



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2017 – 05:13 PM EDT

PDB ID : 1D6R
Title : CRYSTAL STRUCTURE OF CANCER CHEMOPREVENTIVE BOWMAN-BIRK INHIBITOR IN TERNARY COMPLEX WITH BOVINE TRYPSIN AT 2.3 Å RESOLUTION. STRUCTURAL BASIS OF JANUS-FACED SERINE PROTEASE INHIBITOR SPECIFICITY
Authors : Koepke, J.; Ermler, U.; Wenzl, G.; Flecker, P.
Deposited on : unknown
Resolution : 2.30 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

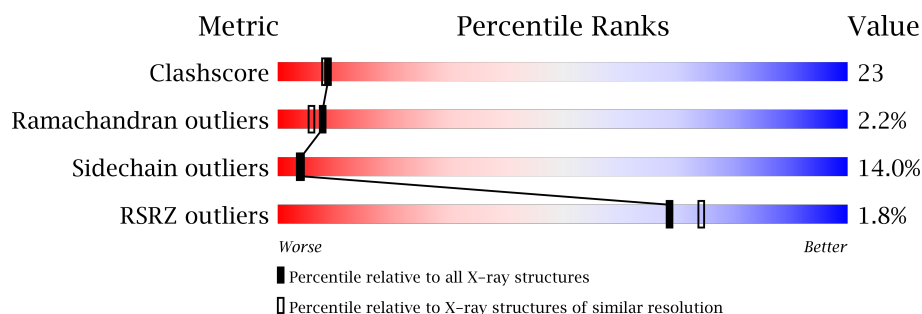
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	223	
2	I	58	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2172 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 TRYPSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1629	1012	279	324	14			

- Molecule 2 is a protein called BOWMAN-BIRK PROTEINASE INHIBITOR PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	58	Total	C	N	O	S	0	0	0
			427	256	74	82	15			

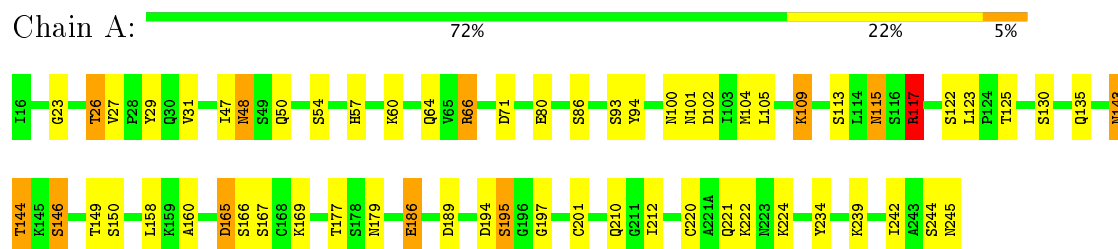
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total	O	0	0
			110	110		
3	I	6	Total	O	0	0
			6	6		

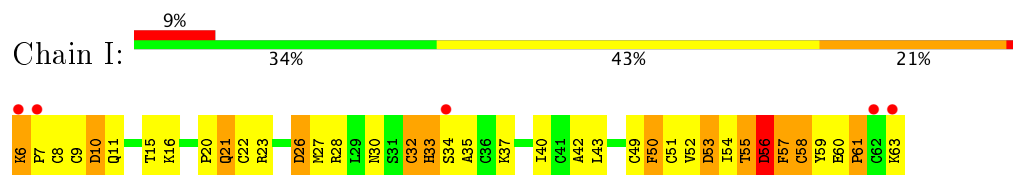
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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: TRYPSINOGEN



