



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:51 PM GMT

PDB ID : 2B5D
Title : Crystal structure of the novel alpha-amylase AmyC from *Thermotoga maritima*
Authors : Dickmanns, A.; Ballschmiter, M.; Liebl, W.; Ficner, R.
Deposited on : 2005-09-28
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

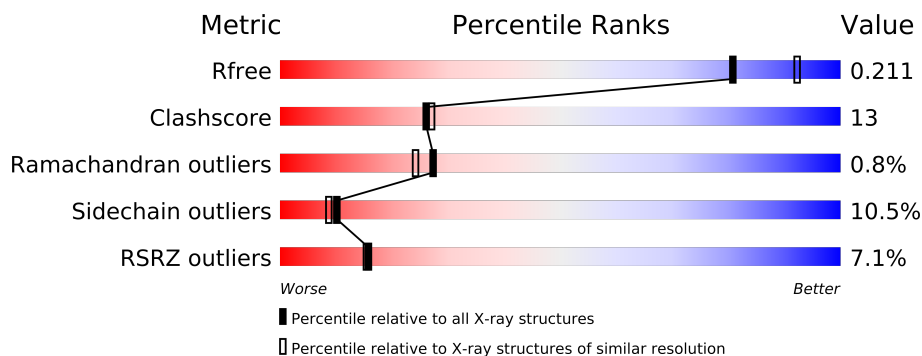
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	X	528	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4660 atoms, of which 0 are hydrogen and 0 are deuterium.

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 alpha-Amylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	518	Total 4343	C 2802	N 728	O 789	S 24	0	4	0

- Molecule 2 is water.

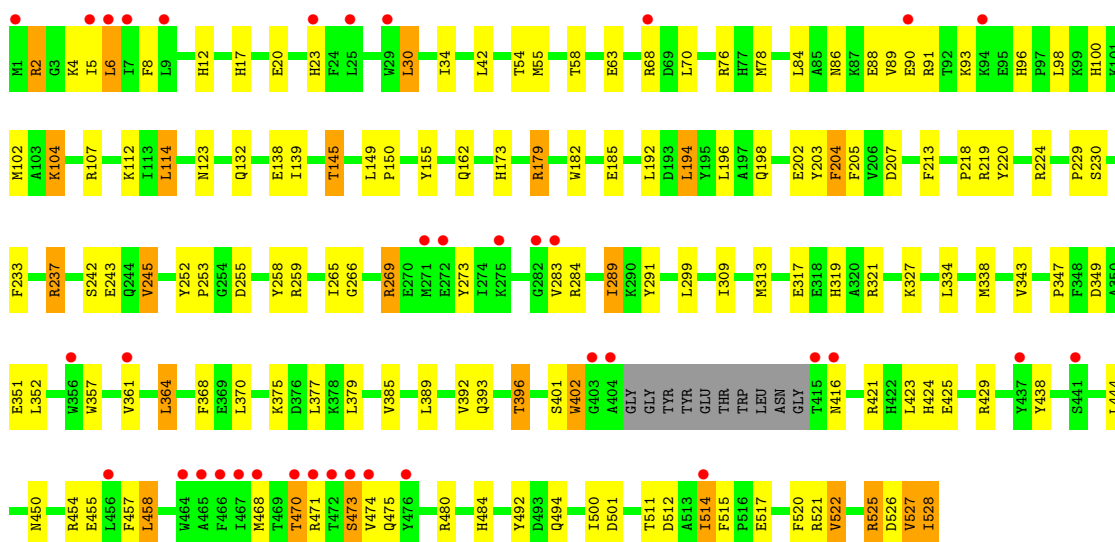
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	317	Total 317	O 317	0	0

