Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 12:30 PM EDT

PDB ID	:	5EZK
Title	:	RNA polymerase model placed by Molecular replacement into X-ray diffraction map of DNA-bound RNA Polymerase-Sigma 54 holoenzyme complex.
Authors	:	Darbari, V.C.; Yang, Y.; Lu, D.; Zhang, N.; Glyde, R.; Wang, Y.; Murakami, K.S.; Buck, M.; Zhang, X.
Deposited on	:	2015-11-26
Resolution	:	8.50 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 (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 (1)) were used in the production of this report:

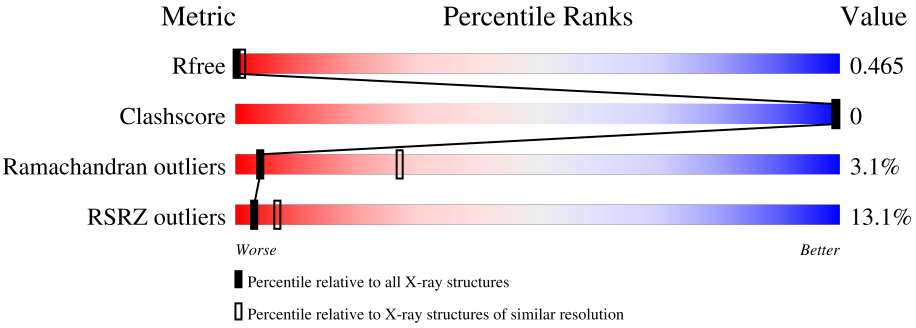
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 8.50 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	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
RSRZ outliers	127900	1004 (9.50-3.80)

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	329	21% 96%
1	B	329	11% 65% 33%
2	C	1342	11% 97%
3	D	1407	11% 79% 18%
4	E	91	7% 97%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15410 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 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	323	1595	949	323	323	0	0	0
1	B	221	1090	648	221	221	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	1335	6569	3899	1335	1335	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	D	1160	5711	3391	1160	1160	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

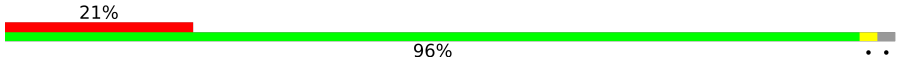
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	90	445	265	90	90	0	0	0

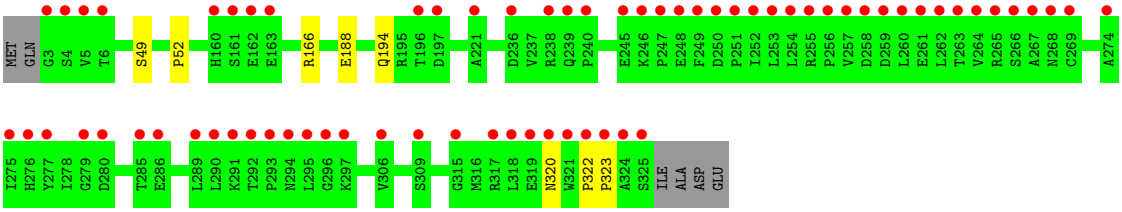
3 Residue-property plots (i)

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: DNA-directed RNA polymerase subunit alpha

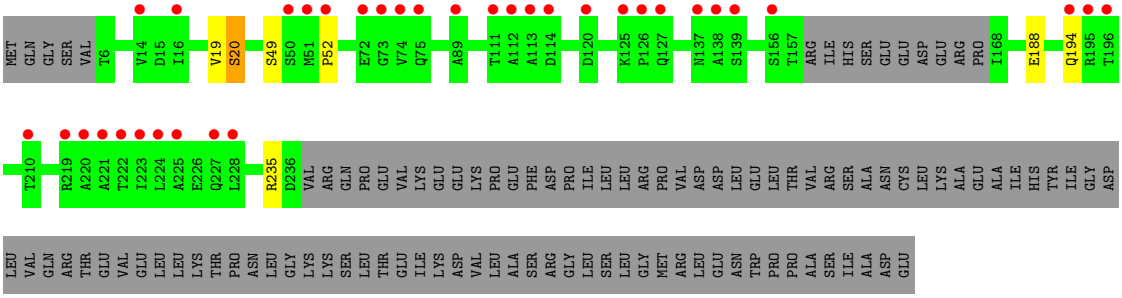
Chain A:





