



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:53 PM GMT

PDB ID : 2J0N
Title : A PROTEOLYTICALLY TRUNCATED FORM OF SHIGELLA FLEXNERI
IPAD
Authors : Johnson, S.; Roversi, P.; Lea, S.M.
Deposited on : 2006-08-03
Resolution : 2.10 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>

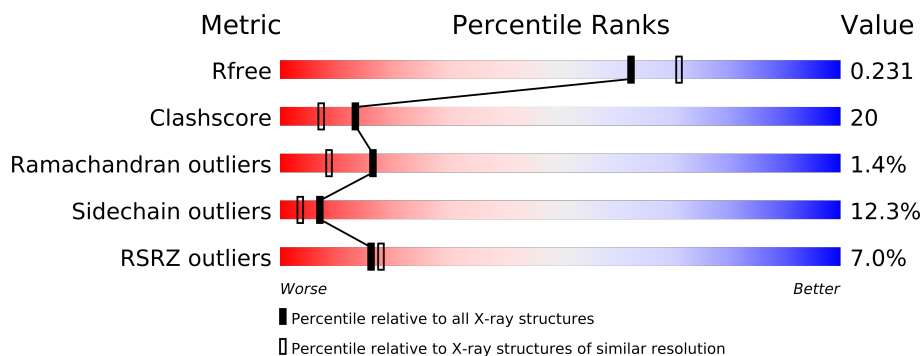
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	A	200	
1	B	200	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2986 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 INVASIN IPAD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1329	835	221	269	4			
1	B	187	Total	C	N	O	S	0	0	0
			1452	914	241	293	4			

- Molecule 2 is water.

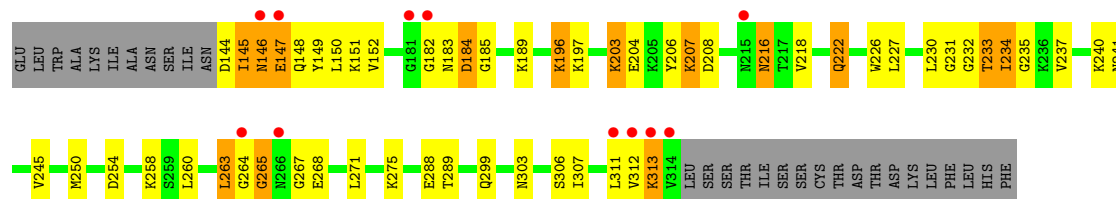
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total	O	0	0
			111	111		
2	B	94	Total	O	0	0
			94	94		

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.

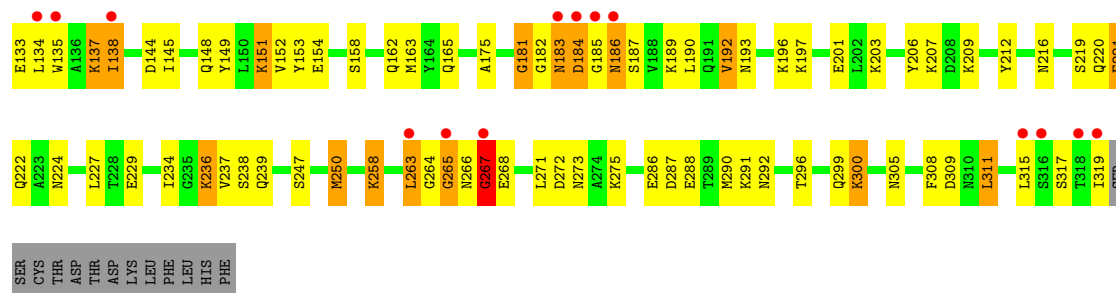
• Molecule 1: INVASIN IPAD

Chain A: 



