



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 04:48 am GMT

PDB ID : 2AS5  
Title : Structure of the DNA binding domains of NFAT and FOXP2 bound specifically to DNA.  
Authors : Wu, Y.; Stroud, J.C.; Borde, M.; Bates, D.L.; Guo, L.; Han, A.; Rao, A.; Chen, L.  
Deposited on : 2005-08-22  
Resolution : 2.70 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](mailto: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.

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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	:	trunk28620
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)	:	recalc28949

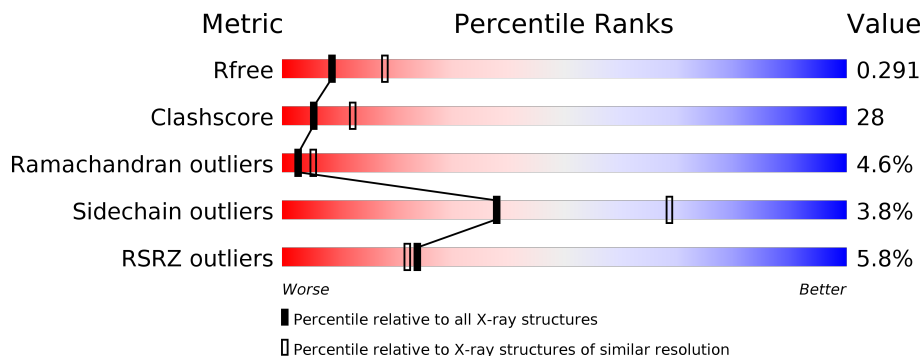
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	21	<div> <div>19%</div> <div>76%</div> <div>5%</div> </div>
1	C	21	<div> <div>19%</div> <div>81%</div> </div>
2	B	21	<div> <div>10%</div> <div>86%</div> <div>5%</div> </div>
2	D	21	<div> <div>24%</div> <div>67%</div> <div>10%</div> </div>
3	M	287	<div> <div>6%</div> <div>52%</div> <div>43%</div> <div>5%</div> </div>
3	N	287	<div> <div>9%</div> <div>55%</div> <div>40%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	93	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>55%</div><div>34%</div><div>11%</div></div></div>
4	G	93	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>61%</div><div>27%</div><div>11%</div></div></div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7821 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 DNA chain called 5'-D(TP\*TP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*GP\*TP\*TP\*TP\*CP\*AP\*TP\*AP\*GP\*)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	21	Total	C	N	O	P	0	0	0
			431	209	76	126	20			
1	C	21	Total	C	N	O	P	0	0	0
			431	209	76	126	20			

- Molecule 2 is a DNA chain called 5'-D(AP\*AP\*CP\*TP\*AP\*TP\*GP\*AP\*AP\*AP\*CP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	21	Total	C	N	O	P	0	0	0
			424	206	76	122	20			
2	D	21	Total	C	N	O	P	0	0	0
			424	206	76	122	20			

- Molecule 3 is a protein called Nuclear factor of activated T-cells, cytoplasmic 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	287	Total	C	N	O	S	0	0	0
			2290	1437	417	427	9			
3	M	287	Total	C	N	O	S	0	0	0
			2290	1437	417	427	9			

- Molecule 4 is a protein called Forkhead box protein P2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	83	Total	C	N	O	S	0	0	0
			707	453	132	120	2			
4	G	83	Total	C	N	O	S	0	0	0
			707	453	132	120	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	502	ILE	ASP	ENGINEERED	UNP O15409
G	502	ILE	ASP	ENGINEERED	UNP O15409

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

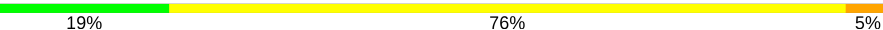
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	17	Total O 17 17	0	0
6	B	10	Total O 10 10	0	0
6	C	19	Total O 19 19	0	0
6	D	10	Total O 10 10	0	0
6	F	8	Total O 8 8	0	0
6	G	8	Total O 8 8	0	0
6	M	18	Total O 18 18	0	0
6	N	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 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.

