



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PQV
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

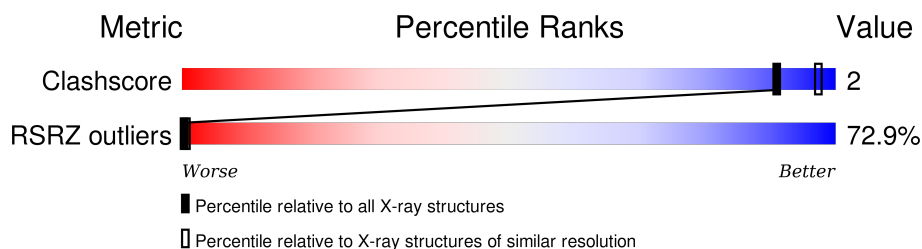
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	102246	1458 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>61%</div> <div>81%</div> <div>19%</div> </div>
2	B	1224	<div> <div>65%</div> <div>90%</div> <div>10%</div> </div>
3	C	318	<div> <div>61%</div> <div>84%</div> <div>16%</div> </div>
4	D	221	<div> <div>39%</div> <div>60%</div> <div>39%</div> </div>
5	E	215	<div> <div>66%</div> <div>99%</div> <div>.</div> </div>
6	F	155	<div> <div>43%</div> <div>54%</div> <div>46%</div> </div>
7	G	171	<div> <div>69%</div> <div>99%</div> <div>.</div> </div>
8	H	146	<div> <div>60%</div> <div>91%</div> <div>9%</div> </div>
9	I	122	<div> <div>66%</div> <div>98%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
10	J	70	<div><div></div><div>73%93%7%</div></div>
11	K	120	<div><div></div><div>76%95%5%</div></div>
12	L	70	<div><div></div><div>41%66%34%</div></div>
13	S	309	<div><div></div><div>41%54%44%</div></div>

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 (three-letter code: MG) (formula: Mg).

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

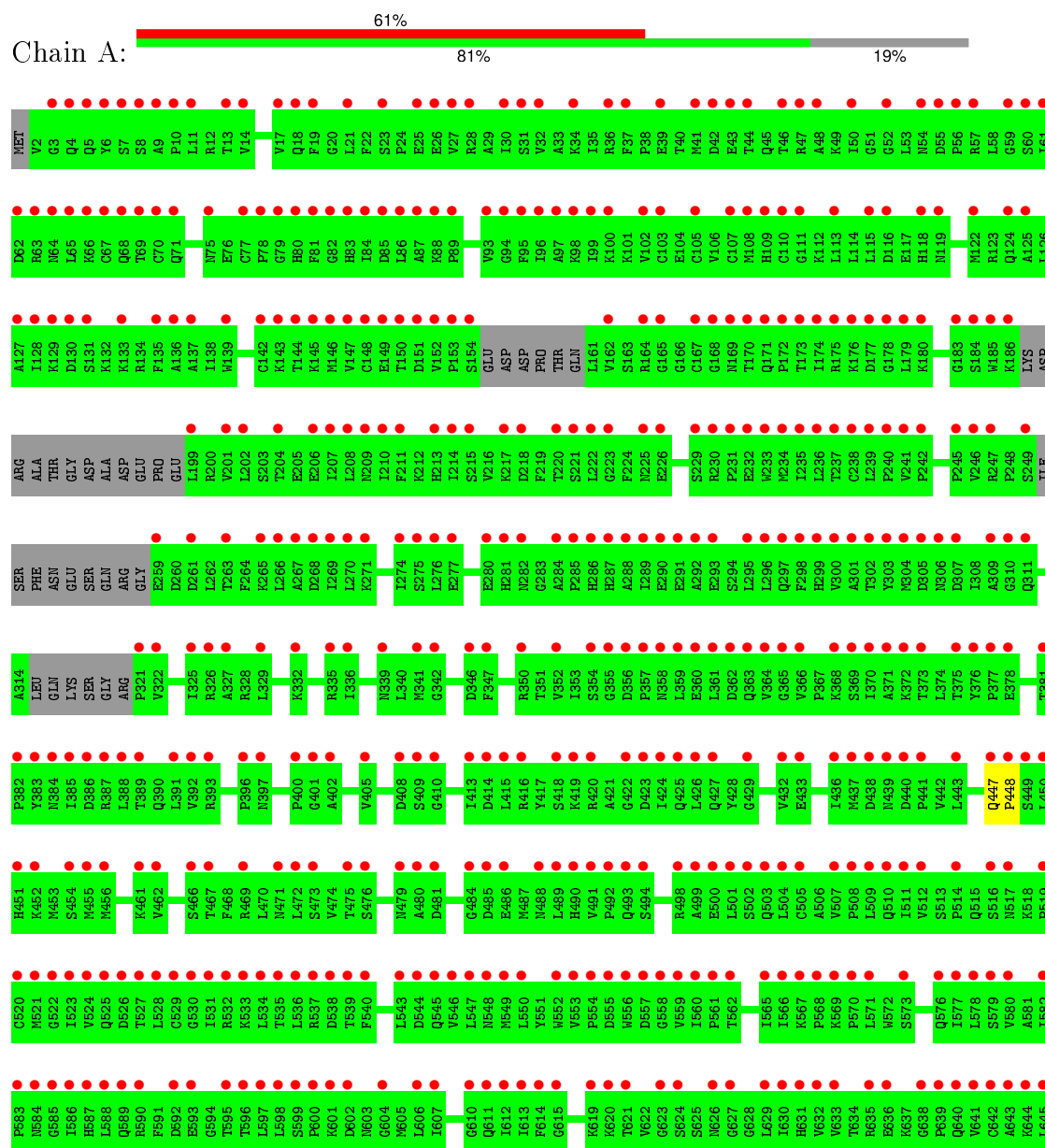
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

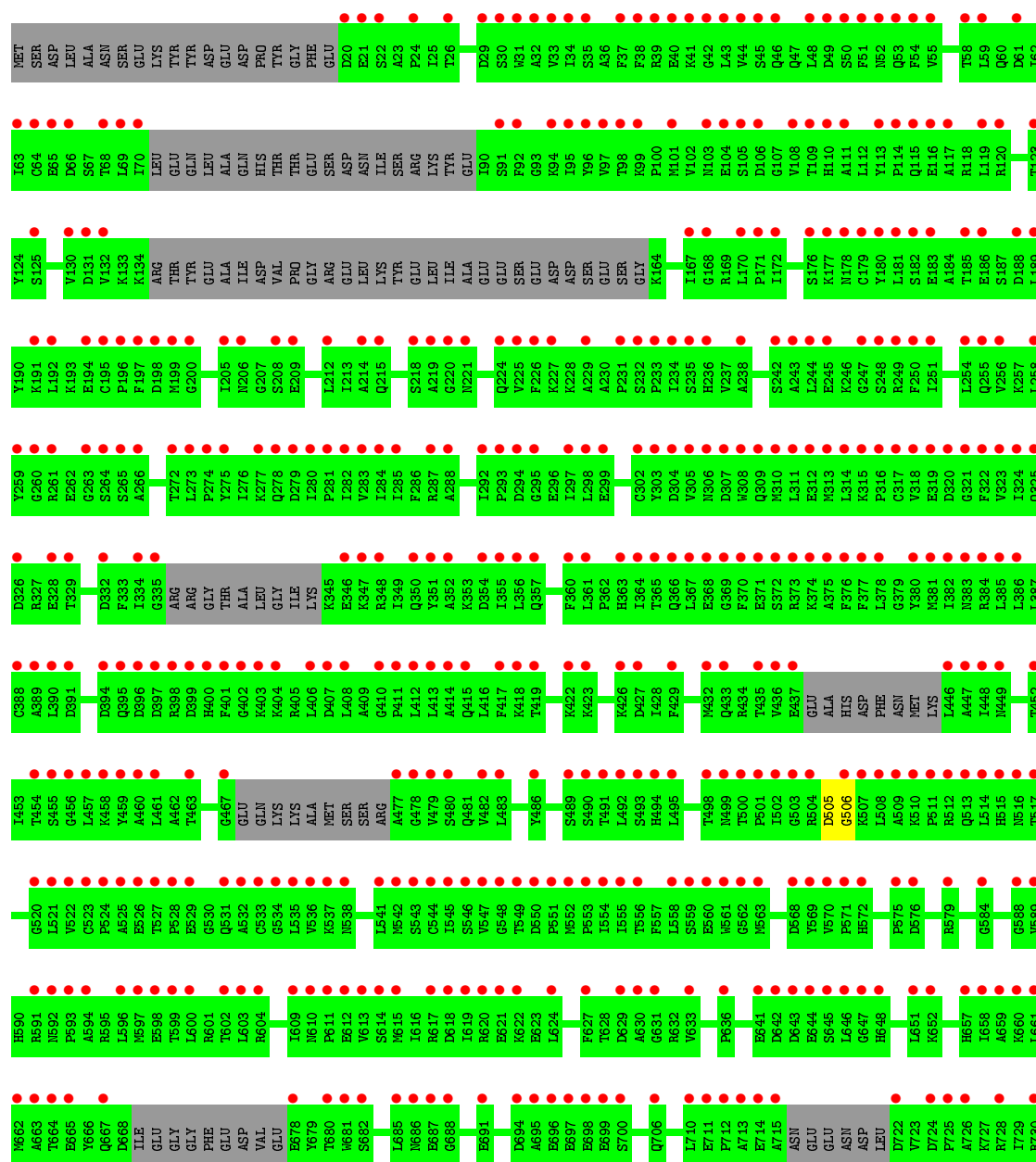
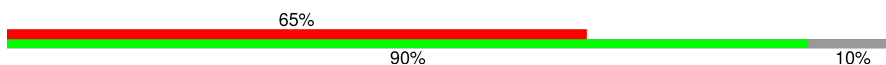
- Molecule 1: DNA-directed RNA polymerase II largest subunit

