:ALA:HA	1:B:220:THR:OG1	2.20	0.41
1:B:455:ASN:ND2	1:B:457:ASP:H	2.18	0.41
1:B:543:ARG:NH1	1:B:573:ASP:O	2.53	0.41
1:B:573:ASP:OD1	2:B:2171:HOH:O	2.21	0.41
1:A:405:ARG:HD3	2:A:2066:HOH:O	2.21	0.41
1:B:158:LYS:NZ	1:B:197:LEU:O	2.35	0.41
1:A:155:VAL:HG22	1:A:316:SER:HB3	2.03	0.41
1:A:495:MSE:HE3	1:A:495:MSE:HB3	2.02	0.41
1:A:124:PHE:CE1	1:A:128:ILE:HD11	2.56	0.41
1:B:158:LYS:HE3	1:B:198:CYS:HA	2.02	0.40
1:B:57:ILE:HG23	1:B:87:VAL:HG22	2.03	0.40
1:B:504:TYR:HB2	1:B:525:TRP:CE2	2.57	0.40
1:B:17:ILE:HG12	1:B:31:TYR:CD1	2.57	0.40
1:B:182:ILE:HG13	1:B:328:ARG:CZ	2.52	0.40
1:A:428:ASP:OD2	2:A:2621:HOH:O	2.22	0.40

All (4) 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)
2:A:2603:HOH:O	2:A:2767:HOH:O[6_555]	2.04	0.16
2:A:2553:HOH:O	2:A:2673:HOH:O[3_654]	2.12	0.08
2:A:2604:HOH:O	2:A:2766:HOH:O[6_555]	2.17	0.03
2:A:2272:HOH:O	2:A:2674:HOH:O[3_654]	2.17	0.03

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	595/597 (100%)	584 (98%)	11 (2%)	0	100	100
1	B	593/597 (99%)	574 (97%)	19 (3%)	0	100	100
All	All	1188/1194 (100%)	1158 (98%)	30 (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	539/522 (103%)	535 (99%)	4 (1%)	88	86
1	B	537/522 (103%)	524 (98%)	13 (2%)	57	41
All	All	1076/1044 (103%)	1059 (98%)	17 (2%)	70	59

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	PHE
1	A	201	LYS
1	A	317	TRP
1	A	488	ASN
1	B	7	TYR
1	B	50	ARG
1	B	54	ARG
1	B	138	LEU
1	B	254	LEU
1	B	304	SER
1	B	317	TRP
1	B	425	HIS
1	B	482	GLU
1	B	556	ASP
1	B	558	ARG
1	B	560	VAL

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Mol	Chain	Res	Type
1	B	561	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	294	ASN
1	B	13	GLN
1	B	356	GLN
1	B	425	HIS
1	B	455	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 ⓘ

