



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:41 PM UTC

PDB ID : 1PQV / pdb_00001pqv
Title : RNA polymerase II-TFIIS complex
Authors : Kettenberger, H.; Armache, K.-J.; Cramer, P.
Deposited on : 2003-06-19
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

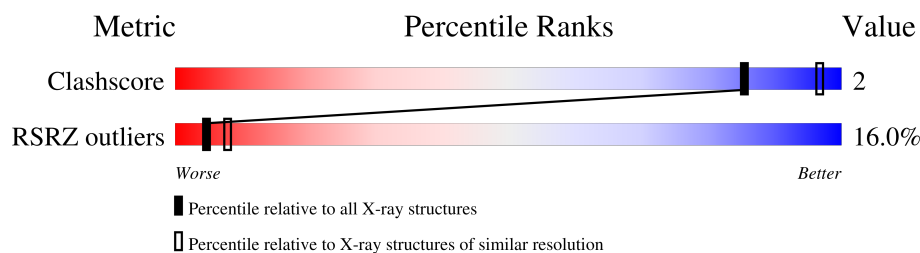
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



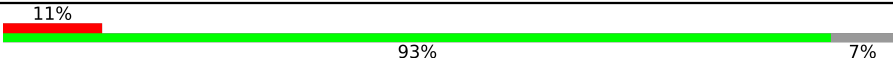
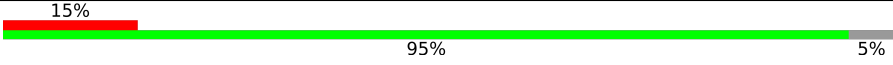
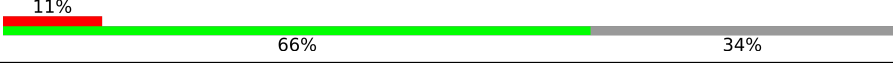
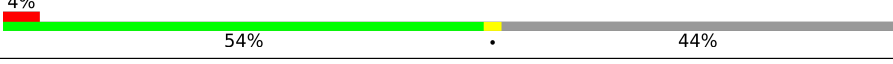
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1012 (3.94-3.66)
RSRZ outliers	180081	1064 (3.96-3.64)

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 $\leq 5\%$. 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	1733	14% 81% 19%
2	B	1224	16% 90% 10%
3	C	318	15% 84% 16%
4	D	221	9% 60% 39%
5	E	215	8% 99% .
6	F	155	11% 54% 46%
7	G	171	23% 99% .
8	H	146	8% 91% 9%
9	I	122	4% 98% .

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Mol	Chain	Length	Quality of chain
10	J	70	
11	K	120	
12	L	70	
13	S	309	

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 4041 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 DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
1	A	1409	Total	C	0	0	1409
			1409	1409			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	B	1103	Total	C	0	0	1103
			1103	1103			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	C	266	Total	C	0	0	266
			266	266			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
4	D	135	Total	C	0	0	135
			135	135			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	86	UNK	-	SEE REMARK 999	UNP P20433
D	87	UNK	-	SEE REMARK 999	UNP P20433
D	88	UNK	-	SEE REMARK 999	UNP P20433
D	89	UNK	-	SEE REMARK 999	UNP P20433
D	90	UNK	-	SEE REMARK 999	UNP P20433
D	91	UNK	-	SEE REMARK 999	UNP P20433
D	92	UNK	-	SEE REMARK 999	UNP P20433
D	93	UNK	-	SEE REMARK 999	UNP P20433

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Chain	Residue	Modelled	Actual	Comment	Reference
D	94	UNK	-	SEE REMARK 999	UNP P20433
D	95	UNK	-	SEE REMARK 999	UNP P20433
D	96	UNK	-	SEE REMARK 999	UNP P20433
D	97	UNK	-	SEE REMARK 999	UNP P20433
D	98	UNK	-	SEE REMARK 999	UNP P20433
D	99	UNK	-	SEE REMARK 999	UNP P20433
D	100	UNK	-	SEE REMARK 999	UNP P20433
D	101	UNK	-	SEE REMARK 999	UNP P20433
D	102	UNK	-	SEE REMARK 999	UNP P20433
D	103	UNK	-	SEE REMARK 999	UNP P20433
D	104	UNK	-	SEE REMARK 999	UNP P20433
D	105	UNK	-	SEE REMARK 999	UNP P20433
D	106	UNK	-	SEE REMARK 999	UNP P20433
D	107	UNK	-	SEE REMARK 999	UNP P20433
D	108	UNK	-	SEE REMARK 999	UNP P20433
D	109	UNK	-	SEE REMARK 999	UNP P20433
D	110	UNK	-	SEE REMARK 999	UNP P20433
D	111	UNK	-	SEE REMARK 999	UNP P20433
D	112	UNK	-	SEE REMARK 999	UNP P20433
D	113	UNK	-	SEE REMARK 999	UNP P20433
D	114	UNK	-	SEE REMARK 999	UNP P20433

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	E	214	Total C 214 214	0	0	214

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	84	Total C 84 84	0	0	84

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	169	Total C 169 169	0	0	169

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
8	H	133	Total	C	0	0	133
			133	133			

- Molecule 9 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
9	I	119	Total	C	0	0	119
			119	119			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
10	J	65	Total	C	0	0	65
			65	65			

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
11	K	114	Total	C	0	0	114
			114	114			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
12	L	46	Total	C	0	0	46
			46	46			

- Molecule 13 is a protein called Transcription elongation factor S-II.

