



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 08:17 AM EDT

PDB ID : 3C3V
Title : Crystal structure of peanut major allergen ara h 3
Authors : Jin, T.; Zhang, Y.
Deposited on : unknown
Resolution : 1.73 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

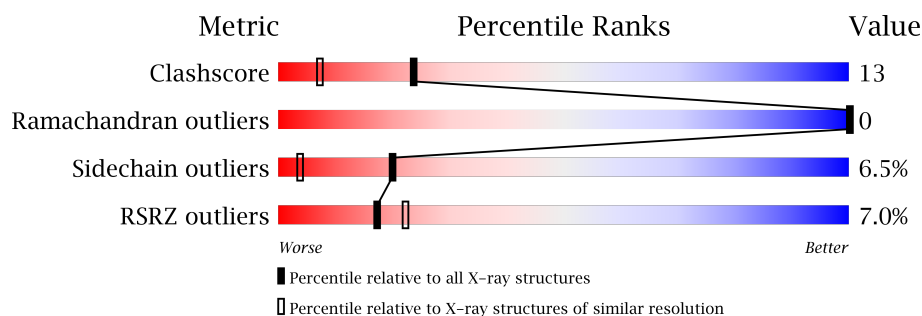
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	2854 (1.76-1.72)
Ramachandran outliers	110173	2824 (1.76-1.72)
Sidechain outliers	110143	2824 (1.76-1.72)
RSRZ outliers	101464	2705 (1.76-1.72)

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	510	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NA	A	1	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3563 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 Arachin Arah3 isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	18	0
			3277	2059	592	622	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	HIS	ASN	SEE REMARK 999	UNP B5TYU1

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

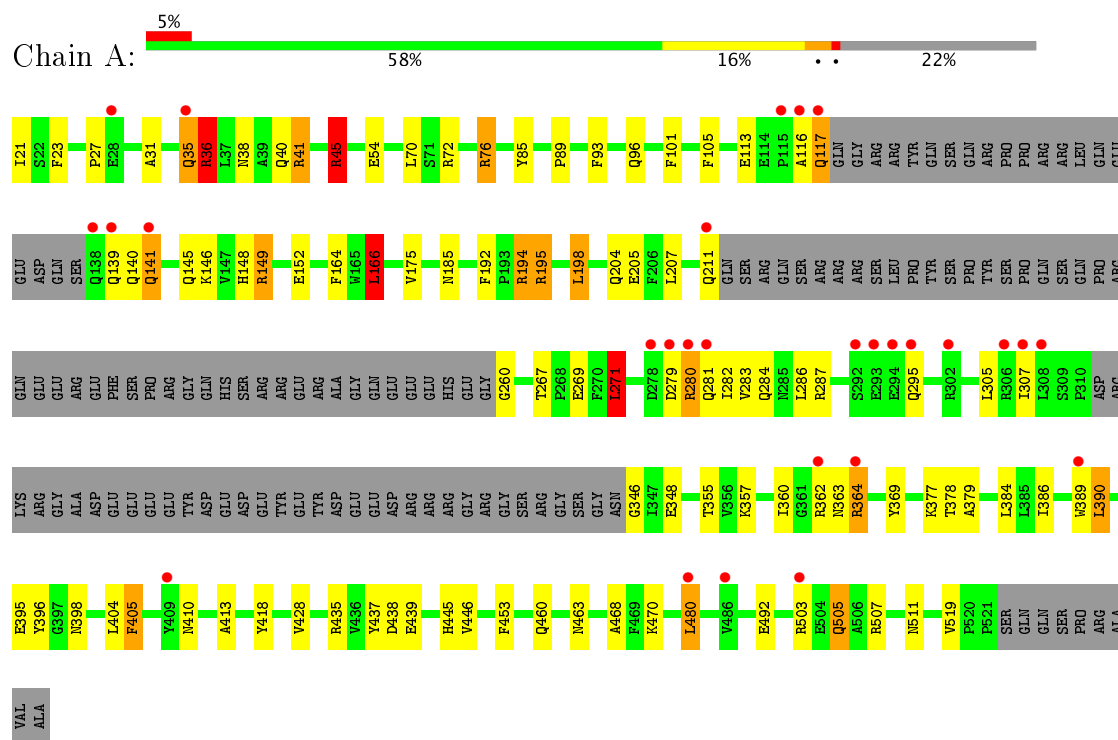
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	285	Total	O	0	0
			285	285		

