



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 08:02 AM BST

PDB ID : 6XY6
Title : Structural insight into sheep-pox virus mediated inhibition of apoptosis
Authors : Suraweera, C.D.; Hinds, M.G.; Kvensakul, M.
Deposited on : 2020-01-29
Resolution : 2.91 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

<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
Xtrriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

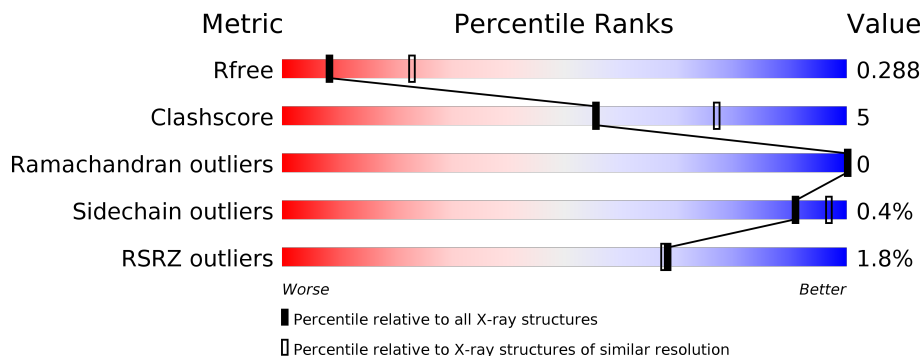
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	150	 3% 78% 12% 10%
1	G	150	 2% 73% 17% 10%
2	B	28	 4% 79% 18%
2	D	28	 4% 82% 18%
2	F	28	 4% 68% 21% 11%
2	H	28	 4% 68% 18% 14%

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Mol	Chain	Length	Quality of chain
2	J	28	
2	L	28	
2	N	28	
2	P	28	
3	C	145	
3	E	145	
3	I	145	
3	K	145	
3	M	145	
3	O	145	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 20675 atoms, of which 10355 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 anti-apoptotic membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	135	2240	706	1129	182	218	5	0	0	0
1	G	135	2262	708	1148	182	218	6	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP A0A3F2YKH3
A	-3	PRO	-	expression tag	UNP A0A3F2YKH3
A	-2	LEU	-	expression tag	UNP A0A3F2YKH3
A	-1	GLY	-	expression tag	UNP A0A3F2YKH3
A	0	SER	-	expression tag	UNP A0A3F2YKH3
G	-4	GLY	-	expression tag	UNP A0A3F2YKH3
G	-3	PRO	-	expression tag	UNP A0A3F2YKH3
G	-2	LEU	-	expression tag	UNP A0A3F2YKH3
G	-1	GLY	-	expression tag	UNP A0A3F2YKH3
G	0	SER	-	expression tag	UNP A0A3F2YKH3

- Molecule 2 is a protein called Apoptosis regulator BAX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	23	344	105	167	30	40	2	0	0	0
2	D	23	349	105	172	31	39	2	0	0	0
2	F	25	368	116	174	33	43	2	0	0	0
2	H	24	376	112	190	32	40	2	0	0	0
2	J	25	388	116	194	33	43	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	L	25	Total	C	H	N	O	S	0	0	0
			388	116	194	33	43	2			
2	N	22	Total	C	H	N	O	S	0	0	0
			337	100	169	29	37	2			
2	P	21	Total	C	H	N	O	S	0	0	0
			320	95	160	28	36	1			

- Molecule 3 is a protein called anti-apoptotic membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
3	C	138	Total	C	H	N	O	S	0	0	0
			2301	722	1164	188	222	5			
3	E	133	Total	C	H	N	O	S	0	0	0
			2210	694	1117	178	216	5			
3	I	133	Total	C	H	N	O	S	0	0	0
			2174	694	1081	178	216	5			
3	K	134	Total	C	H	N	O	S	0	0	0
			2232	700	1130	180	217	5			
3	M	133	Total	C	H	N	O	S	0	1	0
			2218	696	1122	178	216	6			
3	O	132	Total	C	H	N	O	S	0	0	0
			2129	690	1044	176	214	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
4	A	4	Total	O	0	0
			4	4		
4	B	2	Total	O	0	0
			2	2		
4	C	5	Total	O	0	0
			5	5		
4	E	6	Total	O	0	0
			6	6		
4	G	3	Total	O	0	0
			3	3		
4	H	1	Total	O	0	0
			1	1		
4	I	4	Total	O	0	0
			4	4		
4	K	1	Total	O	0	0
			1	1		