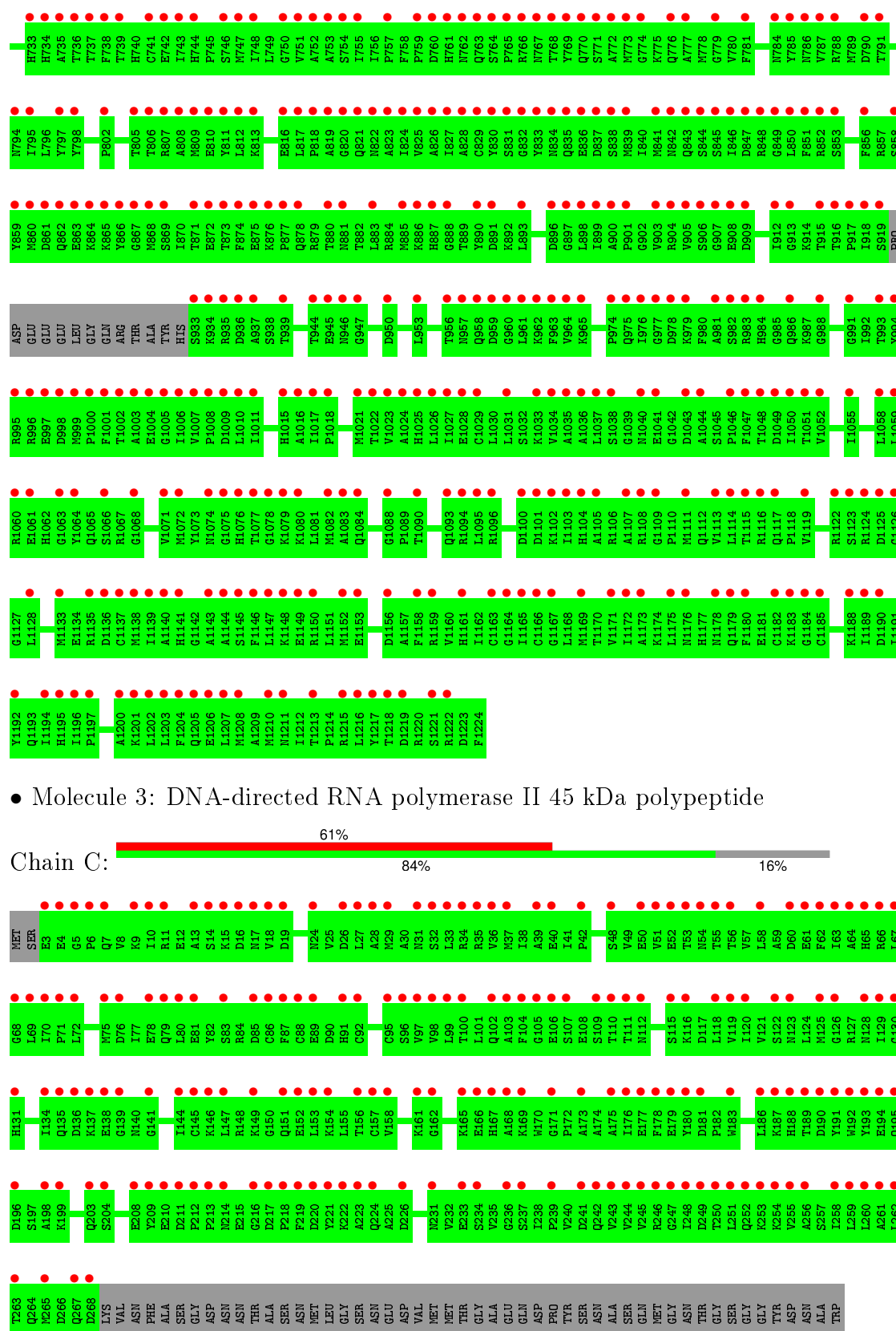


WORLDWIDE
PDB
PROTEIN DATA BANK

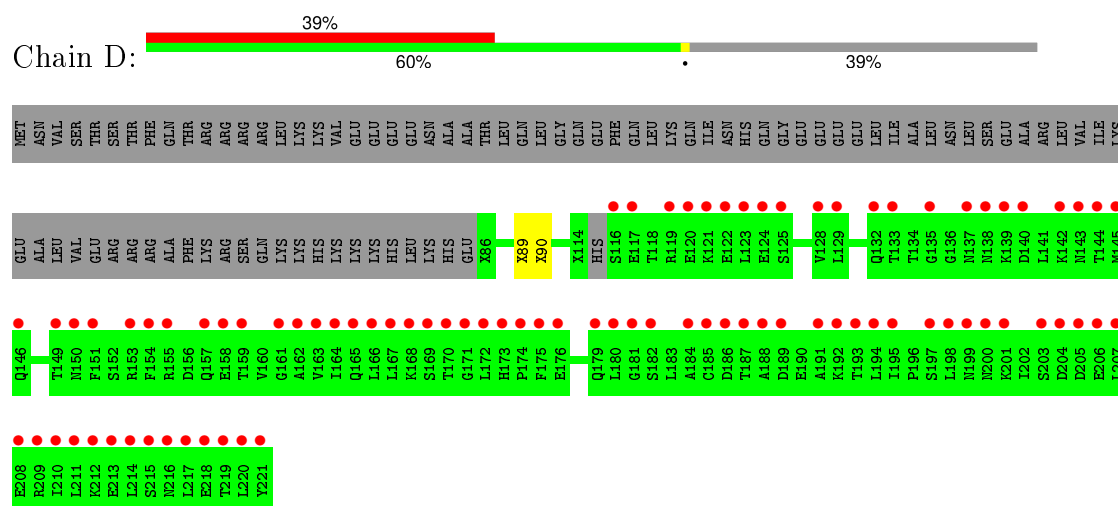
LYS
GLN
ASP
GLU
GLN
LYS
HIS
ASN
GLU
ASN
GLU
ASN
SER
ARG

Chain B:

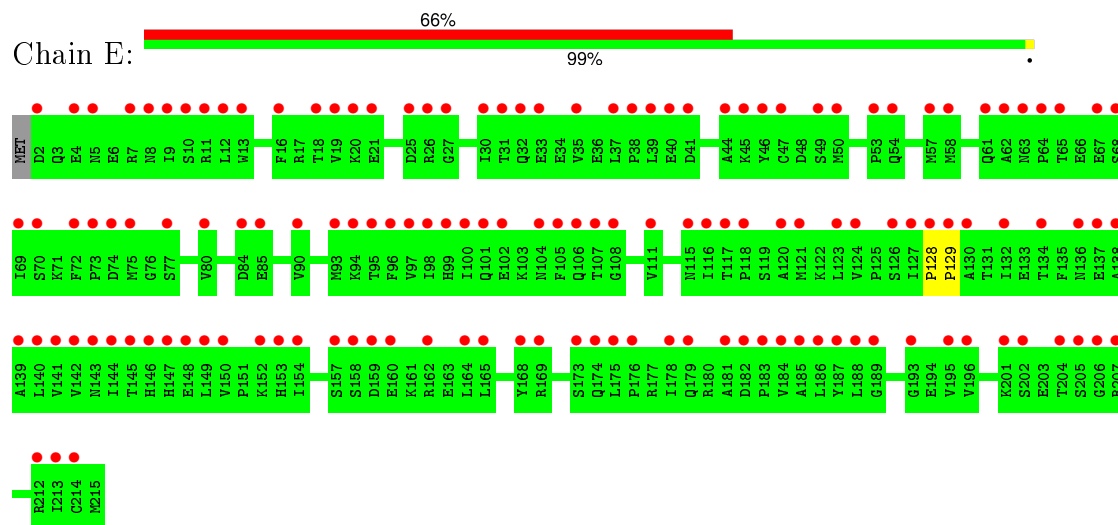




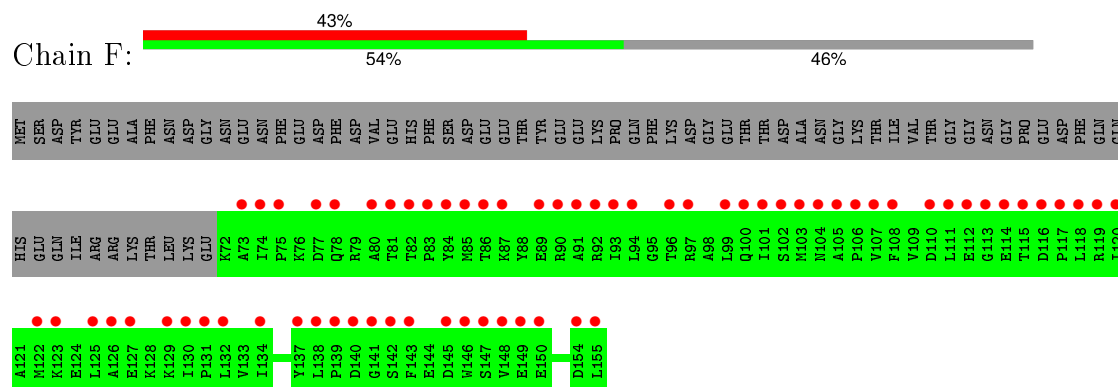
- Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide



- Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

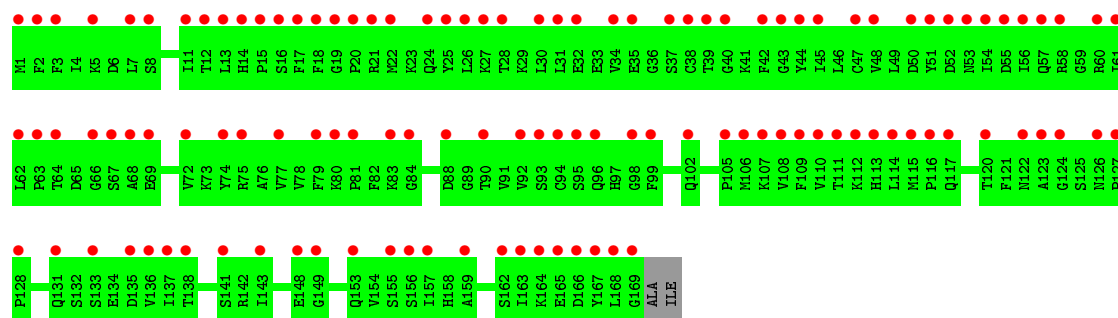


- Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

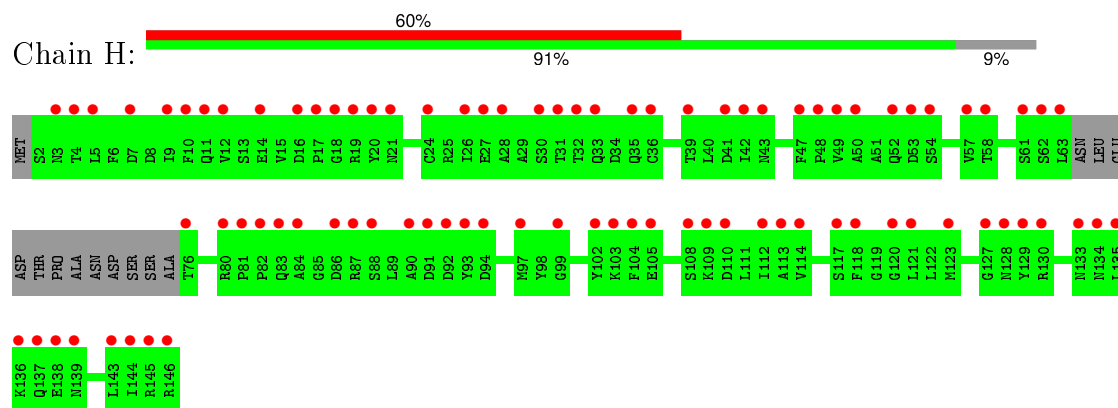


- Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

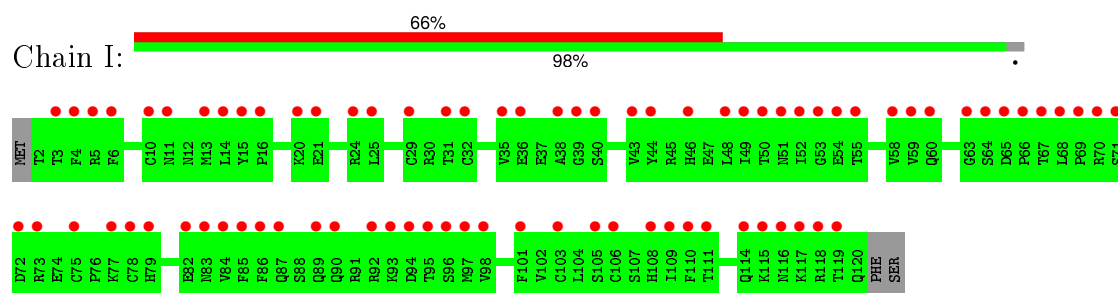




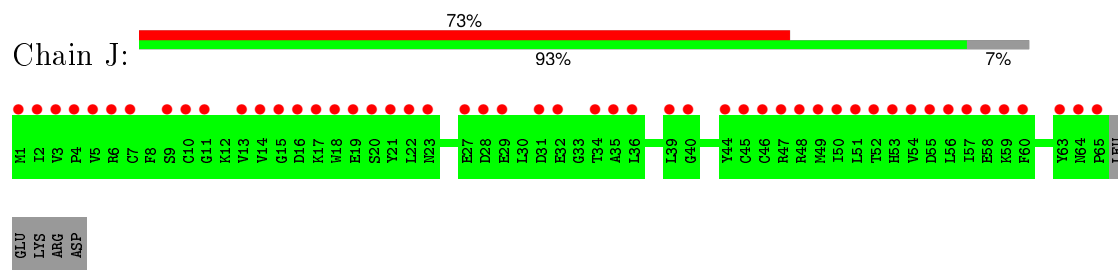
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



