



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2022 – 03:05 pm GMT

PDB ID : 7Q0L
Title : Crystal structure of the peptide transporter YePEPT-K314A at 2.93 Å
Authors : Jeckelmann, J.M.; Stauffer, M.; Ilgue, H.; Boggavarapu, R.; Fotiadis, D.
Deposited on : 2021-10-15
Resolution : 2.71 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

<https://www.wwpdb.org/validation/2017/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) : 1.13
EDS : 2.27
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

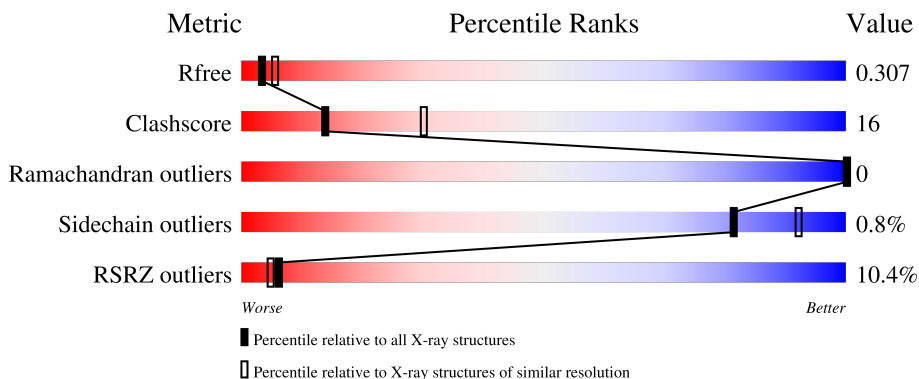
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	519	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3681 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 Peptide transporter YePEPT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	482	3681	2453	593	606	29	0	0	0

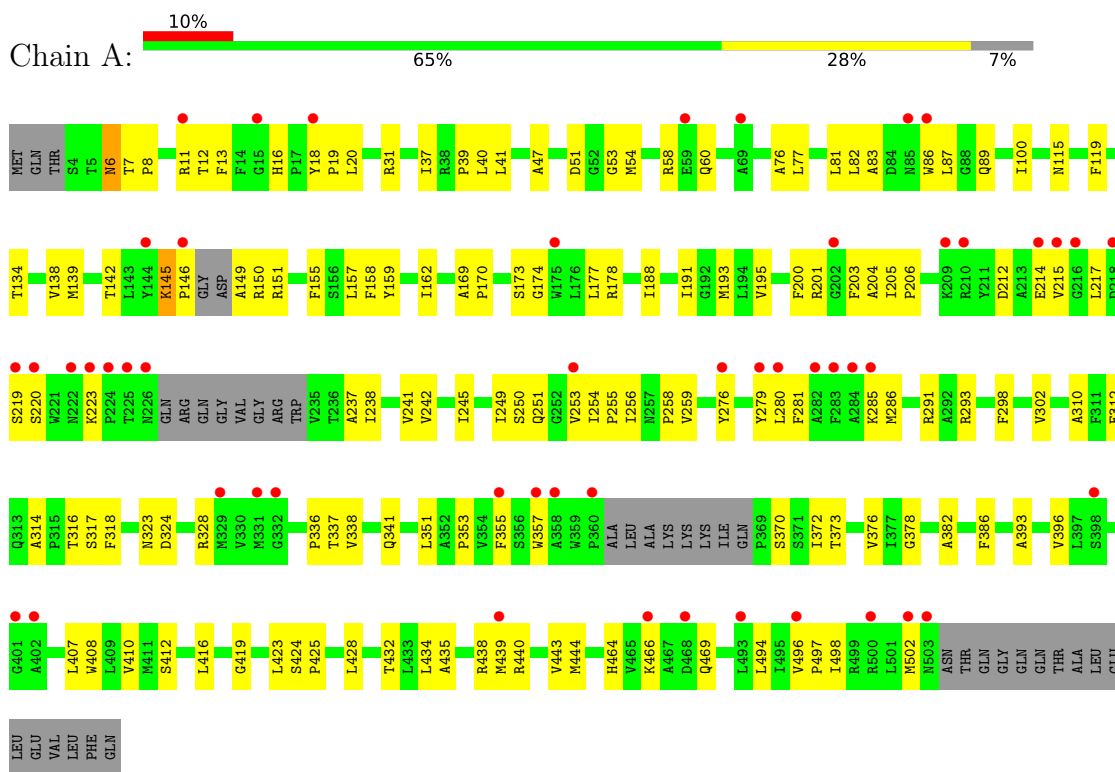
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	314	ALA	LYS	engineered mutation	UNP A0A2R9TD79
A	512	LEU	-	expression tag	UNP A0A2R9TD79
A	513	GLU	-	expression tag	UNP A0A2R9TD79
A	514	LEU	-	expression tag	UNP A0A2R9TD79
A	515	GLU	-	expression tag	UNP A0A2R9TD79
A	516	VAL	-	expression tag	UNP A0A2R9TD79
A	517	LEU	-	expression tag	UNP A0A2R9TD79
A	518	PHE	-	expression tag	UNP A0A2R9TD79
A	519	GLN	-	expression tag	UNP A0A2R9TD79