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	580/597 (97%)	0.14	15 (2%) 59 54	8, 16, 35, 66	0
1	B	578/597 (96%)	1.32	125 (21%) 1 1	26, 45, 63, 72	0
All	All	1158/1194 (96%)	0.73	140 (12%) 6 4	8, 33, 60, 72	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	597	ASP	11.0
1	B	595	GLY	9.1
1	A	199	ASP	8.0
1	B	561	ILE	7.4
1	B	199	ASP	7.2
1	B	348	TRP	6.3
1	A	596	LYS	6.2
1	B	200	GLY	5.9
1	B	590	TRP	5.9
1	B	198	CYS	5.8
1	B	563	THR	5.7
1	B	197	LEU	5.5
1	B	560	VAL	5.5
1	B	143	ARG	5.3
1	B	517	GLY	5.2
1	B	351	GLU	5.1
1	B	44	GLU	4.8
1	B	594	LYS	4.8
1	B	50	ARG	4.7
1	B	564	LEU	4.7
1	B	425	HIS	4.7
1	B	589	GLU	4.7
1	A	483	ASN	4.6
1	B	568	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	585	TRP	4.5
1	B	556	ASP	4.4
1	A	200	GLY	4.3
1	A	595	GLY	4.2
1	A	198	CYS	4.1
1	B	62	TYR	4.1
1	B	410	TYR	4.1
1	B	37	PRO	4.0
1	B	518	TRP	3.9
1	B	587	ASN	3.8
1	B	584	LYS	3.8
1	B	352	ARG	3.8
1	B	46	GLU	3.7
1	B	293	SER	3.7
1	B	385	GLY	3.7
1	B	146	ILE	3.7
1	B	419	TYR	3.7
1	A	143	ARG	3.7
1	B	40	LEU	3.6
1	B	520	THR	3.6
1	B	586	GLU	3.6
1	B	90	TYR	3.6
1	B	289	ARG	3.6
1	B	294	ASN	3.5
1	B	243	GLY	3.5
1	B	515	LEU	3.5
1	B	566	ASP	3.5
1	B	45	GLU	3.5
1	B	483	ASN	3.5
1	B	411	PHE	3.4
1	B	94	ILE	3.4
1	B	353	LYS	3.4
1	B	513	LYS	3.4
1	B	41	GLU	3.4
1	B	559	SER	3.3
1	B	530	ARG	3.3
1	B	292	VAL	3.3
1	A	351	GLU	3.2
1	B	297	LYS	3.2
1	B	536	SER	3.2
1	B	443	LEU	3.1
1	B	555	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	306	SER	3.1
1	B	534	PRO	3.0
1	B	386	VAL	3.0
1	B	100	GLU	3.0
1	B	36	SER	3.0
1	B	387	SER	3.0
1	B	514	GLY	3.0
1	B	382	ARG	3.0
1	B	415	THR	2.9
1	B	416	SER	2.9
1	B	412	GLU	2.9
1	B	537	LYS	2.9
1	B	468	ILE	2.9
1	B	524	ALA	2.9
1	B	54	ARG	2.8
1	A	300	PRO	2.8
1	B	558	ARG	2.8
1	B	17	ILE	2.8
1	B	295	GLU	2.8
1	B	510	PHE	2.8
1	B	588	LYS	2.7
1	B	300	PRO	2.7
1	B	365	LEU	2.7
1	B	521	THR	2.7
1	B	35	LEU	2.7
1	B	93	LYS	2.7
1	B	72	GLU	2.7
1	B	369	LEU	2.7
1	B	418	ASP	2.7
1	A	186	ILE	2.7
1	B	413	LEU	2.6
1	B	444	LEU	2.6
1	B	388	ASP	2.6
1	B	422	GLU	2.6
1	B	169	ASP	2.6
1	B	354	VAL	2.6
1	B	342	ASN	2.5
1	B	366	PHE	2.5
1	B	211	TYR	2.5
1	B	593	HIS	2.5
1	B	592	GLU	2.5
1	B	373	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	533	VAL	2.4
1	A	488	ASN	2.4
1	B	296	TYR	2.4
1	B	562	ASP	2.4
1	B	286	GLU	2.4
1	B	104	THR	2.4
1	B	445	ALA	2.4
1	B	287	PHE	2.4
1	B	565	TYR	2.3
1	B	14	PRO	2.3
1	A	369	LEU	2.3
1	B	403	PHE	2.3
1	B	350	LYS	2.2
1	B	391	LYS	2.2
1	A	241	LYS	2.2
1	B	516	GLU	2.2
1	B	142	ALA	2.2
1	B	488	ASN	2.2
1	B	110	VAL	2.2
1	B	308	ARG	2.2
1	B	89	LYS	2.2
1	B	224	GLU	2.1
1	A	468	ILE	2.1
1	B	12	TYR	2.1
1	B	404	PHE	2.1
1	B	202	SER	2.1
1	B	113	PRO	2.1
1	B	532	GLU	2.0
1	B	511	ARG	2.0
1	B	299	LEU	2.0
1	B	150	TRP	2.0
1	B	310	ASN	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 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.