• Molecule 2: BOWMAN-BIRK PROTEINASE INHIBITOR PRECURSOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	55.60 Å 55.60 Å 183.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 55.60 – 1.80	Depositor EDS
% Data completeness (in resolution range)	82.3 (8.00-2.30) 64.8 (55.60-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.80 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.152 , 0.226 0.140 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 108.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2172	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.93% 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, 0.333 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	2.32	3/1660 (0.2%)	1.42	13/2250 (0.6%)
2	I	7.43	1/436 (0.2%)	1.57	9/589 (1.5%)
All	All	3.97	4/2096 (0.2%)	1.45	22/2839 (0.8%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	63	LYS	C-OXT	154.50	4.16	1.23
1	A	245	ASN	C-OXT	88.59	2.91	1.23
1	A	186	GLU	CD-OE2	6.60	1.32	1.25
1	A	80	GLU	CD-OE2	5.58	1.31	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	ARG	NE-CZ-NH2	-11.13	114.73	120.30
2	I	26	ASP	CB-CG-OD1	9.47	126.83	118.30
1	A	71	ASP	CB-CG-OD1	9.13	126.52	118.30
1	A	66	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	194	ASP	CB-CG-OD2	-8.84	110.34	118.30
2	I	26	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	A	71	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	102	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	A	165	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	165	ASP	CB-CG-OD1	6.84	124.46	118.30
2	I	32	CYS	N-CA-CB	6.43	122.17	110.60
2	I	53	ASP	CB-CG-OD2	-6.39	112.55	118.30
2	I	53	ASP	CB-CG-OD1	6.33	123.99	118.30
1	A	194	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	102	ASP	CB-CG-OD1	5.94	123.64	118.30
2	I	58	CYS	CB-CA-C	-5.92	98.55	110.40
2	I	56	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	I	56	ASP	CB-CG-OD1	5.73	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	10	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	189	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	26	THR	CA-CB-CG2	-5.20	105.13	112.40
1	A	117	ARG	NE-CZ-NH1	5.15	122.87	120.30

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	1629	0	1588	45	0
2	I	427	0	380	48	0
3	A	110	0	0	3	0
3	I	6	0	0	4	0
All	All	2172	0	1968	91	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 23.