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: Arachin Arah3 isoform



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	144.93Å 144.93Å 86.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.63 – 1.73 41.64 – 1.73	Depositor EDS
% Data completeness (in resolution range)	92.8 (41.63-1.73) 92.8 (41.64-1.73)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.248 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.8	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	0.97	EDS
Total number of atoms	3563	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	1.23	11/3394 (0.3%)	1.10	18/4605 (0.4%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	GLU	CD-OE1	6.70	1.33	1.25
1	A	453	PHE	CE2-CZ	6.46	1.49	1.37
1	A	93	PHE	CE1-CZ	6.40	1.49	1.37
1	A	85	TYR	CE1-CZ	5.89	1.46	1.38
1	A	428	VAL	CB-CG2	5.68	1.64	1.52
1	A	396	TYR	CZ-OH	5.56	1.47	1.37
1	A	23	PHE	CE2-CZ	5.41	1.47	1.37
1	A	101	PHE	CE1-CZ	5.40	1.47	1.37
1	A	369	TYR	CD2-CE2	5.36	1.47	1.39
1	A	175	VAL	CB-CG2	5.26	1.63	1.52
1	A	405	PHE	CD1-CE1	5.14	1.49	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	ARG	NE-CZ-NH2	-13.15	113.72	120.30
1	A	45	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	A	76	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	A	76	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	A	166	LEU	CA-CB-CG	7.09	131.60	115.30
1	A	194	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	435	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	435	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	195	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	36	ARG	NE-CZ-NH1	5.77	123.18	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	389	TRP	CA-CB-CG	-5.70	102.86	113.70
1	A	305	LEU	CB-CG-CD1	-5.26	102.07	111.00
1	A	21	ILE	CG1-CB-CG2	-5.25	99.85	111.40
1	A	198	LEU	CB-CG-CD1	-5.20	102.15	111.00
1	A	480	LEU	CB-CG-CD2	5.12	119.71	111.00
1	A	36	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	271[A]	LEU	CA-CB-CG	5.00	126.80	115.30
1	A	271[B]	LEU	CA-CB-CG	5.00	126.80	115.30

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	3277	0	3161	81	0
2	A	1	0	0	0	0
3	A	285	0	0	15	2
All	All	3563	0	3161	81	2

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 13.