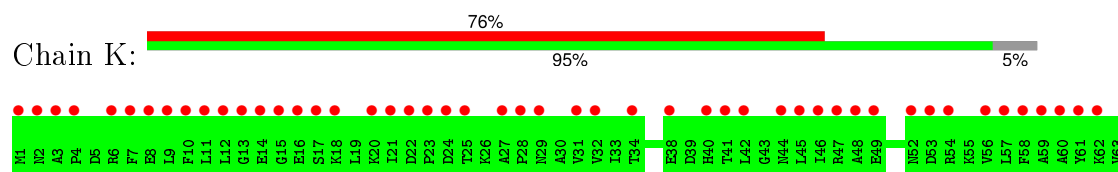
- Molecule 9: DNA-directed RNA polymerase II 14.2 kDa polypeptide

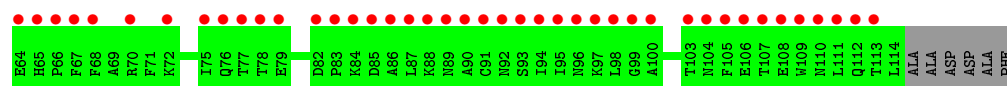


- Molecule 10: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide

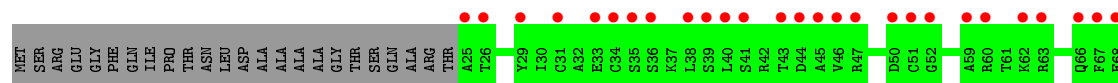
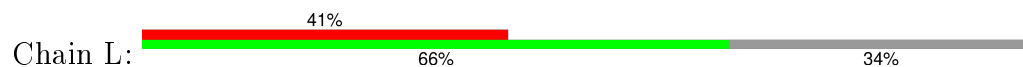


- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

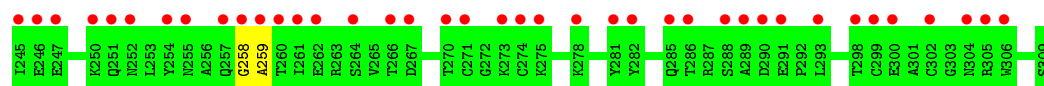
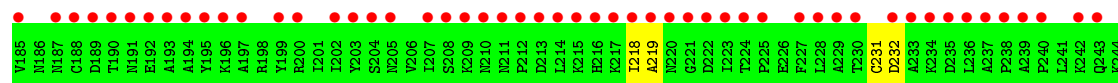
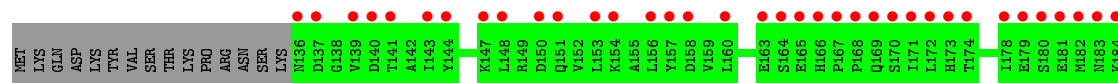




- Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



- Molecule 13: Transcription elongation factor S-II



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 49.41 – 3.79	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-3.80) 89.4 (49.41-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.77Å)	Xtriage
Refinement program	O	Depositor
R, R_{free}	(Not available) , (Not available) 0.464 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	93.6	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 91.3	EDS
Estimated twinning fraction	0.013 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.022 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 115467 reflections	Xtriage
F_o, F_c correlation	0.62	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 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 carbohydrates 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%)	4.65	1052 (74%)  	30, 30, 30, 30	0
2	B	1103/1224 (90%)	4.82	793 (71%)  	30, 30, 30, 30	0
3	C	266/318 (83%)	4.65	194 (72%)  	30, 30, 30, 30	0
4	D	106/221 (47%)	6.19	87 (82%)  	30, 30, 30, 30	0
5	E	214/215 (99%)	4.32	141 (65%)  	30, 30, 30, 30	0
6	F	84/155 (54%)	5.40	67 (79%)  	30, 30, 30, 30	0
7	G	169/171 (98%)	5.60	118 (69%)  	30, 30, 30, 30	0
8	H	133/146 (91%)	4.99	87 (65%)  	30, 30, 30, 30	0
9	I	119/122 (97%)	5.63	80 (67%)  	30, 30, 30, 30	0
10	J	65/70 (92%)	5.73	51 (78%)  	30, 30, 30, 30	0
11	K	114/120 (95%)	5.26	91 (79%)  	30, 30, 30, 30	0
12	L	46/70 (65%)	5.06	29 (63%)  	30, 30, 30, 30	0
13	S	174/309 (56%)	4.97	127 (72%)  	30, 30, 30, 30	0
All	All	4002/4874 (82%)	4.87	2917 (72%)  	30, 30, 30, 30	0

All (2917) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	306	ASN	45.3
2	B	275	TYR	40.2
7	G	113	HIS	36.5
9	I	3	THR	34.4
1	A	1272	THR	33.5
12	L	26	THR	31.6
2	B	735	ALA	30.9
2	B	69	LEU	29.9
2	B	274	PRO	29.3

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Mol	Chain	Res	Type	RSRZ
9	I	51	ASN	28.4
2	B	568	ASP	27.7
5	E	138	ALA	27.6
1	A	423	ASP	26.9
10	J	65	PRO	26.7
1	A	1083	THR	26.6
8	H	90	ALA	25.0
9	I	72	ASP	24.5
1	A	420	ARG	23.6
2	B	515	HIS	23.5
2	B	295	GLY	23.3
2	B	781	PHE	23.0
8	H	121	LEU	22.7
2	B	212	LEU	22.7
3	C	109	SER	22.2
5	E	115	ASN	22.1
13	S	189	ASP	22.0
1	A	555	ASP	22.0
1	A	1320	PRO	21.8
4	D	158	GLU	21.5
8	H	48	PRO	21.5
1	A	214	ILE	21.4
9	I	97	MET	21.3
9	I	58	VAL	21.3
2	B	1108	ARG	21.2
1	A	560	ILE	21.1
3	C	56	THR	21.0
8	H	87	ARG	20.9
7	G	165	GLU	20.7
6	F	115	THR	20.7
13	S	290	ASP	20.6
2	B	279	ASP	20.5
13	S	237	ALA	20.4
13	S	137	ASP	20.4
1	A	64	ASN	20.3
11	K	84	LYS	20.3
9	I	96	SER	20.2
1	A	1186	ASP	20.2
3	C	211	ASP	20.1
1	A	537	ARG	20.0
1	A	1129	GLU	20.0
1	A	702	LEU	20.0

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Mol	Chain	Res	Type	RSRZ
4	D	137	ASN	19.9
2	B	293	PRO	19.9
7	G	18	PHE	19.8
2	B	860	MET	19.7
1	A	955	PRO	19.7
2	B	1190	ASP	19.6
13	S	143	ILE	19.5
2	B	320	ASP	19.5
7	G	28	THR	19.3
10	J	64	ASN	19.2
2	B	886	LYS	19.0
3	C	217	ASP	18.9
1	A	170	THR	18.9
9	I	52	ILE	18.8
2	B	597	MET	18.7
1	A	115	LEU	18.5
2	B	1211	ASN	18.5
1	A	437	MET	18.2
3	C	224	GLN	18.1
1	A	171	GLN	18.1
7	G	96	GLN	18.0
4	D	207	LEU	17.9
4	D	180	LEU	17.9
7	G	31	LEU	17.8
2	B	200	GLY	17.7
8	H	31	THR	17.6
2	B	509	ALA	17.6
2	B	786	ASN	17.5
8	H	4	THR	17.5
1	A	1257	ASP	17.4
4	D	201	LYS	17.4
1	A	108	MET	17.4
4	D	214	LEU	17.3
11	K	25	THR	17.3
4	D	211	LEU	17.3
7	G	135	ASP	17.3
1	A	582	ILE	17.3
2	B	171	PRO	17.2
2	B	334	ILE	17.2
1	A	1112	LYS	17.0
1	A	88	LYS	17.0
3	C	194	GLU	17.0

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Mol	Chain	Res	Type	RSRZ
1	A	103	CYS	17.0
4	D	210	ILE	16.9
13	S	222	ASP	16.9
9	I	78	CYS	16.8
7	G	63	PRO	16.8
13	S	172	LEU	16.5
1	A	215	SER	16.5
3	C	26	ASP	16.5
1	A	996	ASN	16.5
5	E	73	PRO	16.4
11	K	52	ASN	16.3
2	B	533	CYS	16.3
1	A	568	PRO	16.3
12	L	41	SER	16.1
6	F	107	VAL	16.1
2	B	816	GLU	16.0
2	B	711	GLU	16.0
8	H	129	TYR	15.9
8	H	53	ASP	15.9
8	H	35	GLN	15.8
8	H	80	ARG	15.8
2	B	836	GLU	15.7
7	G	120	THR	15.7
2	B	501	PRO	15.7
2	B	546	SER	15.7
4	D	172	LEU	15.6
2	B	354	ASP	15.6
2	B	661	LEU	15.6
11	K	68	PHE	15.6
1	A	1158	PRO	15.5
2	B	525	ALA	15.5
1	A	1254	ALA	15.5
2	B	1048	THR	15.5
7	G	88	ASP	15.5
2	B	866	TYR	15.4
2	B	313	MET	15.3
2	B	554	ILE	15.3
12	L	51	CYS	15.2
2	B	328	GLU	15.2
6	F	82	THR	15.1
2	B	642	ASP	15.0
1	A	597	LEU	15.0

