



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:21 AM GMT

PDB ID : 3EBJ
Title : Crystal structure of an avian influenza virus protein
Authors : Yuan, P.; Bartlam, M.; Lou, Z.; Chen, S.; Rao, Z.; Liu, Y.
Deposited on : 2008-08-27
Resolution : 2.20 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

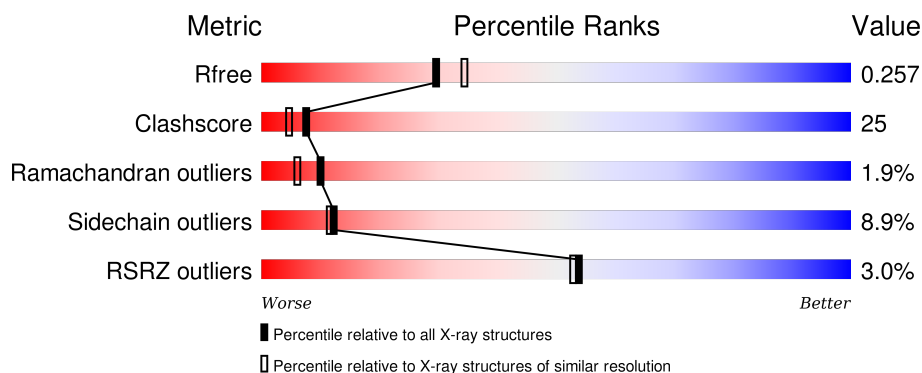
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	259	<div> <div>2%</div> <div> <div></div> <div>39%</div> <div>24%</div> <div>•</div> <div>32%</div> </div> </div>
1	B	259	<div> <div>2%</div> <div> <div></div> <div>39%</div> <div>24%</div> <div>• •</div> <div>32%</div> </div> </div>
1	C	259	<div> <div>2%</div> <div> <div></div> <div>40%</div> <div>23%</div> <div>• •</div> <div>32%</div> </div> </div>
1	D	259	<div> <div>2%</div> <div> <div></div> <div>32%</div> <div>31%</div> <div>5%</div> <div>32%</div> </div> </div>

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	MG	A	999	-	-	-	X
2	MG	C	999	-	-	-	X
2	MG	D	999	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5925 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1446	914	249	272	11			
1	B	175	Total	C	N	O	S	0	0	0
			1458	923	250	274	11			
1	C	176	Total	C	N	O	S	0	0	0
			1456	920	252	273	11			
1	D	175	Total	C	N	O	S	0	0	0
			1446	914	249	272	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
A	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
A	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
A	201	ILE	VAL	ENGINEERED	UNP Q9Q0U9
B	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
B	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
B	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
B	201	ILE	VAL	ENGINEERED	UNP Q9Q0U9
C	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
C	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
C	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
C	201	ILE	VAL	ENGINEERED	UNP Q9Q0U9
D	-2	LEU	-	EXPRESSION TAG	UNP Q9Q0U9
D	-1	GLY	-	EXPRESSION TAG	UNP Q9Q0U9
D	0	SER	-	EXPRESSION TAG	UNP Q9Q0U9
D	201	ILE	VAL	ENGINEERED	UNP Q9Q0U9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