All (81) 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:410[B]:ASN:ND2	1:A:413:ALA:HB3	1.70	1.04
1:A:410[B]:ASN:HD21	1:A:413:ALA:HB3	1.26	1.00
1:A:164:PHE:CE2	1:A:166:LEU:HD12	1.97	0.99
1:A:492:GLU:OE2	1:A:507:ARG:HG2	1.68	0.94
1:A:364[A]:ARG:H	1:A:364[A]:ARG:HE	1.18	0.87
1:A:503:ARG:HD2	1:A:507:ARG:HH21	1.43	0.84
1:A:96:GLN:HA	1:A:152:GLU:CG	2.13	0.78
1:A:164:PHE:HE2	1:A:166:LEU:HD12	1.49	0.76
1:A:404:LEU:HB3	1:A:519[A]:VAL:HG12	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ARG:HH11	1:A:507:ARG:HE	1.35	0.73
1:A:267:THR:O	1:A:271[B]:LEU:HD12	1.88	0.72
1:A:492:GLU:OE2	1:A:507:ARG:CG	2.39	0.71
1:A:76:ARG:HD2	3:A:663:HOH:O	1.93	0.68
1:A:164:PHE:CZ	1:A:166:LEU:HD12	2.30	0.67
1:A:363:ASN:CB	1:A:377:LYS:HE2	2.24	0.66
1:A:96:GLN:HA	1:A:152:GLU:HG2	1.76	0.66
1:A:116:ALA:HA	1:A:141:GLN:HB2	1.78	0.66
1:A:205[B]:GLU:H	1:A:205[B]:GLU:CD	1.94	0.65
1:A:194:ARG:HA	1:A:204:GLN:HE22	1.61	0.65
1:A:149:ARG:O	1:A:357:LYS:HE2	1.97	0.64
1:A:40:GLN:HE21	1:A:40:GLN:HA	1.62	0.64
1:A:395[B]:GLU:HG2	1:A:470:LYS:HE3	1.81	0.63
1:A:195:ARG:H	1:A:204:GLN:NE2	1.98	0.61
1:A:185[A]:ASN:HB3	3:A:871:HOH:O	2.01	0.60
1:A:395[B]:GLU:HG3	1:A:468:ALA:HB3	1.84	0.59
1:A:185[B]:ASN:ND2	3:A:857:HOH:O	2.35	0.59
1:A:105:PHE:H	1:A:145:GLN:HE22	1.51	0.58
1:A:364[A]:ARG:H	1:A:364[A]:ARG:NE	1.96	0.58
1:A:260:GLY:HA3	3:A:744:HOH:O	2.04	0.57
1:A:378:THR:HG23	3:A:855:HOH:O	2.05	0.56
1:A:503:ARG:HH11	1:A:507:ARG:NE	2.03	0.56
1:A:362:ARG:NH2	3:A:633:HOH:O	2.40	0.54
1:A:41:ARG:NH2	1:A:72[B]:ARG:HH22	2.08	0.52
1:A:281:GLN:HG3	1:A:281:GLN:O	2.09	0.52
1:A:211:GLN:HG2	3:A:803:HOH:O	2.08	0.52
1:A:503:ARG:NH1	1:A:507:ARG:HE	2.05	0.51
1:A:364[A]:ARG:NH2	3:A:884:HOH:O	2.44	0.51
1:A:116:ALA:HA	1:A:141:GLN:HE21	1.76	0.51
1:A:41:ARG:HG3	1:A:445:HIS:CD2	2.46	0.51
1:A:355:THR:HG22	1:A:384:LEU:CD1	2.41	0.50
1:A:45:ARG:HD2	1:A:54:GLU:HG2	1.94	0.50
1:A:439:GLU:HB2	3:A:813:HOH:O	2.12	0.49
1:A:40:GLN:NE2	1:A:40:GLN:HA	2.28	0.48
1:A:418:TYR:HD1	1:A:446:VAL:HG22	1.78	0.48
1:A:139:GLN:HB3	3:A:847:HOH:O	2.13	0.47
1:A:146:LYS:HE2	1:A:148:HIS:CD2	2.49	0.47
1:A:505:GLN:HG2	3:A:726:HOH:O	2.14	0.47
1:A:438:ASP:O	1:A:439:GLU:HB3	2.14	0.47
1:A:390:LEU:HD23	1:A:390:LEU:N	2.30	0.47
1:A:398:ASN:HB3	1:A:463:ASN:HD21	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HD2	1:A:54:GLU:CG	2.46	0.46
1:A:194:ARG:HA	1:A:204:GLN:NE2	2.27	0.46
1:A:360:ILE:HG21	1:A:379:ALA:HB2	1.98	0.45
1:A:195:ARG:H	1:A:204:GLN:HE21	1.64	0.45
1:A:346:GLY:N	3:A:725:HOH:O	2.49	0.45
1:A:35[A]:GLN:NE2	3:A:863:HOH:O	2.50	0.44
1:A:141:GLN:HE21	1:A:141:GLN:HB2	1.62	0.44
1:A:70:LEU:CD2	1:A:446:VAL:HG21	2.48	0.44
1:A:271[B]:LEU:HD23	1:A:286[B]:LEU:HD13	1.99	0.43
1:A:27:PRO:HB2	1:A:31:ALA:HB3	2.00	0.43
1:A:164:PHE:CZ	1:A:166:LEU:CD1	3.00	0.43
1:A:364[A]:ARG:N	1:A:364[A]:ARG:HE	2.00	0.43
1:A:279:ASP:HB3	1:A:282:ILE:HD12	2.00	0.43
1:A:117:GLN:HB2	3:A:777:HOH:O	2.18	0.43
1:A:437:TYR:CZ	1:A:439:GLU:HG2	2.54	0.43
1:A:271[A]:LEU:HD23	1:A:287:ARG:HD3	2.01	0.43
1:A:36:ARG:CD	1:A:38:ASN:HD21	2.32	0.43
1:A:70:LEU:HD23	1:A:446:VAL:HG21	2.01	0.42
1:A:507:ARG:O	1:A:511:ASN:ND2	2.52	0.42
1:A:280:ARG:O	1:A:284:GLN:HG3	2.20	0.42
1:A:113:GLU:OE1	1:A:140:GLN:NE2	2.53	0.42
1:A:283:VAL:O	1:A:287:ARG:HG3	2.19	0.42
1:A:89:PRO:HB3	1:A:390:LEU:HD13	2.01	0.42
1:A:117:GLN:H	1:A:141:GLN:NE2	2.19	0.41
1:A:378:THR:CG2	3:A:855:HOH:O	2.67	0.41
1:A:36:ARG:NE	1:A:38:ASN:HD21	2.19	0.41
1:A:280:ARG:O	1:A:280:ARG:HG3	2.21	0.40
1:A:117:GLN:HB3	1:A:117:GLN:HE21	1.56	0.40
1:A:204:GLN:HA	1:A:205[B]:GLU:OE1	2.21	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
3:A:846:HOH:O	3:A:868:HOH:O[2_545]	2.09	0.11
3:A:867:HOH:O	3:A:869:HOH:O[9_555]	2.14	0.06