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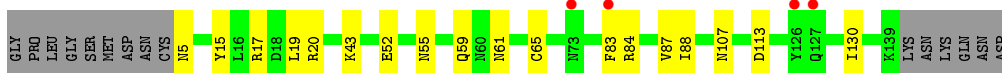
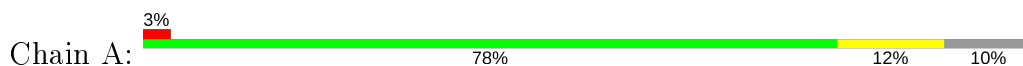
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O 1 1	0	0
4	M	6	Total O 6 6	0	0
4	O	6	Total O 6 6	0	0

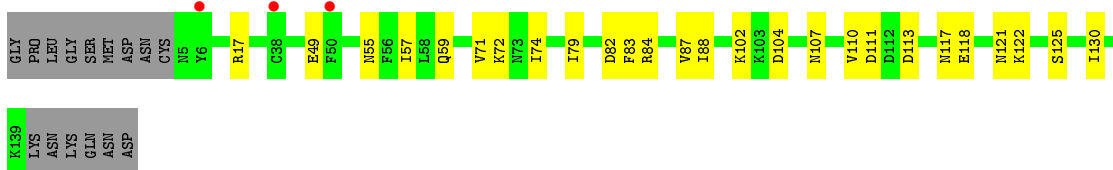
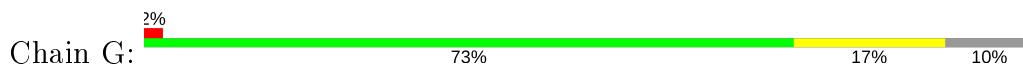
3 Residue-property plots [i](#)

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.

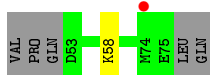
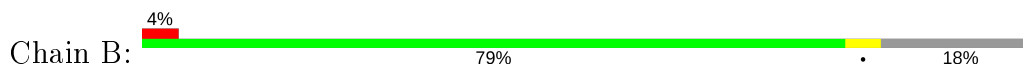
- Molecule 1: anti-apoptotic membrane protein



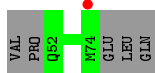
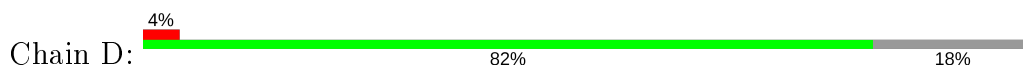
- Molecule 1: anti-apoptotic membrane protein



- Molecule 2: Apoptosis regulator BAX

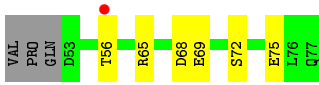


- Molecule 2: Apoptosis regulator BAX

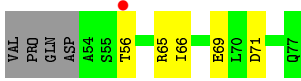


- Molecule 2: Apoptosis regulator BAX





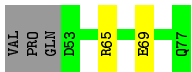
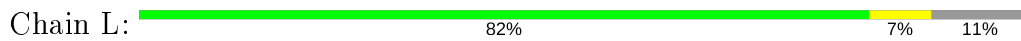
- Molecule 2: Apoptosis regulator BAX



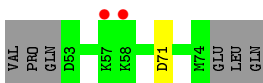
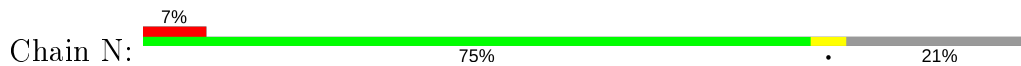
- Molecule 2: Apoptosis regulator BAX



- Molecule 2: Apoptosis regulator BAX



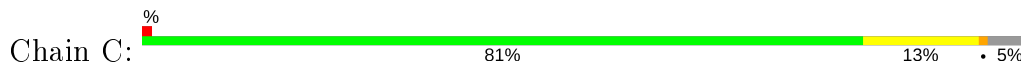
- Molecule 2: Apoptosis regulator BAX



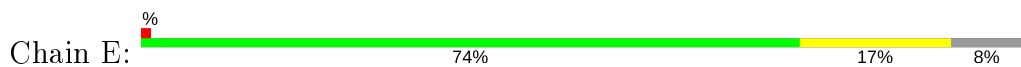
- Molecule 2: Apoptosis regulator BAX

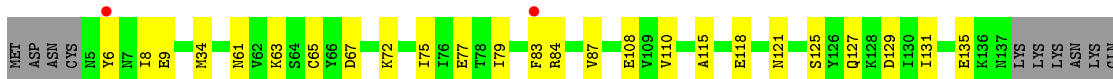


- Molecule 3: anti-apoptotic membrane protein



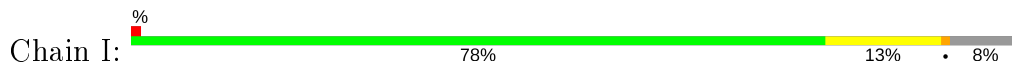
- Molecule 3: anti-apoptotic membrane protein