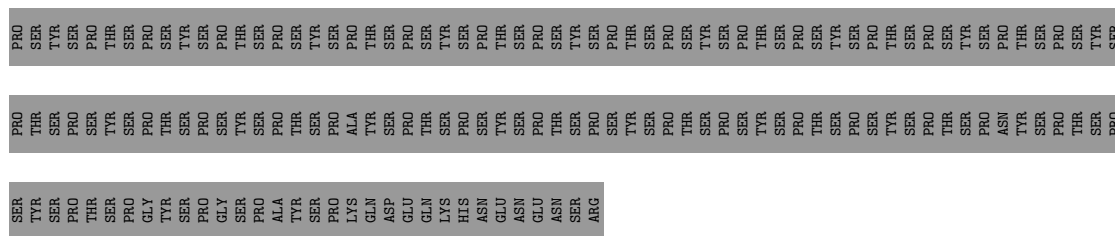
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
13	S	174	Total	C	0	0	174
			174	174			

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

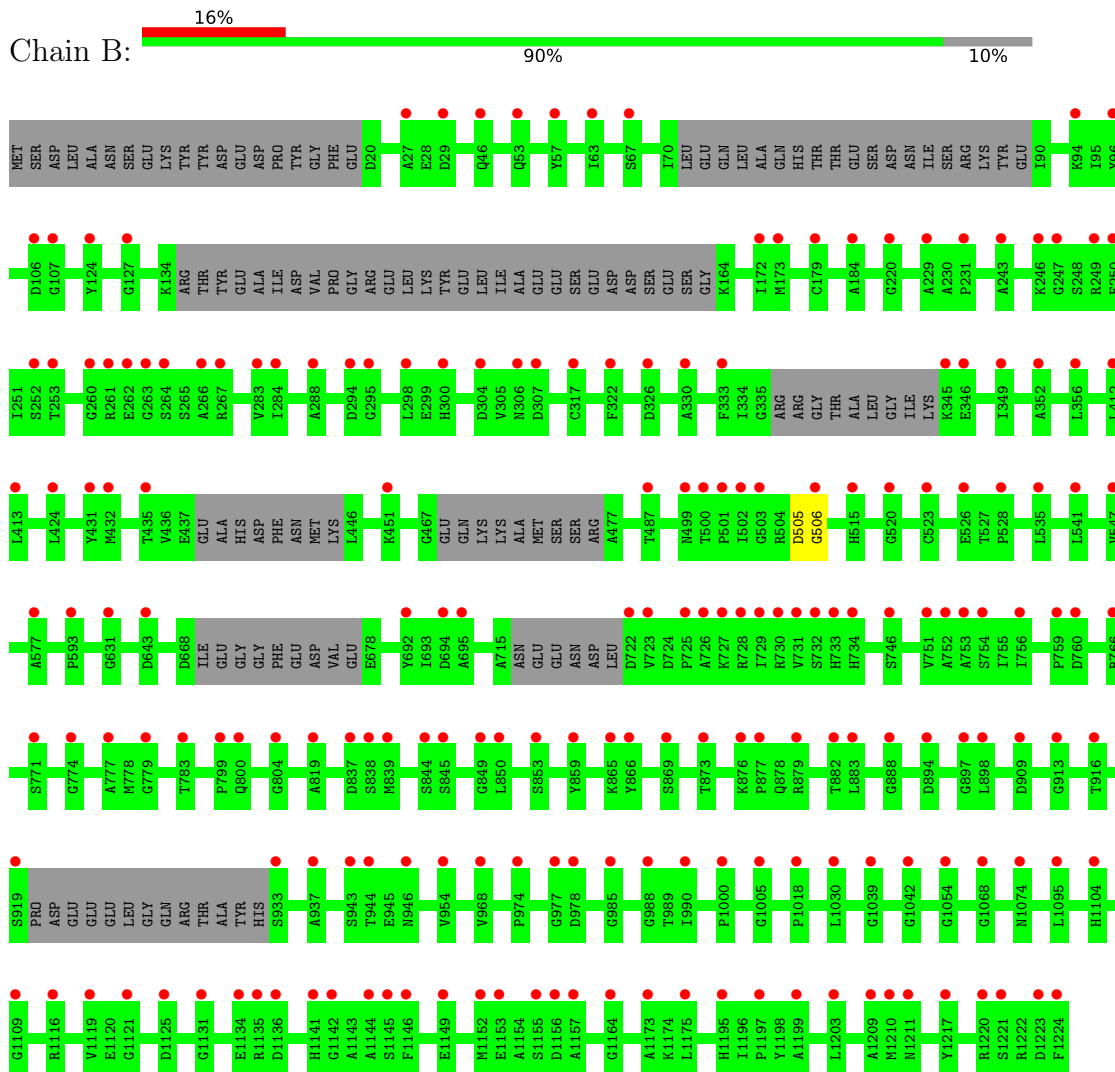
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Mg	0	0
			1	1		