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Peptide transporter YePEPT



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.98Å 101.06Å 103.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.81 – 2.71 46.12 – 2.71	Depositor EDS
% Data completeness (in resolution range)	80.6 (28.81-2.71) 74.5 (46.12-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.73Å)	Xtrriage
Refinement program	PHENIX 1.14	Depositor
R, R_{free}	0.260 , 0.292 0.270 , 0.307	Depositor DCC
R_{free} test set	1048 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	72.9	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for -h,l,k	Xtrriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	3681	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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](#)

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	0.39	0/3780	0.55	0/5139

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 [i](#)

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	3681	0	3794	118	2
All	All	3681	0	3794	118	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 16.

All (118) 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:178:ARG:CD	1:A:336:PRO:HG3	1.75	1.15
1:A:201:ARG:HA	1:A:205:ILE:HD12	1.24	1.11
1:A:178:ARG:HD2	1:A:336:PRO:HG3	1.07	1.02
1:A:178:ARG:HD2	1:A:336:PRO:CG	1.94	0.95
1:A:86:TRP:CE3	1:A:87:LEU:HD23	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:CE2	1:A:157:LEU:HD21	2.10	0.85
1:A:39:PRO:HB3	1:A:341:GLN:HG3	1.58	0.84
1:A:6:ASN:HB2	1:A:11:ARG:HD2	1.59	0.83
1:A:86:TRP:CE3	1:A:87:LEU:CD2	2.64	0.81
1:A:86:TRP:CZ3	1:A:87:LEU:CD2	2.63	0.80
1:A:89:GLN:NE2	1:A:138:VAL:HB	1.97	0.79
1:A:249:ILE:HG22	1:A:254:ILE:HG13	1.65	0.78
1:A:279:TYR:HD1	1:A:280:LEU:HD12	1.47	0.78
1:A:201:ARG:HA	1:A:205:ILE:CD1	2.11	0.78
1:A:86:TRP:CZ3	1:A:87:LEU:HD23	2.23	0.74
1:A:214:GLU:HG2	1:A:215:VAL:HG23	1.71	0.73
1:A:86:TRP:CZ3	1:A:87:LEU:HD21	2.25	0.72
1:A:149:ALA:O	1:A:150:ARG:HB2	1.92	0.69
1:A:250:SER:HB3	1:A:256:ILE:HD11	1.75	0.67
1:A:40:LEU:CD2	1:A:338:VAL:HG11	2.27	0.64
1:A:423:LEU:C	1:A:423:LEU:HD23	2.18	0.64
1:A:249:ILE:CG2	1:A:254:ILE:HG13	2.27	0.64
1:A:314:ALA:HA	1:A:318:PHE:HB2	1.79	0.64
1:A:86:TRP:HZ3	1:A:87:LEU:HD21	1.64	0.62
1:A:432:THR:HG22	1:A:443:VAL:HG21	1.81	0.62
1:A:145:LYS:HG2	1:A:146:PRO:HD2	1.81	0.62
1:A:245:ILE:O	1:A:249:ILE:HG12	2.00	0.62
1:A:13:PHE:CE2	1:A:157:LEU:CD2	2.81	0.62
1:A:159:TYR:O	1:A:162:ILE:HB	2.00	0.61
1:A:178:ARG:CD	1:A:336:PRO:CG	2.66	0.60
1:A:54:MET:HE1	1:A:119:PHE:HZ	1.67	0.60
1:A:89:GLN:HE22	1:A:138:VAL:HB	1.67	0.60
1:A:250:SER:HB3	1:A:256:ILE:CD1	2.32	0.60
1:A:407:LEU:HA	1:A:410:VAL:HB	1.83	0.60
1:A:40:LEU:HD23	1:A:338:VAL:HG11	1.84	0.59
1:A:351:LEU:HB3	1:A:355:PHE:HE2	1.67	0.59
1:A:378:GLY:HA2	1:A:419:GLY:HA2	1.85	0.59
1:A:276:TYR:O	1:A:280:LEU:HD13	2.03	0.59
1:A:12:THR:HB	1:A:16:HIS:O	2.04	0.58
1:A:428:LEU:HD21	1:A:444:MET:HG3	1.86	0.57
1:A:31:ARG:HG3	1:A:162:ILE:HG12	1.86	0.56
1:A:440:ARG:O	1:A:443:VAL:HG22	2.05	0.56
1:A:13:PHE:HE2	1:A:157:LEU:CD2	2.19	0.56
1:A:178:ARG:HD3	1:A:336:PRO:HG3	1.81	0.55
1:A:238:ILE:O	1:A:242:VAL:HG23	2.06	0.55
1:A:54:MET:HE1	1:A:119:PHE:CZ	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:SER:HB3	1:A:223:LYS:HD2	1.88	0.55
