



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 02:39 PM EDT

PDB ID : 3EGB
Title : Structure of Pellino2 FHA domain at 3.3 Angstroms resolution.
Authors : Ferguson, K.M.; Lin, C.; Schmitz, K.R.
Deposited on : unknown
Resolution : 3.25 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

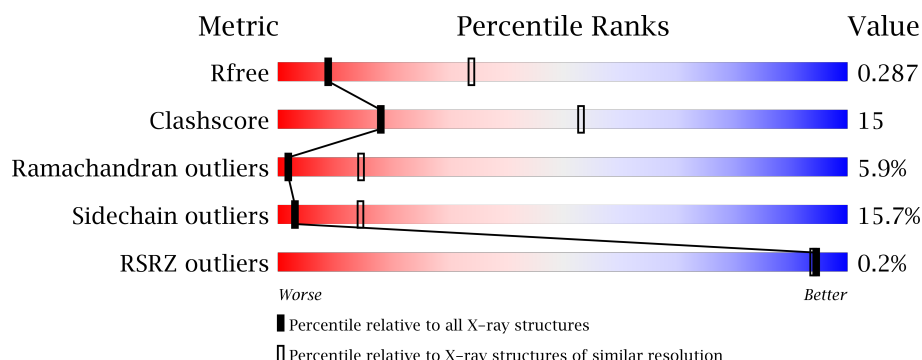
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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. 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	285	
1	B	285	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3244 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 Protein pellino homolog 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1667	1050	298	311	8			
1	B	223	Total	C	N	O	S	0	0	0
			1577	993	278	299	7			

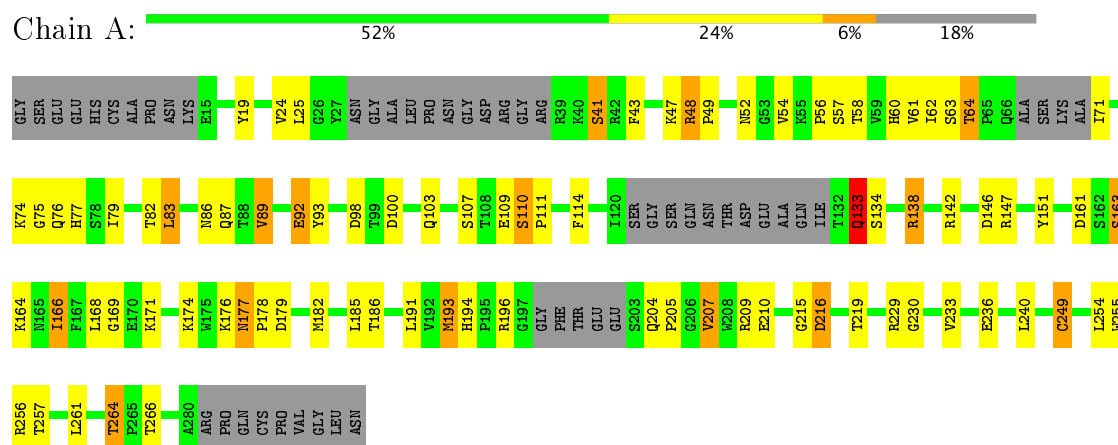
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	EXPRESSION TAG	UNP Q9HAT8
A	6	SER	-	EXPRESSION TAG	UNP Q9HAT8
B	5	GLY	-	EXPRESSION TAG	UNP Q9HAT8
B	6	SER	-	EXPRESSION TAG	UNP Q9HAT8