- Molecule 15 is ZINC ION (CCD ID: ZN) (formula: Zn).

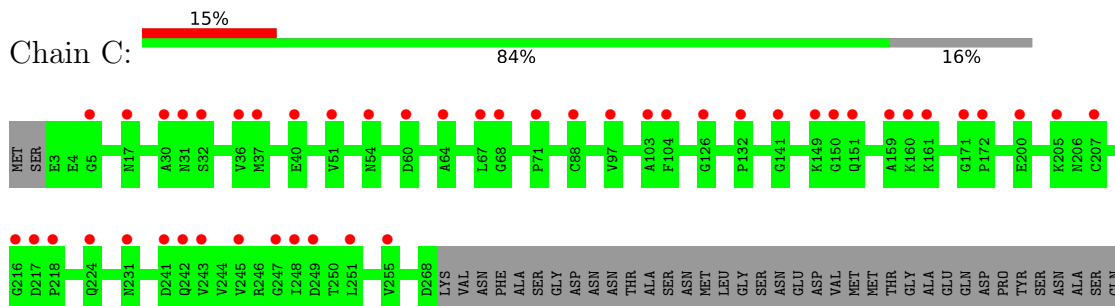
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total 2	Zn 2	0	0
15	B	1	Total 1	Zn 1	0	0
15	C	1	Total 1	Zn 1	0	0
15	I	2	Total 2	Zn 2	0	0
15	J	1	Total 1	Zn 1	0	0
15	L	1	Total 1	Zn 1	0	0
15	S	1	Total 1	Zn 1	0	0



- Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide



- Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	218.90Å 395.30Å 281.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 50.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-3.80) 89.6 (50.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	91.0	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	4041	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	1409	0	0	3	0
2	B	1103	0	0	1	0
3	C	266	0	0	0	0
4	D	135	0	0	1	0
5	E	214	0	0	1	0
6	F	84	0	0	0	0
7	G	169	0	0	0	0
8	H	133	0	0	0	0
9	I	119	0	0	0	0
10	J	65	0	0	0	0
11	K	114	0	0	0	0
12	L	46	0	0	0	0
13	S	174	0	0	3	0
14	A	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
15	S	1	0	0	0	0
All	All	4041	0	0	9	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 2.

All (9) 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:A:1330:ASN:CA	1:A:1331:SER:CA	2.54	0.85
4:D:89:UNK:CA	4:D:90:UNK:CA	2.57	0.83
1:A:1385:THR:CA	1:A:1386:ARG:CA	2.57	0.81
2:B:505:ASP:CA	2:B:506:GLY:CA	2.63	0.76
13:S:218:ILE:CA	13:S:219:ALA:CA	2.73	0.66
13:S:231:CYS:CA	13:S:232:ASP:CA	2.86	0.53
5:E:128:PRO:CA	5:E:129:PRO:CA	2.91	0.49
1:A:447:GLN:CA	1:A:448:PRO:CA	2.90	0.49
13:S:258:GLY:CA	13:S:259:ALA:CA	2.99	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 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 [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, 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	1409/1733 (81%)	0.97	238 (16%) 4 7	30, 30, 30, 30	0
2	B	1103/1224 (90%)	0.97	198 (17%) 3 6	30, 30, 30, 30	0
3	C	266/318 (83%)	0.96	47 (17%) 4 6	30, 30, 30, 30	0
4	D	106/221 (47%)	1.12	19 (17%) 3 6	30, 30, 30, 30	0
5	E	214/215 (99%)	0.34	17 (7%) 18 17	30, 30, 30, 30	0
6	F	84/155 (54%)	1.22	17 (20%) 3 5	30, 30, 30, 30	0
7	G	169/171 (98%)	1.40	40 (23%) 2 3	30, 30, 30, 30	0
8	H	133/146 (91%)	0.38	12 (9%) 15 16	30, 30, 30, 30	0
9	I	119/122 (97%)	0.11	5 (4%) 40 29	30, 30, 30, 30	0
10	J	65/70 (92%)	0.77	8 (12%) 8 12	30, 30, 30, 30	0
11	K	114/120 (95%)	0.89	18 (15%) 5 8	30, 30, 30, 30	0
12	L	46/70 (65%)	0.85	8 (17%) 4 6	30, 30, 30, 30	0
13	S	174/309 (56%)	0.32	12 (6%) 23 20	30, 30, 30, 30	0
All	All	4002/4874 (82%)	0.88	639 (15%) 5 8	30, 30, 30, 30	0