• Molecule 1: INVASIN IPAD

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.79Å 91.36Å 54.91Å 90.00° 96.35° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 41.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.10) 99.7 (41.87-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.89Å)	Xtriage
Refinement program	TNT 5.6.1	Depositor
R, R_{free}	0.189 , (Not available) 0.199 , 0.231	Depositor DCC
R_{free} test set	1112 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30126 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2986	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.49% 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	A	0.44	0/1351	0.69	2/1828 (0.1%)
1	B	0.46	1/1476 (0.1%)	0.72	3/1999 (0.2%)
All	All	0.45	1/2827 (0.0%)	0.70	5/3827 (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	A	0	1
1	B	0	6
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	VAL	CB-CG2	-5.62	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	LEU	N-CA-C	9.48	136.59	111.00
1	B	267	GLY	C-N-CA	7.24	139.80	121.70
1	A	313	LYS	CB-CA-C	6.24	122.88	110.40
1	B	184	ASP	N-CA-C	-6.12	94.48	111.00
1	A	263	LEU	N-CA-C	-5.78	95.38	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	313	LYS	Mainchain
1	B	183	ASN	Mainchain,Peptide
1	B	265	GLY	Mainchain,Peptide
1	B	267	GLY	Mainchain,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	A	1329	0	1303	54	0
1	B	1452	0	1431	70	1
2	A	111	0	0	4	0
2	B	94	0	0	7	0
All	All	2986	0	2734	112	1

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 20.