1:A:498:ILE:O	1:A:502:MET:N	2.34	0.54
1:A:86:TRP:HZ3	1:A:87:LEU:CD2	2.17	0.53
1:A:201:ARG:HD2	1:A:205:ILE:HD12	1.90	0.52
1:A:351:LEU:HB3	1:A:355:PHE:CE2	2.45	0.52
1:A:205:ILE:HB	1:A:206:PRO:HD3	1.93	0.51
1:A:494:LEU:HA	1:A:497:PRO:HG2	1.92	0.51
1:A:139:MET:O	1:A:142:THR:OG1	2.23	0.50
1:A:316:THR:OG1	1:A:317:SER:N	2.43	0.50
1:A:328:ARG:CZ	1:A:337:THR:HG22	2.40	0.50
1:A:86:TRP:CE3	1:A:87:LEU:HD21	2.42	0.50
1:A:200:PHE:HA	1:A:204:ALA:HB3	1.94	0.50
1:A:60:GLN:NE2	1:A:258:PRO:HD2	2.27	0.50
1:A:281:PHE:CE1	1:A:291:ARG:HB2	2.47	0.49
1:A:323:ASN:OD1	1:A:337:THR:HG21	2.12	0.49
1:A:76:ALA:HB1	1:A:134:THR:HG21	1.94	0.49
1:A:372:ILE:O	1:A:376:VAL:HG23	2.11	0.49
1:A:423:LEU:HD23	1:A:423:LEU:O	2.12	0.49
1:A:424:SER:N	1:A:425:PRO:CD	2.75	0.49
1:A:438:ARG:O	1:A:438:ARG:HD2	2.12	0.49
1:A:212:ASP:HB2	1:A:217:LEU:HD12	1.94	0.49
1:A:428:LEU:O	1:A:432:THR:HG23	2.12	0.49
1:A:203:PHE:C	1:A:206:PRO:HD2	2.33	0.48
1:A:220:SER:HA	1:A:223:LYS:O	2.13	0.48
1:A:77:LEU:O	1:A:81:LEU:HG	2.13	0.48
1:A:439:MET:O	1:A:443:VAL:HG13	2.14	0.47
1:A:86:TRP:HE3	1:A:87:LEU:CD2	2.21	0.47
1:A:286:MET:HE3	1:A:438:ARG:HB3	1.96	0.47
1:A:382:ALA:HA	1:A:416:LEU:HD23	1.95	0.47
1:A:83:ALA:HA	1:A:87:LEU:HB2	1.95	0.47
1:A:89:GLN:NE2	1:A:138:VAL:CB	2.74	0.47
1:A:18:TYR:N	1:A:19:PRO:HD2	2.31	0.46
1:A:298:PHE:O	1:A:302:VAL:HG23	2.15	0.46
1:A:174:GLY:O	1:A:177:LEU:HB3	2.15	0.46
1:A:47:ALA:HB3	1:A:53:GLY:HA3	1.97	0.46
1:A:435:ALA:HB2	1:A:443:VAL:HG11	1.96	0.46
1:A:238:ILE:O	1:A:241:VAL:HB	2.15	0.46
1:A:432:THR:HG22	1:A:443:VAL:CG2	2.44	0.46
1:A:54:MET:HG2	1:A:115:ASN:OD1	2.16	0.45
1:A:279:TYR:CD1	1:A:280:LEU:HD12	2.38	0.45
1:A:250:SER:HA	1:A:254:ILE:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:N	1:A:8:PRO:HD2	2.32	0.45
1:A:293:ARG:HB3	1:A:434:LEU:O	2.16	0.45
1:A:37:ILE:O	1:A:41:LEU:HG	2.17	0.45
1:A:310:ALA:HB1	1:A:386:PHE:CE1	2.53	0.44
1:A:7:THR:N	1:A:8:PRO:CD	2.80	0.44
1:A:155:PHE:O	1:A:158:PHE:HB3	2.18	0.44
1:A:253:VAL:O	1:A:255:PRO:HD3	2.17	0.44
1:A:285:LYS:O	1:A:286:MET:HG3	2.18	0.43
1:A:60:GLN:NE2	1:A:259:VAL:HG23	2.33	0.43
1:A:138:VAL:O	1:A:142:THR:HG23	2.18	0.43
1:A:328:ARG:NE	1:A:337:THR:HG22	2.33	0.43
1:A:169:ALA:HB3	1:A:170:PRO:HD3	2.00	0.43
1:A:353:PRO:O	1:A:357:TRP:N	2.48	0.43
1:A:372:ILE:HD11	1:A:498:ILE:HG21	2.01	0.43
1:A:242:VAL:O	1:A:245:ILE:HG13	2.19	0.42
1:A:370:SER:N	1:A:373:THR:OG1	2.52	0.42
1:A:191:ILE:O	1:A:195:VAL:HG23	2.19	0.42
1:A:237:ALA:O	1:A:241:VAL:HG23	2.20	0.42
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.94	0.42
1:A:203:PHE:O	1:A:206:PRO:HD2	2.19	0.41
1:A:188:ILE:HD12	1:A:188:ILE:HA	1.95	0.41
1:A:393:ALA:O	1:A:396:VAL:HB	2.20	0.41
1:A:312:GLU:OE2	1:A:312:GLU:HA	2.21	0.41
1:A:464:HIS:HA	1:A:466:LYS:HZ3	1.86	0.41
1:A:466:LYS:HE2	1:A:469:GLN:HG3	2.02	0.41
1:A:100:ILE:HG22	1:A:193:MET:HG2	2.03	0.41
1:A:58:ARG:NH2	1:A:324:ASP:OD2	2.51	0.40
1:A:149:ALA:O	1:A:150:ARG:CB	2.67	0.40
1:A:408:TRP:O	1:A:412:SER:OG	2.20	0.40
1:A:13:PHE:HD2	1:A:20:LEU:HD23	1.86	0.40
1:A:170:PRO:HA	1:A:173:SER:OG	2.22	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)
1:A:8:PRO:CG	1:A:51:ASP:OD1[2_455]	2.16	0.04
1:A:251:GLN:OE1	1:A:496:VAL:CG2[3_555]	2.17	0.03

