



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2017 – 04:03 PM EDT

PDB ID : 2GD5
Title : Structural basis for budding by the ESCRTIII factor CHMP3
Authors : Muziol, T.M.; Pineda-Molina, E.; Ravelli, R.B.; Zamborlini, A.; Usami, Y.;
Gottlinger, H.; Weissenhorn, W.
Deposited on : unknown
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

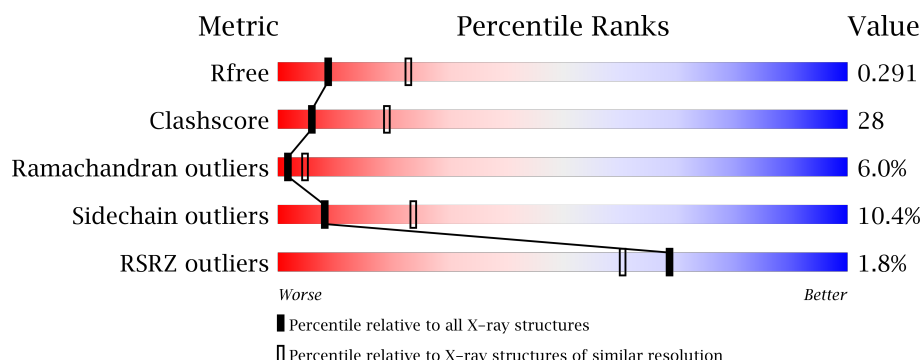
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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. 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	179	<div> <div>2%</div> <div> <div></div> <div>35%</div> <div>36%</div> <div>7%</div> <div>21%</div> </div> </div>
1	B	179	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>29%</div> <div>12%</div> <div>13%</div> </div> </div>
1	C	179	<div> <div>2%</div> <div> <div></div> <div>42%</div> <div>32%</div> <div>•</div> <div>21%</div> </div> </div>
1	D	179	<div> <div></div> <div> <div>45%</div> <div>39%</div> <div>7%</div> <div>9%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4746 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 Charged multivesicular body protein 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	Se	0	0	0
			1134	710	207	205	1	11			
1	B	156	Total	C	N	O	S	Se	0	0	0
			1219	763	223	220	1	12			
1	C	142	Total	C	N	O	S	Se	0	0	0
			1123	703	204	204	1	11			
1	D	162	Total	C	N	O	S	Se	0	0	0
			1270	793	229	234	1	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	CLONING ARTIFACT	UNP Q9Y3E7
A	6	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
A	7	MSE	-	CLONING ARTIFACT	UNP Q9Y3E7
A	8	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
A	27	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	67	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	84	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	89	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	91	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	111	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	114	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	127	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	134	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	135	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	157	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
A	163	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	5	GLY	-	CLONING ARTIFACT	UNP Q9Y3E7
B	6	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
B	7	MSE	-	CLONING ARTIFACT	UNP Q9Y3E7
B	8	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
B	27	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	84	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	89	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	91	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	111	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	114	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	127	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	134	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	135	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	157	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
B	163	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	5	GLY	-	CLONING ARTIFACT	UNP Q9Y3E7
C	6	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
C	7	MSE	-	CLONING ARTIFACT	UNP Q9Y3E7
C	8	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
C	27	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	67	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	84	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	89	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	91	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	111	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	114	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	127	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	134	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	135	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	157	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
C	163	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	5	GLY	-	CLONING ARTIFACT	UNP Q9Y3E7
D	6	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
D	7	MSE	-	CLONING ARTIFACT	UNP Q9Y3E7
D	8	ALA	-	CLONING ARTIFACT	UNP Q9Y3E7
D	27	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	67	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	84	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	89	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	91	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	111	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	114	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	127	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	134	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	135	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7
D	157	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7