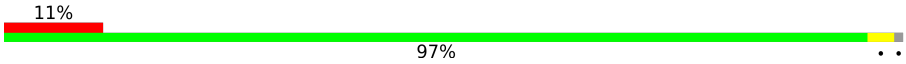
• Molecule 1: DNA-directed RNA polymerase subunit alpha

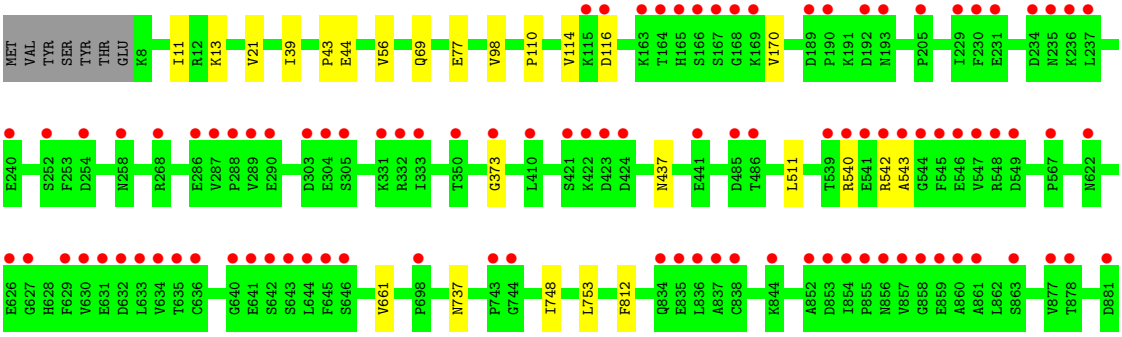
Chain B:

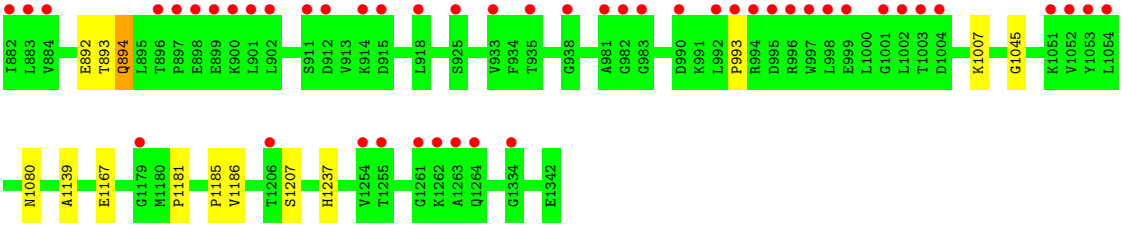


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

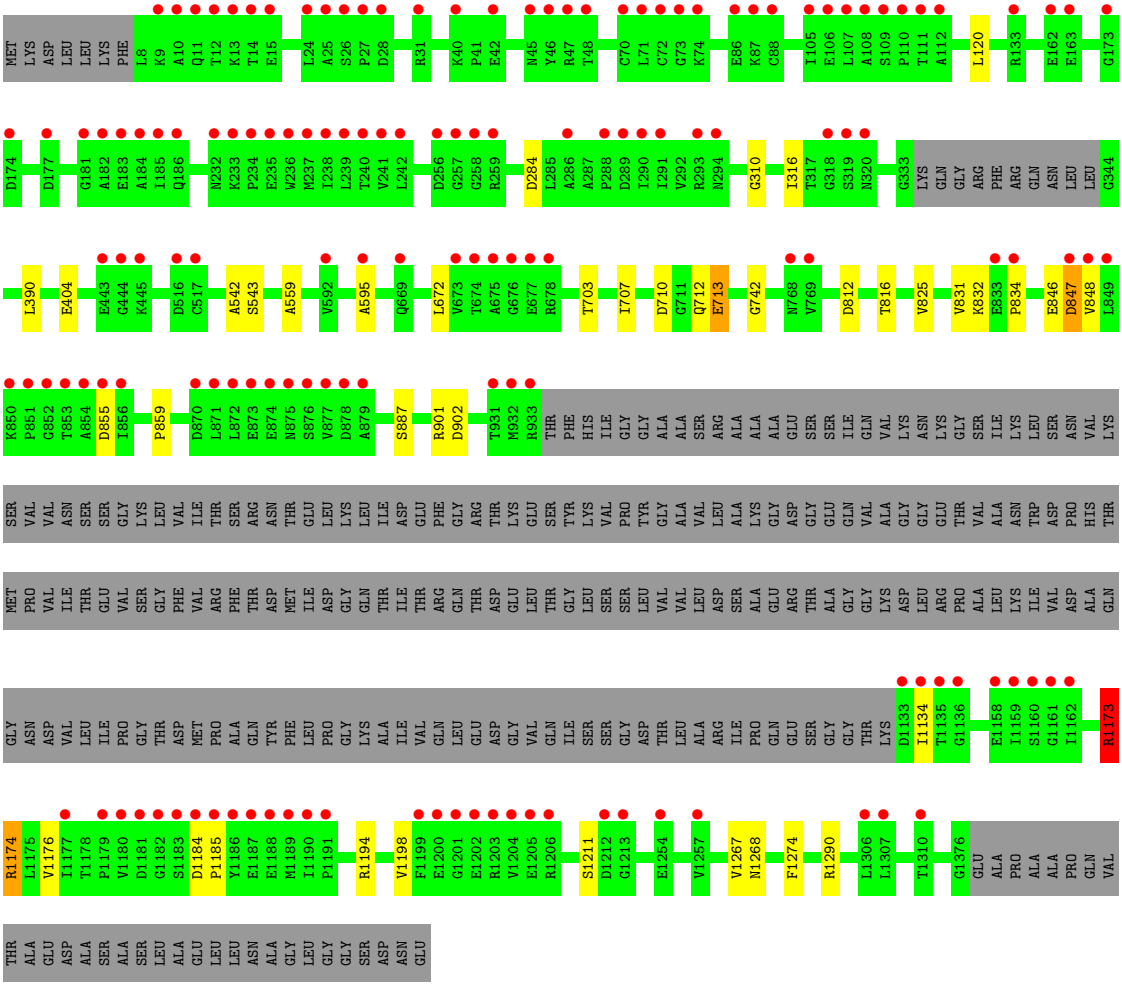






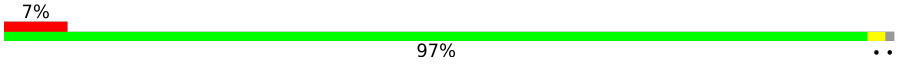
- Molecule 3: DNA-directed RNA polymerase subunit beta'

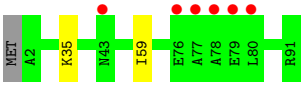
Chain D:



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	255.54Å 255.54Å 189.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	143.89 – 8.50 143.89 – 7.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (143.89-8.50) 99.4 (143.89-7.50)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 7.44Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.470 , 0.470 0.462 , 0.465	Depositor DCC
R_{free} test set	436 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	313.9	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.12 , 999.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.103 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.63	EDS
Total number of atoms	15410	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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 (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	0.30	0/1594	0.49	0/2218
1	B	0.30	0/1088	0.49	0/1511
2	C	0.29	0/6568	0.47	0/9130
3	D	0.29	0/5708	0.47	0/7933
4	E	0.30	0/444	0.46	0/617
All	All	0.29	0/15402	0.47	0/21409

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
3	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1173	ARG	Peptide

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	1595	0	715	0	0
1	B	1090	0	498	1	0
2	C	6569	0	2956	1	0
3	D	5711	0	2659	3	0
4	E	445	0	215	0	0
All	All	15410	0	7043	5	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 0.

All (5) 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:B:19:VAL:O	1:B:20:SER:CB	2.58	0.51
3:D:712:GLN:O	3:D:713:GLU:CB	2.63	0.46
3:D:1173:ARG:O	3:D:1174:ARG:CB	2.67	0.43
3:D:846:GLU:O	3:D:847:ASP:C	2.58	0.41
2:C:893:THR:O	2:C:894:GLN:CB	2.69	0.40

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	321/329 (98%)	276 (86%)	37 (12%)	8 (2%)	5 32
1	B	217/329 (66%)	194 (89%)	17 (8%)	6 (3%)	5 30
2	C	1333/1342 (99%)	1097 (82%)	198 (15%)	38 (3%)	4 29
3	D	1154/1407 (82%)	956 (83%)	156 (14%)	42 (4%)	3 25
4	E	88/91 (97%)	79 (90%)	7 (8%)	2 (2%)	6 34
All	All	3113/3498 (89%)	2602 (84%)	415 (13%)	96 (3%)	4 27

