



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 03:48 AM EDT

PDB ID : 2OL5
Title : Crystal Structure of a protease synthase and sporulation negative regulatory protein PAI 2 from *Bacillus stearothermophilus*
Authors : Brunzelle, J.S.; Cuff, M.E.; Minasov, G.; Li, H.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)
Deposited on : unknown
Resolution : 2.50 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

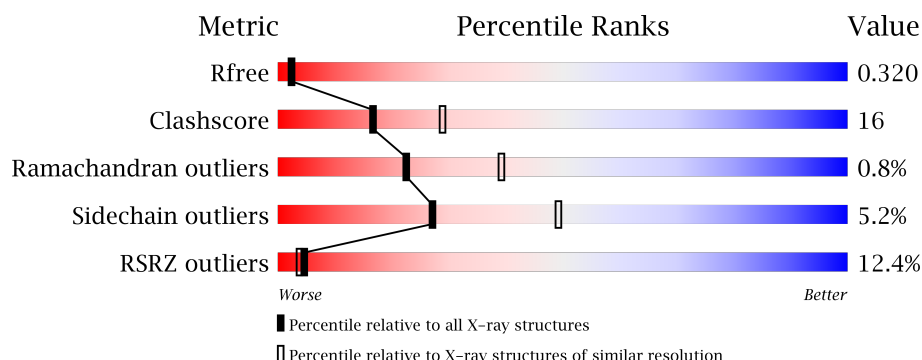
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	202	<div> <div>8%</div> <div>63%</div> <div>25%</div> <div>9%</div> </div>
1	B	202	<div> <div>13%</div> <div>64%</div> <div>24%</div> <div>8%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3120 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 PAI 2 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	Se	0	0	0
			1494	951	265	269	2	7			
1	B	186	Total	C	N	O	S	Se	0	0	0
			1518	963	268	278	2	7			

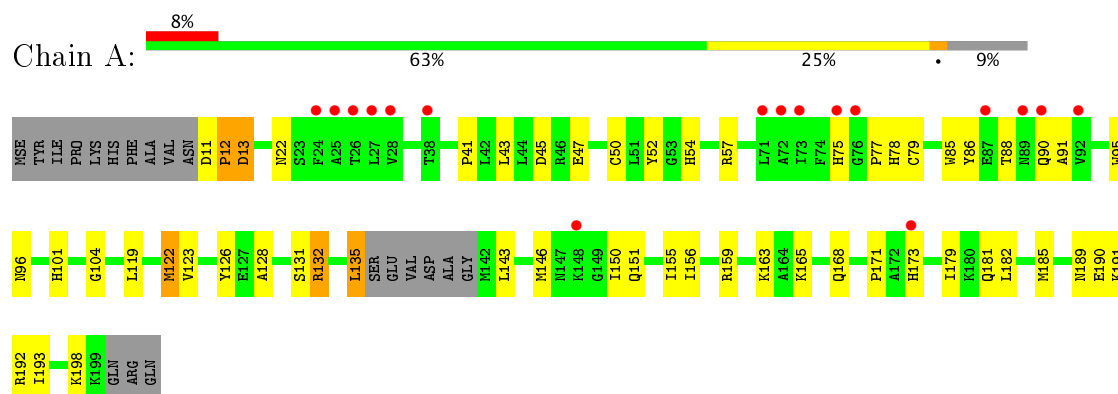
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		
2	B	44	Total	O	0	0
			44	44		

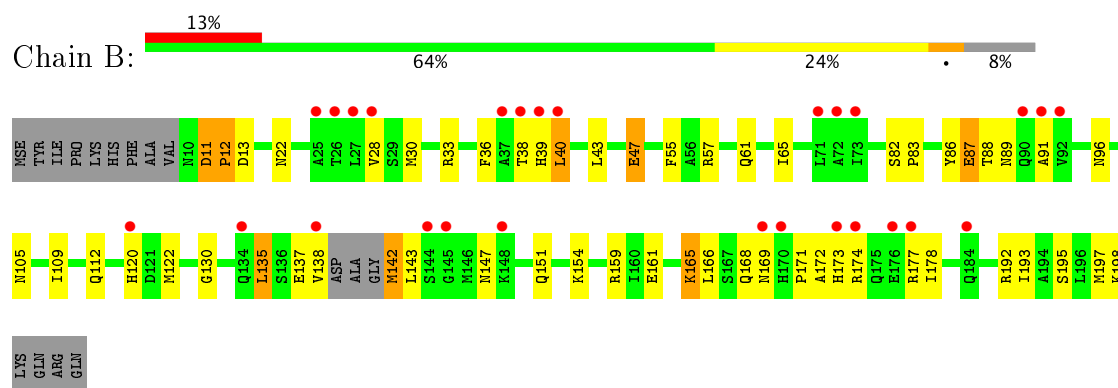
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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: PAI 2 protein



