



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:13 am BST

PDB ID : 6A30
Title : Crystal Structure of Munc13-1 MUN Domain and Synaptobrevin-2 Juxtamembrane Linker Region
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Deposited on : 2018-06-14
Resolution : 2.79 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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

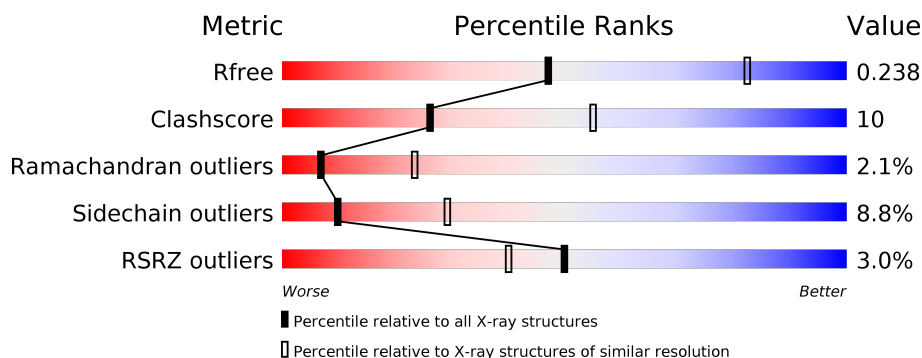
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	537	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>21%</div> <div>• •</div> </div> </div>
2	P	6	<div> <div>50%</div> <div> <div>50%</div> <div>50%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4347 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 unc-13 homolog A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4262	2719	710	805	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1408	GLU	-	linker	UNP Q62768
A	1409	PHE	-	linker	UNP Q62768

- Molecule 2 is a protein called Synaptobrevin-2 juxtamembrane linker peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	6	Total	C	N	O	0	0	0
			66	47	11	8			

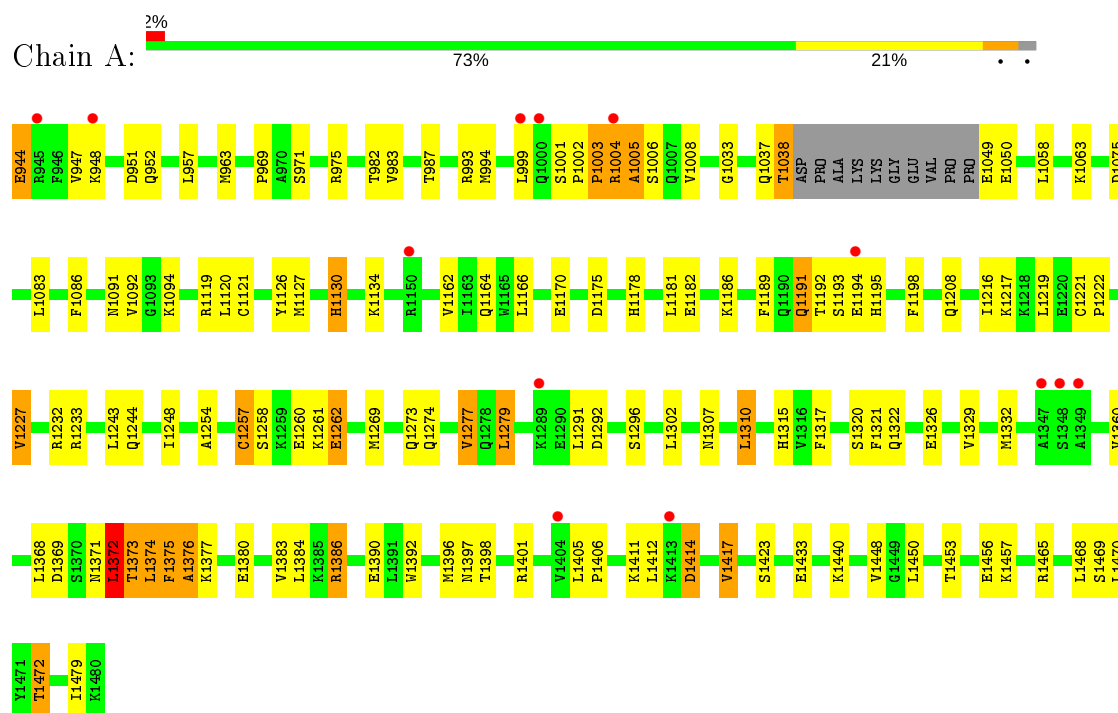
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		