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	PRO
1	B	20	SER
2	C	39	ILE
2	C	43	PRO
2	C	56	VAL
2	C	110	PRO
2	C	661	VAL
2	C	748	ILE
2	C	1181	PRO
2	C	1186	VAL
3	D	120	LEU
3	D	390	LEU
3	D	707	ILE
3	D	713	GLU
3	D	1174	ARG
1	B	52	PRO
1	B	194	GLN
1	B	235	ARG
2	C	170	VAL
2	C	540	ARG
2	C	543	ALA
2	C	894	GLN
2	C	1185	PRO
2	C	1207	SER
3	D	284	ASP
3	D	310	GLY
3	D	316	ILE
3	D	847	ASP
3	D	855	ASP
3	D	901	ARG
3	D	902	ASP
3	D	1274	PHE
1	A	52	PRO
1	A	188	GLU
1	A	194	GLN
1	B	188	GLU
2	C	11	ILE
2	C	13	LYS
2	C	542	ARG
2	C	812	PHE
3	D	543	SER
3	D	672	LEU

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Mol	Chain	Res	Type
3	D	812	ASP
3	D	834	PRO
3	D	1134	ILE
3	D	1211	SER
3	D	1267	VAL
3	D	1268	ASN
1	A	320	ASN
2	C	116	ASP
2	C	511	LEU
2	C	737	ASN
2	C	892	GLU
2	C	993	PRO
2	C	1007	LYS
2	C	1080	ASN
2	C	1167	GLU
2	C	1237	HIS
3	D	404	GLU
3	D	542	ALA
3	D	559	ALA
3	D	595	ALA
3	D	710	ASP
3	D	887	SER
3	D	1173	ARG
3	D	1290	ARG
4	E	35	LYS
1	A	49	SER
1	A	166	ARG
1	B	49	SER
2	C	44	GLU
2	C	114	VAL
2	C	437	ASN
3	D	703	THR
3	D	831	VAL
3	D	1194	ARG
2	C	69	GLN
2	C	77	GLU
2	C	753	LEU
2	C	1139	ALA
3	D	816	THR
3	D	832	LYS
3	D	859	PRO
3	D	1185	PRO

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Mol	Chain	Res	Type
3	D	1198	VAL
2	C	1045	GLY
3	D	848	VAL
4	E	59	ILE
2	C	21	VAL
3	D	742	GLY
3	D	1176	VAL
1	A	323	PRO
2	C	373	GLY
2	C	98	VAL
3	D	825	VAL
3	D	1184	ASP

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 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	323/329 (98%)	0.85	69 (21%) 0 3	6, 56, 135, 172	0
1	B	221/329 (67%)	0.53	35 (15%) 2 5	23, 82, 126, 152	0
2	C	1335/1342 (99%)	0.24	148 (11%) 5 9	3, 40, 141, 193	0
3	D	1160/1407 (82%)	0.49	151 (13%) 3 7	2, 35, 126, 176	0
4	E	90/91 (98%)	0.21	6 (6%) 17 18	4, 34, 66, 94	0
All	All	3129/3498 (89%)	0.42	409 (13%) 3 7	2, 42, 134, 193	0

