wwPDB X-ray Structure Validation Summary Report (i)

Dec 16, 2023 – 11:11 AM EST

PDB ID	:	2O1T
Title	:	Structure of Middle plus C-terminal domains (M+C) of GRP94
Authors	:	Dollins, D.E.; Warren, J.J.; Immormino, R.M.; Gewirth, D.T.
Deposited on	:	2006-11-29
Resolution	:	3.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

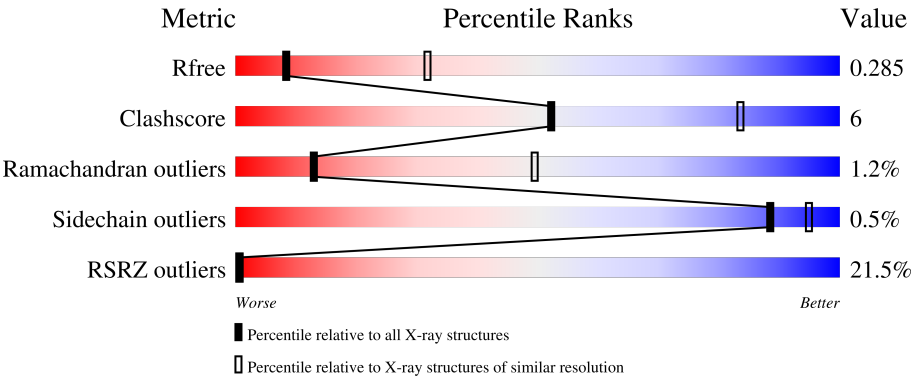
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 of 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 <=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	450	12% 81% 10% • 8%
1	B	450	24% 82% 10% 8%
1	C	450	12% 82% 9% 8%
1	D	450	18% 79% 12% 8%
1	E	450	12% 78% 13% 8%