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Mol	Chain	Res	Type	RSRZ
2	B	432	MET	15.0
13	S	166	HIS	15.0
11	K	79	GLU	15.0
10	J	51	LEU	14.9
7	G	167	TYR	14.9
1	A	36	ARG	14.9
10	J	45	CYS	14.8
7	G	117	GLN	14.8
2	B	724	ASP	14.8
2	B	278	GLN	14.7
1	A	1315	GLU	14.7
6	F	75	PRO	14.6
2	B	504	ARG	14.6
7	G	16	SER	14.5
2	B	285	ILE	14.5
1	A	540	PHE	14.5
7	G	74	TYR	14.4
2	B	1210	MET	14.4
1	A	738	LYS	14.4
4	D	150	ASN	14.4
5	E	84	ASP	14.3
1	A	1390	ASN	14.3
2	B	502	ILE	14.2
1	A	1163	ILE	14.1
2	B	68	THR	14.1
2	B	837	ASP	14.1
2	B	371	GLU	14.1
5	E	85	GLU	14.1
6	F	154	ASP	14.1
7	G	40	GLY	14.0
2	B	570	VAL	14.0
4	D	162	ALA	14.0
1	A	382	PRO	13.9
2	B	97	VAL	13.9
2	B	592	ASN	13.9
1	A	179	LEU	13.9
2	B	411	PRO	13.9
8	H	81	PRO	13.9
11	K	67	PHE	13.9
1	A	583	PRO	13.9
1	A	1231	ASP	13.8
9	I	110	PHE	13.8

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Mol	Chain	Res	Type	RSRZ
1	A	558	GLY	13.8
1	A	1233	ASP	13.8
2	B	192	LEU	13.7
1	A	736	ASN	13.7
9	I	53	GLY	13.7
10	J	10	CYS	13.7
1	A	1216	ILE	13.7
1	A	282	ASN	13.6
1	A	672	ASP	13.6
2	B	798	TYR	13.5
2	B	61	ASP	13.5
5	E	139	ALA	13.5
2	B	64	CYS	13.5
1	A	791	ASP	13.4
8	H	135	LEU	13.4
7	G	12	THR	13.4
7	G	52	ASP	13.4
5	E	5	ASN	13.4
7	G	55	ASP	13.4
7	G	27	LYS	13.4
1	A	1298	TYR	13.3
11	K	2	ASN	13.3
1	A	767	GLN	13.2
4	D	219	THR	13.2
4	D	125	SER	13.2
2	B	206	ASN	13.2
1	A	1162	VAL	13.1
11	K	9	LEU	13.1
13	S	169	GLN	13.1
7	G	22	MET	13.1
2	B	919	SER	13.1
2	B	725	PRO	13.1
2	B	277	LYS	13.0
4	D	122	GLU	13.0
3	C	75	MET	13.0
1	A	1324	PRO	13.0
2	B	529	GLU	13.0
1	A	1085	HIS	12.9
6	F	112	GLU	12.9
5	E	53	PRO	12.9
8	H	7	ASP	12.9
7	G	81	PRO	12.8

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Mol	Chain	Res	Type	RSRZ
10	J	50	ILE	12.8
3	C	203	GLN	12.8
13	S	153	LEU	12.8
2	B	292	ILE	12.8
1	A	358	ASN	12.7
10	J	13	VAL	12.7
8	H	49	VAL	12.7
3	C	131	HIS	12.6
1	A	1377	THR	12.6
2	B	747	MET	12.6
13	S	171	ILE	12.6
2	B	698	GLU	12.6
6	F	130	ILE	12.6
1	A	285	PRO	12.6
2	B	542	MET	12.6
4	D	144	THR	12.6
2	B	614	SER	12.6
1	A	1333	ILE	12.5
2	B	26	THR	12.5
2	B	759	PRO	12.5
3	C	88	CYS	12.5
5	E	126	SER	12.5
2	B	1169	MET	12.5
2	B	736	THR	12.4
8	H	109	LYS	12.4
1	A	786	HIS	12.4
1	A	525	GLN	12.4
2	B	722	ASP	12.4
1	A	1421	CYS	12.3
6	F	108	PHE	12.3
2	B	65	GLU	12.3
1	A	853	ASP	12.2
1	A	1105	LEU	12.2
2	B	812	LEU	12.2
7	G	47	CYS	12.2
1	A	1210	GLY	12.2
2	B	937	ALA	12.2
1	A	362	ASP	12.2
5	E	49	SER	12.2
9	I	10	CYS	12.2
2	B	324	ILE	12.2
2	B	524	PRO	12.2

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Mol	Chain	Res	Type	RSRZ
1	A	1230	GLU	12.1
6	F	93	ILE	12.1
1	A	302	THR	12.1
1	A	670	ILE	12.1
7	G	24	GLN	12.0
4	D	215	SER	12.0
1	A	1228	TRP	12.0
3	C	95	CYS	12.0
10	J	40	GLY	12.0
1	A	781	ASP	12.0
1	A	234	MET	12.0
11	K	64	GLU	12.0
1	A	549	MET	12.0
1	A	110	CYS	12.0
5	E	38	PRO	11.9
1	A	909	ASP	11.9
7	G	108	VAL	11.9
4	D	142	LYS	11.9
6	F	110	ASP	11.9
2	B	768	THR	11.8
4	D	133	THR	11.8
11	K	92	ASN	11.8
3	C	204	SER	11.8
12	L	63	ARG	11.8
5	E	50	MET	11.8
1	A	815	PHE	11.8
1	A	538	ASP	11.7
1	A	70	CYS	11.7
5	E	7	ARG	11.7
9	I	83	ASN	11.7
2	B	297	ILE	11.7
1	A	400	PRO	11.7
2	B	317	CYS	11.7
5	E	104	ASN	11.7
1	A	266	LEU	11.7
2	B	96	TYR	11.6
1	A	4	GLN	11.6
3	C	262	LEU	11.6
3	C	125	MET	11.6
3	C	256	ALA	11.6
2	B	95	ILE	11.5
2	B	1052	VAL	11.5

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Mol	Chain	Res	Type	RSRZ
3	C	192	TRP	11.5
1	A	1082	ASN	11.5
2	B	305	VAL	11.4
1	A	820	GLY	11.4
1	A	239	LEU	11.4
5	E	149	LEU	11.4
2	B	123	THR	11.4
2	B	678	GLU	11.4
2	B	547	VAL	11.4
4	D	140	ASP	11.3
2	B	369	GLY	11.3
1	A	1124	HIS	11.3
1	A	600	PRO	11.3
2	B	251	ILE	11.3
3	C	72	LEU	11.3
3	C	60	ASP	11.3
2	B	183	GLU	11.3
10	J	39	LEU	11.3
1	A	52	GLY	11.3
2	B	763	GLN	11.3
1	A	959	ASN	11.3
1	A	758	ILE	11.3
1	A	728	LYS	11.3
2	B	802	PRO	11.2
1	A	1028	THR	11.2
1	A	231	PRO	11.2
7	G	19	GLY	11.1
1	A	1200	ALA	11.1
13	S	234	LYS	11.1
2	B	900	ALA	11.1
2	B	224	GLN	11.1
2	B	613	VAL	11.1
13	S	180	SER	11.1
5	E	69	ILE	11.1
2	B	199	MET	11.1
13	S	163	GLU	11.1
5	E	13	TRP	11.1
1	A	978	PRO	11.1
8	H	136	LYS	11.1
2	B	752	ALA	11.1
11	K	85	ASP	11.0
1	A	94	GLY	11.0

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Mol	Chain	Res	Type	RSRZ
1	A	755	PHE	11.0
1	A	1157	ASP	11.0
1	A	1074	GLU	11.0
9	I	118	ARG	11.0
2	B	188	ASP	11.0
2	B	329	THR	11.0
1	A	930	ASP	11.0
8	H	58	THR	11.0
1	A	1317	MET	11.0
4	D	164	ILE	11.0
3	C	29	MET	10.9
2	B	514	LEU	10.9
4	D	200	ASN	10.9
2	B	248	SER	10.9
13	S	262	GLU	10.9
2	B	1185	CYS	10.9
2	B	433	GLN	10.9
1	A	974	ASP	10.8
2	B	24	PRO	10.8
7	G	105	PRO	10.8
13	S	178	ILE	10.8
1	A	450	LEU	10.8
9	I	106	CYS	10.8
10	J	58	GLU	10.8
1	A	290	GLU	10.8
1	A	557	ASP	10.8
1	A	1048	ASN	10.7
1	A	75	ASN	10.7
2	B	831	SER	10.7
1	A	61	ILE	10.6
1	A	678	GLU	10.6
1	A	396	PRO	10.6
2	B	399	ASP	10.6
9	I	32	CYS	10.6
2	B	218	SER	10.6
1	A	615	GLY	10.6
2	B	304	ASP	10.6
3	C	253	LYS	10.6
7	G	26	LEU	10.6
1	A	476	SER	10.6
1	A	953	ASN	10.6
1	A	480	ALA	10.5

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Mol	Chain	Res	Type	RSRZ
3	C	130	GLY	10.5
12	L	33	GLU	10.5
1	A	656	TRP	10.5
2	B	571	PRO	10.5
5	E	146	HIS	10.5
5	E	12	LEU	10.5
11	K	4	PRO	10.5
7	G	123	ALA	10.5
8	H	88	SER	10.5
1	A	1295	THR	10.5
11	K	29	ASN	10.5
1	A	288	ALA	10.5
5	E	39	LEU	10.5
3	C	191	TYR	10.4
6	F	139	PRO	10.4
2	B	456	GLY	10.4
2	B	787	VAL	10.4
12	L	62	LYS	10.4
2	B	1104	HIS	10.4
1	A	569	LYS	10.4
1	A	970	THR	10.4
2	B	20	ASP	10.4
1	A	7	SER	10.4
2	B	869	SER	10.4
2	B	1047	PHE	10.4
7	G	126	ASN	10.4
1	A	1138	ILE	10.4
11	K	13	GLY	10.3
9	I	29	CYS	10.3
6	F	77	ASP	10.3
2	B	1038	SER	10.3
1	A	826	ASP	10.3
2	B	593	PRO	10.3
2	B	167	ILE	10.3
9	I	116	ASN	10.3
1	A	717	ASN	10.2
1	A	438	ASP	10.2
3	C	212	PRO	10.2
8	H	19	ARG	10.2
1	A	873	MET	10.2
2	B	774	GLY	10.2
5	E	143	ASN	10.2

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Mol	Chain	Res	Type	RSRZ
1	A	854	ASN	10.2
1	A	949	ASP	10.2
9	I	55	THR	10.1
9	I	103	CYS	10.1
2	B	611	PRO	10.1
13	S	282	TYR	10.1
2	B	790	ASP	10.1
4	D	218	GLU	10.1
5	E	173	SER	10.1
7	G	35	GLU	10.1
11	K	14	GLU	10.1
5	E	40	GLU	10.1
2	B	452	THR	10.1
5	E	140	LEU	10.1
2	B	503	GLY	10.1
3	C	92	CYS	10.0
2	B	975	GLN	10.0
3	C	190	ASP	10.0
5	E	16	PHE	10.0
3	C	17	ASN	10.0
3	C	110	THR	10.0
1	A	425	GLN	10.0
12	L	39	SER	10.0
2	B	712	PRO	10.0
5	E	19	VAL	10.0
2	B	1195	HIS	10.0
1	A	178	GLY	10.0
5	E	124	VAL	10.0
1	A	1439	GLY	10.0
13	S	209	LYS	9.9
2	B	315	LYS	9.9
13	S	148	LEU	9.9
1	A	1255	GLU	9.9
3	C	10	ILE	9.9
2	B	699	GLU	9.9
1	A	43	GLU	9.8
13	S	260	THR	9.8
3	C	33	LEU	9.8
1	A	1361	SER	9.8
13	S	167	PRO	9.8
2	B	356	LEU	9.8
7	G	106	MET	9.8