All (112) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:192:VAL:HG21	1:B:265:GLY:O	1.58	1.03
1:B:192:VAL:CG2	1:B:267:GLY:H	1.76	0.97
1:A:233:THR:HG22	1:B:165:GLN:HE22	1.40	0.87
1:A:233:THR:HG22	1:B:165:GLN:NE2	1.90	0.86
1:A:147:GLU:HB3	1:A:148:GLN:NE2	1.90	0.85
1:B:192:VAL:CG2	1:B:267:GLY:N	2.47	0.77
1:B:163:MET:SD	1:B:290:MET:HE1	2.25	0.76
1:B:227:LEU:HD22	1:B:237:VAL:HG23	1.68	0.75
1:B:209:LYS:HD2	2:B:2044:HOH:O	1.87	0.75
1:B:197:LYS:O	1:B:201:GLU:HG3	1.86	0.75
1:B:134:LEU:HB2	2:B:2002:HOH:O	1.87	0.73
1:A:307:ILE:O	1:A:311:LEU:HD23	1.90	0.71
1:B:192:VAL:HG22	1:B:267:GLY:H	1.53	0.70
1:A:230:LEU:HB3	1:A:234:ILE:HD11	1.75	0.68
1:A:203:LYS:HE3	1:A:254:ASP:OD1	1.93	0.68
1:A:258:LYS:NZ	2:A:2087:HOH:O	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:236:LYS:HE3	1:B:247:SER:HB2	1.76	0.68
1:B:133:GLU:HG2	1:B:134:LEU:N	2.09	0.67
1:A:289:THR:HG21	1:B:165:GLN:HG2	1.76	0.66
1:B:133:GLU:HG3	2:B:2003:HOH:O	1.96	0.65
1:A:299:GLN:O	1:B:305:ASN:ND2	2.30	0.65
1:A:288:GLU:HG3	1:B:291:LYS:HE2	1.79	0.64
1:B:292:ASN:O	1:B:296:THR:HG23	1.98	0.63
1:B:192:VAL:HG22	1:B:267:GLY:N	2.13	0.62
1:A:231:GLY:O	1:A:233:THR:N	2.27	0.62
1:B:189:LYS:HD3	1:B:268:GLU:CD	2.19	0.62
1:B:189:LYS:HD3	1:B:268:GLU:OE2	1.99	0.62
1:A:204:GLU:O	1:A:207:LYS:HD2	2.00	0.60
1:A:307:ILE:HG22	1:A:311:LEU:CD2	2.30	0.60
1:B:236:LYS:CE	1:B:247:SER:HB2	2.33	0.58
1:A:234:ILE:HB	2:A:2106:HOH:O	2.03	0.58
1:A:230:LEU:HB3	1:A:234:ILE:CD1	2.35	0.56
1:A:307:ILE:HG22	1:A:311:LEU:HD21	1.86	0.56
1:B:182:GLY:O	1:B:184:ASP:HA	2.05	0.56
1:A:184:ASP:CG	1:A:185:GLY:N	2.59	0.56
1:B:206:TYR:HB2	1:B:250:MET:CE	2.36	0.56
1:A:233:THR:HG22	1:B:165:GLN:CD	2.25	0.55
1:A:234:ILE:HG12	1:A:235:GLY:N	2.21	0.54
1:A:207:LYS:HG2	1:A:208:ASP:N	2.23	0.54
1:A:241:ASN:ND2	2:A:2075:HOH:O	2.40	0.54
1:B:192:VAL:HG23	1:B:267:GLY:N	2.22	0.54
1:A:288:GLU:HG2	2:A:2100:HOH:O	2.06	0.54
1:A:254:ASP:O	1:A:258:LYS:HG2	2.08	0.53
1:B:288:GLU:HG3	2:B:2087:HOH:O	2.08	0.53
1:B:311:LEU:HD22	1:B:315:LEU:CD2	2.39	0.53
1:A:233:THR:HG23	1:B:162:GLN:HG2	1.89	0.53
1:B:272:ASP:OD2	1:B:275:LYS:HD3	2.09	0.53
1:B:151:LYS:HE2	2:B:2011:HOH:O	2.09	0.51
1:B:192:VAL:HG22	1:B:267:GLY:HA2	1.91	0.51
1:B:222:GLN:OE1	1:B:222:GLN:HA	2.11	0.51
1:B:192:VAL:HG22	1:B:267:GLY:CA	2.40	0.51
1:A:307:ILE:HG23	1:A:311:LEU:HD22	1.92	0.51
1:A:240:LYS:HD2	1:A:245:VAL:HG11	1.91	0.51
1:A:307:ILE:CG2	1:A:311:LEU:HD22	2.39	0.51
1:B:158:SER:O	1:B:162:GLN:HG3	2.11	0.50
1:B:133:GLU:HG2	2:B:2002:HOH:O	2.10	0.50
1:A:271:LEU:HD22	1:A:275:LYS:HG2	1.92	0.50
1:B:263:LEU:N	1:B:264:GLY:HA2	2.24	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:181:GLY:HA3	1:B:187:SER:OG	2.12	0.50
1:B:220:GLN:O	1:B:224:ASN:OD1	2.30	0.50
1:A:312:VAL:HG12	1:A:312:VAL:O	2.12	0.49
1:B:219:SER:OG	1:B:221:GLU:HG2	2.13	0.49
1:A:303:ASN:ND2	1:B:309:ASP:OD2	2.46	0.49
1:B:152:VAL:HG13	1:B:212:TYR:HD2	1.77	0.49
1:A:189:LYS:HD2	1:A:268:GLU:CD	2.33	0.49
1:B:190:LEU:HD23	1:B:192:VAL:HG12	1.95	0.48
1:B:236:LYS:HE2	1:B:236:LYS:HB3	1.61	0.47
1:B:145:ILE:O	1:B:149:TYR:HB3	2.15	0.47
1:A:206:TYR:HB2	1:A:250:MET:CE	2.45	0.47
1:A:218:VAL:HG21	1:A:222:GLN:HG2	1.96	0.47
1:B:137:LYS:HA	1:B:137:LYS:HD2	1.49	0.47
1:A:307:ILE:CG2	1:A:311:LEU:CD2	2.93	0.46
1:A:146:ASN:HB3	1:A:148:GLN:H	1.81	0.46
1:A:184:ASP:OD1	1:A:185:GLY:N	2.48	0.46
1:A:182:GLY:HA3	1:A:183:ASN:HA	1.53	0.46
1:B:300:LYS:HE2	2:B:2093:HOH:O	2.15	0.46
1:B:311:LEU:HD22	1:B:315:LEU:HD23	1.97	0.46
1:B:258:LYS:HD2	1:B:258:LYS:HA	1.47	0.46
1:B:144:ASP:O	1:B:148:GLN:HG3	2.17	0.45
1:A:189:LYS:HB2	1:A:189:LYS:HE2	1.72	0.44
1:A:196:LYS:HB3	1:A:196:LYS:HE3	1.28	0.44
1:A:233:THR:HG22	1:B:165:GLN:OE1	2.18	0.44
1:A:227:LEU:HD22	1:A:237:VAL:HG23	2.00	0.44
1:A:312:VAL:CG1	1:A:312:VAL:O	2.65	0.44
1:A:145:ILE:HD11	1:A:150:LEU:HD21	2.00	0.44
1:B:163:MET:CE	1:B:290:MET:HE3	2.49	0.43
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.82	0.43
1:A:204:GLU:HG3	1:A:207:LYS:NZ	2.34	0.43
1:A:260:LEU:O	1:A:263:LEU:O	2.37	0.43
1:B:153:TYR:CE2	1:B:300:LYS:HG2	2.53	0.43
1:B:196:LYS:HE2	1:B:196:LYS:HB3	1.82	0.43
1:A:146:ASN:H	1:A:149:TYR:HB3	1.84	0.42
1:A:275:LYS:HE3	1:B:175:ALA:O	2.20	0.42
1:B:315:LEU:HD22	1:B:315:LEU:N	2.33	0.42
1:B:138:ILE:HD12	1:B:138:ILE:HA	1.84	0.42
1:A:307:ILE:O	1:A:311:LEU:CD2	2.65	0.42
1:B:184:ASP:OD2	1:B:185:GLY:HA2	2.19	0.42
1:A:289:THR:CG2	1:B:165:GLN:HG2	2.47	0.42
1:B:153:TYR:OH	1:B:229:GLU:OE1	2.33	0.42
1:A:152:VAL:HG11	1:A:226:TRP:CH2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:151:LYS:HD2	1:B:154:GLU:OE1	2.19	0.42
1:A:265:GLY:C	1:A:267:GLY:H	2.23	0.42
1:B:152:VAL:HG13	1:B:212:TYR:CD2	2.54	0.41
1:A:307:ILE:HD11	1:B:308:PHE:HE2	1.85	0.41
1:B:286:GLU:OE1	1:B:286:GLU:HA	2.19	0.41
1:B:151:LYS:HA	1:B:151:LYS:HD2	1.87	0.41
1:B:315:LEU:HA	1:B:315:LEU:HD13	1.52	0.41
1:A:197:LYS:HB2	1:A:197:LYS:HE2	1.58	0.41
1:A:206:TYR:HB2	1:A:250:MET:HE1	2.02	0.41
1:B:186:ASN:HD22	1:B:186:ASN:HA	1.64	0.40
1:B:193:ASN:H	1:B:267:GLY:HA3	1.86	0.40
1:B:163:MET:CE	1:B:290:MET:CE	2.99	0.40