All (91) 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)
2:I:7:PRO:HG3	2:I:35:ALA:HB3	1.32	1.10
1:A:143:ASN:HD22	1:A:144:THR:H	1.18	0.92
2:I:7:PRO:HG3	2:I:35:ALA:CB	2.05	0.85
2:I:50:PHE:HE2	2:I:52:VAL:HA	1.40	0.84
1:A:64:GLN:HE22	1:A:66:ARG:HH21	1.25	0.80
2:I:50:PHE:CE2	2:I:52:VAL:HG12	2.17	0.80
2:I:7:PRO:HA	2:I:33:HIS:CE1	2.16	0.79
1:A:48:ASN:HD22	1:A:50:GLN:H	1.31	0.77
1:A:48:ASN:ND2	1:A:50:GLN:H	1.82	0.77
1:A:143:ASN:HD22	1:A:144:THR:N	1.84	0.75
1:A:64:GLN:NE2	1:A:66:ARG:HH21	1.88	0.72
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:6:LYS:N	2:I:6:LYS:HD3	2.08	0.67
1:A:221:GLN:HB2	1:A:224:LYS:HB2	1.77	0.67
2:I:35:ALA:N	3:I:69:HOH:O	2.28	0.65
2:I:34:SER:N	3:I:69:HOH:O	2.29	0.65
1:A:143:ASN:ND2	1:A:150:SER:H	1.96	0.63
1:A:146:SER:HB3	1:A:220:CYS:O	1.99	0.63
2:I:27:MET:CE	2:I:50:PHE:HD1	2.11	0.63
2:I:21:GLN:HB2	2:I:54:ILE:CG2	2.30	0.62
2:I:6:LYS:CB	2:I:7:PRO:HD2	2.29	0.61
2:I:50:PHE:CD2	2:I:52:VAL:HG12	2.34	0.61
2:I:26:ASP:OD2	2:I:28:ARG:NH2	2.33	0.60
1:A:210:GLN:NE2	3:A:261:HOH:O	2.34	0.59
1:A:47:ILE:HD11	1:A:242:ILE:HD11	1.85	0.59
2:I:8:CYS:HB2	2:I:60:GLU:O	2.03	0.59
1:A:197:GLY:HA3	3:A:251:HOH:O	2.03	0.58
2:I:33:HIS:C	2:I:35:ALA:H	2.06	0.57
2:I:37:LYS:N	2:I:53:ASP:OD2	2.29	0.56
1:A:143:ASN:ND2	1:A:144:THR:N	2.54	0.56
2:I:23:ARG:NH2	2:I:50:PHE:HZ	2.03	0.56
1:A:48:ASN:C	1:A:48:ASN:HD22	2.09	0.56
2:I:50:PHE:HD2	2:I:50:PHE:C	2.09	0.56
2:I:21:GLN:HB2	2:I:54:ILE:HG21	1.88	0.56
2:I:50:PHE:C	2:I:50:PHE:CD2	2.79	0.55
1:A:117:ARG:HH11	1:A:117:ARG:CG	2.19	0.55
2:I:27:MET:HE1	2:I:50:PHE:HD1	1.71	0.55
2:I:20:PRO:O	2:I:56:ASP:HA	2.07	0.55
2:I:34:SER:C	3:I:69:HOH:O	2.46	0.54
2:I:23:ARG:NH2	2:I:50:PHE:CZ	2.76	0.53
2:I:6:LYS:HB2	2:I:7:PRO:HD2	1.89	0.53
2:I:55:THR:C	2:I:57:PHE:H	2.11	0.53
2:I:7:PRO:CG	2:I:35:ALA:HB3	2.23	0.52
2:I:6:LYS:CB	2:I:7:PRO:CD	2.87	0.52
2:I:54:ILE:O	2:I:55:THR:HG22	2.10	0.52
2:I:9:CYS:N	2:I:60:GLU:O	2.37	0.51
2:I:7:PRO:CG	2:I:35:ALA:CB	2.84	0.51
2:I:50:PHE:HE2	2:I:52:VAL:CA	2.17	0.51
1:A:100:ASN:HD21	1:A:179:ASN:HD22	1.59	0.51
1:A:23:GLY:O	1:A:26:THR:HG23	2.11	0.51
1:A:135:GLN:HE22	1:A:160:ALA:C	2.14	0.51
2:I:50:PHE:CE2	2:I:52:VAL:HA	2.32	0.50
2:I:55:THR:OG1	2:I:57:PHE:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASN:ND2	1:A:144:THR:H	1.99	0.50
1:A:143:ASN:HD21	1:A:150:SER:H	1.59	0.50
2:I:60:GLU:O	2:I:61:PRO:O	2.30	0.49
2:I:50:PHE:CD2	2:I:51:CYS:N	2.80	0.49
2:I:56:ASP:O	2:I:57:PHE:HB3	2.11	0.49
1:A:64:GLN:HE21	1:A:66:ARG:HE	1.60	0.49
1:A:195:SER:HB2	2:I:16:LYS:O	2.13	0.48
1:A:221:GLN:OE1	1:A:221:GLN:HA	2.14	0.48
2:I:42:ALA:C	2:I:43:LEU:HD12	2.34	0.48
1:A:149:THR:HG23	1:A:149:THR:O	2.14	0.47
2:I:22:CYS:N	2:I:55:THR:O	2.36	0.47
2:I:16:LYS:NZ	3:I:65:HOH:O	2.27	0.47
1:A:115:ASN:HD22	1:A:117:ARG:H	1.62	0.47
1:A:27:VAL:HG13	1:A:29:TYR:CZ	2.51	0.46
1:A:64:GLN:NE2	1:A:66:ARG:HE	2.13	0.46
2:I:43:LEU:CD1	2:I:43:LEU:N	2.79	0.45
1:A:115:ASN:C	1:A:115:ASN:HD22	2.20	0.45
1:A:86:SER:HB3	1:A:109:LYS:HD2	1.97	0.45
1:A:57:HIS:CD2	2:I:15:THR:HB	2.52	0.45
1:A:135:GLN:HE22	1:A:160:ALA:CA	2.29	0.45
2:I:50:PHE:HD2	2:I:51:CYS:N	2.15	0.44
1:A:54:SER:HB3	1:A:104:MET:CE	2.47	0.44
1:A:101:ASN:HA	1:A:234:TYR:OH	2.18	0.44
1:A:224:LYS:HD3	1:A:224:LYS:HA	1.82	0.44
1:A:115:ASN:ND2	1:A:117:ARG:H	2.16	0.44
1:A:48:ASN:HD22	1:A:50:GLN:N	2.09	0.43
1:A:242:ILE:HD13	1:A:242:ILE:HG21	1.67	0.43
2:I:32:CYS:SG	2:I:49:CYS:HB3	2.59	0.43
2:I:37:LYS:HB2	2:I:37:LYS:HE2	1.72	0.43
1:A:94:TYR:HA	1:A:101:ASN:HB2	2.01	0.42
1:A:144:THR:HG21	3:A:332:HOH:O	2.19	0.42
1:A:117:ARG:NH1	1:A:117:ARG:CG	2.79	0.42
2:I:59:TYR:CD2	2:I:59:TYR:N	2.88	0.42
1:A:239:LYS:HB2	1:A:239:LYS:HE2	1.73	0.42
1:A:86:SER:HB3	1:A:109:LYS:HA	2.02	0.41
1:A:100:ASN:ND2	1:A:177:THR:OG1	2.53	0.41
2:I:57:PHE:HD2	2:I:58:CYS:O	2.04	0.41
1:A:212:ILE:HG21	1:A:212:ILE:HD13	1.83	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	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
2	I	56/58 (97%)	42 (75%)	8 (14%)	6 (11%)	0	0
All	All	277/281 (99%)	256 (92%)	15 (5%)	6 (2%)	8	6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	33	HIS
2	I	61	PRO
2	I	56	ASP
2	I	57	PHE
2	I	10	ASP
2	I	30	ASN