• Molecule 1: PAI 2 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.60Å 77.95Å 89.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 2.50 38.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.81-2.50) 86.4 (38.79-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.276 0.278 , 0.320	Depositor DCC
R_{free} test set	1556 reflections (10.16%)	DCC
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.968	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3120	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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	0.73	0/1525	0.84	3/2052 (0.1%)
1	B	0.67	0/1549	0.74	1/2086 (0.0%)
All	All	0.70	0/3074	0.79	4/4138 (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	B	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	132	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	13	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	11	ASP	CB-CG-OD2	5.24	123.02	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	130	GLY	Peptide
1	B	55	PHE	Peptide
1	B	65	ILE	Peptide

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	1494	0	1468	48	0
1	B	1518	0	1483	48	0
2	A	64	0	0	8	0
2	B	44	0	0	1	0
All	All	3120	0	2951	94	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 16.

All (94) 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:135:LEU:C	1:A:135:LEU:HD22	1.54	1.28
1:B:86:TYR:CE1	1:B:91:ALA:HB3	1.89	1.06
1:A:135:LEU:CD2	1:A:135:LEU:C	2.30	0.95
1:A:11:ASP:CB	1:A:12:PRO:HD3	1.97	0.95
1:B:86:TYR:HE1	1:B:91:ALA:HB3	1.33	0.92
1:B:135:LEU:O	1:B:135:LEU:HD12	1.71	0.90
1:B:11:ASP:OD1	1:B:12:PRO:HD2	1.75	0.86
1:A:78:HIS:O	1:A:189:ASN:HB3	1.77	0.84
1:A:135:LEU:O	1:A:135:LEU:HD22	1.88	0.73
1:A:57:ARG:HH11	1:A:151:GLN:HE21	1.37	0.73
1:A:57:ARG:HH11	1:A:151:GLN:NE2	1.88	0.70
1:A:54:HIS:ND1	2:A:205:HOH:O	2.25	0.70
1:A:22:ASN:HD21	1:A:192:ARG:HH22	1.38	0.67
1:B:47:GLU:HG3	1:B:47:GLU:O	1.94	0.67
1:B:159:ARG:NH1	1:B:161:GLU:OE2	2.27	0.67
1:B:22:ASN:HD21	1:B:192:ARG:HH22	1.43	0.65
1:B:137:GLU:HG2	1:B:143:LEU:HG	1.76	0.65
1:A:122:MSE:HE2	1:A:123:VAL:HA	1.78	0.65
1:B:197:MSE:O	1:B:198:LYS:HD2	1.98	0.64
1:B:57:ARG:HH12	1:B:151:GLN:HE21	1.46	0.61
1:B:11:ASP:O	1:B:12:PRO:C	2.40	0.60
1:A:50:CYS:HB3	1:A:156:ILE:HA	1.85	0.59
1:B:166:LEU:HB2	1:B:168:GLN:HE21	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LEU:O	1:B:135:LEU:CD1	2.49	0.58
1:A:78:HIS:HA	1:A:96:ASN:O	2.03	0.58
1:B:120:HIS:HE1	1:B:135:LEU:HB3	1.70	0.57
1:A:122:MSE:HE3	1:A:126:TYR:HD2	1.69	0.56
1:B:40:LEU:HD23	1:B:40:LEU:N	2.21	0.56
1:B:83:PRO:HA	1:B:86:TYR:CZ	2.40	0.56
1:A:101:HIS:NE2	1:B:39:HIS:HE1	2.03	0.56
1:B:138:VAL:O	1:B:143:LEU:HB2	2.08	0.54
1:B:57:ARG:NH1	1:B:151:GLN:HE21	2.05	0.54
1:B:173:HIS:HD2	1:B:174:ARG:HG2	1.72	0.54
1:A:77:PRO:HB2	1:A:193:ILE:HG12	1.89	0.54