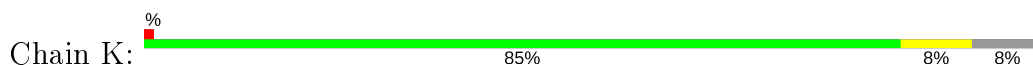


ASN
ASP

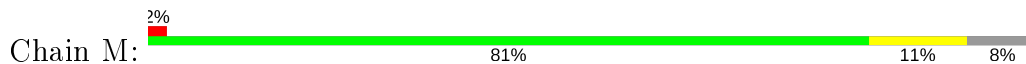
● Molecule 3: anti-apoptotic membrane protein



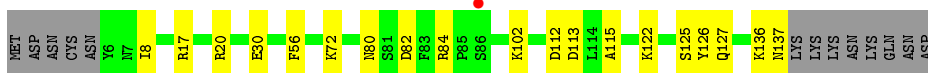
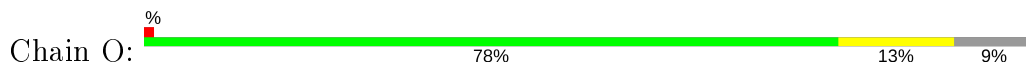
● Molecule 3: anti-apoptotic membrane protein



● Molecule 3: anti-apoptotic membrane protein



● Molecule 3: anti-apoptotic membrane protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.28Å 78.56Å 107.77Å 90.00° 110.97° 90.00°	Depositor
Resolution (Å)	46.82 – 2.91 46.82 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.82-2.91) 99.3 (46.82-2.91)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.239 , 0.288 0.239 , 0.288	Depositor DCC
R_{free} test set	1784 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtrriage
Anisotropy	0.288	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20675	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.11% 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	0.27	0/1121	0.44	0/1508
1	G	0.27	0/1127	0.43	0/1516
2	B	0.26	0/176	0.39	0/232
2	D	0.24	0/176	0.42	0/232
2	F	0.25	0/193	0.44	0/255
2	H	0.25	0/185	0.43	0/244
2	J	0.23	0/193	0.46	0/255
2	L	0.25	0/193	0.40	0/255
2	N	0.25	0/167	0.39	0/220
2	P	0.26	0/159	0.41	0/210
3	C	0.27	0/1147	0.43	0/1541
3	E	0.27	0/1103	0.45	0/1486
3	I	0.26	0/1103	0.42	0/1486
3	K	0.28	0/1112	0.44	0/1497
3	M	0.28	0/1109	0.46	0/1494
3	O	0.27	0/1095	0.44	0/1475
All	All	0.27	0/10359	0.43	0/13906

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	1111	1129	1143	13	0
1	G	1114	1148	1148	18	0
2	B	177	167	175	1	0
2	D	177	172	177	0	0
2	F	194	174	194	5	0
2	H	186	190	190	4	0
2	J	194	194	194	6	0
2	L	194	194	194	1	0
2	N	168	169	169	1	0
2	P	160	160	160	4	0
3	C	1137	1164	1175	13	0
3	E	1093	1117	1117	15	0
3	I	1093	1081	1117	14	0
3	K	1102	1130	1130	6	0
3	M	1096	1122	1122	12	0
3	O	1085	1044	1111	15	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	5	0	0	0	0
4	E	6	0	0	0	0
4	G	3	0	0	0	0
4	H	1	0	0	0	0
4	I	4	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	6	0	0	0	0
4	O	6	0	0	0	0
All	All	10320	10355	10516	107	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 5.