All (639) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	197	SER	16.8
2	B	882	THR	15.9
1	A	665	GLY	15.0
2	B	722	ASP	12.4
1	A	1178	ASP	12.0
2	B	220	GLY	11.7
4	D	177	VAL	11.4
1	A	1122	PRO	11.3
3	C	5	GLY	10.7

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Mol	Chain	Res	Type	RSRZ
1	A	1014	ALA	10.1
1	A	1188	GLN	10.0
3	C	200	GLU	9.8
1	A	153	PRO	9.7
7	G	23	LYS	9.6
2	B	283	VAL	9.3
2	B	295	GLY	9.0
2	B	779	GLY	8.9
2	B	330	ALA	8.9
2	B	262	GLU	8.7
6	F	140	ASP	8.7
1	A	647	GLY	8.6
2	B	733	HIS	8.5
11	K	2	ASN	8.2
1	A	707	GLY	8.2
2	B	250	PHE	8.0
2	B	247	GLY	7.9
1	A	730	GLY	7.8
1	A	44	THR	7.8
7	G	76	ALA	7.6
5	E	108	GLY	7.5
7	G	34	VAL	7.4
2	B	1164	GLY	7.3
1	A	1395	GLY	7.2
2	B	1042	GLY	7.1
1	A	687	LYS	7.0
1	A	733	ALA	6.9
7	G	97	HIS	6.9
2	B	774	GLY	6.8
1	A	778	GLY	6.8
4	D	167	LEU	6.8
1	A	1380	GLY	6.8
2	B	865	LYS	6.8
4	D	181	GLY	6.6
2	B	307	ASP	6.5
1	A	152	VAL	6.5
1	A	483	ASP	6.5
1	A	1396	ALA	6.4
6	F	93	ILE	6.4
1	A	286	HIS	6.4
1	A	3	GLY	6.4
1	A	921	GLY	6.4

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Mol	Chain	Res	Type	RSRZ
2	B	883	LEU	6.3
1	A	1123	GLY	6.2
2	B	294	ASP	6.2
1	A	338	GLY	6.2
1	A	399	HIS	6.2
2	B	937	ALA	6.1
11	K	3	ALA	6.0
2	B	231	PRO	6.0
7	G	131	GLN	6.0
2	B	263	GLY	6.0
1	A	1231	ASP	5.9
1	A	69	THR	5.8
6	F	72	LYS	5.8
1	A	110	CYS	5.8
7	G	26	LEU	5.8
2	B	577	ALA	5.7
2	B	643	ASP	5.7
7	G	43	GLY	5.6
2	B	346	GLU	5.6
1	A	871	ASP	5.5
3	C	126	GLY	5.5
1	A	1256	GLU	5.5
7	G	69	GLU	5.5
7	G	32	GLU	5.4
1	A	422	GLY	5.4
7	G	168	LEU	5.4
2	B	96	TYR	5.4
4	D	160	VAL	5.3
2	B	897	GLY	5.3
10	J	18	TRP	5.3
1	A	716	ASP	5.2
2	B	913	GLY	5.2
2	B	1224	PHE	5.2
2	B	723	VAL	5.1
1	A	980	ASP	5.1
1	A	1156	PRO	5.1
1	A	1221	LYS	5.1
2	B	266	ALA	5.1
11	K	13	GLY	5.0
1	A	1345	ARG	5.0
2	B	1223	ASP	5.0
7	G	120	THR	5.0