1:A:122:MSE:HE2	1:A:123:VAL:CA	2.37	0.53
1:A:13:ASP:HA	2:A:244:HOH:O	2.07	0.53
1:A:104:GLY:HA3	1:A:156:ILE:O	2.08	0.53
1:B:57:ARG:HH12	1:B:151:GLN:NE2	2.06	0.53
1:B:177:ARG:HD2	2:B:235:HOH:O	2.09	0.52
1:A:132:ARG:HD3	2:A:206:HOH:O	2.09	0.52
1:A:41:PRO:HD2	2:A:235:HOH:O	2.09	0.51
1:B:138:VAL:HG22	1:B:142:MSE:HB2	1.92	0.51
1:A:78:HIS:O	1:A:79:CYS:HB3	2.10	0.51
1:A:45:ASP:HB3	1:A:52:TYR:HE1	1.75	0.51
1:B:86:TYR:CZ	1:B:91:ALA:HB3	2.43	0.51
1:A:171:PRO:HB2	1:A:173:HIS:CE1	2.47	0.50
1:B:11:ASP:O	1:B:13:ASP:N	2.44	0.50
1:A:122:MSE:HE2	1:A:123:VAL:N	2.27	0.50
1:A:43:LEU:HD11	1:A:122:MSE:HA	1.92	0.50
1:B:38:THR:OG1	1:B:61:GLN:NE2	2.44	0.50
1:B:40:LEU:HD23	1:B:40:LEU:H	1.78	0.49
1:A:101:HIS:NE2	1:B:39:HIS:CE1	2.80	0.49
1:B:86:TYR:CE1	1:B:91:ALA:CB	2.80	0.49
1:B:11:ASP:C	1:B:11:ASP:OD1	2.51	0.49
1:B:30:MSE:HE3	1:B:33:ARG:HA	1.94	0.49
1:B:83:PRO:HA	1:B:86:TYR:CE1	2.49	0.48
1:B:88:THR:O	1:B:89:ASN:HB2	2.12	0.48
1:B:40:LEU:CD2	1:B:40:LEU:N	2.77	0.48
1:B:195:SER:O	1:B:198:LYS:HD3	2.14	0.47
1:B:43:LEU:HD11	1:B:122:MSE:HA	1.97	0.47
1:A:75:HIS:HD2	2:A:230:HOH:O	1.96	0.47
1:A:182:LEU:HD22	1:A:190:GLU:HG3	1.96	0.47
1:B:138:VAL:HG22	1:B:142:MSE:CB	2.44	0.47
1:B:28:VAL:HA	1:B:36:PHE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:CYS:HB2	1:A:155:ILE:O	2.16	0.46
1:A:179:ILE:HD13	1:A:198:LYS:HG3	1.98	0.45
1:A:189:ASN:ND2	2:A:229:HOH:O	2.44	0.45
1:A:86:TYR:HD2	1:A:91:ALA:CB	2.29	0.45
1:B:86:TYR:CE2	1:B:178:ILE:HD11	2.52	0.45
1:B:96:ASN:HA	1:B:165:LYS:O	2.16	0.45
1:A:45:ASP:HB3	1:A:52:TYR:CE1	2.51	0.45
1:A:143:LEU:HA	1:A:146:MSE:HE3	1.98	0.45
1:A:86:TYR:CD2	1:A:91:ALA:HB1	2.52	0.45
1:A:185:MSE:O	1:A:191:LYS:HE3	2.17	0.44
1:A:86:TYR:CD2	1:A:91:ALA:CB	3.00	0.44
1:A:128:ALA:O	1:A:131:SER:N	2.43	0.44
1:B:137:GLU:O	1:B:143:LEU:HD12	2.18	0.44
1:A:132:ARG:NH2	2:A:216:HOH:O	2.43	0.43
1:A:88:THR:HB	1:A:90:GLN:H	1.83	0.43
1:A:86:TYR:CE2	1:A:91:ALA:HB1	2.54	0.43
1:A:57:ARG:NH1	1:A:151:GLN:NE2	2.61	0.43
1:B:82:SER:HA	1:B:83:PRO:HD3	1.78	0.42
1:A:95:TRP:O	1:A:165:LYS:HD2	2.19	0.42
1:B:109:ILE:HD11	1:B:154:LYS:HB2	2.01	0.42
1:B:87:GLU:HB2	1:B:174:ARG:HH12	1.85	0.42
1:A:50:CYS:CB	1:A:155:ILE:O	2.69	0.41
1:A:122:MSE:HG3	2:A:257:HOH:O	2.20	0.41
1:B:197:MSE:C	1:B:198:LYS:HD2	2.41	0.41
1:A:119:LEU:O	1:A:123:VAL:HG23	2.21	0.41
1:B:193:ILE:HA	1:B:193:ILE:HD13	1.90	0.41
1:B:171:PRO:HD2	1:B:174:ARG:HG3	2.03	0.41
1:A:86:TYR:HD2	1:A:91:ALA:HB2	1.85	0.40
1:A:85:TRP:CE2	1:A:181:GLN:HG2	2.57	0.40
1:B:173:HIS:CD2	1:B:174:ARG:HG2	2.56	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	179/202 (89%)	171 (96%)	7 (4%)	1 (1%)	28	48
1	B	182/202 (90%)	167 (92%)	13 (7%)	2 (1%)	17	29
All	All	361/404 (89%)	338 (94%)	20 (6%)	3 (1%)	22	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	B	12	PRO
1	B	172	ALA