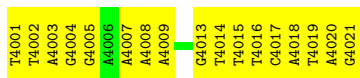
- Molecule 1: 5'-D(TP\*TP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*GP\*TP\*TP\*TP\*CP\*AP\*TP\*AP\*GP\*)-3'

Chain A: 



- Molecule 1: 5'-D(TP\*TP\*AP\*GP\*GP\*AP\*AP\*AP\*AP\*TP\*TP\*TP\*GP\*TP\*TP\*TP\*CP\*AP\*TP\*AP\*GP\*)-3'

Chain C: 




- Molecule 2: 5'-D(AP\*AP\*CP\*TP\*AP\*TP\*GP\*AP\*AP\*AP\*CP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*)-3'

Chain B: 



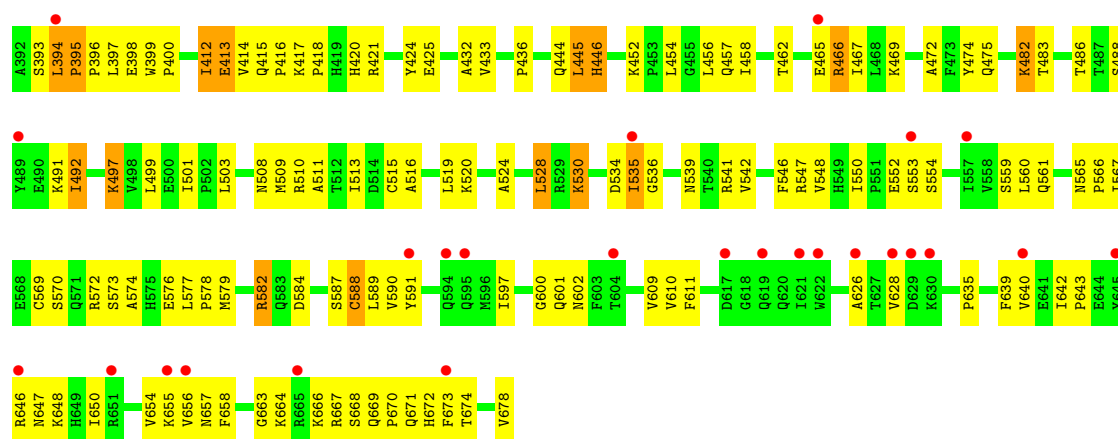
- Molecule 2: 5'-D(AP\*AP\*CP\*TP\*AP\*TP\*GP\*AP\*AP\*AP\*CP\*AP\*AP\*AP\*TP\*TP\*TP\*TP\*CP\*CP\*TP\*)-3'

Chain D: 