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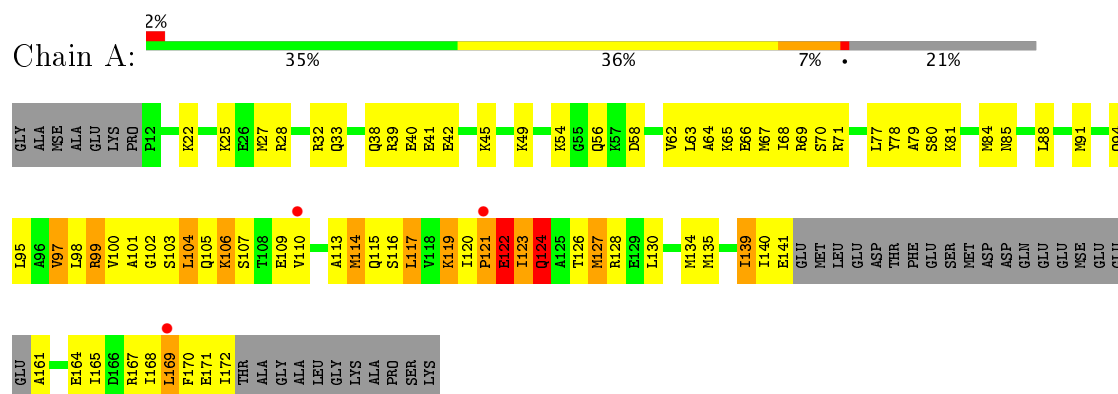
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Chain	Residue	Modelled	Actual	Comment	Reference
D	163	MSE	MET	MODIFIED RESIDUE	UNP Q9Y3E7

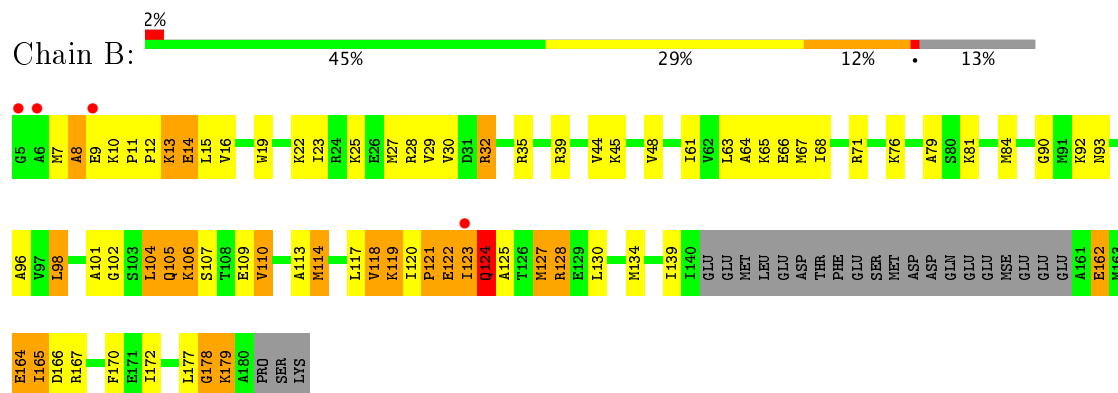
3 Residue-property plots [i](#)

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.

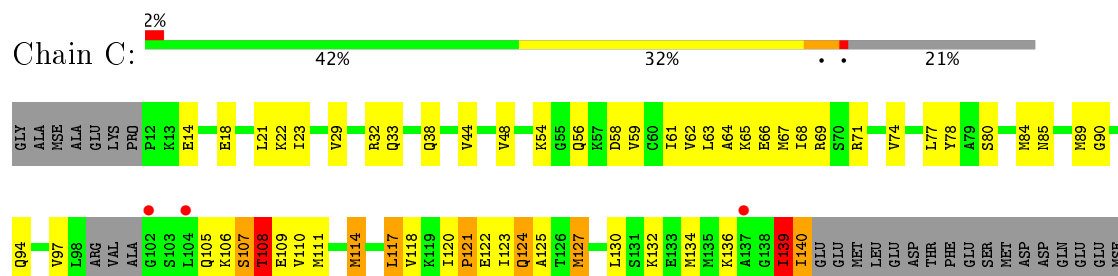
• Molecule 1: Charged multivesicular body protein 3



• Molecule 1: Charged multivesicular body protein 3



• Molecule 1: Charged multivesicular body protein 3



GLU	GLU	GLU	A161	E162	M163	E164	I165	D166	R167	L168	L169	F170	E171	I172	T173	G175	A174	A176	LEU	GLY	LYS	ALA	PRO	SER	LYS
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● Molecule 1: Charged multivesicular body protein 3