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	162/171 (95%)	155 (96%)	7 (4%)	33	58
1	B	166/171 (97%)	156 (94%)	10 (6%)	22	41
All	All	328/342 (96%)	311 (95%)	17 (5%)	27	49

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

Mol	Chain	Res	Type
1	A	47	GLU
1	A	122	MSE
1	A	135	LEU
1	A	150	ILE
1	A	159	ARG
1	A	163	LYS
1	A	168	GLN
1	B	40	LEU
1	B	47	GLU
1	B	87	GLU

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Mol	Chain	Res	Type
1	B	105	ASN
1	B	112	GLN
1	B	135	LEU
1	B	142	MSE
1	B	147	ASN
1	B	165	LYS
1	B	169	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	66	GLN
1	A	75	HIS
1	A	110	ASN
1	A	134	GLN
1	A	151	GLN
1	A	184	GLN
1	A	189	ASN
1	B	22	ASN
1	B	39	HIS
1	B	61	GLN
1	B	78	HIS
1	B	110	ASN
1	B	112	GLN
1	B	120	HIS
1	B	151	GLN
1	B	168	GLN
1	B	169	ASN
1	B	173	HIS
1	B	175	GLN

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 [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	176/202 (87%)	0.60	17 (9%) 8 8	23, 41, 50, 60	0
1	B	179/202 (88%)	0.69	27 (15%) 3 2	25, 39, 47, 64	0
All	All	355/404 (87%)	0.64	44 (12%) 4 4	23, 40, 48, 64	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	HIS	6.2
1	B	145	GLY	4.2
1	B	91	ALA	3.9
1	B	174	ARG	3.9
1	A	26	THR	3.9
1	B	73	ILE	3.7
1	B	28	VAL	3.7
1	B	177	ARG	3.7
1	B	144	SER	3.5
1	B	27	LEU	3.5
1	B	26	THR	3.5
1	A	173	HIS	3.5
1	A	25	ALA	3.3
1	A	89	ASN	3.2
1	A	27	LEU	3.1
1	B	169	ASN	3.1
1	A	73	ILE	3.0
1	B	170	HIS	2.9
1	B	72	ALA	2.8
1	A	28	VAL	2.8
1	A	72	ALA	2.8
1	B	92	VAL	2.8
1	A	38	THR	2.8
1	A	90	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	148	LYS	2.8
1	A	92	VAL	2.8
1	B	90	GLN	2.7
1	B	37	ALA	2.7
1	A	71	LEU	2.7
1	B	25	ALA	2.6
1	B	71	LEU	2.6
1	B	148	LYS	2.5
1	B	38	THR	2.5
1	B	39	HIS	2.4
1	B	184	GLN	2.4
1	B	134	GLN	2.4
1	B	138	VAL	2.4
1	A	76	GLY	2.3
1	A	75	HIS	2.3
1	B	40	LEU	2.2
1	A	24	PHE	2.2
1	A	87	GLU	2.2
1	B	176	GLU	2.2
1	B	120	HIS	2.1

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.