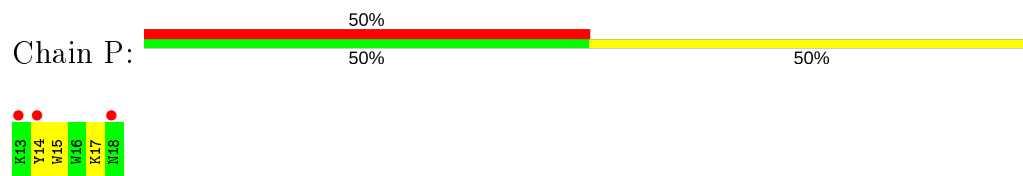
3 Residue-property plots [i](#)

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: Protein unc-13 homolog A



- Molecule 2: Synaptobrevin-2 juxtamembrane linker peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	114.48 Å 270.97 Å 47.91 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.01 – 2.79 42.01 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (42.01-2.79) 99.4 (42.01-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.81 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.207 , 0.239 0.207 , 0.238	Depositor DCC
R_{free} test set	1900 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	80.8	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4347	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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	0.29	0/4348	0.45	0/5873
2	P	0.24	0/70	0.32	0/94
All	All	0.29	0/4418	0.45	0/5967

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	4262	0	4261	88	0
2	P	66	0	60	4	0
3	A	19	0	0	2	0
All	All	4347	0	4321	90	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 10.