Chain D:

45%

39%

7%

9%

R5	E9	P12	M19	K22	K25	R28	N29	V30	I34	Q38	V44	K45	V48	K49	G55	Q56	K57	I61	N62	L63	A64	K65	E66	N67	L68	S75	K76	A79	S80	R81	A82	R83	N84	N89	G90	N91	K92	N93	Q94	L95	A96	N97	L98
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A101	G102	S103	L104	Q105	K106	V110	M111	K112	A113	M114	Q115	S116	L117	V118	K119	I120	P121	E122	I123	Q124	A125	T126	M127	R128	E129	L130	S131	M134	G138	I139	I140	E141	GLU	MET	LEU	GLU	ASP	THR	PHE	GLU	SER	MET	ASP	ASP	GLN	GLU	GLU	M157	E158	E159	E160	A161	E162	M163	E164	I165
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------

D166	R167	I168	L169	F170	E171	I172	T173	A174	A176	A180	P181	SER	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	33.58Å 72.57Å 89.23Å 68.68° 83.61° 76.70°	Depositor
Resolution (Å)	20.00 – 2.80 33.09 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-2.80) 84.9 (33.09-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.259 , 0.301 0.251 , 0.291	Depositor DCC
R_{free} test set	909 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4746	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.63% 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	0.72	0/1128	0.74	0/1476
1	B	0.72	0/1213	0.76	0/1589
1	C	0.71	0/1116	0.70	0/1459
1	D	0.73	0/1265	0.74	0/1659
All	All	0.72	0/4722	0.74	0/6183

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	1134	0	1232	78	0
1	B	1219	0	1325	78	0
1	C	1123	0	1218	68	0
1	D	1270	0	1365	68	0
All	All	4746	0	5140	273	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 28.

The worst 5 of 273 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:D:169:LEU:O	1:D:173:THR:HG22	1.37	1.20
1:C:33:GLN:HE22	1:C:122:GLU:HG2	1.16	1.09
1:C:33:GLN:NE2	1:C:122:GLU:HG2	1.74	1.00
1:D:160:GLU:HB3	1:D:163:MSE:HE2	1.40	1.00
1:C:71:ARG:NH2	1:D:101:ALA:HB2	1.77	0.99

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	138/179 (77%)	118 (86%)	12 (9%)	8 (6%)	2	5
1	B	152/179 (85%)	121 (80%)	20 (13%)	11 (7%)	1	3
1	C	136/179 (76%)	108 (79%)	16 (12%)	12 (9%)	1	2
1	D	158/179 (88%)	143 (90%)	11 (7%)	4 (2%)	6	22
All	All	584/716 (82%)	490 (84%)	59 (10%)	35 (6%)	2	5

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PRO
1	A	122	GLU
1	B	8	ALA
1	B	122	GLU
1	B	124	GLN

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	126/142 (89%)	112 (89%)	14 (11%)	7	21
1	B	132/142 (93%)	118 (89%)	14 (11%)	8	23
1	C	124/142 (87%)	112 (90%)	12 (10%)	9	27
1	D	138/142 (97%)	124 (90%)	14 (10%)	9	25
All	All	520/568 (92%)	466 (90%)	54 (10%)	8	24

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	162	GLU
1	C	105	GLN
1	D	157	MSE
1	B	164	GLU
1	B	179	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	GLN
1	B	94	GLN
1	D	83	HIS
1	A	124	GLN
1	D	17	ASN

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 ⓘ

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	131/179 (73%)	0.02	3 (2%) 61 51	23, 56, 91, 93	0
1	B	144/179 (80%)	0.08	4 (2%) 53 43	38, 58, 82, 90	0
1	C	131/179 (73%)	0.04	3 (2%) 61 51	34, 61, 92, 98	0
1	D	149/179 (83%)	-0.08	0 100 100	29, 55, 71, 82	0
All	All	555/716 (77%)	0.02	10 (1%) 69 60	23, 58, 88, 98	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	137	ALA	4.2
1	B	9	GLU	3.1
1	A	110	VAL	2.5
1	A	121	PRO	2.4
1	B	5	GLY	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.