All (409) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	233	LYS	13.0
1	A	294	ASN	12.0
2	C	631	GLU	11.2
1	A	4	SER	10.7
3	D	1160	SER	10.6
2	C	835	GLU	9.7
1	A	292	THR	9.7
2	C	166	SER	9.6
1	A	295	LEU	9.4
3	D	236	TRP	9.2
2	C	632	ASP	9.2
3	D	235	GLU	9.1
3	D	1181	ASP	9.1
1	A	293	PRO	9.0
2	C	836	LEU	8.9
3	D	1182	GLY	8.9
3	D	1184	ASP	8.6
2	C	167	SER	8.5
2	C	168	GLY	8.3
2	C	995	ASP	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	247	PRO	8.2
1	A	3	GLY	8.1
1	A	250	ASP	8.0
3	D	853	THR	7.9
3	D	1161	GLY	7.8
1	A	246	LYS	7.8
3	D	234	PRO	7.7
3	D	1204	VAL	7.7
2	C	630	VAL	7.6
1	A	256	PRO	7.5
3	D	1183	SER	7.5
3	D	14	THR	7.5
3	D	256	ASP	7.4
3	D	875	ASN	7.4
3	D	850	LYS	7.4
1	A	320	ASN	7.3
3	D	241	VAL	7.2
1	A	259	ASP	7.1
1	A	276	HIS	7.1
3	D	873	GLU	7.1
3	D	1203	ARG	7.0
3	D	107	LEU	7.0
2	C	993	PRO	7.0
3	D	109	SER	7.0
2	C	633	LEU	7.0
2	C	235	ASN	6.9
3	D	11	GLN	6.9
3	D	851	PRO	6.7
2	C	834	GLN	6.6
1	A	251	PRO	6.6
3	D	258	GLY	6.5
3	D	676	GLY	6.5
3	D	852	GLY	6.4
3	D	675	ALA	6.4
3	D	108	ALA	6.3
2	C	994	ARG	6.3
1	A	258	ASP	6.3
3	D	876	SER	6.3
3	D	874	GLU	6.2
3	D	26	SER	6.2
3	D	1133	ASP	6.1
1	A	277	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	255	ARG	6.0
2	C	1262	LYS	6.0
3	D	72	CYS	5.9
3	D	1202	GLU	5.9
3	D	1189	MET	5.8
3	D	854	ALA	5.7
1	A	323	PRO	5.7
3	D	257	GLY	5.7
1	A	249	PHE	5.7
2	C	1052	VAL	5.7
3	D	10	ALA	5.6
3	D	27	PRO	5.6
1	A	257	VAL	5.6
3	D	237	MET	5.6
2	C	634	VAL	5.6
1	A	261	GLU	5.5
3	D	242	LEU	5.5
3	D	13	LYS	5.5
2	C	1261	GLY	5.4
2	C	544	GLY	5.4
1	A	318	LEU	5.4
1	A	5	VAL	5.4
3	D	855	ASP	5.4
3	D	1185	PRO	5.4
3	D	1205	GLU	5.3
1	A	319	GLU	5.3
2	C	899	GLU	5.3
3	D	319	SER	5.3
3	D	15	GLU	5.3
3	D	106	GLU	5.2
3	D	238	ILE	5.2
1	A	6	THR	5.1
1	A	296	GLY	5.1
3	D	674	THR	5.1
3	D	47	ARG	5.1
3	D	677	GLU	5.0
3	D	1159	ILE	5.0
2	C	543	ALA	5.0
1	B	73	GLY	5.0
2	C	982	GLY	4.9
2	C	858	GLY	4.9
3	D	443	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
3	D	933	ARG	4.8
3	D	110	PRO	4.8
2	C	898	GLU	4.8
2	C	236	LYS	4.7
3	D	1134	ILE	4.7
3	D	232	ASN	4.6
1	A	252	ILE	4.6
2	C	165	HIS	4.6
4	E	77	ALA	4.6
3	D	1186	TYR	4.6
2	C	288	PRO	4.6
3	D	849	LEU	4.6
3	D	1179	PRO	4.5
2	C	1254	VAL	4.5
1	A	253	LEU	4.5
3	D	9	LYS	4.5
2	C	883	LEU	4.5
1	A	324	ALA	4.5
3	D	872	LEU	4.5
2	C	992	LEU	4.5
1	A	321	TRP	4.5
3	D	240	THR	4.4
1	A	248	GLU	4.4
2	C	169	LYS	4.4
3	D	73	GLY	4.4
3	D	1213	GLY	4.3
1	B	220	ALA	4.3
3	D	871	LEU	4.3
2	C	859	GLU	4.3
1	A	254	LEU	4.3
3	D	1187	GLU	4.3
3	D	12	THR	4.3
2	C	643	SER	4.2