All (90) 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:1375:PHE:O	1:A:1377:LYS:N	1.71	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1374:LEU:O	1:A:1374:LEU:HD12	1.36	1.22
1:A:1374:LEU:C	1:A:1374:LEU:HD12	1.77	0.94
1:A:1258:SER:HA	1:A:1320:SER:HB2	1.60	0.81
1:A:1310:LEU:HD13	1:A:1386:ARG:HH12	1.46	0.81
1:A:1372:LEU:HD13	1:A:1372:LEU:H	1.54	0.73
1:A:1003:PRO:HB3	1:A:1008:VAL:HG23	1.72	0.71
1:A:1269:MET:HE2	1:A:1383:VAL:HG13	1.72	0.70
1:A:1405:LEU:HD23	1:A:1406:PRO:HD2	1.75	0.69
1:A:1371:ASN:O	1:A:1372:LEU:C	2.30	0.68
1:A:1374:LEU:O	1:A:1374:LEU:CD1	2.30	0.68
1:A:1440:LYS:NZ	1:A:1465:ARG:HH22	1.93	0.66
1:A:969:PRO:HD2	1:A:975:ARG:HG2	1.76	0.66
1:A:1130:HIS:NE2	3:A:1503:HOH:O	2.29	0.65
1:A:1371:ASN:O	1:A:1374:LEU:N	2.29	0.65
1:A:951:ASP:OD1	1:A:993:ARG:NH2	2.29	0.65
1:A:1371:ASN:O	1:A:1373:THR:N	2.30	0.65
1:A:1372:LEU:CD1	1:A:1372:LEU:N	2.59	0.65
1:A:1310:LEU:HD13	1:A:1386:ARG:NH1	2.11	0.65
1:A:1469:SER:HA	1:A:1472:THR:HG22	1.81	0.62
1:A:1375:PHE:CD1	1:A:1375:PHE:N	2.66	0.61
1:A:1033:GLY:HA2	1:A:1037:GLN:HG2	1.82	0.60
1:A:1372:LEU:HD13	1:A:1372:LEU:N	2.14	0.59
1:A:1332:MET:HB2	1:A:1360:VAL:HG13	1.88	0.56
1:A:1315:HIS:HA	1:A:1390:GLU:HG2	1.87	0.55
1:A:1191:GLN:OE1	1:A:1193:SER:N	2.41	0.54
1:A:1121:CYS:HB2	1:A:1126:TYR:CZ	2.43	0.54
1:A:1063:LYS:NZ	3:A:1501:HOH:O	2.00	0.54
1:A:1004:ARG:O	1:A:1006:SER:N	2.40	0.54
1:A:1257:CYS:SG	1:A:1258:SER:N	2.81	0.53
1:A:1375:PHE:C	1:A:1377:LYS:N	2.54	0.53
1:A:1192:THR:HG23	1:A:1198:PHE:O	2.08	0.53
1:A:1232:ARG:NE	1:A:1292:ASP:OD2	2.42	0.52
1:A:1371:ASN:C	1:A:1373:THR:N	2.61	0.52
1:A:1002:PRO:HG2	1:A:1003:PRO:HD3	1.92	0.52
1:A:1440:LYS:HZ1	1:A:1465:ARG:HH22	1.56	0.52
1:A:1279:LEU:HD11	1:A:1302:LEU:HD23	1.90	0.51
1:A:1274:GLN:HA	1:A:1277:VAL:HG13	1.93	0.50
1:A:1260:GLU:CD	1:A:1261:LYS:HA	2.33	0.50
1:A:1193:SER:O	1:A:1195:HIS:N	2.43	0.49
1:A:1119:ARG:NH1	1:A:1164:GLN:OE1	2.42	0.49
1:A:1003:PRO:HD2	1:A:1004:ARG:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1374:LEU:O	1:A:1375:PHE:O	2.30	0.49
1:A:1329:VAL:HA	1:A:1332:MET:HG2	1.94	0.48
1:A:1397:ASN:HB3	1:A:1401:ARG:NH2	2.27	0.48
1:A:1440:LYS:NZ	1:A:1456:GLU:OE2	2.47	0.48
1:A:1134:LYS:HD2	1:A:1219:LEU:O	2.13	0.48
1:A:1091:ASN:HB3	1:A:1094:LYS:HB2	1.95	0.48
1:A:1166:LEU:HD21	1:A:1216:ILE:HD11	1.96	0.47
1:A:957:LEU:HD22	1:A:982:THR:HG23	1.95	0.47
1:A:1004:ARG:HD2	1:A:1004:ARG:O	2.15	0.47
1:A:1414:ASP:OD1	1:A:1414:ASP:N	2.47	0.47
1:A:1369:ASP:O	1:A:1373:THR:HB	2.15	0.47
1:A:987:THR:HG22	1:A:1005:ALA:HB1	1.96	0.46
1:A:1376:ALA:H	1:A:1384:LEU:HD13	1.81	0.46
1:A:1186:LYS:NZ	1:A:1186:LYS:HB2	2.31	0.46
2:P:14:TYR:CD1	2:P:17:LYS:HE3	2.51	0.46
1:A:1273:GLN:HB2	1:A:1310:LEU:HD11	1.98	0.46
1:A:1119:ARG:O	1:A:1126:TYR:OH	2.34	0.45
1:A:1372:LEU:HB3	2:P:15:TRP:CE3	2.51	0.45
1:A:1392:TRP:O	1:A:1396:MET:HG2	2.16	0.45
1:A:1127:MET:HE1	1:A:1162:VAL:HG22	1.99	0.45
1:A:1121:CYS:HB2	1:A:1126:TYR:CE2	2.52	0.45
1:A:1321:PHE:HE1	1:A:1371:ASN:ND2	2.14	0.45
1:A:1440:LYS:HZ1	1:A:1465:ARG:NH2	2.15	0.45
1:A:1075:ASP:HB3	1:A:1092:VAL:HG12	2.00	0.44
1:A:1326:GLU:HA	1:A:1398:THR:HG21	1.99	0.44
1:A:1262:GLU:HG3	1:A:1317:PHE:CE1	2.53	0.43
1:A:1373:THR:HG22	1:A:1374:LEU:N	2.34	0.43
1:A:1372:LEU:HD12	1:A:1372:LEU:HA	1.53	0.43
1:A:1244:GLN:O	1:A:1248:ILE:HG12	2.19	0.43
1:A:1291:LEU:HD23	1:A:1296:SER:HB3	2.01	0.43
1:A:1412:LEU:HB3	1:A:1417:VAL:HG13	2.00	0.42
1:A:1373:THR:OG1	2:P:15:TRP:O	2.35	0.42
2:P:14:TYR:HB2	2:P:17:LYS:HG3	2.00	0.42
1:A:1221:CYS:HB3	1:A:1227:VAL:HG23	2.02	0.41
1:A:1170:GLU:OE1	1:A:1233:ARG:NH2	2.51	0.41
1:A:944:GLU:O	1:A:947:VAL:HG12	2.20	0.41
1:A:1037:GLN:HB3	1:A:1038:THR:H	1.63	0.41
1:A:1221:CYS:HA	1:A:1222:PRO:HD3	1.77	0.41
1:A:1003:PRO:CD	1:A:1004:ARG:HA	2.51	0.40
1:A:1119:ARG:HD3	1:A:1119:ARG:HA	1.80	0.40
1:A:1217:LYS:HA	1:A:1217:LYS:HD2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:LEU:HB3	1:A:1372:LEU:HD22	2.03	0.40
1:A:1374:LEU:C	1:A:1375:PHE:O	2.59	0.40
1:A:983:VAL:O	1:A:987:THR:HG23	2.21	0.40
1:A:1254:ALA:HA	1:A:1257:CYS:SG	2.61	0.40
1:A:1457:LYS:HA	1:A:1457:LYS:HD3	1.90	0.40
1:A:1181:LEU:HD23	1:A:1181:LEU:HA	1.95	0.40
1:A:1243:LEU:HA	1:A:1243:LEU:HD23	1.91	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	523/537 (97%)	480 (92%)	32 (6%)	11 (2%)	7	23
2	P	4/6 (67%)	4 (100%)	0	0	100	100
All	All	527/543 (97%)	484 (92%)	32 (6%)	11 (2%)	7	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1003	PRO
1	A	1005	ALA
1	A	1375	PHE
1	A	1376	ALA
1	A	1178	HIS
1	A	1189	PHE
1	A	1194	GLU
1	A	1372	LEU
1	A	1001	SER
1	A	1414	ASP
1	A	1479	ILE