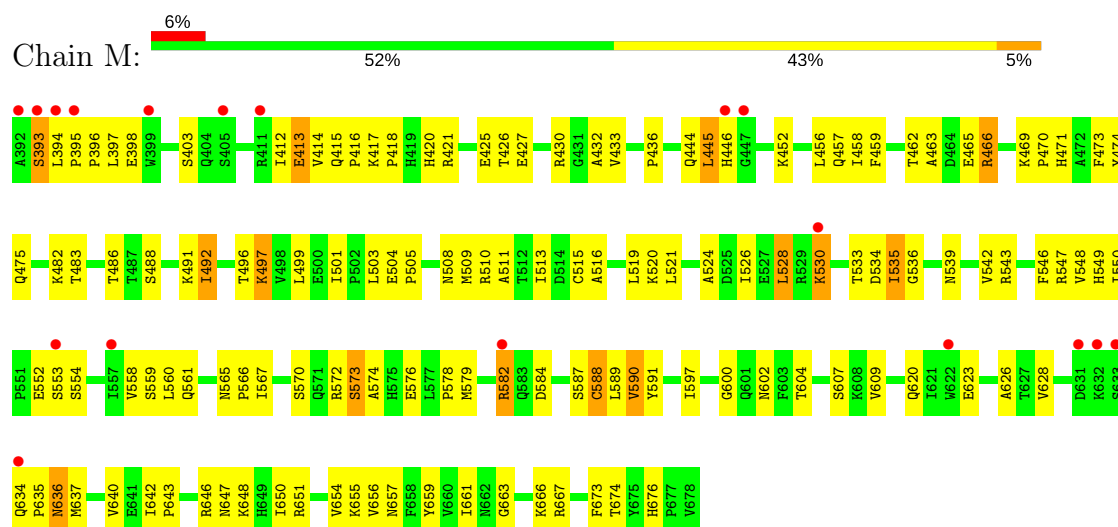


- Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2

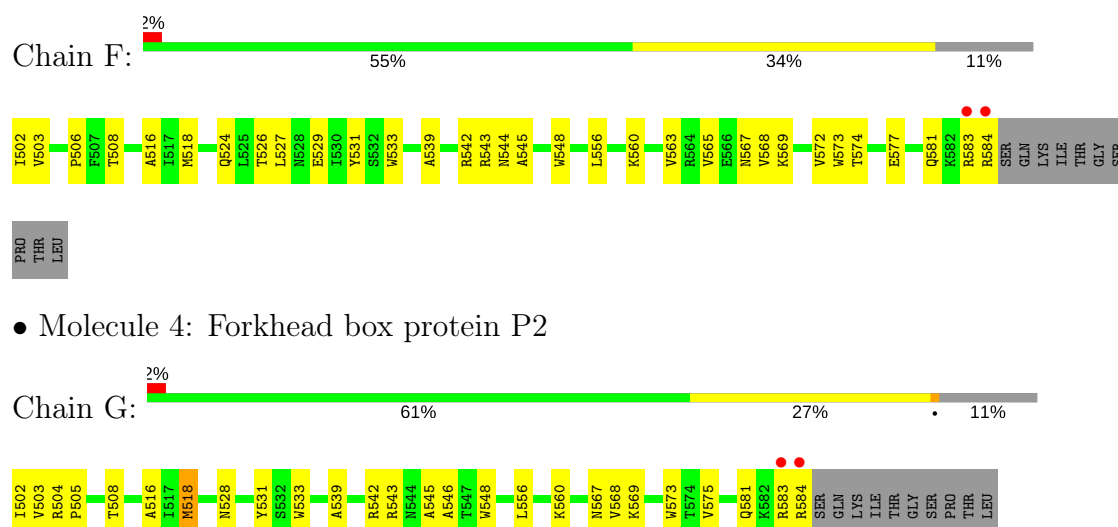
Chain N: 



• Molecule 3: Nuclear factor of activated T-cells, cytoplasmic 2



• Molecule 4: Forkhead box protein P2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.45Å 157.45Å 67.67Å 90.00° 118.67° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 39.32 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 94.8 (39.32-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.238 , 0.287 0.246 , 0.291	Depositor DCC
$R_{free}$ test set	3160 reflections (9.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	1.186	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 28.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.056 for -h-l,k,h 0.056 for l,k,-h-l 0.200 for h,-k,-h-l 0.067 for -h-l,-k,l 0.066 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7821	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.83	0/483	0.92	0/745
1	C	0.68	0/483	0.86	0/745
2	B	0.75	0/475	0.83	0/730
2	D	0.65	0/475	0.84	0/730
3	M	0.38	0/2341	0.64	0/3168
3	N	0.42	0/2341	0.69	1/3168 (0.0%)
4	F	0.49	0/725	0.69	0/982
4	G	0.50	0/725	0.65	0/982
All	All	0.51	0/8048	0.72	1/11250 (0.0%)