2	C	1334	GLY	4.2
2	C	645	PHE	4.2
2	C	996	ARG	4.2
2	C	837	ALA	4.2
2	C	190	PRO	4.2
2	C	421	SER	4.2
1	A	162	GLU	4.2
3	D	1188	GLU	4.2
1	A	260	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
3	D	320	ASN	4.1
3	D	182	ALA	4.1
2	C	896	THR	4.1
2	C	897	PRO	4.1
2	C	548	ARG	4.1
3	D	1190	ILE	4.1
2	C	287	VAL	4.1
2	C	1263	ALA	4.1
1	B	112	ALA	4.1
3	D	289	ASP	4.1
2	C	289	VAL	4.0
3	D	877	VAL	4.0
3	D	848	VAL	4.0
1	A	161	SER	4.0
2	C	901	LEU	4.0
2	C	332	ARG	4.0
3	D	184	ALA	4.0
3	D	286	ALA	4.0
2	C	884	VAL	4.0
4	E	78	ALA	3.9
2	C	997	TRP	3.9
2	C	234	ASP	3.9
2	C	644	LEU	3.9
1	A	325	SER	3.8
3	D	46	TYR	3.8
2	C	252	SER	3.8
2	C	857	VAL	3.8
1	B	195	ARG	3.7
2	C	1003	THR	3.7
1	B	223	ILE	3.7
2	C	642	SER	3.7
1	B	126	PRO	3.7
3	D	1201	GLY	3.7
1	A	236	ASP	3.7
1	A	275	ILE	3.6
2	C	635	THR	3.6
3	D	48	THR	3.6
4	E	79	GLU	3.6
2	C	983	GLY	3.6
2	C	549	ASP	3.6
3	D	678	ARG	3.6
2	C	854	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	322	PRO	3.6
3	D	86	GLU	3.6
3	D	87	LYS	3.6
1	B	221	ALA	3.5
3	D	71	LEU	3.5
3	D	318	GLY	3.5
2	C	254	ASP	3.5
2	C	1004	ASP	3.4
2	C	115	LYS	3.4
2	C	539	THR	3.4
1	A	240	PRO	3.4
2	C	915	ASP	3.4
2	C	422	LYS	3.4
3	D	1177	ILE	3.3
2	C	231	GLU	3.3
3	D	833	GLU	3.3
1	A	196	THR	3.3
3	D	88	CYS	3.3
1	A	197	ASP	3.3
1	A	291	LYS	3.3
2	C	304	GLU	3.3
1	B	194	GLN	3.3
2	C	331	LYS	3.2
2	C	900	LYS	3.2
3	D	1191	PRO	3.2
3	D	183	GLU	3.2
1	B	113	ALA	3.2
2	C	230	PHE	3.2
2	C	925	SER	3.2
3	D	517	CYS	3.2
1	B	72	GLU	3.2
3	D	856	ILE	3.2
2	C	485	ASP	3.1
2	C	902	LEU	3.1
2	C	441	GLU	3.1
2	C	540	ARG	3.1
2	C	542	ARG	3.1
2	C	646	SER	3.1
2	C	999	GLU	3.1
1	A	263	THR	3.1
1	A	285	THR	3.1
2	C	1179	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	935	THR	3.0
3	D	878	ASP	3.0
1	A	269	CYS	3.0
2	C	290	GLU	3.0
2	C	882	ILE	3.0
1	B	16	ILE	3.0
1	B	196	THR	3.0
2	C	424	ASP	3.0
3	D	239	LEU	3.0
3	D	1158	GLU	3.0
3	D	847	ASP	2.9
2	C	856	ASN	2.9
2	C	164	THR	2.9
2	C	486	THR	2.9
3	D	174	ASP	2.9
4	E	43	ASN	2.9
2	C	911	SER	2.9
4	E	76	GLU	2.9
3	D	1306	LEU	2.9
2	C	240	GLU	2.9
2	C	838	CYS	2.9
2	C	333	ILE	2.9
3	D	444	GLY	2.8
1	A	274	ALA	2.8
2	C	981	ALA	2.8
2	C	423	ASP	2.8
2	C	1053	TYR	2.8
3	D	870	ASP	2.8
2	C	629	PHE	2.8
3	D	1307	LEU	2.8
2	C	641	GLU	2.8
1	B	127	GLN	2.8
1	A	266	SER	2.8
3	D	288	PRO	2.8
2	C	189	ASP	2.8
3	D	1162	ILE	2.8
2	C	193	ASN	2.8
3	D	45	ASN	2.8
1	B	222	THR	2.8
1	B	227	GLN	2.8
3	D	1135	THR	2.8
1	B	74	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	1054	LEU	2.8
2	C	990	ASP	2.7