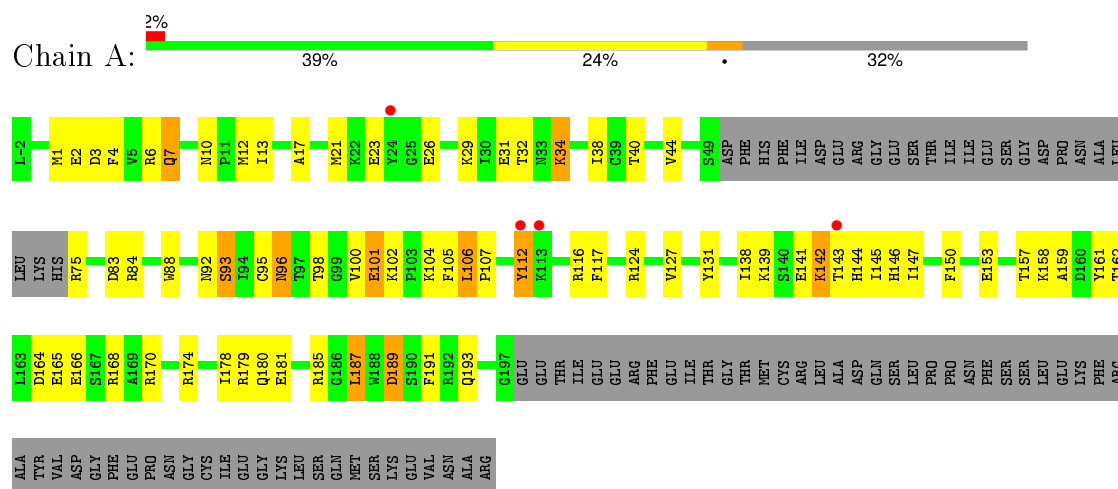
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	40	Total O 40 40	0	0
3	B	28	Total O 28 28	0	0
3	C	22	Total O 22 22	0	0
3	D	25	Total O 25 25	0	0

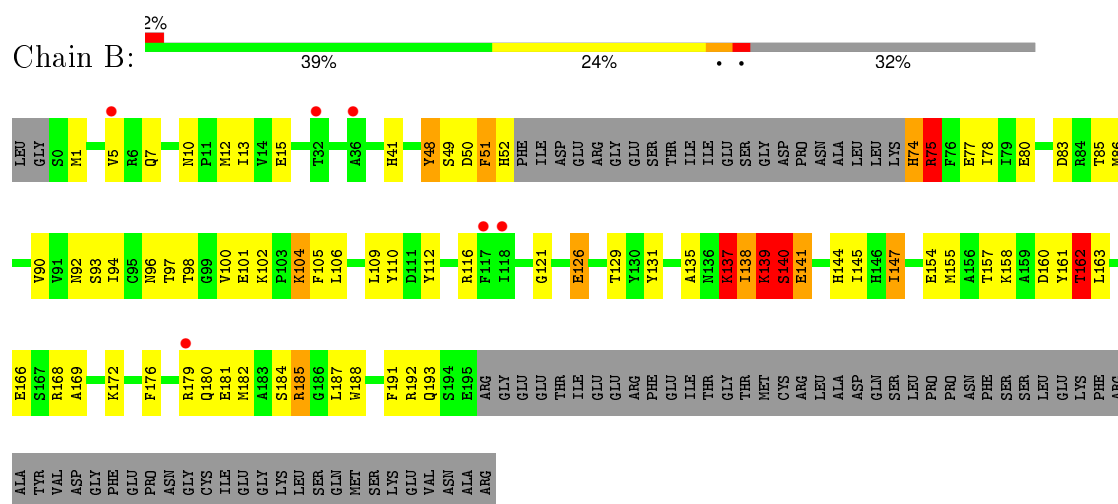
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