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Mol	Chain	Res	Type	RSRZ
7	G	167	TYR	5.0
2	B	1142	GLY	5.0
1	A	1235	LYS	5.0
1	A	1077	THR	5.0
2	B	249	ARG	5.0
1	A	111	GLY	4.9
11	K	16	GLU	4.9
1	A	872	GLY	4.9
1	A	683	ILE	4.8
1	A	686	ALA	4.8
2	B	431	TYR	4.8
2	B	306	ASN	4.8
2	B	729	ILE	4.8
7	G	111	THR	4.8
1	A	168	GLY	4.7
1	A	1126	ALA	4.7
1	A	36	ARG	4.7
5	E	121	MET	4.7
11	K	7	PHE	4.7
7	G	119	LEU	4.7
1	A	127	ALA	4.7
1	A	272	ALA	4.7
11	K	10	PHE	4.6
10	J	51	LEU	4.6
1	A	740	LEU	4.6
3	C	104	PHE	4.6
1	A	835	GLY	4.6
3	C	171	GLY	4.6
1	A	952	ALA	4.6
1	A	1337	GLU	4.6
2	B	526	GLU	4.6
2	B	1156	ASP	4.5
2	B	888	GLY	4.5
7	G	121	PHE	4.5
6	F	121	ALA	4.5
3	C	150	GLY	4.5
1	A	365	GLY	4.4
2	B	725	PRO	4.4
1	A	749	ALA	4.4
12	L	63	ARG	4.4
2	B	1131	GLY	4.4
5	E	183	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	732	SER	4.4
9	I	116	ASN	4.3
2	B	734	HIS	4.3
2	B	804	GLY	4.3
7	G	161	GLY	4.3
12	L	26	THR	4.3
5	E	2	ASP	4.3
1	A	776	ALA	4.3
1	A	1357	ALA	4.3
2	B	1121	GLY	4.3
7	G	98	GLY	4.2
7	G	156	SER	4.2
1	A	1180	GLU	4.2
1	A	1183	GLN	4.2
2	B	1146	PHE	4.2
2	B	877	PRO	4.2
8	H	120	GLY	4.2
1	A	1179	GLU	4.2
1	A	1243	VAL	4.2
2	B	252	SER	4.2
1	A	744	LYS	4.2
1	A	519	PRO	4.1
1	A	1010	ALA	4.1
2	B	503	GLY	4.1
10	J	48	ARG	4.1
11	K	69	ALA	4.1
1	A	97	ALA	4.1
1	A	798	GLY	4.0
2	B	261	ARG	4.0
4	D	196	PRO	4.0
12	L	48	CYS	4.0
1	A	154	SER	4.0
2	B	944	THR	4.0
2	B	988	GLY	4.0
2	B	300	HIS	4.0
1	A	2	VAL	3.9
1	A	1182	GLU	3.9
3	C	141	GLY	3.9
2	B	333	PHE	3.9
2	B	304	ASP	3.9
3	C	249	ASP	3.9
11	K	9	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	849	GLY	3.9
1	A	1366	ARG	3.9
2	B	1141	HIS	3.9
2	B	746	SER	3.9
1	A	671	ALA	3.9
7	G	9	LEU	3.8
2	B	933	SER	3.8
2	B	943	SER	3.8
11	K	80	GLY	3.8
2	B	1195	HIS	3.8
2	B	866	TYR	3.8
7	G	157	ILE	3.8
2	B	506	GLY	3.8
11	K	4	PRO	3.8
2	B	1145	SER	3.8
1	A	165	GLY	3.8
1	A	694	THR	3.8
1	A	753	GLY	3.8
1	A	888	GLY	3.8
1	A	1076	ALA	3.8
2	B	1039	GLY	3.8
2	B	1173	ALA	3.8
1	A	1065	GLY	3.7
1	A	1346	ALA	3.7
1	A	1431	GLY	3.7
13	S	175	ALA	3.7
2	B	985	GLY	3.7
1	A	667	GLY	3.7
2	B	1054	GLY	3.7
1	A	388	LEU	3.7
3	C	231	ASN	3.7
2	B	1144	ALA	3.6
8	H	84	ALA	3.6
2	B	844	SER	3.6
1	A	1050	GLU	3.5
1	A	1437	GLY	3.5
1	A	1212	VAL	3.5
1	A	1438	THR	3.5
8	H	108	SER	3.5
11	K	11	LEU	3.5
3	C	40	GLU	3.5
5	E	139	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	435	THR	3.5
2	B	876	LYS	3.5
8	H	102	TYR	3.5
1	A	1213	GLY	3.5
2	B	127	GLY	3.5
6	F	96	THR	3.5
1	A	517	ASN	3.5
2	B	730	ARG	3.5
1	A	1201	ALA	3.5
2	B	753	ALA	3.5