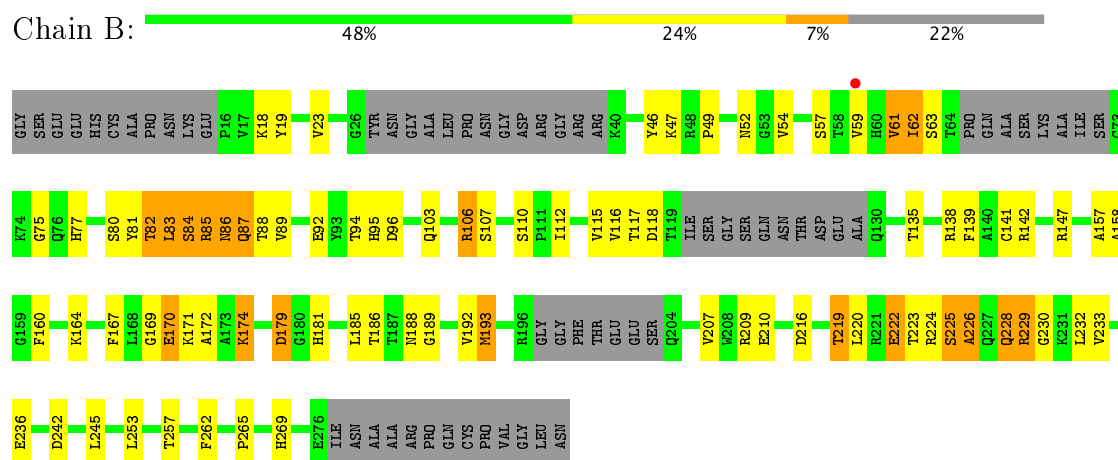
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Protein pellino homolog 2



• Molecule 1: Protein pellino homolog 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.68 Å 89.48 Å 125.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.00 – 3.25 41.25 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.00-3.25) 100.0 (41.25-3.25)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.26 (at 3.25 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.238 , 0.315 0.234 , 0.287	Depositor DCC
R_{free} test set	380 reflections (4.84%)	DCC
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.1	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	3244	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.22% 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	0.49	0/1697	0.65	0/2315
1	B	0.49	0/1607	0.66	0/2196
All	All	0.49	0/3304	0.65	0/4511

There are no bond length outliers.

There are no bond angle outliers.

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	1667	0	1511	51	0
1	B	1577	0	1400	44	0
All	All	3244	0	2911	93	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 15.