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Mol	Chain	Length	Quality of chain
1	F	450	12% 76% 15% 8%
1	G	450	22% 80% 12% 8%
1	H	450	32% 79% 12% 8%
1	I	450	40% 82% 10% 8%
1	J	450	14% 80% 12% 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 33009 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 Endoplasmin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	B	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	C	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	D	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	E	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	F	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	G	413	Total	C	N	O	S	0	0	0
			3300	2101	548	638	13			
1	H	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	I	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			
1	J	413	Total	C	N	O	S	0	0	0
			3301	2101	549	638	13			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	MET	-	expression tag	UNP P41148
A	317	GLY	-	expression tag	UNP P41148
A	318	SER	-	expression tag	UNP P41148
A	319	SER	-	expression tag	UNP P41148
A	320	HIS	-	expression tag	UNP P41148
A	321	HIS	-	expression tag	UNP P41148
A	322	HIS	-	expression tag	UNP P41148
A	323	HIS	-	expression tag	UNP P41148
A	324	HIS	-	expression tag	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
A	325	HIS	-	expression tag	UNP P41148
A	326	SER	-	expression tag	UNP P41148
A	327	SER	-	expression tag	UNP P41148
A	328	GLY	-	expression tag	UNP P41148
A	329	LEU	-	expression tag	UNP P41148
A	330	VAL	-	expression tag	UNP P41148
A	331	PRO	-	expression tag	UNP P41148
A	332	ARG	-	expression tag	UNP P41148
A	333	GLY	-	expression tag	UNP P41148
A	334	SER	-	expression tag	UNP P41148
A	335	HIS	-	expression tag	UNP P41148
B	316	MET	-	expression tag	UNP P41148
B	317	GLY	-	expression tag	UNP P41148
B	318	SER	-	expression tag	UNP P41148
B	319	SER	-	expression tag	UNP P41148
B	320	HIS	-	expression tag	UNP P41148
B	321	HIS	-	expression tag	UNP P41148
B	322	HIS	-	expression tag	UNP P41148
B	323	HIS	-	expression tag	UNP P41148
B	324	HIS	-	expression tag	UNP P41148
B	325	HIS	-	expression tag	UNP P41148
B	326	SER	-	expression tag	UNP P41148
B	327	SER	-	expression tag	UNP P41148
B	328	GLY	-	expression tag	UNP P41148
B	329	LEU	-	expression tag	UNP P41148
B	330	VAL	-	expression tag	UNP P41148
B	331	PRO	-	expression tag	UNP P41148
B	332	ARG	-	expression tag	UNP P41148
B	333	GLY	-	expression tag	UNP P41148
B	334	SER	-	expression tag	UNP P41148
B	335	HIS	-	expression tag	UNP P41148
C	316	MET	-	expression tag	UNP P41148
C	317	GLY	-	expression tag	UNP P41148
C	318	SER	-	expression tag	UNP P41148
C	319	SER	-	expression tag	UNP P41148
C	320	HIS	-	expression tag	UNP P41148
C	321	HIS	-	expression tag	UNP P41148
C	322	HIS	-	expression tag	UNP P41148
C	323	HIS	-	expression tag	UNP P41148
C	324	HIS	-	expression tag	UNP P41148
C	325	HIS	-	expression tag	UNP P41148
C	326	SER	-	expression tag	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
C	327	SER	-	expression tag	UNP P41148
C	328	GLY	-	expression tag	UNP P41148
C	329	LEU	-	expression tag	UNP P41148
C	330	VAL	-	expression tag	UNP P41148
C	331	PRO	-	expression tag	UNP P41148
C	332	ARG	-	expression tag	UNP P41148
C	333	GLY	-	expression tag	UNP P41148
C	334	SER	-	expression tag	UNP P41148
C	335	HIS	-	expression tag	UNP P41148
D	316	MET	-	expression tag	UNP P41148
D	317	GLY	-	expression tag	UNP P41148
D	318	SER	-	expression tag	UNP P41148
D	319	SER	-	expression tag	UNP P41148
D	320	HIS	-	expression tag	UNP P41148
D	321	HIS	-	expression tag	UNP P41148
D	322	HIS	-	expression tag	UNP P41148
D	323	HIS	-	expression tag	UNP P41148
D	324	HIS	-	expression tag	UNP P41148
D	325	HIS	-	expression tag	UNP P41148
D	326	SER	-	expression tag	UNP P41148
D	327	SER	-	expression tag	UNP P41148
D	328	GLY	-	expression tag	UNP P41148
D	329	LEU	-	expression tag	UNP P41148
D	330	VAL	-	expression tag	UNP P41148
D	331	PRO	-	expression tag	UNP P41148
D	332	ARG	-	expression tag	UNP P41148
D	333	GLY	-	expression tag	UNP P41148
D	334	SER	-	expression tag	UNP P41148
D	335	HIS	-	expression tag	UNP P41148
E	316	MET	-	expression tag	UNP P41148
E	317	GLY	-	expression tag	UNP P41148
E	318	SER	-	expression tag	UNP P41148
E	319	SER	-	expression tag	UNP P41148
E	320	HIS	-	expression tag	UNP P41148
E	321	HIS	-	expression tag	UNP P41148
E	322	HIS	-	expression tag	UNP P41148
E	323	HIS	-	expression tag	UNP P41148
E	324	HIS	-	expression tag	UNP P41148
E	325	HIS	-	expression tag	UNP P41148
E	326	SER	-	expression tag	UNP P41148
E	327	SER	-	expression tag	UNP P41148
E	328	GLY	-	expression tag	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
E	329	LEU	-	expression tag	UNP P41148
E	330	VAL	-	expression tag	UNP P41148
E	331	PRO	-	expression tag	UNP P41148
E	332	ARG	-	expression tag	UNP P41148
E	333	GLY	-	expression tag	UNP P41148
E	334	SER	-	expression tag	UNP P41148
E	335	HIS	-	expression tag	UNP P41148
F	316	MET	-	expression tag	UNP P41148
F	317	GLY	-	expression tag	UNP P41148
F	318	SER	-	expression tag	UNP P41148
F	319	SER	-	expression tag	UNP P41148
F	320	HIS	-	expression tag	UNP P41148
F	321	HIS	-	expression tag	UNP P41148
F	322	HIS	-	expression tag	UNP P41148
F	323	HIS	-	expression tag	UNP P41148
F	324	HIS	-	expression tag	UNP P41148
F	325	HIS	-	expression tag	UNP P41148
F	326	SER	-	expression tag	UNP P41148
F	327	SER	-	expression tag	UNP P41148
F	328	GLY	-	expression tag	UNP P41148
F	329	LEU	-	expression tag	UNP P41148
F	330	VAL	-	expression tag	UNP P41148
F	331	PRO	-	expression tag	UNP P41148
F	332	ARG	-	expression tag	UNP P41148
F	333	GLY	-	expression tag	UNP P41148
F	334	SER	-	expression tag	UNP P41148
F	335	HIS	-	expression tag	UNP P41148
G	316	MET	-	expression tag	UNP P41148
G	317	GLY	-	expression tag	UNP P41148
G	318	SER	-	expression tag	UNP P41148
G	319	SER	-	expression tag	UNP P41148
G	320	HIS	-	expression tag	UNP P41148
G	321	HIS	-	expression tag	UNP P41148
G	322	HIS	-	expression tag	UNP P41148
G	323	HIS	-	expression tag	UNP P41148
G	324	HIS	-	expression tag	UNP P41148
G	325	HIS	-	expression tag	UNP P41148
G	326	SER	-	expression tag	UNP P41148
G	327	SER	-	expression tag	UNP P41148
G	328	GLY	-	expression tag	UNP P41148
G	329	LEU	-	expression tag	UNP P41148
G	330	VAL	-	expression tag	UNP P41148