3 Residue-property plots

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: alpha-Amylase

Chain X: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	112.16Å 112.16Å 335.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (30.00-2.20) 90.8 (29.97-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0013	Depositor
R, R_{free}	0.219 , 0.257 0.220 , 0.211	Depositor DCC
R_{free} test set	2488 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	6 of 49689 reflections (0.012%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4660	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	X	0.84	1/4486 (0.0%)	0.85	6/6059 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	517	GLU	CB-CG	5.14	1.61	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	237	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	X	525	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	X	338	MET	CG-SD-CE	-6.21	90.26	100.20
1	X	6	LEU	CA-CB-CG	5.88	128.84	115.30
1	X	525	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	X	458	LEU	CB-CG-CD1	5.44	120.25	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	402	TRP	Peptide
1	X	527	VAL	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	4343	0	4177	114	0
2	X	317	0	0	16	0
All	All	4660	0	4177	114	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (114) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:179:ARG:NH2	1:X:202:GLU:OE2	1.83	1.10
1:X:63:GLU:OE2	1:X:514:ILE:O	1.74	1.06
1:X:219:ARG:H	1:X:393:GLN:HE22	1.04	1.02
1:X:5:ILE:HD11	1:X:379:LEU:CD2	1.93	0.98
1:X:526:ASP:HB2	2:X:565:HOH:O	1.62	0.97
1:X:352:LEU:HB3	2:X:650:HOH:O	1.65	0.97
1:X:145:THR:HG21	1:X:457:PHE:O	1.67	0.95
1:X:207:ASP:OD1	1:X:237:ARG:NH2	2.03	0.91
1:X:2:ARG:HH11	1:X:2:ARG:HB3	1.39	0.86
1:X:179:ARG:NE	2:X:709:HOH:O	2.08	0.86
1:X:351:GLU:HB3	2:X:666:HOH:O	1.78	0.84
1:X:179:ARG:CZ	2:X:709:HOH:O	2.24	0.83
1:X:179:ARG:NH1	2:X:709:HOH:O	2.12	0.82
1:X:5:ILE:HD11	1:X:379:LEU:HD23	1.63	0.81
1:X:454[B]:ARG:HH21	1:X:514:ILE:N	1.82	0.77
1:X:219:ARG:N	1:X:393:GLN:HE22	1.82	0.75
1:X:179:ARG:NH2	1:X:202:GLU:CD	2.41	0.75
1:X:2:ARG:HH11	1:X:2:ARG:CB	2.00	0.73
1:X:377:LEU:O	2:X:529:HOH:O	2.09	0.70
1:X:269:ARG:HG2	1:X:273:TYR:CD1	2.26	0.69
1:X:96:HIS:HD2	1:X:98:LEU:H	1.39	0.69
1:X:526:ASP:CB	2:X:565:HOH:O	2.28	0.68
1:X:2:ARG:HH11	1:X:2:ARG:CG	2.06	0.67
1:X:219:ARG:H	1:X:393:GLN:NE2	1.86	0.67
1:X:454[B]:ARG:NH1	1:X:515:PHE:O	2.26	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:5:ILE:CD1	1:X:379:LEU:HD23	2.26	0.64
1:X:179:ARG:HH22	1:X:202:GLU:CD	2.00	0.64
1:X:12:HIS:HD2	1:X:58:THR:OG1	1.80	0.63
1:X:224:ARG:NH2	1:X:389:LEU:HG	2.13	0.63
1:X:185:GLU:O	1:X:401:SER:HB2	1.99	0.62
1:X:258:TYR:OH	1:X:319:HIS:HD2	1.83	0.62
1:X:100:HIS:CE1	1:X:104:LYS:HD3	2.35	0.61
1:X:526:ASP:CG	2:X:565:HOH:O	2.39	0.61
1:X:438:TYR:O	1:X:521:ARG:HD3	2.00	0.60
1:X:454[B]:ARG:NH1	1:X:454[B]:ARG:HG2	2.15	0.60
1:X:266:GLY:O	1:X:284:ARG:HD2	2.01	0.59
1:X:155:TYR:OH	1:X:424:HIS:HD2	1.85	0.59
1:X:454[B]:ARG:HH12	1:X:515:PHE:HB2	1.66	0.58
1:X:416:ASN:HB3	2:X:663:HOH:O	2.02	0.58
1:X:309:ILE:O	1:X:313:MET:HG2	2.03	0.58
1:X:132:GLN:NE2	1:X:139:ILE:H	2.02	0.58
1:X:317:GLU:HG3	1:X:321:ARG:NH1	2.19	0.58