All (1) 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	Distance(Å)	Clash(Å)
1:B:216:ASN:OD1	1:B:263:LEU:O[4_455]	2.08	0.12

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	169/200 (84%)	159 (94%)	6 (4%)	4 (2%)	9	3
1	B	185/200 (92%)	172 (93%)	12 (6%)	1 (0%)	38	33
All	All	354/400 (88%)	331 (94%)	18 (5%)	5 (1%)	16	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	GLY
1	A	216	ASN
1	A	264	GLY
1	B	181	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	265	GLY

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	147/174 (84%)	133 (90%)	14 (10%)	12	8
1	B	161/174 (92%)	137 (85%)	24 (15%)	4	2
All	All	308/348 (88%)	270 (88%)	38 (12%)	7	3

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ASP
1	A	145	ILE
1	A	146	ASN
1	A	147	GLU
1	A	151	LYS
1	A	184	ASP
1	A	196	LYS
1	A	203	LYS
1	A	207	LYS
1	A	216	ASN
1	A	222	GLN
1	A	233	THR
1	A	234	ILE
1	A	306	SER
1	B	135	TRP
1	B	137	LYS
1	B	138	ILE
1	B	151	LYS
1	B	183	ASN
1	B	186	ASN
1	B	203	LYS
1	B	207	LYS
1	B	221	GLU
1	B	234	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	236	LYS
1	B	238	SER
1	B	239	GLN
1	B	250	MET
1	B	258	LYS
1	B	266	ASN
1	B	271	LEU
1	B	273	ASN
1	B	287	ASP
1	B	299	GLN
1	B	300	LYS
1	B	311	LEU
1	B	317	SER
1	B	319	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	148	GLN
1	A	183	ASN
1	A	216	ASN
1	A	295	GLN
1	B	186	ASN
1	B	262	ASN

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	A	171/200 (85%)	0.07	11 (6%) 19 21	17, 37, 84, 92	0
1	B	187/200 (93%)	0.14	14 (7%) 14 16	20, 44, 77, 98	0
All	All	358/400 (89%)	0.11	25 (6%) 16 18	17, 41, 82, 98	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	LEU	7.9
1	A	314	VAL	6.8
1	B	135	TRP	6.5
1	A	182	GLY	6.1
1	A	266	ASN	5.7
1	B	319	ILE	5.5
1	A	312	VAL	5.5
1	B	315	LEU	5.0
1	B	183	ASN	4.9
1	B	184	ASP	4.6
1	A	313	LYS	4.5
1	B	318	THR	4.2
1	B	138	ILE	3.5
1	A	146	ASN	3.5
1	A	264	GLY	3.2
1	B	186	ASN	3.1
1	B	267	GLY	2.9
1	B	134	LEU	2.8
1	B	185	GLY	2.7
1	B	316	SER	2.4
1	B	263	LEU	2.3
1	B	265	GLY	2.3
1	A	147	GLU	2.2
1	A	181	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	215	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.