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Chain	Residue	Modelled	Actual	Comment	Reference
G	331	PRO	-	expression tag	UNP P41148
G	332	ARG	-	expression tag	UNP P41148
G	333	GLY	-	expression tag	UNP P41148
G	334	SER	-	expression tag	UNP P41148
G	335	HIS	-	expression tag	UNP P41148
H	316	MET	-	expression tag	UNP P41148
H	317	GLY	-	expression tag	UNP P41148
H	318	SER	-	expression tag	UNP P41148
H	319	SER	-	expression tag	UNP P41148
H	320	HIS	-	expression tag	UNP P41148
H	321	HIS	-	expression tag	UNP P41148
H	322	HIS	-	expression tag	UNP P41148
H	323	HIS	-	expression tag	UNP P41148
H	324	HIS	-	expression tag	UNP P41148
H	325	HIS	-	expression tag	UNP P41148
H	326	SER	-	expression tag	UNP P41148
H	327	SER	-	expression tag	UNP P41148
H	328	GLY	-	expression tag	UNP P41148
H	329	LEU	-	expression tag	UNP P41148
H	330	VAL	-	expression tag	UNP P41148
H	331	PRO	-	expression tag	UNP P41148
H	332	ARG	-	expression tag	UNP P41148
H	333	GLY	-	expression tag	UNP P41148
H	334	SER	-	expression tag	UNP P41148
H	335	HIS	-	expression tag	UNP P41148
I	316	MET	-	expression tag	UNP P41148
I	317	GLY	-	expression tag	UNP P41148
I	318	SER	-	expression tag	UNP P41148
I	319	SER	-	expression tag	UNP P41148
I	320	HIS	-	expression tag	UNP P41148
I	321	HIS	-	expression tag	UNP P41148
I	322	HIS	-	expression tag	UNP P41148
I	323	HIS	-	expression tag	UNP P41148
I	324	HIS	-	expression tag	UNP P41148
I	325	HIS	-	expression tag	UNP P41148
I	326	SER	-	expression tag	UNP P41148
I	327	SER	-	expression tag	UNP P41148
I	328	GLY	-	expression tag	UNP P41148
I	329	LEU	-	expression tag	UNP P41148
I	330	VAL	-	expression tag	UNP P41148
I	331	PRO	-	expression tag	UNP P41148
I	332	ARG	-	expression tag	UNP P41148

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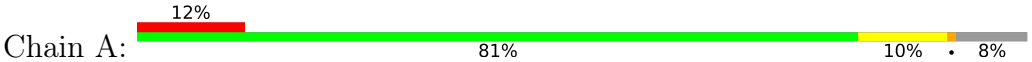
Chain	Residue	Modelled	Actual	Comment	Reference
I	333	GLY	-	expression tag	UNP P41148
I	334	SER	-	expression tag	UNP P41148
I	335	HIS	-	expression tag	UNP P41148
J	316	MET	-	expression tag	UNP P41148
J	317	GLY	-	expression tag	UNP P41148
J	318	SER	-	expression tag	UNP P41148
J	319	SER	-	expression tag	UNP P41148
J	320	HIS	-	expression tag	UNP P41148
J	321	HIS	-	expression tag	UNP P41148
J	322	HIS	-	expression tag	UNP P41148
J	323	HIS	-	expression tag	UNP P41148
J	324	HIS	-	expression tag	UNP P41148
J	325	HIS	-	expression tag	UNP P41148
J	326	SER	-	expression tag	UNP P41148
J	327	SER	-	expression tag	UNP P41148
J	328	GLY	-	expression tag	UNP P41148
J	329	LEU	-	expression tag	UNP P41148
J	330	VAL	-	expression tag	UNP P41148
J	331	PRO	-	expression tag	UNP P41148
J	332	ARG	-	expression tag	UNP P41148
J	333	GLY	-	expression tag	UNP P41148
J	334	SER	-	expression tag	UNP P41148
J	335	HIS	-	expression tag	UNP P41148

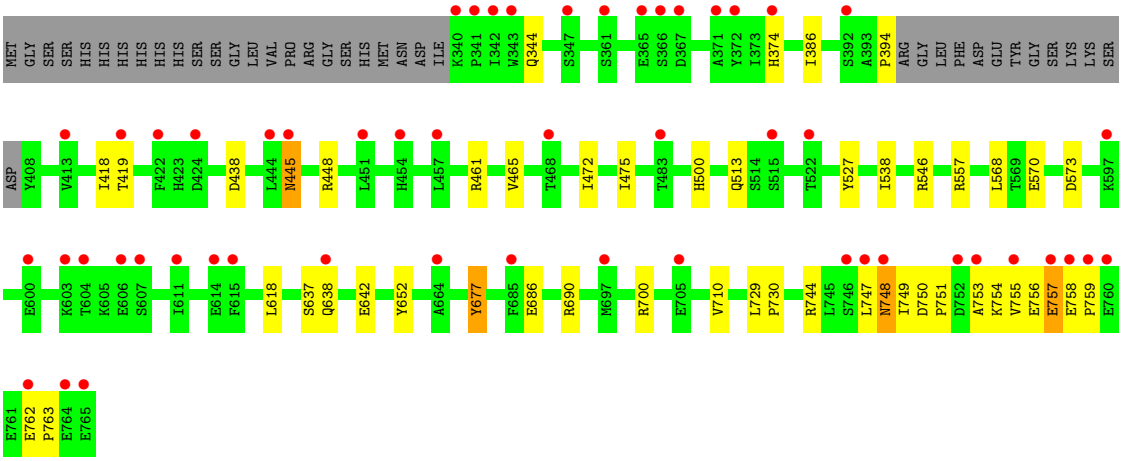
3 Residue-property plots (i)

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: Endoplasmin

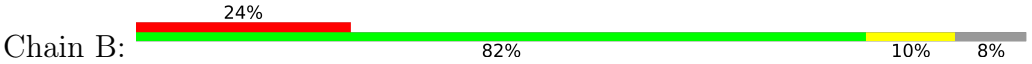
Chain A:

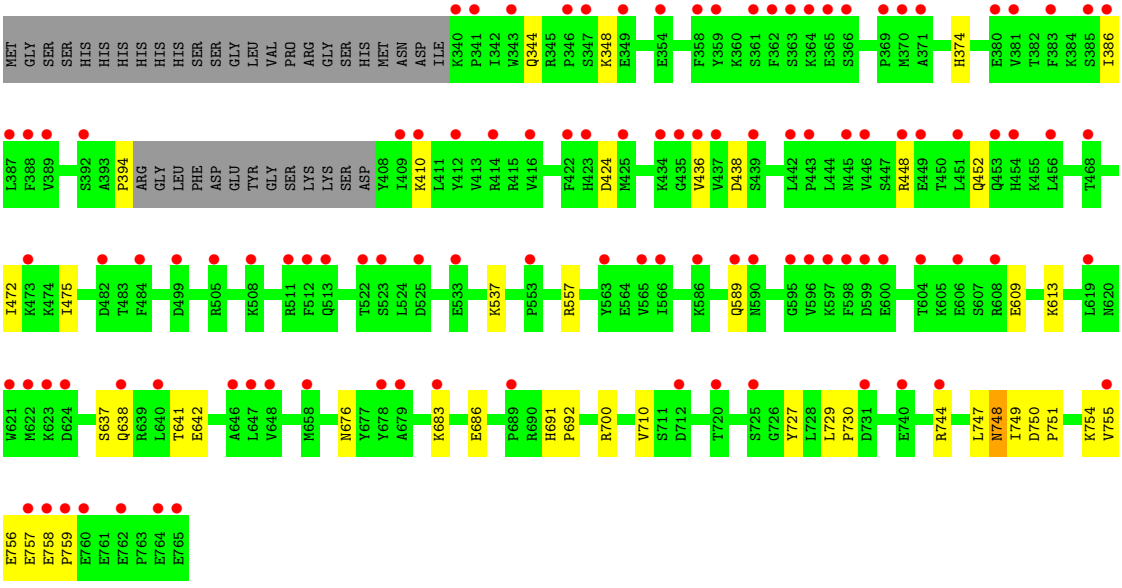




• Molecule 1: Endoplasmin

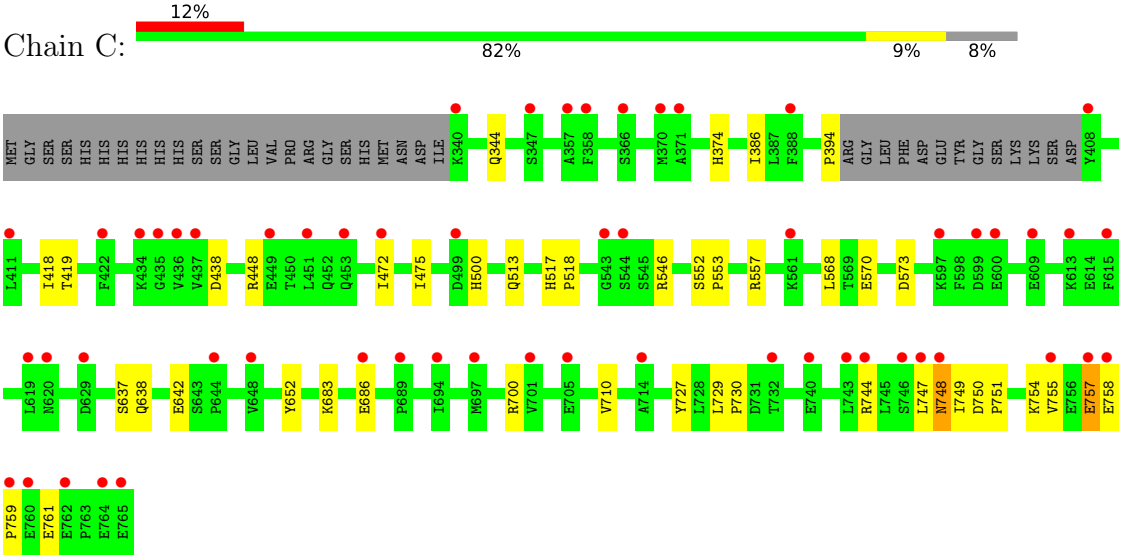
Chain B:





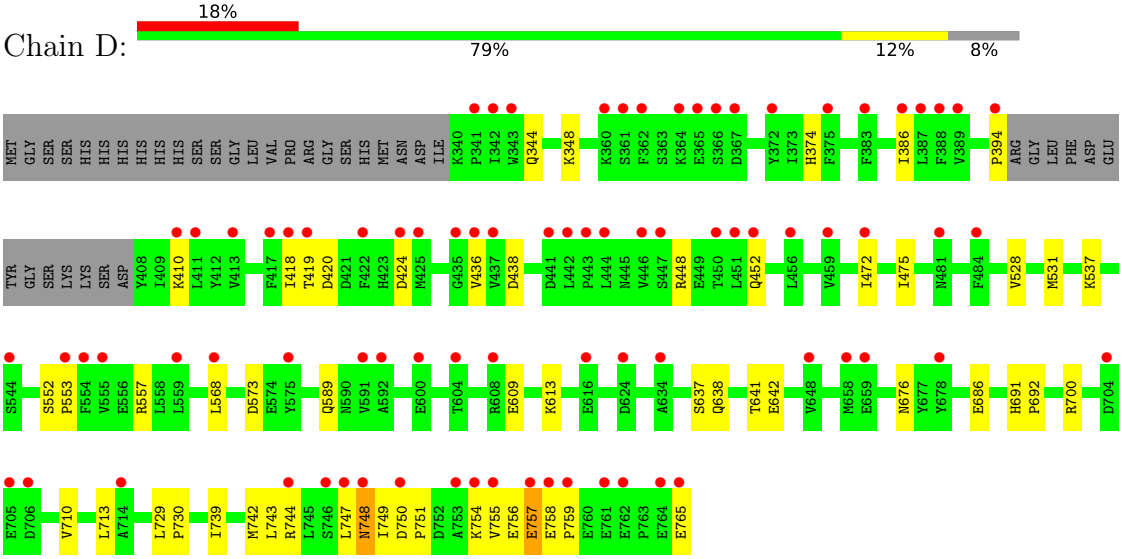
• Molecule 1: Endoplasmin

Chain C:



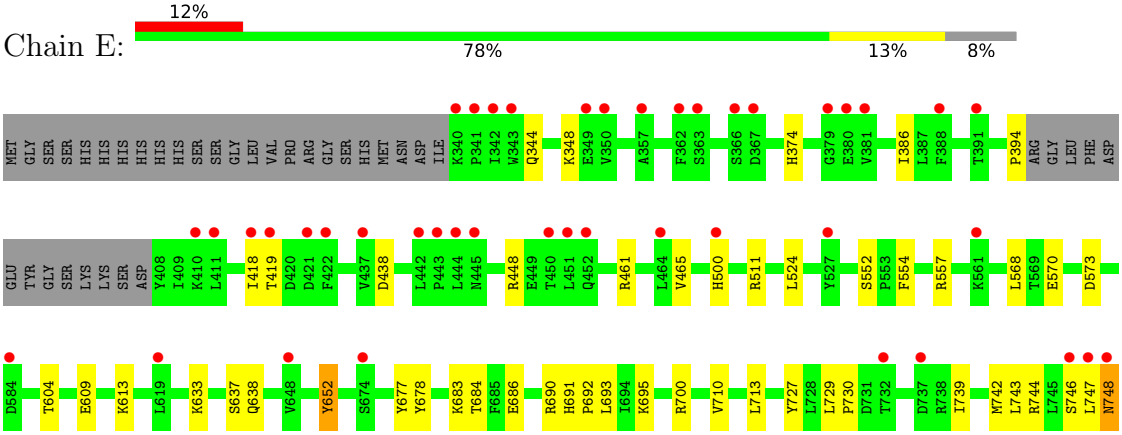
• Molecule 1: Endoplasmin

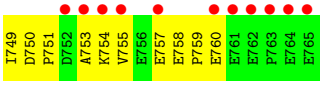
Chain D:



• Molecule 1: Endoplasmin

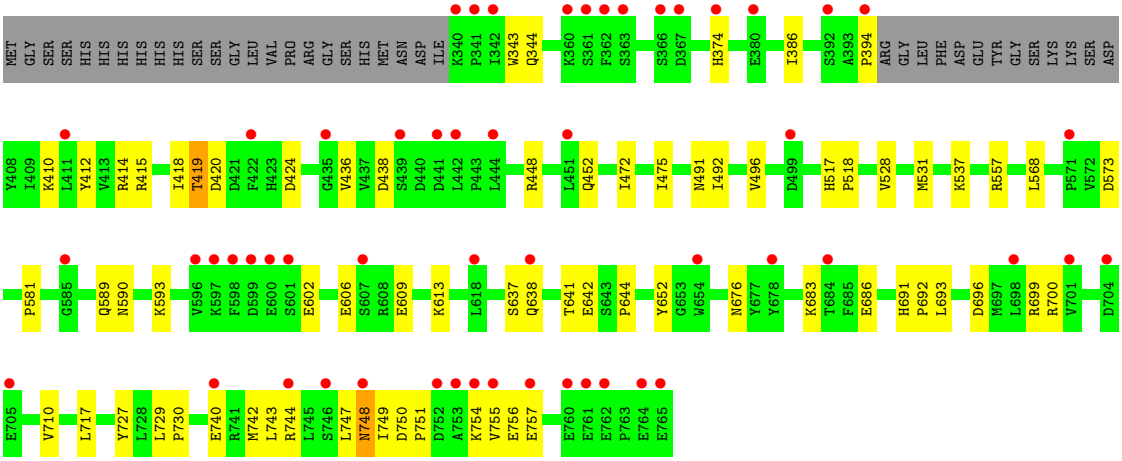
Chain E:





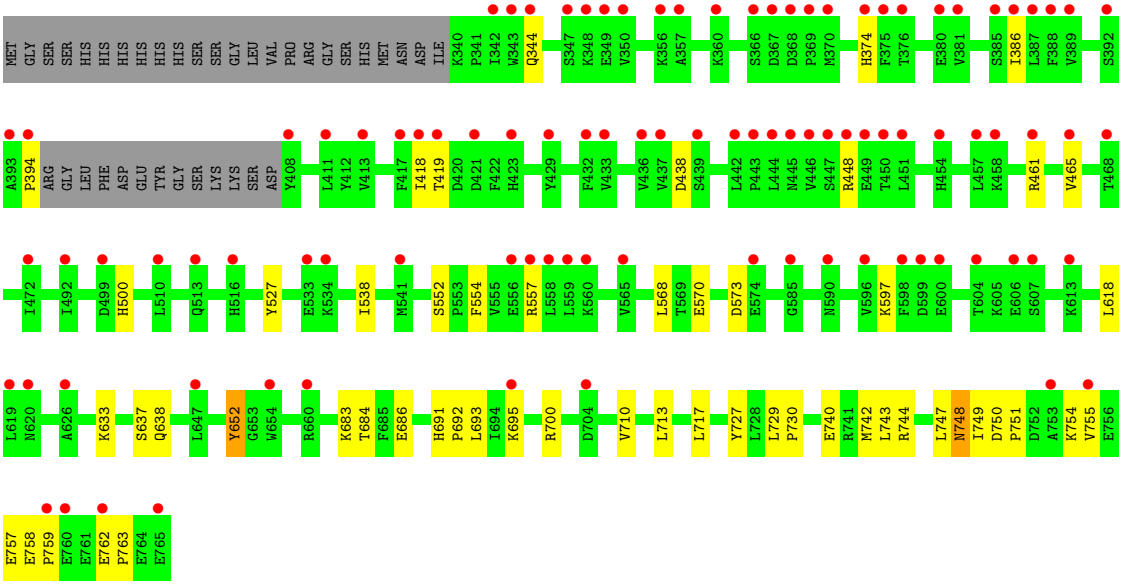
• Molecule 1: Endoplasmin

Chain F:



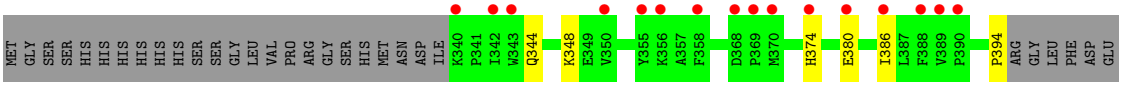
• Molecule 1: Endoplasmin

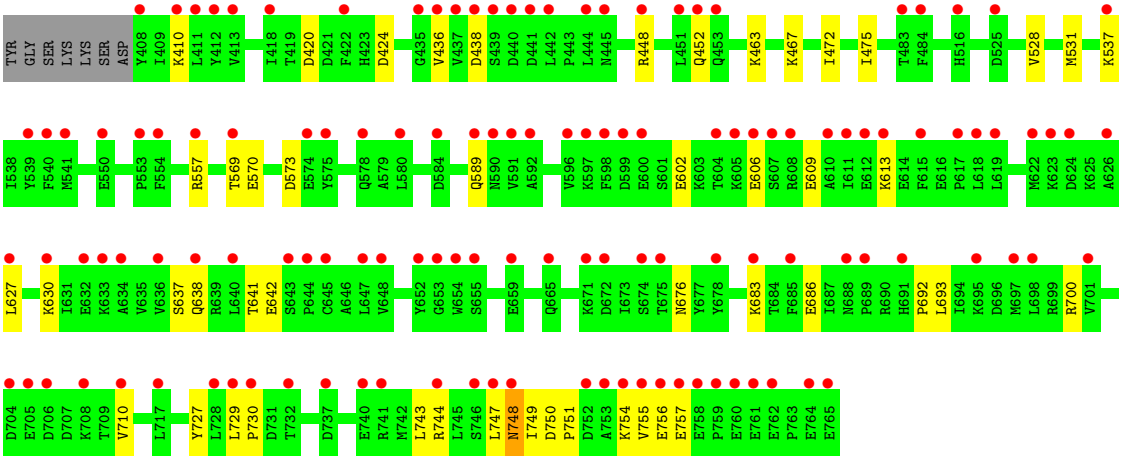
Chain G:



• Molecule 1: Endoplasmin

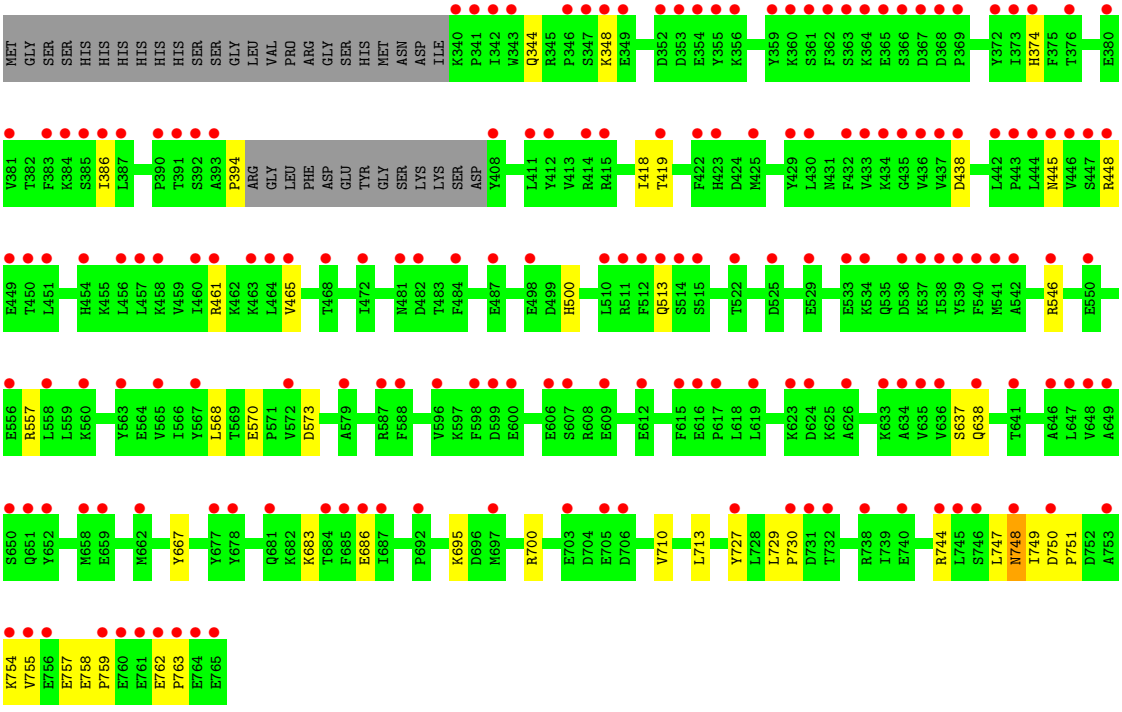
Chain H:





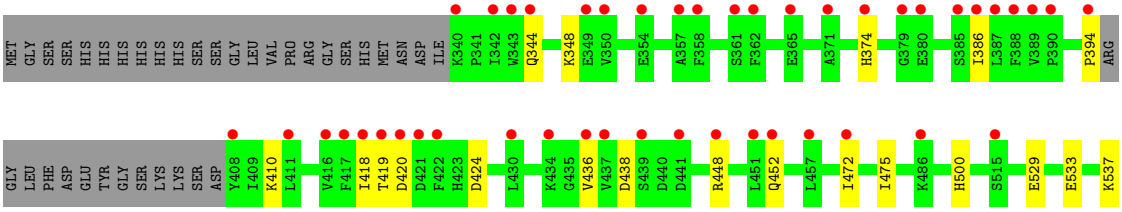
• Molecule 1: Endoplasmin

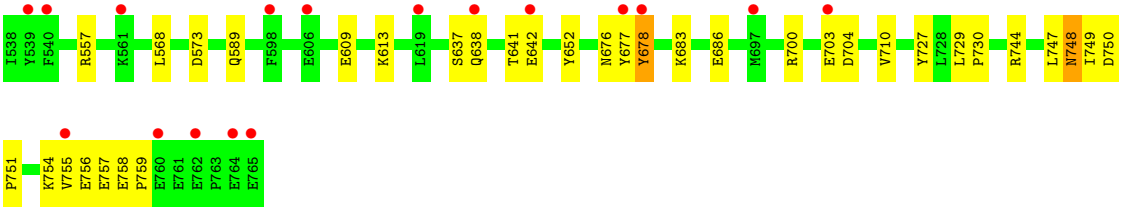
Chain I:



• Molecule 1: Endoplasmin

Chain J:




I538
Y539
F540
R557
K561
L568
D573
Q589
F598
E606
E609
K613
L619
S637
Q638
T641
E642
Y652
N676
Y677
Y678
K683
E686
M697
R700
E703
D704
V710
Y727
L728
L729
P730
R744
L747
N748
I749
D750
P751
K754
V755
E756
E757
E758
P759
E760
E761
E762
P763
E764
E765

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	131.30Å 129.54Å 184.78Å 90.00° 99.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 45.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-3.20) 99.6 (45.52-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.284 , 0.294 0.273 , 0.285	Depositor DCC
R_{free} test set	5021 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	109.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 163.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	33009	wwPDB-VP
Average B, all atoms (Å^2)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	1/3368 (0.0%)	0.68	2/4543 (0.0%)
1	B	0.37	0/3368	0.61	1/4543 (0.0%)
1	C	0.42	0/3368	0.64	1/4543 (0.0%)
1	D	0.43	0/3368	0.64	1/4543 (0.0%)
1	E	0.53	0/3368	0.68	1/4543 (0.0%)
1	F	0.51	0/3368	0.66	1/4543 (0.0%)
1	G	0.43	0/3366	0.65	2/4540 (0.0%)
1	H	0.36	0/3368	0.61	1/4543 (0.0%)
1	I	0.35	0/3368	0.62	1/4543 (0.0%)
1	J	0.48	0/3368	0.65	1/4543 (0.0%)
All	All	0.45	1/33678 (0.0%)	0.64	12/45427 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	677	TYR	CA-CB	-6.37	1.40	1.53

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	394	PRO	N-CA-CB	7.79	112.64	103.30
1	B	394	PRO	N-CA-CB	7.39	112.16	103.30
1	E	394	PRO	N-CA-CB	7.35	112.12	103.30
1	A	394	PRO	N-CA-CB	7.34	112.11	103.30
1	J	394	PRO	N-CA-CB	7.33	112.10	103.30

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	3301	0	3196	44	4
1	B	3301	0	3196	25	0
1	C	3301	0	3196	40	0
1	D	3301	0	3196	51	1
1	E	3301	0	3196	69	1
1	F	3301	0	3196	59	5
1	G	3300	0	3194	47	1
1	H	3301	0	3196	36	0
1	I	3301	0	3196	29	2
1	J	3301	0	3196	62	0
All	All	33009	0	31958	360	7

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 6.