All (93) 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:48:ARG:HD2	1:A:52:ASN:HB2	1.33	1.04
1:A:82:THR:CG2	1:A:169:GLY:HA2	1.99	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ARG:HE	1:B:233:VAL:HG21	1.40	0.86
1:B:103:GLN:HE22	1:B:160:PHE:H	1.21	0.84
1:B:185:LEU:HD11	1:B:229:ARG:HB3	1.63	0.79
1:A:48:ARG:CD	1:A:52:ASN:HB2	2.15	0.77
1:B:233:VAL:HG11	1:B:236:GLU:OE1	1.85	0.77
1:A:103:GLN:HE21	1:A:142:ARG:HG2	1.52	0.73
1:B:61:VAL:O	1:B:62:ILE:CB	2.37	0.73
1:B:179:ASP:OD2	1:B:181:HIS:ND1	2.25	0.70
1:A:79:ILE:HG12	1:A:166:ILE:HG13	1.76	0.68
1:A:82:THR:HG23	1:A:169:GLY:HA2	1.74	0.68
1:A:60:HIS:HE1	1:A:92:GLU:OE2	1.79	0.66
1:B:103:GLN:NE2	1:B:160:PHE:H	1.91	0.64
1:A:257:THR:O	1:A:261:LEU:HD12	1.98	0.63
1:B:23:VAL:O	1:B:253:LEU:HA	1.98	0.63
1:A:176:LYS:HB2	1:A:182:MET:CE	2.31	0.61
1:A:240:LEU:HB3	1:A:255:TRP:CD1	2.37	0.59
1:B:18:LYS:HB2	1:B:46:TYR:CE2	2.37	0.59
1:A:256:ARG:HH22	1:A:264:THR:HG23	1.68	0.59
1:B:167:PHE:CZ	1:B:169:GLY:HA3	2.38	0.59
1:A:82:THR:HG22	1:A:168:LEU:O	2.04	0.58
1:B:185:LEU:HB3	1:B:210:GLU:OE1	2.05	0.57
1:B:219:THR:O	1:B:230:GLY:HA3	2.04	0.57
1:B:81:TYR:O	1:B:89:VAL:N	2.30	0.57
1:B:172:ALA:O	1:B:174:LYS:HE2	2.06	0.56
1:A:64:THR:O	1:A:86:ASN:HA	2.07	0.55
1:B:82:THR:OG1	1:B:170:GLU:N	2.32	0.54
1:B:84:SER:O	1:B:86:ASN:N	2.42	0.53
1:A:177:ASN:HB2	1:A:178:PRO:CD	2.38	0.53
1:B:82:THR:HA	1:B:88:THR:HA	1.91	0.53
1:A:43:PHE:HB2	1:A:114:PHE:CD1	2.44	0.53
1:B:192:VAL:HA	1:B:245:LEU:O	2.08	0.53
1:A:219:THR:O	1:A:230:GLY:HA3	2.08	0.52
1:B:103:GLN:HE22	1:B:160:PHE:N	2.00	0.52
1:A:71:ILE:N	1:B:106:ARG:HH22	2.07	0.52
1:A:48:ARG:HD2	1:A:52:ASN:CB	2.23	0.52
1:A:24:VAL:HG23	1:A:41:SER:O	2.11	0.51
1:B:82:THR:HG22	1:B:88:THR:HG23	1.92	0.51
1:A:215:GLY:O	1:A:216:ASP:O	2.29	0.50
1:A:233:VAL:HG11	1:A:236:GLU:OE1	2.11	0.50
1:A:107:SER:HB2	1:A:138:ARG:HG2	1.94	0.49
1:B:18:LYS:HD2	1:B:46:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD11	1:A:89:VAL:HG22	1.95	0.48
1:B:242:ASP:HB2	1:B:257:THR:CB	2.44	0.48
1:A:82:THR:O	1:A:174:LYS:HE3	2.13	0.48
1:A:161:ASP:C	1:A:163:SER:H	2.16	0.47
1:A:61:VAL:HG12	1:A:89:VAL:HG13	1.97	0.47
1:A:256:ARG:HH21	1:A:261:LEU:HA	1.78	0.47
1:A:249:CYS:O	1:A:249:CYS:SG	2.73	0.46
1:A:60:HIS:CE1	1:A:92:GLU:OE2	2.65	0.46
1:A:176:LYS:HB2	1:A:182:MET:HE1	1.98	0.46
1:B:19:TYR:CE1	1:B:47:LYS:HA	2.51	0.46
1:A:256:ARG:NH2	1:A:264:THR:O	2.49	0.45
1:B:106:ARG:HA	1:B:116:VAL:O	2.16	0.45
1:A:138:ARG:NH2	1:B:112:ILE:O	2.47	0.45
1:A:56:PRO:HA	1:A:93:TYR:HA	1.98	0.45
1:B:47:LYS:HE3	1:B:147:ARG:NH2	2.31	0.45
1:A:19:TYR:CD2	1:A:151:TYR:HB3	2.51	0.45
1:A:54:VAL:HG11	1:A:77:HIS:CD2	2.51	0.45
1:A:191:LEU:HA	1:A:209:ARG:O	2.15	0.45
1:B:141:CYS:HA	1:B:158:ALA:O	2.16	0.45
1:B:226:ALA:HB1	1:B:228:GLN:O	2.17	0.45
1:B:77:HIS:HA	1:B:164:LYS:O	2.16	0.45
1:A:25:LEU:HD11	1:A:254:LEU:HB2	1.99	0.44
1:A:57:SER:OG	1:A:58:THR:N	2.50	0.44
1:B:112:ILE:HD11	1:B:139:PHE:HA	1.98	0.44
1:B:222:GLU:O	1:B:224:ARG:N	2.50	0.44
1:A:193:MET:HB2	1:A:207:VAL:O	2.17	0.44
1:B:54:VAL:HA	1:B:96:ASP:H	1.83	0.44
1:A:74:LYS:C	1:A:76:GLN:H	2.21	0.44
1:A:110:SER:N	1:A:111:PRO:CD	2.81	0.43
1:A:58:THR:HB	1:A:92:GLU:OE2	2.18	0.43
1:B:107:SER:HB3	1:B:138:ARG:O	2.18	0.43
1:B:193:MET:HB2	1:B:207:VAL:O	2.18	0.43
1:B:83:LEU:HG	1:B:87:GLN:O	2.19	0.43
1:B:47:LYS:HE3	1:B:147:ARG:CZ	2.48	0.43
1:A:76:GLN:O	1:A:164:LYS:HB2	2.19	0.42
1:B:222:GLU:O	1:B:225:SER:N	2.52	0.42
1:A:63:SER:HA	1:A:87:GLN:HA	1.99	0.42
1:B:169:GLY:O	1:B:171:LYS:N	2.52	0.42
1:A:177:ASN:CB	1:A:178:PRO:CD	2.96	0.42
1:A:109:GLU:C	1:A:111:PRO:HD2	2.41	0.41
1:B:83:LEU:O	1:B:84:SER:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ASN:HB2	1:A:178:PRO:HD2	2.02	0.41
1:B:103:GLN:HG2	1:B:142:ARG:HG2	2.02	0.41
1:B:85:ARG:O	1:B:86:ASN:HB2	2.21	0.41
1:A:62:ILE:HD12	1:A:63:SER:H	1.86	0.41
1:A:133:GLN:HB3	1:A:134:SER:H	1.66	0.40
1:B:157:ALA:O	1:B:158:ALA:HB3	2.22	0.40
1:B:188:ASN:HB3	1:B:189:GLY:H	1.67	0.40
1:A:100:ASP:OD1	1:A:147:ARG:HD2	2.22	0.40
1:A:185:LEU:HD22	1:A:210:GLU:HG2	2.04	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	225/285 (79%)	189 (84%)	26 (12%)	10 (4%)	3	21
1	B	213/285 (75%)	173 (81%)	24 (11%)	16 (8%)	1	8
All	All	438/570 (77%)	362 (83%)	50 (11%)	26 (6%)	2	14