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	408/510 (80%)	390 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	355/441 (80%)	329 (93%)	26 (7%)	16	2

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35[A]	GLN
1	A	35[B]	GLN
1	A	36	ARG
1	A	41	ARG
1	A	45	ARG
1	A	117	GLN
1	A	141	GLN
1	A	149	ARG
1	A	166	LEU
1	A	192	PHE
1	A	198	LEU
1	A	207	LEU
1	A	269	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	271[A]	LEU
1	A	271[B]	LEU
1	A	280	ARG
1	A	295[A]	GLN
1	A	295[B]	GLN
1	A	307	ILE
1	A	364[A]	ARG
1	A	364[B]	ARG
1	A	390	LEU
1	A	405	PHE
1	A	460	GLN
1	A	480	LEU
1	A	505	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	38	ASN
1	A	40	GLN
1	A	60	ASN
1	A	117	GLN
1	A	140	GLN
1	A	141	GLN
1	A	145	GLN
1	A	191	GLN
1	A	204	GLN
1	A	460	GLN
1	A	463	ASN
1	A	484	ASN
1	A	505	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	398/510 (78%)	0.30	28 (7%)	17 22	20, 32, 56, 81	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	117	GLN	6.6
1	A	116	ALA	6.3
1	A	364[A]	ARG	5.2
1	A	280	ARG	4.4
1	A	294	GLU	4.3
1	A	293	GLU	3.9
1	A	306	ARG	3.9
1	A	139	GLN	3.7
1	A	308	LEU	3.7
1	A	211	GLN	3.7
1	A	281	GLN	3.6
1	A	278	ASP	3.5
1	A	138	GLN	3.5
1	A	292	SER	3.4
1	A	141	GLN	3.2
1	A	389	TRP	3.2
1	A	480	LEU	3.1
1	A	35[A]	GLN	3.1
1	A	295[A]	GLN	3.0
1	A	28	GLU	2.7
1	A	362	ARG	2.7
1	A	115	PRO	2.5
1	A	409	TYR	2.4
1	A	486	VAL	2.3
1	A	503	ARG	2.3
1	A	302	ARG	2.2
1	A	307	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	279	ASP	2.0

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NA	A	1	1/1	0.99	0.15	2.56	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.