4	D	221	TYR	3.5
2	B	771	SER	3.5
3	C	68	GLY	3.5
2	B	1203	LEU	3.5
7	G	114	LEU	3.5
1	A	650	GLN	3.5
5	E	174	GLN	3.4
1	A	1222	ASN	3.4
4	D	143	ASN	3.4
2	B	800	GLN	3.4
1	A	804	TYR	3.4
2	B	1153	GLU	3.4
2	B	631	GLY	3.4
1	A	826	ASP	3.4
1	A	703	THR	3.4
3	C	149	LYS	3.4
1	A	1176	LEU	3.4
3	C	224	GLN	3.4
1	A	337	ARG	3.4
1	A	1288	ASP	3.3
7	G	96	GLN	3.3
2	B	288	ALA	3.3
3	C	159	ALA	3.3
2	B	243	ALA	3.3
1	A	908	LEU	3.3
1	A	530	GLY	3.3
7	G	33	GLU	3.3
11	K	8	GLU	3.3
3	C	103	ALA	3.3
2	B	968	VAL	3.3
1	A	1189	SER	3.3
1	A	869	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	45	GLN	3.3
1	A	1070	GLN	3.3
2	B	27	ALA	3.3
6	F	83	PRO	3.3
2	B	839	MET	3.3
1	A	331	GLY	3.3
1	A	144	THR	3.3
1	A	809	THR	3.3
2	B	179	CYS	3.3
4	D	179	GLN	3.3
1	A	421	ALA	3.2
2	B	1220	ARG	3.2
11	K	83	PRO	3.2
1	A	593	GLU	3.2
1	A	29	ALA	3.2
2	B	246	LYS	3.2
13	S	274	CYS	3.2
1	A	1304	TRP	3.2
2	B	535	LEU	3.2
6	F	151	LEU	3.2
8	H	142	LEU	3.2
2	B	754	SER	3.2
1	A	1131	ALA	3.2
2	B	229	ALA	3.2
2	B	1210	MET	3.2
1	A	56	PRO	3.2
1	A	52	GLY	3.2
1	A	811	GLN	3.2
12	L	49	LYS	3.2
1	A	301	ALA	3.2
3	C	36	VAL	3.2
2	B	759	PRO	3.2
1	A	1400	CYS	3.1
2	B	728	ARG	3.1
1	A	676	MET	3.1
3	C	216	GLY	3.1
1	A	1187	GLN	3.1
1	A	1381	LEU	3.1
2	B	731	VAL	3.1
4	D	200	ASN	3.1
2	B	879	ARG	3.1
3	C	217	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	107	GLY	3.1
1	A	354	SER	3.0
1	A	850	VAL	3.0
3	C	64	ALA	3.0
1	A	1294	PRO	3.0
3	C	132	PRO	3.0
1	A	1275	GLY	3.0
3	C	247	GLY	3.0
2	B	783	THR	3.0
11	K	27	ALA	3.0
2	B	67	SER	3.0
2	B	499	ASN	3.0
2	B	94	LYS	3.0
2	B	845	SER	3.0
2	B	799	PRO	3.0
3	C	161	LYS	3.0
8	H	85	GLY	3.0
1	A	1177	LEU	3.0
1	A	1125	ALA	3.0
2	B	1199	ALA	3.0
1	A	700	ASN	3.0
2	B	1217	TYR	3.0
2	B	106	ASP	3.0
2	B	727	LYS	2.9
8	H	131	ASN	2.9
1	A	514	PRO	2.9
1	A	374	LEU	2.9
1	A	847	ASP	2.9
1	A	659	HIS	2.9
2	B	451	LYS	2.9
1	A	79	GLY	2.9
1	A	1355	VAL	2.9
1	A	1440	ALA	2.9
2	B	726	ALA	2.9
4	D	198	LEU	2.9
1	A	1255	GLU	2.9
1	A	1324	PRO	2.9
1	A	1061	GLY	2.9
2	B	919	SER	2.9
3	C	151	GLN	2.9
2	B	487	THR	2.9
2	B	172	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	267	ARG	2.9
4	D	161	GLY	2.9
7	G	36	GLY	2.9
1	A	88	LYS	2.9
3	C	205	LYS	2.9
3	C	71	PRO	2.9
1	A	704	ALA	2.8
2	B	523	CYS	2.8
5	E	124	VAL	2.8
2	B	752	ALA	2.8
2	B	432	MET	2.8
4	D	138	ASN	2.8
3	C	88	CYS	2.8
6	F	100	GLN	2.8
10	J	26	GLN	2.8
13	S	283	GLN	2.8
1	A	1067	LEU	2.8
2	B	1000	PRO	2.8
3	C	32	SER	2.8
1	A	282	ASN	2.8
3	C	251	LEU	2.8
2	B	869	SER	2.8
7	G	81	PRO	2.8
2	B	692	TYR	2.8
1	A	621	THR	2.8
2	B	349	ILE	2.7