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	184/184 (100%)	158 (86%)	26 (14%)	4	4
2	I	52/54 (96%)	45 (86%)	7 (14%)	4	4
All	All	236/238 (99%)	203 (86%)	33 (14%)	4	4

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	48	ASN
1	A	60	LYS
1	A	93	SER
1	A	105	LEU
1	A	109	LYS
1	A	113	SER
1	A	115	ASN
1	A	117	ARG
1	A	122	SER
1	A	123	LEU
1	A	125	THR
1	A	130	SER
1	A	143	ASN
1	A	144	THR
1	A	146	SER
1	A	158	LEU
1	A	165	ASP
1	A	166	SER
1	A	167	SER
1	A	169	LYS
1	A	186	GLU
1	A	195	SER
1	A	201	CYS
1	A	222	LYS
1	A	244	SER
2	I	6	LYS
2	I	11	GLN
2	I	21	GLN
2	I	40	ILE
2	I	50	PHE
2	I	55	THR
2	I	56	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	48	ASN
1	A	64	GLN
1	A	74	ASN
1	A	100	ASN
1	A	115	ASN

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Mol	Chain	Res	Type
1	A	135	GLN
1	A	143	ASN
1	A	210	GLN
1	A	223	ASN
1	A	233	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	223/223 (100%)	-1.08	0 100 100	3, 16, 44, 64	0
2	I	58/58 (100%)	0.13	5 (8%) 11 16	2, 27, 66, 82	58 (100%)
All	All	281/281 (100%)	-0.83	5 (1%) 69 74	2, 17, 50, 82	58 (20%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	6	LYS	5.9
2	I	34	SER	5.1
2	I	63	LYS	5.0
2	I	62	CYS	2.9
2	I	7	PRO	2.2

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.