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Mol	Chain	Res	Type	RSRZ
1	A	1154	TYR	9.8
5	E	159	ASP	9.7
3	C	6	PRO	9.7
1	A	1084	PHE	9.7
1	A	859	SER	9.7
2	B	1123	SER	9.7
4	D	186	ASP	9.7
2	B	730	ARG	9.6
1	A	1325	THR	9.6
1	A	383	TYR	9.6
1	A	1090	ALA	9.6
1	A	1359	ASP	9.6
1	A	565	ILE	9.6
11	K	22	ASP	9.6
2	B	170	LEU	9.6
1	A	1208	THR	9.6
1	A	199	LEU	9.6
2	B	412	LEU	9.6
13	S	193	ALA	9.6
13	S	224	THR	9.6
1	A	118	HIS	9.6
9	I	115	LYS	9.6
1	A	745	GLN	9.6
2	B	843	GLN	9.5
1	A	1382	THR	9.5
2	B	401	PHE	9.5
1	A	481	ASP	9.5
1	A	694	THR	9.5
6	F	126	ALA	9.5
1	A	801	GLU	9.5
4	D	195	ILE	9.5
2	B	347	LYS	9.5
3	C	118	LEU	9.5
1	A	1235	LYS	9.5
7	G	155	SER	9.5
8	H	17	PRO	9.5
3	C	208	GLU	9.5
12	L	50	ASP	9.4
7	G	13	LEU	9.4
1	A	707	GLY	9.4
1	A	1001	ARG	9.4
1	A	218	ASP	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	41	MET	9.4
1	A	680	THR	9.4
2	B	576	ASP	9.4
11	K	86	ALA	9.4
1	A	62	ASP	9.3
3	C	123	ASN	9.3
3	C	86	CYS	9.3
1	A	23	SER	9.3
2	B	1124	ARG	9.3
1	A	54	ASN	9.3
7	G	51	TYR	9.3
1	A	310	GLY	9.3
2	B	168	GLY	9.3
6	F	149	GLU	9.3
2	B	382	ILE	9.3
1	A	6	TYR	9.3
2	B	819	ALA	9.3
1	A	1059	HIS	9.3
8	H	134	ASN	9.2
4	D	149	THR	9.2
6	F	84	TYR	9.2
2	B	905	VAL	9.2
1	A	887	GLY	9.2
1	A	1145	SER	9.2
2	B	552	MET	9.2
1	A	436	ILE	9.2
3	C	3	GLU	9.2
2	B	449	ASN	9.2
3	C	189	THR	9.2
1	A	409	SER	9.2
1	A	494	SER	9.1
13	S	203	TYR	9.1
1	A	877	HIS	9.1
11	K	89	ASN	9.1
1	A	369	SER	9.1
2	B	427	ASP	9.1
13	S	289	ALA	9.1
5	E	2	ASP	9.0
1	A	1113	THR	9.0
7	G	25	TYR	9.0
2	B	180	TYR	9.0
5	E	204	THR	9.0

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Mol	Chain	Res	Type	RSRZ
7	G	7	LEU	9.0
1	A	1111	MET	9.0
2	B	746	SER	9.0
5	E	153	HIS	9.0
13	S	220	ASN	9.0
2	B	364	ILE	9.0
2	B	198	ASP	9.0
3	C	210	GLU	9.0
13	S	217	LYS	9.0
1	A	905	ASP	9.0
1	A	1072	ILE	9.0
2	B	862	GLN	8.9
2	B	106	ASP	8.9
2	B	298	LEU	8.9
1	A	475	THR	8.9
3	C	67	LEU	8.9
6	F	119	ARG	8.9
10	J	15	GLY	8.9
1	A	695	LYS	8.9
2	B	646	LEU	8.9
1	A	276	LEU	8.9
1	A	174	ILE	8.8
1	A	1010	ALA	8.8
5	E	152	LYS	8.8
2	B	250	PHE	8.8
1	A	807	GLY	8.8
5	E	74	ASP	8.8
2	B	499	ASN	8.8
4	D	193	THR	8.8
1	A	919	ILE	8.8
9	I	93	LYS	8.8
1	A	1347	ALA	8.8
1	A	843	LYS	8.8
9	I	44	TYR	8.8
9	I	64	SER	8.8
5	E	96	PHE	8.7
2	B	569	TYR	8.7
9	I	39	GLY	8.7
1	A	1453	TYR	8.7
1	A	1076	ALA	8.7
1	A	113	LEU	8.7
9	I	60	GLN	8.7

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Mol	Chain	Res	Type	RSRZ
3	C	134	ILE	8.7
2	B	325	GLN	8.7
9	I	59	VAL	8.7
8	H	86	ASP	8.7
9	I	4	PHE	8.7
13	S	257	GLN	8.7
7	G	20	PRO	8.7
1	A	1242	VAL	8.7
11	K	11	LEU	8.7
1	A	392	VAL	8.7
2	B	43	LEU	8.6
13	S	214	LEU	8.6
2	B	791	THR	8.6
1	A	829	VAL	8.6
1	A	129	LYS	8.6
1	A	209	ASN	8.6
2	B	713	ALA	8.6
2	B	1149	GLU	8.6
2	B	457	LEU	8.6
11	K	109	TRP	8.6
1	A	77	CYS	8.6
1	A	1264	GLU	8.6
1	A	275	SER	8.5
3	C	186	LEU	8.5
1	A	732	LEU	8.5
13	S	144	TYR	8.5
1	A	1203	ASN	8.5
1	A	1316	VAL	8.5
3	C	180	TYR	8.5
1	A	419	LYS	8.5
1	A	589	GLN	8.5
2	B	221	ASN	8.5
10	J	46	CYS	8.5
2	B	105	SER	8.5
2	B	520	GLY	8.5
2	B	302	CYS	8.5
13	S	202	ILE	8.5
10	J	16	ASP	8.4
11	K	59	ALA	8.4
13	S	261	ILE	8.4
1	A	1040	GLN	8.4
1	A	673	GLY	8.4

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Mol	Chain	Res	Type	RSRZ
13	S	273	LYS	8.4
11	K	40	HIS	8.4
7	G	149	GLY	8.4
1	A	1077	THR	8.4
13	S	208	SER	8.4
2	B	437	GLU	8.4
11	K	113	THR	8.4
1	A	397	ASN	8.4
2	B	1125	ASP	8.4
8	H	110	ASP	8.4
2	B	917	PRO	8.3
10	J	6	ARG	8.3
7	G	138	THR	8.3
2	B	806	THR	8.3
2	B	414	ALA	8.3
1	A	1110	ASN	8.3
1	A	284	ALA	8.3
3	C	214	ASN	8.3
13	S	251	GLN	8.3
2	B	396	ASP	8.3
2	B	517	THR	8.3
2	B	744	HIS	8.3
4	D	181	GLY	8.3
8	H	47	PHE	8.3
2	B	859	TYR	8.3
1	A	1055	ARG	8.3
12	L	34	CYS	8.3
2	B	534	GLY	8.3
1	A	1448	GLU	8.2
13	S	168	PRO	8.2
11	K	112	GLN	8.2
13	S	221	GLY	8.2
10	J	3	VAL	8.2
11	K	49	GLU	8.2
2	B	435	THR	8.2
1	A	649	ILE	8.2
12	L	25	ALA	8.2
1	A	1341	ILE	8.2
1	A	1353	TYR	8.2
2	B	1114	LEU	8.2
7	G	45	ILE	8.2
1	A	833	GLU	8.2

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Mol	Chain	Res	Type	RSRZ
9	I	86	PHE	8.2
7	G	48	VAL	8.2
8	H	102	TYR	8.2
1	A	378	GLU	8.2
2	B	29	ASP	8.2
3	C	249	ASP	8.2
1	A	722	LEU	8.2
1	A	989	GLY	8.1
2	B	875	GLU	8.1
1	A	109	HIS	8.1
4	D	198	LEU	8.1
1	A	291	GLU	8.1
1	A	69	THR	8.1
2	B	346	GLU	8.1
1	A	1017	LEU	8.1
2	B	658	ILE	8.1
2	B	856	PHE	8.1
2	B	873	THR	8.1
1	A	1006	ILE	8.1
2	B	284	ILE	8.0
1	A	1213	GLY	8.0
2	B	939	THR	8.0
8	H	76	THR	8.0
6	F	143	PHE	8.0
13	S	164	SER	8.0
1	A	1219	THR	8.0
1	A	792	TYR	8.0
3	C	34	ARG	8.0
12	L	66	GLN	8.0
1	A	1000	LEU	8.0
2	B	1077	THR	8.0
1	A	862	ASN	8.0
13	S	218	ILE	8.0
2	B	1156	ASP	7.9
1	A	148	CYS	7.9
6	F	97	ARG	7.9
1	A	261	ASP	7.9
1	A	903	ASN	7.9
1	A	1116	LEU	7.9
1	A	714	PHE	7.9
1	A	167	CYS	7.9
2	B	312	GLU	7.9

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Mol	Chain	Res	Type	RSRZ
3	C	144	ILE	7.9
1	A	168	GLY	7.9
2	B	219	ALA	7.9
9	I	90	GLN	7.9
2	B	849	GLY	7.9
3	C	5	GLY	7.9
13	S	160	LEU	7.9
2	B	314	LEU	7.9
9	I	75	CYS	7.9
1	A	601	LYS	7.8
1	A	5	GLN	7.8
2	B	754	SER	7.8
1	A	274	ILE	7.8
1	A	1374	VAL	7.8
4	D	185	CYS	7.8
1	A	1277	GLU	7.8
2	B	657	HIS	7.8
1	A	834	THR	7.8
2	B	622	LYS	7.8
1	A	780	VAL	7.8
1	A	1127	ASP	7.8
7	G	164	LYS	7.8
3	C	91	HIS	7.8
1	A	1161	THR	7.8
2	B	114	PRO	7.7
7	G	30	LEU	7.7
1	A	965	GLN	7.7
1	A	201	VAL	7.7
3	C	209	TYR	7.7
2	B	830	TYR	7.7
3	C	176	ILE	7.7
2	B	417	PHE	7.7
4	D	184	ALA	7.7
1	A	472	LEU	7.7
2	B	619	ILE	7.7
2	B	1050	ILE	7.7
10	J	52	THR	7.7
13	S	196	LYS	7.7
1	A	1215	ARG	7.7
1	A	1292	PRO	7.7
1	A	971	PHE	7.7
10	J	27	GLU	7.7