4	D	189	ASP	2.7
3	C	37	MET	2.7
1	A	610	GLY	2.7
6	F	95	GLY	2.7
1	A	825	ILE	2.7
8	H	140	ALA	2.7
2	B	1116	ARG	2.7
1	A	572	TRP	2.7
1	A	1392	SER	2.7
5	E	110	PHE	2.7
1	A	1073	GLY	2.7
1	A	1370	LEU	2.7
2	B	1175	LEU	2.7
3	C	30	ALA	2.7
8	H	98	TYR	2.7
1	A	857	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	1134	GLU	2.7
5	E	169	ARG	2.7
1	A	302	THR	2.7
13	S	309	SER	2.7
3	C	172	PRO	2.7
1	A	1023	ARG	2.7
1	A	54	ASN	2.7
7	G	95	SER	2.7
5	E	118	PRO	2.7
13	S	137	ASP	2.7
2	B	695	ALA	2.7
2	B	1109	GLY	2.7
1	A	1209	MET	2.7
2	B	424	LEU	2.7
7	G	136	VAL	2.6
2	B	1155	SER	2.6
7	G	113	HIS	2.6
1	A	941	LYS	2.6
2	B	352	ALA	2.6
6	F	78	GLN	2.6
12	L	32	ALA	2.6
2	B	1152	MET	2.6
1	A	657	LEU	2.6
2	B	356	LEU	2.6
2	B	894	ASP	2.6
2	B	1221	SER	2.6
9	I	12	ASN	2.6
2	B	63	ILE	2.6
6	F	129	LYS	2.6
1	A	313	GLN	2.6
1	A	1108	ALA	2.6
1	A	824	LEU	2.6
2	B	298	LEU	2.6
13	S	235	ASP	2.6
3	C	31	ASN	2.6
1	A	1283	VAL	2.6
6	F	118	LEU	2.6
1	A	161	LEU	2.6
1	A	1098	VAL	2.5
3	C	255	VAL	2.5
2	B	184	ALA	2.5
2	B	1018	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	1157	ALA	2.5
1	A	624	SER	2.5
1	A	1372	VAL	2.5
1	A	768	GLN	2.5
12	L	55	ILE	2.5
2	B	873	THR	2.5
3	C	243	VAL	2.5
7	G	101	VAL	2.5
2	B	326	ASP	2.5
1	A	772	GLY	2.5
10	J	40	GLY	2.5
1	A	690	VAL	2.5
8	H	51	ALA	2.5
1	A	950	GLY	2.5
2	B	260	GLY	2.5
1	A	65	LEU	2.5
1	A	1199	ARG	2.5
4	D	159	THR	2.5
2	B	547	VAL	2.5
7	G	130	TYR	2.5
9	I	102	VAL	2.5
2	B	345	LYS	2.5
3	C	54	ASN	2.5
1	A	643	ALA	2.5
1	A	1200	ALA	2.5
2	B	694	ASP	2.5
5	E	112	TYR	2.5
7	G	41	LYS	2.4
13	S	165	GLU	2.4
1	A	725	ALA	2.4
1	A	563	PRO	2.4
2	B	541	LEU	2.4
1	A	521	MET	2.4
1	A	761	MET	2.4
1	A	1198	ASP	2.4
12	L	45	ALA	2.4
13	S	304	ASN	2.4
1	A	831	THR	2.4
3	C	60	ASP	2.4
1	A	789	LYS	2.4
3	C	248	ILE	2.4
1	A	120	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	515	HIS	2.4
2	B	777	ALA	2.4
3	C	242	GLN	2.4
4	D	174	PRO	2.4
1	A	1097	GLY	2.4
3	C	160	LYS	2.4
2	B	751	VAL	2.4
2	B	954	VAL	2.4
1	A	336	ILE	2.4
2	B	990	ILE	2.4
1	A	550	LEU	2.4
2	B	1030	LEU	2.4
3	C	218	PRO	2.4
5	E	206	GLY	2.4
6	F	139	PRO	2.4
1	A	1071	SER	2.4
7	G	8	SER	2.4
2	B	322	PHE	2.4
1	A	864	ILE	2.4
2	B	284	ILE	2.4
2	B	412	LEU	2.4
6	F	155	LEU	2.4
11	K	12	LEU	2.4
1	A	469	ARG	2.4
1	A	299	HIS	2.4
1	A	480	ALA	2.4
11	K	91	CYS	2.4
10	J	60	PHE	2.4
3	C	97	VAL	2.4
1	A	200	ARG	2.4
1	A	967	ALA	2.4
1	A	1069	ALA	2.4
5	E	66	GLU	2.4
11	K	14	GLU	2.4
1	A	406	ILE	2.3
6	F	94	LEU	2.3
2	B	124	TYR	2.3
1	A	790	ASP	2.3
4	D	151	PHE	2.3
2	B	502	ILE	2.3
2	B	1074	ASN	2.3
1	A	1142	THR	2.3