3	D	290	ILE	2.7
3	D	834	PRO	2.7
2	C	546	GLU	2.7
1	A	317	ARG	2.7
1	B	225	ALA	2.7
1	A	221	ALA	2.7
3	D	181	GLY	2.7
2	C	286	GLU	2.7
1	B	224	LEU	2.7
3	D	162	GLU	2.7
2	C	844	LYS	2.7
2	C	163	LYS	2.7
1	A	306	VAL	2.6
3	D	163	GLU	2.6
3	D	445	LYS	2.6
1	A	309	SER	2.6
1	A	163	GLU	2.6
1	B	52	PRO	2.6
2	C	410	LEU	2.6
2	C	878	THR	2.6
2	C	373	GLY	2.6
3	D	768	ASN	2.6
2	C	627	GLY	2.5
2	C	192	ASP	2.5
3	D	595	ALA	2.5
2	C	622	ASN	2.5
3	D	1200	GLU	2.5
3	D	185	ILE	2.5
1	A	262	LEU	2.5
3	D	1199	PHE	2.5
1	A	268	ASN	2.5
2	C	1206	THR	2.5
1	B	137	ASN	2.5
2	C	1264	GLN	2.5
3	D	177	ASP	2.5
2	C	855	PRO	2.5
1	B	14	VAL	2.4
2	C	1051	LYS	2.4
3	D	769	VAL	2.4
3	D	932	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	160	HIS	2.4
2	C	640	GLY	2.4
2	C	116	ASP	2.4
3	D	111	THR	2.4
1	A	280	ASP	2.4
3	D	931	THR	2.4
2	C	237	LEU	2.4
3	D	1136	GLY	2.4
1	A	264	VAL	2.4
2	C	1002	LEU	2.4
3	D	293	ARG	2.4
2	C	541	GLU	2.4
2	C	877	VAL	2.4
1	B	50	SER	2.4
3	D	879	ALA	2.4
2	C	229	ILE	2.4
1	A	238	ARG	2.4
1	B	120	ASP	2.4
3	D	42	GLU	2.4
2	C	863	SER	2.4
3	D	105	ILE	2.4
1	A	290	LEU	2.4
2	C	305	SER	2.3
1	B	111	THR	2.3
2	C	258	ASN	2.3
2	C	938	GLY	2.3
2	C	860	ALA	2.3
1	B	138	ALA	2.3
1	A	315	GLY	2.3
1	B	210	THR	2.3
2	C	626	GLU	2.3
3	D	1180	VAL	2.3
3	D	1212	ASP	2.3
2	C	547	VAL	2.3
2	C	912	ASP	2.3
1	B	125	LYS	2.3
3	D	25	ALA	2.3
1	A	267	ALA	2.3
1	B	139	SER	2.3
3	D	294	ASN	2.3
3	D	70	CYS	2.2
1	A	279	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	914	LYS	2.2
3	D	74	LYS	2.2
3	D	259	ARG	2.2
1	A	286	GLU	2.2
3	D	669	GLN	2.2
1	B	156	SER	2.2
2	C	861	ALA	2.2
2	C	350	THR	2.2
3	D	24	LEU	2.2
2	C	205	PRO	2.2
3	D	592	VAL	2.2
2	C	545	PHE	2.2
2	C	918	LEU	2.2
2	C	698	PRO	2.2
3	D	1254	GLU	2.2
3	D	1206	ARG	2.2
4	E	80	LEU	2.2
1	B	228	LEU	2.2
2	C	743	PRO	2.2
3	D	28	ASP	2.2
2	C	881	ASP	2.1
3	D	186	GLN	2.1
1	A	265	ARG	2.1
1	B	219	ARG	2.1
2	C	744	GLY	2.1
2	C	567	PRO	2.1
3	D	516	ASP	2.1
3	D	112	ALA	2.1
1	A	289	LEU	2.1
2	C	853	ASP	2.1
3	D	291	ILE	2.1
1	B	114	ASP	2.1
3	D	673	VAL	2.1
1	B	51	MET	2.1
3	D	133	ARG	2.1
3	D	40	LYS	2.1
3	D	31	ARG	2.1
2	C	933	VAL	2.1
3	D	1257	VAL	2.1
1	B	75	GLN	2.1
1	A	297	LYS	2.0
2	C	636	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	239	GLN	2.0
2	C	852	ALA	2.0
2	C	998	LEU	2.0
1	B	89	ALA	2.0
2	C	268	ARG	2.0
2	C	1255	THR	2.0
2	C	303	ASP	2.0
3	D	1310	THR	2.0
1	A	245	GLU	2.0
2	C	1001	GLY	2.0
3	D	173	GLY	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 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.