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Mol	Chain	Res	Type	RSRZ
11	K	15	GLY	7.7
2	B	448	ILE	7.7
2	B	665	GLU	7.6
2	B	1202	LEU	7.6
11	K	110	ASN	7.6
5	E	158	SER	7.6
2	B	621	GLU	7.6
2	B	1063	GLY	7.6
1	A	37	PHE	7.6
6	F	102	SER	7.6
1	A	580	VAL	7.6
1	A	286	HIS	7.6
2	B	288	ALA	7.6
1	A	735	VAL	7.6
2	B	1216	LEU	7.6
7	G	34	VAL	7.6
2	B	647	GLY	7.6
1	A	1012	ARG	7.6
2	B	1189	ILE	7.6
9	I	48	LEU	7.6
8	H	54	SER	7.5
2	B	308	TRP	7.5
1	A	1122	PRO	7.5
1	A	1065	GLY	7.5
8	H	50	ALA	7.5
1	A	1184	SER	7.5
9	I	40	SER	7.5
11	K	54	ARG	7.5
2	B	961	LEU	7.5
8	H	32	THR	7.5
8	H	28	ALA	7.5
1	A	99	ILE	7.5
1	A	935	GLN	7.5
1	A	1269	GLU	7.5
1	A	992	ASP	7.5
2	B	332	ASP	7.5
5	E	106	GLN	7.5
6	F	94	LEU	7.5
11	K	53	ASP	7.5
1	A	742	ASN	7.5
2	B	1035	ALA	7.5
3	C	222	LYS	7.5

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Mol	Chain	Res	Type	RSRZ
6	F	104	ASN	7.4
1	A	1130	GLN	7.4
1	A	705	LYS	7.4
2	B	429	PHE	7.4
1	A	413	ILE	7.4
1	A	1397	LEU	7.4
2	B	1031	LEU	7.4
2	B	350	GLN	7.4
3	C	62	PHE	7.4
10	J	36	LEU	7.4
3	C	63	ILE	7.4
1	A	347	PHE	7.4
2	B	773	MET	7.4
7	G	50	ASP	7.4
1	A	709	THR	7.4
5	E	145	THR	7.4
1	A	1101	LEU	7.4
2	B	1221	SER	7.4
12	L	31	CYS	7.4
2	B	1166	CYS	7.3
11	K	98	LEU	7.3
2	B	299	GLU	7.3
2	B	1136	ASP	7.3
2	B	455	SER	7.3
2	B	531	GLN	7.3
1	A	1232	ASN	7.3
1	A	986	ILE	7.3
2	B	1138	MET	7.3
13	S	267	ASP	7.3
1	A	105	CYS	7.3
7	G	56	ILE	7.3
13	S	298	THR	7.2
4	D	191	ALA	7.2
3	C	78	GLU	7.2
5	E	32	GLN	7.2
2	B	42	GLY	7.2
2	B	559	SER	7.2
8	H	83	GLN	7.2
2	B	1147	LEU	7.2
2	B	389	ALA	7.2
1	A	683	ILE	7.2
1	A	447	GLN	7.2

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Mol	Chain	Res	Type	RSRZ
1	A	969	GLN	7.2
8	H	118	PHE	7.2
1	A	1079	MET	7.2
2	B	652	LYS	7.2
4	D	161	GLY	7.2
5	E	179	GLN	7.2
6	F	127	GLU	7.2
1	A	1205	LYS	7.2
13	S	204	SER	7.2
6	F	131	PRO	7.2
1	A	298	PHE	7.2
4	D	199	ASN	7.2
1	A	1166	ASP	7.2
2	B	739	THR	7.2
1	A	1052	GLN	7.1
4	D	167	LEU	7.1
1	A	1132	LYS	7.1
4	D	204	ASP	7.1
12	L	44	ASP	7.1
1	A	491	VAL	7.1
2	B	256	VAL	7.1
3	C	244	VAL	7.1
1	A	1342	GLU	7.1
1	A	1435	PRO	7.1
2	B	120	ARG	7.1
2	B	1137	CYS	7.1
5	E	184	VAL	7.1
1	A	1131	ALA	7.1
13	S	179	GLU	7.1
13	S	266	THR	7.1
9	I	68	LEU	7.1
10	J	20	SER	7.1
1	A	287	HIS	7.1
2	B	178	ASN	7.1
2	B	934	LYS	7.1
7	G	43	GLY	7.1
6	F	123	LYS	7.1
5	E	101	GLN	7.1
2	B	751	VAL	7.1
2	B	627	PHE	7.1
1	A	226	GLU	7.1
2	B	864	LYS	7.1

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Mol	Chain	Res	Type	RSRZ
11	K	8	GLU	7.1
1	A	645	LEU	7.0
9	I	38	ALA	7.0
1	A	1429	ILE	7.0
2	B	181	LEU	7.0
2	B	493	SER	7.0
2	B	618	ASP	7.0
2	B	912	ILE	7.0
2	B	1036	ALA	7.0
2	B	22	SER	7.0
1	A	860	LEU	7.0
1	A	31	SER	7.0
4	D	203	SER	7.0
1	A	1143	LEU	7.0
1	A	698	GLN	7.0
3	C	58	LEU	7.0
3	C	255	VAL	7.0
8	H	117	SER	7.0
11	K	3	ALA	7.0
1	A	499	ALA	7.0
1	A	185	TRP	7.0
2	B	232	SER	7.0
1	A	1173	HIS	7.0
10	J	5	VAL	7.0
1	A	756	ILE	7.0
2	B	946	ASN	6.9
10	J	17	LYS	6.9
2	B	233	PRO	6.9
13	S	225	PRO	6.9
4	D	176	GLU	6.9
1	A	309	ALA	6.9
2	B	891	ASP	6.9
2	B	811	TYR	6.9
7	G	75	ARG	6.9
8	H	113	ALA	6.9
1	A	977	LYS	6.9
2	B	99	LYS	6.9
2	B	272	THR	6.9
10	J	57	ILE	6.9
1	A	790	ASP	6.9
2	B	209	GLU	6.9
3	C	166	GLU	6.9

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Mol	Chain	Res	Type	RSRZ
2	B	579	ARG	6.9
1	A	629	LEU	6.9
7	G	11	ILE	6.9
13	S	238	PRO	6.9
2	B	226	PHE	6.9
1	A	1403	GLU	6.9
5	E	18	THR	6.9
2	B	820	GLY	6.9
1	A	727	ASP	6.9
10	J	19	GLU	6.8
5	E	189	GLY	6.8
1	A	677	ARG	6.8
1	A	932	GLU	6.8
3	C	243	VAL	6.8
2	B	280	ILE	6.8
2	B	1026	LEU	6.8
6	F	92	ARG	6.8
11	K	76	GLN	6.8
2	B	197	PHE	6.8
1	A	1344	GLY	6.8
3	C	165	LYS	6.8
9	I	82	GLU	6.8
1	A	1225	PHE	6.8
2	B	390	LEU	6.8
1	A	545	GLN	6.8
1	A	1376	THR	6.8
7	G	64	THR	6.8
2	B	373	ARG	6.7
2	B	58	THR	6.7
3	C	236	GLY	6.7
3	C	250	THR	6.7
2	B	1066	SER	6.7
2	B	394	ASP	6.7
5	E	144	ILE	6.7
2	B	878	GLN	6.7
5	E	99	HIS	6.7
2	B	283	VAL	6.7
1	A	1042	PHE	6.7
2	B	832	GLY	6.7
1	A	356	ASP	6.7
3	C	237	SER	6.7
9	I	36	GLU	6.7

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Mol	Chain	Res	Type	RSRZ
11	K	91	CYS	6.7
1	A	370	ILE	6.7
1	A	1394	THR	6.7
1	A	823	GLY	6.7
7	G	93	SER	6.7
2	B	1182	CYS	6.7
1	A	1430	LEU	6.6
8	H	52	GLN	6.6
1	A	654	ASN	6.6
8	H	120	GLY	6.6
2	B	1153	GLU	6.6
1	A	795	GLU	6.6
2	B	92	PHE	6.6
11	K	7	PHE	6.6
2	B	880	THR	6.6
2	B	633	VAL	6.6
1	A	1371	LEU	6.6
12	L	46	VAL	6.6
2	B	383	ASN	6.6
2	B	125	SER	6.6
1	A	150	THR	6.6
2	B	916	THR	6.6
1	A	692	ASP	6.6
5	E	68	SER	6.6
9	I	65	ASP	6.6
13	S	141	THR	6.6
1	A	1058	VAL	6.6
5	E	185	ALA	6.6
1	A	821	ARG	6.6
7	G	99	PHE	6.6
1	A	1022	LEU	6.6
2	B	887	HIS	6.6
7	G	38	CYS	6.6
1	A	144	THR	6.6
3	C	16	ASP	6.6
1	A	164	ARG	6.5
3	C	258	ILE	6.5
1	A	514	PRO	6.5
1	A	1302	PRO	6.5
7	G	141	SER	6.5
1	A	386	ASP	6.5
1	A	408	ASP	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	595	THR	6.5
1	A	1286	LYS	6.5
10	J	4	PRO	6.5
2	B	867	GLY	6.5
4	D	173	HIS	6.5
5	E	10	SER	6.5
8	H	41	ASP	6.5
1	A	999	VAL	6.5
6	F	122	MET	6.5
1	A	578	LEU	6.5
11	K	82	ASP	6.5
1	A	1199	ARG	6.5
2	B	489	SER	6.5
1	A	660	ASN	6.5
4	D	165	GLN	6.5
5	E	123	LEU	6.5
2	B	35	SER	6.5
2	B	1082	MET	6.5
1	A	162	VAL	6.5
1	A	576	GLN	6.5
7	G	32	GLU	6.4
2	B	1034	VAL	6.4
9	I	89	GLN	6.4
1	A	1385	THR	6.4
2	B	103	ASN	6.4
1	A	924	LYS	6.4
2	B	1183	LYS	6.4
2	B	1133	MET	6.4
3	C	198	ALA	6.4
1	A	771	GLU	6.4
1	A	1109	LYS	6.4
2	B	682	SER	6.4
2	B	631	GLY	6.4
1	A	172	PRO	6.4
2	B	667	GLN	6.4
1	A	68	GLN	6.4
2	B	1100	ASP	6.4
1	A	1117	THR	6.4
13	S	207	ILE	6.4
3	C	241	ASP	6.4
1	A	774	ARG	6.3
5	E	132	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
11	K	45	LEU	6.3
6	F	74	ILE	6.3
2	B	1007	VAL	6.3
12	L	35	SER	6.3
1	A	640	GLN	6.3
2	B	311	LEU	6.3
4	D	194	LEU	6.3
1	A	839	ARG	6.3
3	C	219	PHE	6.3
4	D	220	LEU	6.3
1	A	650	GLN	6.3
1	A	1420	ASP	6.3
13	S	271	CYS	6.3
2	B	962	LYS	6.3
3	C	65	HIS	6.3
2	B	38	PHE	6.3
13	S	182	MET	6.3
1	A	1019	CYS	6.3
1	A	1223	ASP	6.3
2	B	1178	ASN	6.2
3	C	42	PRO	6.2
1	A	128	ILE	6.2
1	A	1263	ILE	6.2
5	E	72	PHE	6.2
2	B	863	GLU	6.2
2	B	1111	MET	6.2
11	K	95	ILE	6.2
1	A	124	GLN	6.2
5	E	174	GLN	6.2
13	S	185	VAL	6.2
1	A	1410	PHE	6.2
2	B	662	MET	6.2
1	A	1002	GLY	6.2
3	C	242	GLN	6.2
10	J	63	TYR	6.2
1	A	381	THR	6.2
1	A	1068	ALA	6.2
7	G	166	ASP	6.2
1	A	306	ASN	6.2
1	A	268	ASP	6.2
1	A	726	ARG	6.2
11	K	96	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	1141	THR	6.2
13	S	140	ASP	6.2
2	B	109	THR	6.2
2	B	645	SER	6.2
3	C	167	HIS	6.2
2	B	323	VAL	6.2
5	E	148	GLU	6.2
1	A	1373	ASP	6.2
2	B	51	PHE	6.2
2	B	598	GLU	6.1
10	J	2	ILE	6.1
13	S	157	TYR	6.1
8	H	3	ASN	6.1
6	F	146	TRP	6.1
5	E	67	GLU	6.1
1	A	222	LEU	6.1
2	B	651	LEU	6.1
1	A	1387	HIS	6.1
1	A	1362	TYR	6.1
1	A	86	LEU	6.1
13	S	192	GLU	6.1
8	H	33	GLN	6.1
2	B	648	HIS	6.1
1	A	9	ALA	6.1
1	A	55	ASP	6.1
1	A	806	ARG	6.1
1	A	67	CYS	6.1
6	F	106	PRO	6.1
2	B	615	MET	6.1
1	A	503	GLN	6.1
2	B	760	ASP	6.1
9	I	94	ASP	6.1
13	S	281	TYR	6.1
2	B	537	LYS	6.1
7	G	136	VAL	6.1
2	B	918	ILE	6.1
1	A	151	ASP	6.1
3	C	31	ASN	6.1
1	A	241	VAL	6.0
2	B	986	GLN	6.0
1	A	891	ALA	6.0
4	D	168	LYS	6.0