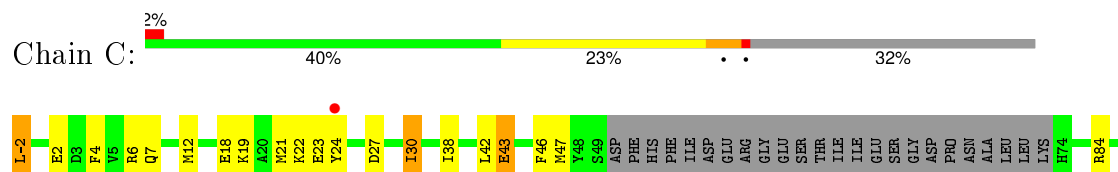
• Molecule 1: Polymerase acidic protein

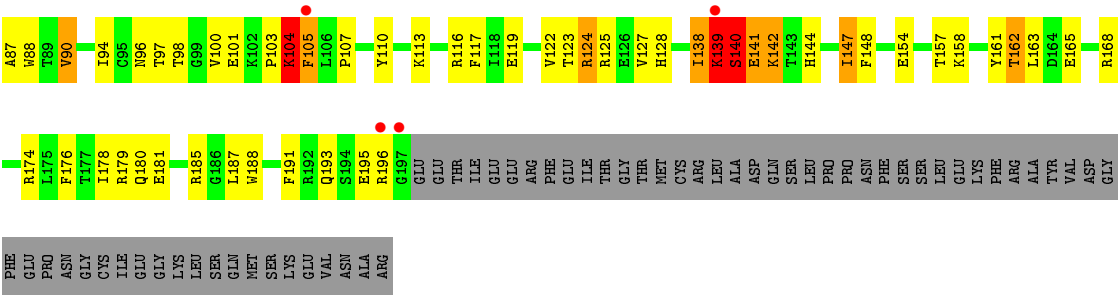


• Molecule 1: Polymerase acidic protein

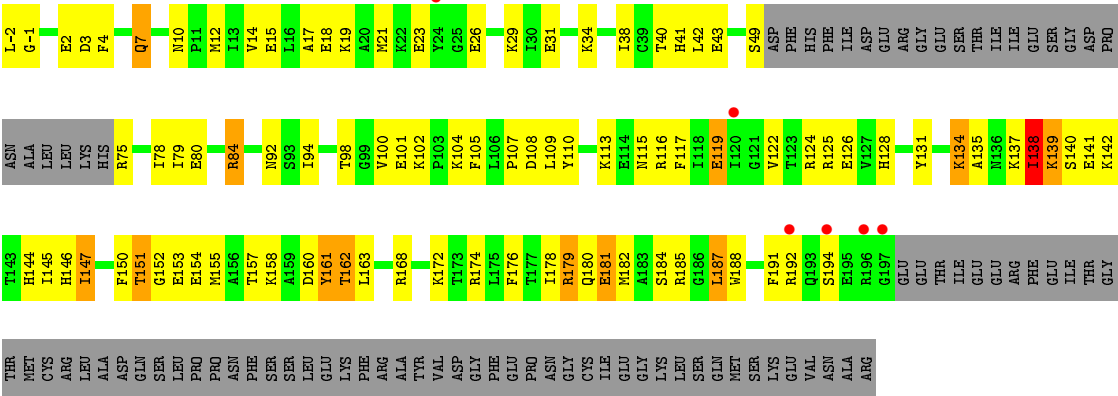
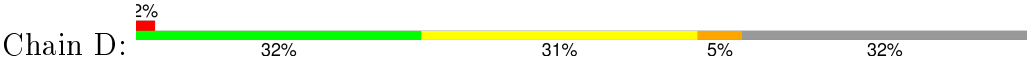


• Molecule 1: Polymerase acidic protein





● Molecule 1: Polymerase acidic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.05Å 59.83Å 67.17Å 96.55° 96.82° 109.51°	Depositor
Resolution (Å)	50.00 – 2.20 21.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 76.5 (21.93-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.19Å)	Xtriage
Refinement program	CNS1.2	Depositor
R, R_{free}	0.231 , 0.252 0.234 , 0.257	Depositor DCC
R_{free} test set	1487 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33576 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5925	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.66% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