The worst 5 of 360 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:757:GLU:OE2	1:J:677:TYR:HA	1.21	1.31
1:E:500:HIS:CE1	1:J:704:ASP:HB2	1.80	1.16
1:D:759:PRO:HD3	1:E:692:PRO:HD3	1.38	1.05
1:A:754:LYS:HD3	1:E:678:TYR:OH	1.61	1.00
1:C:757:GLU:OE2	1:J:677:TYR:CA	2.11	0.98

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:753:ALA:O	1:G:652:TYR:OH[1_455]	1.62	0.58
1:A:677:TYR:CB	1:D:757:GLU:OE1[2_655]	1.73	0.47
1:F:699:ARG:NH2	1:I:445:ASN:O[1_655]	1.74	0.46
1:A:445:ASN:ND2	1:F:412:TYR:CD1[1_565]	1.91	0.29
1:F:696:ASP:OD2	1:I:445:ASN:ND2[1_655]	2.03	0.17

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	409/450 (91%)	361 (88%)	44 (11%)	4 (1%)	15	54
1	B	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	13	49
1	C	409/450 (91%)	365 (89%)	40 (10%)	4 (1%)	15	54
1	D	409/450 (91%)	368 (90%)	35 (9%)	6 (2%)	10	44
1	E	409/450 (91%)	357 (87%)	47 (12%)	5 (1%)	13	49
1	F	409/450 (91%)	365 (89%)	36 (9%)	8 (2%)	7	38
1	G	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	15	54
1	H	409/450 (91%)	367 (90%)	36 (9%)	6 (2%)	10	44
1	I	409/450 (91%)	363 (89%)	42 (10%)	4 (1%)	15	54
1	J	409/450 (91%)	364 (89%)	40 (10%)	5 (1%)	13	49
All	All	4090/4500 (91%)	3637 (89%)	402 (10%)	51 (1%)	13	49

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	749	ILE
1	C	749	ILE
1	D	757	GLU
1	E	749	ILE
1	I	749	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
1	A	352/410 (86%)	349 (99%)	3 (1%)	78 91
1	B	352/410 (86%)	351 (100%)	1 (0%)	92 96
1	C	352/410 (86%)	350 (99%)	2 (1%)	86 94
1	D	352/410 (86%)	351 (100%)	1 (0%)	92 96
1	E	352/410 (86%)	349 (99%)	3 (1%)	78 91
1	F	352/410 (86%)	350 (99%)	2 (1%)	86 94
1	G	352/410 (86%)	350 (99%)	2 (1%)	86 94
1	H	352/410 (86%)	351 (100%)	1 (0%)	92 96
1	I	352/410 (86%)	351 (100%)	1 (0%)	92 96
1	J	352/410 (86%)	350 (99%)	2 (1%)	86 94
All	All	3520/4100 (86%)	3502 (100%)	18 (0%)	88 95

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	448	ARG
1	J	678	TYR
1	J	448	ARG
1	E	652	TYR
1	G	652	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	452	GLN
1	H	452	GLN
1	J	452	GLN
1	D	452	GLN
1	B	452	GLN

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

6.1 Protein, DNA and RNA chains

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^{th} 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	413/450 (91%)	0.88	53 (12%)	3 2	129, 151, 152, 165	0
1	B	413/450 (91%)	1.52	109 (26%)	0 0	129, 151, 152, 165	0
1	C	413/450 (91%)	0.94	56 (13%)	3 2	129, 151, 152, 165	0
1	D	413/450 (91%)	1.21	82 (19%)	1 1	129, 151, 152, 165	0
1	E	413/450 (91%)	1.01	54 (13%)	3 2	129, 151, 152, 165	0
1	F	413/450 (91%)	0.88	54 (13%)	3 2	129, 151, 152, 165	0
1	G	413/450 (91%)	1.50	98 (23%)	0 0	129, 151, 152, 165	0
1	H	413/450 (91%)	1.82	144 (34%)	0 0	129, 151, 152, 165	0
1	I	413/450 (91%)	2.63	178 (43%)	0 0	129, 151, 152, 165	0
1	J	413/450 (91%)	0.88	62 (15%)	2 1	129, 151, 152, 165	0
All	All	4130/4500 (91%)	1.33	890 (21%)	0 1	129, 151, 153, 165	0

The worst 5 of 890 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	443	PRO	20.1
1	I	437	VAL	19.2
1	I	443	PRO	18.9
1	I	363	SER	17.4
1	D	765	GLU	17.1

6.2 Non-standard residues in protein, DNA, RNA chains

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.