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Mol	Chain	Res	Type	RSRZ
5	E	90	VAL	2.3
2	B	57	TYR	2.3
1	A	876	ALA	2.3
9	I	56	ALA	2.3
1	A	758	ILE	2.3
1	A	762	SER	2.3
1	A	1143	LEU	2.3
1	A	1260	LEU	2.3
1	A	586	ILE	2.3
1	A	1441	PHE	2.3
2	B	29	ASP	2.3
2	B	977	GLY	2.3
2	B	500	THR	2.3
1	A	335	ARG	2.3
1	A	1313	LEU	2.3
7	G	17	PHE	2.3
2	B	46	GLN	2.3
2	B	53	GLN	2.3
1	A	734	GLU	2.3
1	A	663	SER	2.3
2	B	974	PRO	2.3
2	B	1068	GLY	2.3
3	C	241	ASP	2.3
7	G	104	GLY	2.3
1	A	631	HIS	2.3
2	B	916	THR	2.3
1	A	817	ALA	2.3
1	A	1369	ALA	2.3
2	B	819	ALA	2.3
6	F	105	ALA	2.3
1	A	334	GLY	2.3
2	B	760	ASP	2.3
1	A	314	ALA	2.2
7	G	74	TYR	2.2
4	D	139	LYS	2.2
1	A	1234	GLU	2.2
2	B	1005	GLY	2.2
3	C	245	VAL	2.2
7	G	84	GLY	2.2
1	A	1127	ASP	2.2
2	B	898	LEU	2.2
2	B	978	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	946	ASN	2.2
1	A	8	SER	2.2
1	A	1287	TYR	2.2
2	B	1095	LEU	2.2
1	A	1078	GLN	2.2
2	B	853	SER	2.2
2	B	520	GLY	2.2
2	B	317	CYS	2.2
3	C	207	CYS	2.2
2	B	837	ASP	2.2
3	C	17	ASN	2.2
1	A	83	HIS	2.2
2	B	838	SER	2.2
3	C	67	LEU	2.2
3	C	51	VAL	2.2
7	G	123	ALA	2.2
2	B	1135	ARG	2.2
1	A	370	ILE	2.2
1	A	149	GLU	2.2
1	A	243	PRO	2.2
9	I	18	GLU	2.2
2	B	1211	ASN	2.2
2	B	413	LEU	2.2
5	E	138	ALA	2.1
8	H	116	TYR	2.1
1	A	242	PRO	2.1
2	B	1149	GLU	2.1
2	B	253	THR	2.1
1	A	488	ASN	2.1
1	A	502	SER	2.1
13	S	145	HIS	2.1
1	A	531	ILE	2.1
2	B	1119	VAL	2.1
5	E	122	LYS	2.1
11	K	58	PHE	2.1
2	B	1197	PRO	2.1
1	A	339	ASN	2.1
1	A	775	ILE	2.1
1	A	609	ASP	2.1
13	S	232	ASP	2.1
1	A	868	TYR	2.1
13	S	306	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	238	CYS	2.1
2	B	528	PRO	2.1
2	B	264	SER	2.1
7	G	145	VAL	2.1
7	G	14	HIS	2.1
1	A	1035	TYR	2.1
2	B	859	TYR	2.1
2	B	593	PRO	2.1
6	F	106	PRO	2.1
8	H	82	PRO	2.1
4	D	118	THR	2.1
2	B	1104	HIS	2.1
1	A	604	GLY	2.1
1	A	810	PRO	2.1
1	A	1359	ASP	2.1
2	B	909	ASP	2.1
2	B	1136	ASP	2.1
1	A	1103	GLU	2.1
12	L	68	GLU	2.1
5	E	200	ARG	2.1
2	B	756	ILE	2.1
1	A	943	LEU	2.1
1	A	166	GLY	2.0
1	A	351	THR	2.0
2	B	1209	ALA	2.0
1	A	597	LEU	2.0
2	B	173	MET	2.0
2	B	501	PRO	2.0
1	A	1104	ILE	2.0
10	J	12	LYS	2.0
1	A	117	GLU	2.0
2	B	1125	ASP	2.0
1	A	74	MET	2.0
1	A	549	MET	2.0
1	A	1423	GLY	2.0
2	B	766	ARG	2.0
2	B	850	LEU	2.0
10	J	32	GLU	2.0
1	A	1373	ASP	2.0
7	G	159	ALA	2.0
13	S	177	ALA	2.0
1	A	364	VAL	2.0

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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
14	MG	A	1734	1/1	0.72	0.36	61,61,61,61	0
15	ZN	B	1300	1/1	0.74	0.16	30,30,30,30	0
15	ZN	S	400	1/1	0.89	0.19	30,30,30,30	0
15	ZN	J	100	1/1	0.90	0.13	30,30,30,30	0
15	ZN	A	1735	1/1	0.90	0.23	30,30,30,30	0
15	ZN	L	100	1/1	0.92	0.23	30,30,30,30	0
15	ZN	I	201	1/1	0.94	0.25	30,30,30,30	0
15	ZN	C	319	1/1	0.94	0.17	30,30,30,30	0
15	ZN	A	1736	1/1	0.95	0.17	30,30,30,30	0
15	ZN	I	200	1/1	0.97	0.17	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.