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	1.02	13/1474 (0.9%)	0.77	2/1977 (0.1%)
1	B	1.41	33/1489 (2.2%)	0.93	8/1999 (0.4%)
1	C	1.09	21/1485 (1.4%)	0.87	6/1992 (0.3%)
1	D	0.45	0/1474	0.64	0/1977
All	All	1.05	67/5922 (1.1%)	0.81	16/7945 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	PHE	CD2-CE2	-15.77	1.07	1.39
1	B	51	PHE	CE2-CZ	-15.09	1.08	1.37
1	A	105	PHE	CE2-CZ	-13.37	1.11	1.37
1	A	105	PHE	CD1-CE1	-13.28	1.12	1.39
1	C	138	ILE	CB-CG2	-11.26	1.18	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	ASP	CB-CG-OD2	9.04	126.44	118.30
1	C	138	ILE	CG1-CB-CG2	-9.01	91.58	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	SER	N-CA-C	8.24	133.24	111.00
1	B	160	ASP	CB-CG-OD1	-7.84	111.25	118.30
1	B	50	ASP	CB-CG-OD1	7.54	125.09	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	48	TYR	Mainchain
1	D	161	TYR	Sidechain

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	1446	0	1422	63	0
1	B	1458	0	1418	66	0
1	C	1456	0	1429	79	0
1	D	1446	0	1422	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	40	0	0	3	0
3	B	28	0	0	0	0
3	C	22	0	0	5	0
3	D	25	0	0	3	0
All	All	5925	0	5691	292	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 25.

The worst 5 of 292 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:C:139:LYS:CG	1:C:140:SER:HA	1.41	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LYS:HG2	1:C:140:SER:CA	1.59	1.30
1:C:139:LYS:CG	1:C:140:SER:CA	2.12	1.21
1:C:139:LYS:CB	1:C:140:SER:HA	1.75	1.16
1:C:104:LYS:NZ	1:C:139:LYS:HB2	1.66	1.08

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	171/259 (66%)	159 (93%)	11 (6%)	1 (1%)	30	29
1	B	171/259 (66%)	159 (93%)	8 (5%)	4 (2%)	8	4
1	C	172/259 (66%)	155 (90%)	13 (8%)	4 (2%)	8	4
1	D	171/259 (66%)	154 (90%)	13 (8%)	4 (2%)	8	4
All	All	685/1036 (66%)	627 (92%)	45 (7%)	13 (2%)	10	6

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	THR
1	B	139	LYS
1	B	140	SER
1	C	139	LYS
1	C	162	THR

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	157/231 (68%)	146 (93%)	11 (7%)	19	19
1	B	159/231 (69%)	146 (92%)	13 (8%)	14	13
1	C	158/231 (68%)	141 (89%)	17 (11%)	8	7
1	D	157/231 (68%)	142 (90%)	15 (10%)	10	9
All	All	631/924 (68%)	575 (91%)	56 (9%)	12	11

5 of 56 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	7	GLN
1	C	100	VAL
1	D	162	THR
1	C	12	MET
1	C	30	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	74	HIS
1	B	92	ASN
1	D	10	ASN
1	B	41	HIS
1	D	92	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

Of 4 ligands modelled in this entry, 4 are 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

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	175/259 (67%)	-0.00	4 (2%) 64 63	25, 45, 62, 69	0
1	B	175/259 (67%)	0.15	6 (3%) 49 47	28, 47, 66, 81	0
1	C	176/259 (67%)	0.22	5 (2%) 56 55	31, 52, 68, 83	0
1	D	175/259 (67%)	0.39	6 (3%) 49 47	33, 52, 75, 94	0
All	All	701/1036 (67%)	0.19	21 (2%) 54 53	25, 48, 69, 94	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	GLY	10.4
1	C	197	GLY	5.4
1	D	196	ARG	4.3
1	A	112	TYR	4.1
1	C	105	PHE	3.6

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(\AA^2)	Q<0.9
2	MG	D	999	1/1	0.72	0.52	10.76	67,67,67,67	0
2	MG	A	999	1/1	0.95	0.25	3.64	45,45,45,45	0
2	MG	C	999	1/1	0.84	0.22	2.57	46,46,46,46	0
2	MG	B	999	1/1	0.89	0.20	1.20	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.