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ASP
1	B	62	ILE
1	B	84	SER
1	B	85	ARG
1	B	86	ASN
1	B	170	GLU
1	A	75	GLY
1	B	75	GLY
1	B	225	SER

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Mol	Chain	Res	Type
1	B	226	ALA
1	A	171	LYS
1	A	204	GLN
1	B	49	PRO
1	B	87	GLN
1	B	95	HIS
1	B	223	THR
1	B	228	GLN
1	B	222	GLU
1	A	47	LYS
1	A	49	PRO
1	A	133	GLN
1	A	196	ARG
1	B	269	HIS
1	A	179	ASP
1	A	205	PRO
1	B	265	PRO

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	157/242 (65%)	135 (86%)	22 (14%)	4	19
1	B	148/242 (61%)	122 (82%)	26 (18%)	2	10
All	All	305/484 (63%)	257 (84%)	48 (16%)	3	14

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	SER
1	A	48	ARG
1	A	64	THR
1	A	83	LEU
1	A	89	VAL
1	A	92	GLU

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Mol	Chain	Res	Type
1	A	98	ASP
1	A	110	SER
1	A	133	GLN
1	A	138	ARG
1	A	146	ASP
1	A	163	SER
1	A	166	ILE
1	A	177	ASN
1	A	186	THR
1	A	193	MET
1	A	194	HIS
1	A	207	VAL
1	A	229	ARG
1	A	249	CYS
1	A	264	THR
1	A	266	THR
1	B	52	ASN
1	B	57	SER
1	B	59	VAL
1	B	61	VAL
1	B	63	SER
1	B	80	SER
1	B	82	THR
1	B	83	LEU
1	B	92	GLU
1	B	94	THR
1	B	106	ARG
1	B	110	SER
1	B	115	VAL
1	B	117	THR
1	B	118	ASP
1	B	135	THR
1	B	174	LYS
1	B	179	ASP
1	B	186	THR
1	B	193	MET
1	B	216	ASP
1	B	219	THR
1	B	220	LEU
1	B	229	ARG
1	B	232	LEU
1	B	262	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	77	HIS
1	A	103	GLN
1	A	165	ASN
1	A	241	GLN
1	B	76	GLN
1	B	95	HIS
1	B	103	GLN

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	235/285 (82%)	-0.15	0	100 100	27, 44, 68, 82	0
1	B	223/285 (78%)	-0.17	1 (0%)	92 90	28, 49, 76, 84	0
All	All	458/570 (80%)	-0.16	1 (0%)	94 94	27, 46, 70, 84	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	59	VAL	2.3

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.