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	474/519 (91%)	464 (98%)	10 (2%)	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	382/412 (93%)	379 (99%)	3 (1%)	81 92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	145	LYS
1	A	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	85	ASN
1	A	89	GLN
1	A	90	GLN
1	A	464	HIS

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Mol	Chain	Res	Type
1	A	469	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 monosaccharides 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	482/519 (92%)	0.68	50 (10%) 6 5	45, 75, 120, 152	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	ASN	7.8
1	A	219	SER	7.1
1	A	220	SER	6.3
1	A	223	LYS	6.3
1	A	331	MET	5.7
1	A	357	TRP	5.3
1	A	224	PRO	5.2
1	A	285	LYS	5.1
1	A	226	ASN	4.6
1	A	225	THR	4.6
1	A	502	MET	4.6
1	A	360	PRO	4.3
1	A	216	GLY	4.3
1	A	218	ASP	4.2
1	A	283	PHE	3.9
1	A	86	TRP	3.7
1	A	332	GLY	3.4
1	A	466	LYS	3.3
1	A	146	PRO	3.2
1	A	279	TYR	3.1
1	A	11	ARG	3.1
1	A	214	GLU	2.9
1	A	69	ALA	2.9
1	A	402	ALA	2.9
1	A	253	VAL	2.9
1	A	144	TYR	2.9
1	A	59	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	280	LEU	2.8
1	A	493	LEU	2.8
1	A	398	SER	2.7
1	A	210	ARG	2.7
1	A	276	TYR	2.6
1	A	18	TYR	2.6
1	A	202	GLY	2.6
1	A	85	ASN	2.5
1	A	358	ALA	2.4
1	A	329	MET	2.4
1	A	15	GLY	2.4
1	A	222	ASN	2.4
1	A	282	ALA	2.3
1	A	284	ALA	2.3
1	A	355	PHE	2.2
1	A	209	LYS	2.2
1	A	401	GLY	2.1
1	A	496	VAL	2.1
1	A	500	ARG	2.1
1	A	468	ASP	2.1
1	A	215	VAL	2.0
1	A	439	MET	2.0
1	A	175	TRP	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 monosaccharides 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.