The worst 5 of 107 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)
2:L:65:ARG:NH1	2:L:69:GLU:OE2	1.97	0.97
2:F:65:ARG:NH1	2:F:69:GLU:OE2	2.08	0.87
3:O:102:LYS:NZ	3:O:112:ASP:OD1	2.08	0.86
2:H:65:ARG:NH2	2:H:69:GLU:OE1	2.15	0.79
3:M:84:ARG:NH1	2:N:71:ASP:OD2	2.16	0.78

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	133/150 (89%)	133 (100%)	0	0	100	100
1	G	134/150 (89%)	133 (99%)	1 (1%)	0	100	100
2	B	21/28 (75%)	20 (95%)	1 (5%)	0	100	100
2	D	21/28 (75%)	20 (95%)	1 (5%)	0	100	100
2	F	23/28 (82%)	23 (100%)	0	0	100	100
2	H	22/28 (79%)	22 (100%)	0	0	100	100
2	J	23/28 (82%)	23 (100%)	0	0	100	100
2	L	23/28 (82%)	22 (96%)	1 (4%)	0	100	100
2	N	20/28 (71%)	20 (100%)	0	0	100	100
2	P	19/28 (68%)	18 (95%)	1 (5%)	0	100	100
3	C	136/145 (94%)	135 (99%)	1 (1%)	0	100	100
3	E	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
3	I	131/145 (90%)	130 (99%)	1 (1%)	0	100	100
3	K	132/145 (91%)	132 (100%)	0	0	100	100
3	M	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
3	O	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
All	All	1231/1394 (88%)	1221 (99%)	10 (1%)	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	133/146 (91%)	133 (100%)	0	100	100
1	G	134/146 (92%)	134 (100%)	0	100	100
2	B	21/26 (81%)	21 (100%)	0	100	100
2	D	21/26 (81%)	21 (100%)	0	100	100
2	F	23/26 (88%)	23 (100%)	0	100	100
2	H	22/26 (85%)	22 (100%)	0	100	100
2	J	23/26 (88%)	23 (100%)	0	100	100
2	L	23/26 (88%)	23 (100%)	0	100	100
2	N	20/26 (77%)	20 (100%)	0	100	100
2	P	19/26 (73%)	19 (100%)	0	100	100
3	C	136/143 (95%)	135 (99%)	1 (1%)	84	95
3	E	131/143 (92%)	129 (98%)	2 (2%)	65	86
3	I	131/143 (92%)	130 (99%)	1 (1%)	81	93
3	K	132/143 (92%)	131 (99%)	1 (1%)	81	93
3	M	132/143 (92%)	132 (100%)	0	100	100
3	O	130/143 (91%)	130 (100%)	0	100	100
All	All	1231/1358 (91%)	1226 (100%)	5 (0%)	91	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	128	LYS
3	E	125	SER
3	E	129	ASP
3	I	83	PHE
3	K	125	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	51	ASN
3	E	121	ASN
3	I	137	ASN
3	K	59	GLN
3	O	80	ASN

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 [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	135/150 (90%)	0.28	4 (2%) 50 46	47, 64, 89, 108	0
1	G	135/150 (90%)	0.25	3 (2%) 62 60	41, 63, 86, 94	0
2	B	23/28 (82%)	0.30	1 (4%) 35 32	66, 81, 103, 109	0
2	D	23/28 (82%)	0.46	1 (4%) 35 32	61, 78, 99, 106	0
2	F	25/28 (89%)	0.33	1 (4%) 38 35	68, 86, 101, 122	0
2	H	24/28 (85%)	0.03	1 (4%) 36 33	65, 79, 99, 108	0
2	J	25/28 (89%)	0.29	0 100 100	54, 69, 94, 100	0
2	L	25/28 (89%)	0.26	0 100 100	65, 78, 95, 100	0
2	N	22/28 (78%)	0.46	2 (9%) 9 7	66, 81, 98, 103	0
2	P	21/28 (75%)	0.22	0 100 100	66, 84, 94, 97	0
3	C	138/145 (95%)	0.25	2 (1%) 75 76	42, 62, 84, 103	0
3	E	133/145 (91%)	0.28	2 (1%) 73 73	41, 68, 86, 97	0
3	I	133/145 (91%)	0.29	1 (0%) 86 86	36, 56, 76, 89	0
3	K	134/145 (92%)	0.26	1 (0%) 87 88	38, 56, 78, 95	0
3	M	133/145 (91%)	0.38	3 (2%) 60 59	45, 66, 90, 98	0
3	O	132/145 (91%)	0.33	1 (0%) 86 86	46, 67, 88, 95	0
All	All	1261/1394 (90%)	0.29	23 (1%) 68 67	36, 65, 91, 122	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	74	MET	3.4
3	C	5	ASN	3.1
3	M	134	VAL	2.9
1	A	127	GLN	2.9
3	O	86	SER	2.9

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.