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Mol	Chain	Res	Type	RSRZ
4	D	216	ASN	6.0
7	G	102	GLN	6.0
1	A	1189	SER	6.0
13	S	170	SER	6.0
2	B	738	PHE	6.0
2	B	235	SER	6.0
3	C	112	ASN	6.0
5	E	196	VAL	6.0
2	B	575	PRO	6.0
13	S	199	TYR	6.0
1	A	501	LEU	6.0
1	A	1348	LEU	6.0
10	J	56	LEU	6.0
2	B	98	THR	6.0
1	A	526	ASP	6.0
7	G	143	ILE	6.0
1	A	533	LYS	6.0
2	B	321	GLY	6.0
1	A	805	LEU	6.0
5	E	120	ALA	6.0
1	A	585	GLY	6.0
1	A	1169	ILE	6.0
1	A	1098	VAL	6.0
2	B	737	THR	6.0
3	C	115	SER	6.0
9	I	54	GLU	6.0
1	A	882	SER	5.9
10	J	53	HIS	5.9
1	A	176	LYS	5.9
7	G	124	GLY	5.9
3	C	268	ASP	5.9
1	A	897	TYR	5.9
3	C	66	ARG	5.9
1	A	1088	GLY	5.9
1	A	277	GLU	5.9
9	I	95	THR	5.9
2	B	663	ALA	5.9
2	B	743	ILE	5.9
13	S	254	TYR	5.9
11	K	93	SER	5.9
1	A	643	ALA	5.9
5	E	100	ILE	5.9

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Mol	Chain	Res	Type	RSRZ
3	C	52	GLU	5.9
1	A	130	ASP	5.9
1	A	1067	LEU	5.9
13	S	136	ASN	5.9
13	S	139	VAL	5.9
7	G	39	THR	5.9
6	F	90	ARG	5.9
3	C	89	GLU	5.9
4	D	119	ARG	5.9
1	A	951	GLU	5.9
1	A	837	ILE	5.9
2	B	380	TYR	5.9
7	G	80	LYS	5.9
4	D	197	SER	5.9
2	B	753	ALA	5.9
1	A	685	GLU	5.8
1	A	939	ASP	5.8
1	A	941	LYS	5.8
11	K	103	THR	5.8
1	A	213	HIS	5.8
3	C	102	GLN	5.8
2	B	395	GLN	5.8
2	B	734	HIS	5.8
4	D	154	PHE	5.8
11	K	10	PHE	5.8
1	A	1118	VAL	5.8
8	H	138	GLU	5.8
1	A	1123	GLY	5.8
9	I	109	ILE	5.8
1	A	1202	MET	5.8
1	A	238	CYS	5.8
2	B	131	ASP	5.8
13	S	219	ALA	5.8
2	B	1139	ILE	5.7
1	A	1207	LEU	5.7
1	A	116	ASP	5.7
1	A	1349	TYR	5.7
6	F	129	LYS	5.7
1	A	1364	ASN	5.7
2	B	45	SER	5.7
1	A	57	ARG	5.7
1	A	1197	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	448	PRO	5.7
2	B	245	GLU	5.7
1	A	439	ASN	5.7
7	G	57	GLN	5.7
2	B	1207	LEU	5.7
2	B	998	ASP	5.7
5	E	129	PRO	5.7
1	A	1005	GLU	5.7
1	A	175	ARG	5.7
1	A	871	ASP	5.7
1	A	297	GLN	5.7
1	A	938	LYS	5.7
8	H	91	ASP	5.7
1	A	146	MET	5.7
5	E	45	LYS	5.7
11	K	105	PHE	5.7
1	A	479	ASN	5.7
2	B	398	ARG	5.7
1	A	335	ARG	5.7
3	C	70	ILE	5.7
9	I	119	THR	5.7
2	B	944	THR	5.6
5	E	182	ASP	5.6
2	B	467	GLY	5.6
1	A	783	THR	5.6
2	B	351	TYR	5.6
1	A	393	ARG	5.6
1	A	452	LYS	5.6
2	B	888	GLY	5.6
11	K	28	PRO	5.6
2	B	933	SER	5.6
2	B	391	ASP	5.6
12	L	38	LEU	5.6
7	G	153	GLN	5.6
1	A	289	ILE	5.6
1	A	721	PHE	5.6
2	B	189	LEU	5.6
1	A	60	SER	5.6
1	A	1412	ALA	5.6
6	F	73	ALA	5.6
6	F	147	SER	5.6
7	G	37	SER	5.6