1:X:527:VAL:O	1:X:528:ILE:HB	2.06	0.56
1:X:88:GLU:OE2	1:X:269:ARG:HD3	2.06	0.55
1:X:5:ILE:CD1	1:X:379:LEU:CD2	2.76	0.55
1:X:8:PHE:O	1:X:347:PRO:HA	2.07	0.54
1:X:473:SER:O	1:X:475:GLN:N	2.40	0.54
1:X:78:MET:HB3	1:X:114:LEU:HG	1.90	0.54
1:X:265:ILE:HD13	1:X:289:ILE:CD1	2.39	0.53
1:X:63:GLU:OE1	1:X:173:HIS:CE1	2.61	0.53
1:X:86:ASN:HA	1:X:89:VAL:HG12	1.91	0.53
1:X:494:GLN:NE2	1:X:501:ASP:H	2.07	0.53
1:X:450:ASN:ND2	1:X:520:PHE:H	2.06	0.53
1:X:2:ARG:HH22	1:X:375:LYS:HA	1.75	0.52
1:X:78:MET:CB	1:X:114:LEU:HG	2.39	0.52
1:X:429:ARG:HG2	1:X:492:TYR:CE1	2.46	0.51
1:X:253:PRO:HG3	1:X:357:TRP:CD2	2.46	0.51
1:X:203:TYR:HA	1:X:233:PHE:O	2.09	0.51
1:X:455:GLU:OE1	1:X:512:ASP:OD2	2.28	0.51
1:X:450:ASN:O	1:X:454[A]:ARG:HG3	2.10	0.51
1:X:522:VAL:O	1:X:525:ARG:HD2	2.11	0.51
1:X:8:PHE:CZ	1:X:182[B]:TRP:CD1	2.99	0.50
1:X:494:GLN:HB3	1:X:500:ILE:HA	1.94	0.50
1:X:5:ILE:HD11	1:X:379:LEU:HD22	1.91	0.50
1:X:17:HIS:O	2:X:665:HOH:O	2.19	0.50
1:X:30:LEU:O	1:X:34:ILE:HG13	2.11	0.50
1:X:480:ARG:CZ	1:X:484:HIS:HE1	2.24	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:2:ARG:NH1	1:X:2:ARG:HG2	2.26	0.49
1:X:237:ARG:HG2	2:X:562:HOH:O	2.13	0.49
1:X:89:VAL:HG21	1:X:107:ARG:HH21	1.77	0.49
1:X:93:LYS:HA	1:X:100:HIS:CD2	2.48	0.49
1:X:258:TYR:OH	1:X:319:HIS:CD2	2.65	0.48
1:X:2:ARG:CG	1:X:2:ARG:NH1	2.68	0.48
1:X:455:GLU:OE2	1:X:484:HIS:HD2	1.97	0.48
1:X:450:ASN:HD21	1:X:520:PHE:H	1.60	0.48
1:X:361:VAL:HG22	2:X:532:HOH:O	2.14	0.48
1:X:327:LYS:HE2	1:X:327:LYS:HA	1.97	0.47
1:X:229:PRO:CD	1:X:396:THR:HG22	2.44	0.47
1:X:480:ARG:HA	1:X:480:ARG:HD2	1.70	0.47
1:X:242:SER:O	1:X:245:VAL:HG13	2.14	0.47
1:X:317:GLU:HG3	1:X:321:ARG:HH11	1.78	0.47
1:X:2:ARG:HH12	1:X:375:LYS:C	2.18	0.46
1:X:132:GLN:HE21	1:X:139:ILE:H	1.62	0.46
1:X:182[B]:TRP:HD1	1:X:205:PHE:CD1	2.34	0.46
1:X:55:MET:O	1:X:139:ILE:HA	2.15	0.45
1:X:289:ILE:HD11	1:X:291:TYR:CZ	2.52	0.45
1:X:218:PRO:HA	1:X:393:GLN:NE2	2.31	0.45
1:X:237:ARG:HD3	1:X:237:ARG:HH21	1.58	0.45
1:X:54:THR:HG23	1:X:138:GLU:HG3	1.99	0.44
1:X:179:ARG:NH2	1:X:202:GLU:OE1	2.47	0.44
1:X:450:ASN:O	1:X:454[B]:ARG:HG3	2.18	0.44
1:X:255:ASP:HB3	1:X:258:TYR:CD1	2.52	0.44
1:X:2:ARG:HH11	1:X:2:ARG:HG2	1.82	0.44
1:X:252:TYR:HB2	1:X:253:PRO:HD3	1.99	0.44
1:X:63:GLU:OE1	1:X:173:HIS:HE1	2.00	0.43
1:X:528:ILE:O	2:X:843:HOH:O	2.21	0.43
1:X:265:ILE:HD13	1:X:289:ILE:HD12	2.00	0.43
1:X:204:PHE:N	1:X:204:PHE:CD2	2.86	0.43
1:X:237:ARG:HD2	1:X:402:TRP:CE2	2.54	0.43
1:X:194:LEU:O	1:X:198:GLN:HG3	2.18	0.43
1:X:54:THR:HA	1:X:138:GLU:O	2.19	0.43
1:X:149:LEU:N	1:X:150:PRO:CD	2.83	0.42
1:X:145:THR:CG2	1:X:162:GLN:HE22	2.32	0.42
1:X:182[B]:TRP:CD1	1:X:205:PHE:CD1	3.08	0.42
1:X:364:LEU:HD12	1:X:368:PHE:CZ	2.55	0.42
1:X:425:GLU:O	1:X:429:ARG:HD3	2.20	0.41
1:X:289:ILE:HD11	1:X:291:TYR:CE1	2.56	0.41
1:X:182[B]:TRP:HZ3	2:X:673:HOH:O	2.04	0.41
1:X:88:GLU:CD	1:X:269:ARG:HH11	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:470:THR:OG1	1:X:471:ARG:N	2.51	0.40
1:X:220:TYR:CD1	1:X:224:ARG:HD3	2.57	0.40
1:X:511:THR:O	2:X:665:HOH:O	2.22	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	X	518/528 (98%)	484 (93%)	30 (6%)	4 (1%)	27 24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	474	VAL
1	X	470	THR
1	X	514	ILE
1	X	473	SER