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	A	0	1
2	B	0	2
2	D	0	2
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	394	LEU	C-N-CD	-11.79	94.67	120.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4005	DG	Sidechain
2	B	5016	DT	Sidechain
2	B	5018	DT	Sidechain
2	D	5014	DA	Sidechain
2	D	5016	DT	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	431	0	242	37	0
1	C	431	0	242	39	0
2	B	424	0	240	32	0
2	D	424	0	240	24	0
3	M	2290	0	2297	131	0
3	N	2290	0	2297	124	0
4	F	707	0	704	27	0
4	G	707	0	704	20	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	A	17	0	0	1	0
6	B	10	0	0	1	0
6	C	19	0	0	1	0
6	D	10	0	0	0	0
6	F	8	0	0	1	0
6	G	8	0	0	0	0
6	M	18	0	0	4	0
6	N	25	0	0	11	0
All	All	7821	0	6966	417	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 417 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)
3:N:578:PRO:HG2	6:N:114:HOH:O	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4016:DT:H2''	1:A:4017:DC:H5''	1.47	0.97
2:B:5010:DA:H2''	2:B:5011:DC:H5'	1.45	0.97
2:D:5010:DA:H2''	2:D:5011:DC:H5'	1.47	0.94
1:A:4014:DT:H2''	1:A:4015:DT:H5''	1.51	0.90

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	
3	M	285/287 (99%)	238 (84%)	33 (12%)	14 (5%)	2	5
3	N	285/287 (99%)	229 (80%)	38 (13%)	18 (6%)	1	2
4	F	81/93 (87%)	73 (90%)	7 (9%)	1 (1%)	15	37
4	G	81/93 (87%)	71 (88%)	9 (11%)	1 (1%)	15	37
All	All	732/760 (96%)	611 (84%)	87 (12%)	34 (5%)	3	5

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	N	395	PRO
3	N	413	GLU
3	N	466	ARG
3	N	482	LYS
3	N	513	ILE

### 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	
3	M	256/256 (100%)	247 (96%)	9 (4%)	41	72
3	N	256/256 (100%)	247 (96%)	9 (4%)	41	72
4	F	75/84 (89%)	71 (95%)	4 (5%)	26	54
4	G	75/84 (89%)	72 (96%)	3 (4%)	36	67
All	All	662/680 (97%)	637 (96%)	25 (4%)	38	68

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	497	LYS
3	M	534	ASP
4	G	560	LYS
3	M	508	ASN
3	M	539	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	404	GLN
3	M	423	HIS
4	F	567	ASN
3	M	420	HIS
3	M	440	HIS

### 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 2 ligands modelled in this entry, 2 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9	
1	A	21/21 (100%)	-0.62	0	100	100	19, 38, 67, 74	0
1	C	21/21 (100%)	-0.40	0	100	100	28, 45, 67, 73	0
2	B	21/21 (100%)	-0.65	0	100	100	18, 40, 56, 64	0
2	D	21/21 (100%)	-0.46	0	100	100	27, 48, 62, 69	0
3	M	287/287 (100%)	0.39	18 (6%)	21	19	30, 70, 111, 135	0
3	N	287/287 (100%)	0.59	26 (9%)	10	7	12, 69, 115, 130	0
4	F	83/93 (89%)	0.00	2 (2%)	59	60	22, 46, 92, 137	0
4	G	83/93 (89%)	0.03	2 (2%)	59	60	20, 42, 93, 141	0
All	All	824/844 (97%)	0.29	48 (5%)	24	22	12, 63, 111, 141	0

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	646	ARG	7.2
3	N	629	ASP	6.8
4	F	584	ARG	6.3
3	M	392	ALA	6.2
3	N	617	ASP	4.9

### 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 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
5	MG	G	202	1/1	0.82	0.14	-0.83	56,56,56,56	0
5	MG	F	201	1/1	0.97	0.09	-3.12	59,59,59,59	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.