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	483/491 (98%)	440 (91%)	43 (9%)	9	28
2	P	6/6 (100%)	6 (100%)	0	100	100
All	All	489/497 (98%)	446 (91%)	43 (9%)	10	29

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	944	GLU
1	A	948	LYS
1	A	952	GLN
1	A	963	MET
1	A	971	SER
1	A	994	MET
1	A	999	LEU
1	A	1004	ARG
1	A	1038	THR
1	A	1049	GLU
1	A	1050	GLU
1	A	1058	LEU
1	A	1083	LEU
1	A	1086	PHE
1	A	1120	LEU
1	A	1130	HIS
1	A	1175	ASP
1	A	1182	GLU
1	A	1191	GLN
1	A	1208	GLN
1	A	1227	VAL
1	A	1257	CYS
1	A	1262	GLU
1	A	1277	VAL
1	A	1279	LEU
1	A	1307	ASN
1	A	1310	LEU

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Mol	Chain	Res	Type
1	A	1322	GLN
1	A	1372	LEU
1	A	1373	THR
1	A	1374	LEU
1	A	1380	GLU
1	A	1386	ARG
1	A	1411	LYS
1	A	1417	VAL
1	A	1423	SER
1	A	1433	GLU
1	A	1448	VAL
1	A	1450	LEU
1	A	1453	THR
1	A	1468	LEU
1	A	1470	LEU
1	A	1472	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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	527/537 (98%)	0.17	13 (2%) 57 47	49, 82, 134, 185	0
2	P	6/6 (100%)	1.62	3 (50%) 0 0	122, 135, 141, 145	0
All	All	533/543 (98%)	0.19	16 (3%) 50 40	49, 83, 137, 185	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1348	SER	5.1
2	P	18	ASN	3.6
1	A	1000	GLN	3.5
1	A	1289	LYS	2.9
1	A	1413	LYS	2.9
1	A	999	LEU	2.6
2	P	13	LYS	2.4
1	A	948	LYS	2.4
1	A	1404	VAL	2.3
1	A	1347	ALA	2.3
1	A	1150	ARG	2.3
1	A	1004	ARG	2.2
1	A	1194	GLU	2.1
1	A	1349	ALA	2.1
1	A	945	ARG	2.1
2	P	14	TYR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.