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	X	462/474 (98%)	413 (89%)	49 (11%)	10 8

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	2	ARG

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Mol	Chain	Res	Type
1	X	4	LYS
1	X	6	LEU
1	X	20	GLU
1	X	23	HIS
1	X	30	LEU
1	X	42	LEU
1	X	68	ARG
1	X	70	LEU
1	X	76	ARG
1	X	84	LEU
1	X	90[A]	GLU
1	X	90[B]	GLU
1	X	91	ARG
1	X	102	MET
1	X	104	LYS
1	X	112	LYS
1	X	114	LEU
1	X	123	ASN
1	X	145	THR
1	X	179	ARG
1	X	192	LEU
1	X	194	LEU
1	X	196	LEU
1	X	204	PHE
1	X	213	PHE
1	X	230	SER
1	X	243	GLU
1	X	245	VAL
1	X	259	ARG
1	X	269	ARG
1	X	283	VAL
1	X	289	ILE
1	X	299	LEU
1	X	334	LEU
1	X	343	VAL
1	X	349	ASP
1	X	364	LEU
1	X	370	LEU
1	X	385	VAL
1	X	392	VAL
1	X	396	THR
1	X	421	ARG

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Mol	Chain	Res	Type
1	X	423	LEU
1	X	444	LEU
1	X	458	LEU
1	X	468	MET
1	X	522	VAL
1	X	528	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	12	HIS
1	X	71	GLN
1	X	86	ASN
1	X	96	HIS
1	X	100	HIS
1	X	109	HIS
1	X	123	ASN
1	X	132	GLN
1	X	169	ASN
1	X	173	HIS
1	X	198	GLN
1	X	199	ASN
1	X	217	GLN
1	X	244	GLN
1	X	286	ASN
1	X	319	HIS
1	X	372	ASN
1	X	393	GLN
1	X	424	HIS
1	X	450	ASN
1	X	484	HIS
1	X	494	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	X	518/528 (98%)	0.35	37 (7%) 16 15	36, 58, 91, 108	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	404	ALA	9.2
1	X	283	VAL	5.2
1	X	94	LYS	5.0
1	X	466	PHE	4.7
1	X	468	MET	4.5
1	X	470	THR	4.4
1	X	29	TRP	4.2
1	X	476	TYR	4.1
1	X	472	THR	3.7
1	X	465	ALA	3.7
1	X	275	LYS	3.3
1	X	471	ARG	3.1
1	X	467	ILE	3.0
1	X	474	VAL	3.0
1	X	90[A]	GLU	3.0
1	X	23	HIS	2.9
1	X	403	GLY	2.8
1	X	1	MET	2.7
1	X	272	GLU	2.6
1	X	416	ASN	2.6
1	X	356	TRP	2.6
1	X	473	SER	2.6
1	X	7	ILE	2.6
1	X	68	ARG	2.5
1	X	25	LEU	2.5
1	X	361	VAL	2.5
1	X	464	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	X	9	LEU	2.3
1	X	271	MET	2.3
1	X	282	GLY	2.3
1	X	514	ILE	2.3
1	X	441	SER	2.3
1	X	6	LEU	2.2
1	X	456	LEU	2.2
1	X	5	ILE	2.1
1	X	415	THR	2.1
1	X	437	TYR	2.1

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.