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Mol	Chain	Res	Type	RSRZ
13	S	158	ASP	5.6
4	D	153	ARG	5.6
3	C	68	GLY	5.6
10	J	22	LEU	5.6
1	A	809	THR	5.6
9	I	70	ARG	5.6
12	L	70	ARG	5.6
8	H	20	TYR	5.6
2	B	1109	GLY	5.6
2	B	885	MET	5.6
6	F	113	GLY	5.6
1	A	1229	SER	5.6
5	E	93	MET	5.6
2	B	52	ASN	5.5
4	D	163	VAL	5.5
1	A	1368	MET	5.5
1	A	484	GLY	5.5
1	A	573	SER	5.5
2	B	548	GLY	5.5
3	C	199	LYS	5.5
4	D	159	THR	5.5
1	A	493	GLN	5.5
3	C	261	ALA	5.5
1	A	793	SER	5.5
9	I	13	MET	5.5
1	A	440	ASP	5.5
6	F	105	ALA	5.5
1	A	1218	GLN	5.5
2	B	861	ASP	5.5
1	A	1400	CYS	5.5
11	K	42	LEU	5.5
2	B	785	TYR	5.5
2	B	249	ARG	5.5
2	B	761	HIS	5.5
2	B	177	LYS	5.4
11	K	56	VAL	5.4
1	A	794	PRO	5.4
11	K	21	ILE	5.4
5	E	4	GLU	5.4
1	A	1176	LEU	5.4
2	B	1217	TYR	5.4
2	B	516	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
8	H	5	LEU	5.4
2	B	555	ILE	5.4
7	G	1	MET	5.4
1	A	995	GLU	5.4
13	S	216	HIS	5.4
2	B	868	MET	5.4
2	B	1175	LEU	5.4
1	A	710	LEU	5.4
2	B	419	THR	5.4
1	A	885	THR	5.4
2	B	898	LEU	5.4
2	B	374	LYS	5.4
1	A	1104	ILE	5.4
2	B	890	TYR	5.4
7	G	62	LEU	5.4
5	E	11	ARG	5.4
1	A	923	LEU	5.4
5	E	105	PHE	5.4
1	A	659	HIS	5.4
2	B	117	ALA	5.4
1	A	529	CYS	5.4
4	D	120	GLU	5.4
1	A	10	PRO	5.3
1	A	946	VAL	5.3
2	B	1029	CYS	5.3
1	A	883	LEU	5.3
1	A	904	THR	5.3
1	A	937	VAL	5.3
1	A	8	SER	5.3
2	B	562	GLY	5.3
1	A	173	THR	5.3
1	A	183	GLY	5.3
1	A	918	GLU	5.3
1	A	1172	LEU	5.3
1	A	1381	LEU	5.3
2	B	229	ALA	5.3
7	G	42	PHE	5.3
1	A	418	SER	5.3
5	E	195	VAL	5.3
5	E	63	ASN	5.3
1	A	373	THR	5.3
3	C	53	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	449	SER	5.3
2	B	715	ALA	5.3
10	J	7	CYS	5.3
3	C	97	VAL	5.2
1	A	1331	SER	5.2
1	A	210	ILE	5.2
1	A	1128	GLN	5.2
2	B	1145	SER	5.2
3	C	223	ALA	5.2
2	B	899	ILE	5.2
2	B	1180	PHE	5.2
2	B	996	ARG	5.2
13	S	228	LEU	5.2
1	A	1378	GLN	5.2
1	A	321	PRO	5.2
1	A	519	PRO	5.2
1	A	665	GLY	5.2
2	B	413	LEU	5.2
7	G	3	PHE	5.2
1	A	42	ASP	5.2
1	A	973	ILE	5.2
1	A	184	SER	5.2
1	A	827	THR	5.2
8	H	93	TYR	5.2
1	A	85	ASP	5.2
1	A	1013	ASP	5.2
6	F	78	GLN	5.2
2	B	779	GLY	5.2
3	C	171	GLY	5.2
4	D	171	GLY	5.2
2	B	742	GLU	5.2
5	E	27	GLY	5.2
2	B	527	THR	5.2
2	B	1159	ARG	5.2
1	A	687	LYS	5.2
9	I	114	GLN	5.2
4	D	182	SER	5.1
1	A	1319	VAL	5.1
2	B	402	GLY	5.1
2	B	418	LYS	5.1
1	A	149	GLU	5.1
1	A	346	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	95	PHE	5.1
8	H	130	ARG	5.1
1	A	917	SER	5.1
7	G	61	ILE	5.1
2	B	1061	GLU	5.1
1	A	71	GLN	5.1
1	A	831	THR	5.1
2	B	196	PRO	5.1
1	A	426	LEU	5.1
2	B	1023	VAL	5.1
2	B	1206	GLU	5.1
7	G	156	SER	5.1
1	A	1402	PHE	5.1
8	H	18	GLY	5.1
4	D	116	SER	5.1
2	B	988	GLY	5.1
9	I	87	GLN	5.1
1	A	1343	ALA	5.1
1	A	96	ILE	5.1
2	B	983	ARG	5.1
7	G	127	PRO	5.1
2	B	807	ARG	5.1
3	C	4	GLU	5.1
1	A	1060	PRO	5.0
2	B	538	ASN	5.0
2	B	963	PHE	5.0
1	A	235	ILE	5.0
1	A	731	ARG	5.0
13	S	243	GLN	5.0
2	B	1017	ILE	5.0
2	B	1022	THR	5.0
1	A	3	GLY	5.0
1	A	511	ILE	5.0
1	A	1425	SER	5.0
3	C	168	ALA	5.0
2	B	1204	PHE	5.0
1	A	1428	VAL	5.0
2	B	845	SER	5.0
13	S	252	ASN	5.0
1	A	816	HIS	5.0
2	B	710	LEU	5.0
3	C	135	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
13	S	154	LYS	5.0
2	B	851	PHE	5.0
2	B	561	TRP	5.0
1	A	675	THR	5.0
7	G	8	SER	5.0
1	A	136	ALA	5.0
2	B	1101	ASP	5.0
10	J	44	TYR	5.0
11	K	87	LEU	5.0
7	G	14	HIS	5.0
7	G	54	ILE	5.0
7	G	58	ARG	5.0
8	H	84	ALA	5.0
1	A	1182	GLU	5.0
2	B	953	LEU	5.0
3	C	216	GLY	5.0
13	S	258	GLY	5.0
13	S	187	ASN	5.0
2	B	660	LYS	5.0
9	I	117	LYS	5.0
1	A	979	SER	5.0
1	A	1311	VAL	5.0
1	A	1115	SER	5.0
1	A	993	LEU	5.0
1	A	220	THR	5.0
1	A	424	ILE	5.0
1	A	1038	THR	5.0
2	B	594	ALA	4.9
7	G	148	GLU	4.9
1	A	669	THR	4.9
2	B	59	LEU	4.9
4	D	213	GLU	4.9
1	A	485	ASP	4.9
2	B	1205	GLN	4.9
1	A	211	PHE	4.9
1	A	360	GLU	4.9
3	C	80	LEU	4.9
1	A	80	HIS	4.9
3	C	50	GLU	4.9
8	H	11	GLN	4.9
1	A	48	ALA	4.9
1	A	125	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	1066	VAL	4.9
1	A	1095	THR	4.9
1	A	1388	GLY	4.9
7	G	94	CYS	4.9
2	B	132	VAL	4.9
8	H	62	SER	4.9
1	A	957	PRO	4.9
1	A	842	VAL	4.9
3	C	51	VAL	4.9
2	B	322	PHE	4.9
1	A	910	PRO	4.9
11	K	46	ILE	4.9
1	A	530	GLY	4.9
2	B	617	ARG	4.9
13	S	156	LEU	4.9
7	G	114	LEU	4.9
13	S	205	ASN	4.9
2	B	835	GLN	4.9
2	B	1107	ALA	4.9
2	B	491	THR	4.9
2	B	1046	PRO	4.9
7	G	128	PRO	4.9
1	A	611	GLN	4.9
1	A	1427	ASN	4.9
1	A	1261	LYS	4.8
1	A	1449	SER	4.8
2	B	588	GLY	4.8
2	B	282	ILE	4.8
1	A	723	ASN	4.8
2	B	808	ALA	4.8
1	A	626	ASN	4.8
1	A	1075	PRO	4.8
1	A	623	GLY	4.8
1	A	733	ALA	4.8
9	I	73	ARG	4.8
13	S	245	ILE	4.8
2	B	1103	ILE	4.8
1	A	1258	HIS	4.8
1	A	567	LYS	4.8
1	A	835	GLY	4.8
1	A	1148	ILE	4.8
2	B	1058	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
9	I	31	THR	4.8
2	B	700	SER	4.8
7	G	98	GLY	4.8
1	A	270	LEU	4.8
5	E	128	PRO	4.8
8	H	36	CYS	4.8
11	K	66	PRO	4.8
1	A	1321	GLY	4.8
12	L	40	LEU	4.8
6	F	89	GLU	4.8
1	A	206	GLU	4.8
1	A	1406	VAL	4.8
1	A	674	PRO	4.8
3	C	139	GLY	4.8
1	A	1102	LYS	4.8
1	A	975	HIS	4.8
9	I	69	PRO	4.8
1	A	502	SER	4.7
2	B	367	LEU	4.7
2	B	406	LEU	4.7
4	D	212	LYS	4.7
1	A	510	GLN	4.7
2	B	847	ASP	4.7
9	I	50	THR	4.7
1	A	1144	LYS	4.7
2	B	30	SER	4.7
1	A	1334	ASP	4.7
1	A	30	ILE	4.7
3	C	259	LEU	4.7
2	B	977	GLY	4.7
1	A	245	PRO	4.7
1	A	249	SER	4.7
2	B	896	ASP	4.7
1	A	787	PHE	4.7
6	F	140	ASP	4.7
9	I	71	SER	4.7
2	B	247	GLY	4.7
1	A	27	VAL	4.7
2	B	984	HIS	4.7
1	A	785	PRO	4.7
2	B	266	ALA	4.7
2	B	1015	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1168	GLU	4.7
1	A	729	ALA	4.7
1	A	388	LEU	4.7
1	A	1312	ASN	4.7
2	B	486	TYR	4.7
1	A	894	GLU	4.7
1	A	1314	SER	4.7
2	B	1102	LYS	4.7
1	A	704	ALA	4.7
1	A	641	VAL	4.7
1	A	1188	GLN	4.7
3	C	83	SER	4.7
1	A	762	SER	4.7
1	A	102	VAL	4.7
7	G	116	PRO	4.7
8	H	14	GLU	4.7
9	I	5	ARG	4.6
13	S	183	ASN	4.6
1	A	703	THR	4.6
1	A	784	LEU	4.6
1	A	958	VAL	4.6
2	B	844	SER	4.6
1	A	836	TYR	4.6
1	A	1330	ASN	4.6
2	B	318	VAL	4.6
2	B	510	LYS	4.6
3	C	252	GLN	4.6
2	B	604	ARG	4.6
7	G	53	ASN	4.6
1	A	221	SER	4.6
1	A	1142	THR	4.6
3	C	265	MET	4.6
3	C	152	GLU	4.6
5	E	157	SER	4.6
1	A	845	LEU	4.6
2	B	66	ASP	4.6
6	F	150	GLU	4.6
1	A	336	ILE	4.6
2	B	116	GLU	4.6
2	B	309	GLN	4.6
2	B	907	GLY	4.6
4	D	174	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
10	J	11	GLY	4.6
1	A	280	GLU	4.6
2	B	696	GLU	4.6
12	L	43	THR	4.6
2	B	397	ASP	4.6
8	H	108	SER	4.6
1	A	744	LYS	4.6
7	G	60	ARG	4.6
2	B	422	LYS	4.6
1	A	577	ILE	4.6
2	B	370	PHE	4.5
9	I	67	THR	4.5
5	E	41	ASP	4.5
2	B	1027	ILE	4.5
2	B	1116	ARG	4.5
1	A	1405	THR	4.5
2	B	404	LYS	4.5
2	B	130	VAL	4.5
5	E	75	MET	4.5
10	J	49	MET	4.5
1	A	627	GLY	4.5
2	B	386	LEU	4.5
1	A	691	LEU	4.5
2	B	1040	ASN	4.5
3	C	196	ASP	4.5
1	A	1268	LEU	4.5
2	B	254	LEU	4.5
1	A	632	VAL	4.5
2	B	993	THR	4.5
5	E	54	GLN	4.5
3	C	14	SER	4.5
1	A	307	ASP	4.5
2	B	368	GLU	4.5
1	A	1187	GLN	4.5
2	B	255	GLN	4.5
7	G	112	LYS	4.5
1	A	1367	HIS	4.5
1	A	681	GLU	4.5
1	A	311	GLN	4.5
1	A	1193	LEU	4.5
4	D	128	VAL	4.5
2	B	824	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	1135	ARG	4.5
2	B	521	LEU	4.5
1	A	766	GLY	4.4
2	B	913	GLY	4.4
5	E	37	LEU	4.4
3	C	156	THR	4.4
1	A	901	LEU	4.4
2	B	335	GLY	4.4
3	C	137	LYS	4.4
6	F	142	SER	4.4
6	F	114	GLU	4.4
10	J	55	ASP	4.4
1	A	63	ARG	4.4
2	B	901	PRO	4.4
2	B	265	SER	4.4
1	A	864	ILE	4.4
5	E	94	LYS	4.4
1	A	684	ALA	4.4
1	A	972	HIS	4.4
1	A	655	PHE	4.4
1	A	269	ILE	4.4
1	A	1265	ASN	4.4
1	A	13	THR	4.4
1	A	706	HIS	4.4
2	B	37	PHE	4.4
1	A	636	GLU	4.4
1	A	657	LEU	4.4
1	A	1025	ARG	4.4
1	A	325	ILE	4.4
2	B	1064	TYR	4.4
1	A	556	TRP	4.4
2	B	688	GLY	4.4
1	A	588	LEU	4.4
1	A	915	SER	4.3
1	A	1329	THR	4.3
2	B	108	VAL	4.3
1	A	1222	ASN	4.3
1	A	1175	SER	4.3
2	B	935	ARG	4.3
2	B	1122	ARG	4.3
2	B	1200	ALA	4.3
2	B	436	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	B	366	GLN	4.3
3	C	105	GLY	4.3
1	A	849	MET	4.3
1	A	1011	GLN	4.3
3	C	136	ASP	4.3
2	B	1044	ALA	4.3
3	C	246	ARG	4.3
5	E	130	ALA	4.3
2	B	881	ASN	4.3
1	A	401	GLY	4.3
4	D	166	LEU	4.3
2	B	1084	GLN	4.3
8	H	24	CYS	4.3
2	B	1080	LYS	4.3
1	A	998	LEU	4.3
2	B	31	TRP	4.3
9	I	21	GLU	4.3
7	G	77	VAL	4.3
13	S	300	GLU	4.3
3	C	120	ILE	4.3
9	I	105	SER	4.3
2	B	101	MET	4.3
5	E	154	ILE	4.3
7	G	115	MET	4.3
2	B	523	CYS	4.3
9	I	63	GLY	4.3
2	B	236	HIS	4.3
2	B	70	ILE	4.3
11	K	94	ILE	4.3
1	A	1135	ARG	4.3
8	H	146	ARG	4.3
2	B	39	ARG	4.3
2	B	733	HIS	4.3
3	C	146	LYS	4.3
1	A	858	ASN	4.2
13	S	151	GLN	4.2
1	A	26	GLU	4.2
1	A	868	TYR	4.2
10	J	31	ASP	4.2
1	A	1020	CYS	4.2
2	B	281	PRO	4.2
9	I	14	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
9	I	43	VAL	4.2
1	A	152	VAL	4.2
1	A	592	ASP	4.2
9	I	46	HIS	4.2
1	A	570	PRO	4.2
1	A	1021	LEU	4.2
6	F	85	MET	4.2
13	S	246	GLU	4.2
13	S	236	LEU	4.2
2	B	49	ASP	4.2
8	H	112	ILE	4.2
1	A	878	ILE	4.2
4	D	146	GLN	4.2
5	E	31	THR	4.2
1	A	1133	LEU	4.2
1	A	964	ILE	4.2
1	A	1004	ASN	4.2
1	A	1009	ASN	4.2
1	A	1404	GLU	4.2
1	A	1443	VAL	4.2
2	B	377	PHE	4.2
2	B	630	ALA	4.2
2	B	1009	ASP	4.2
1	A	653	VAL	4.2
9	I	49	ILE	4.2
6	F	103	MET	4.2
11	K	41	THR	4.2
1	A	666	ILE	4.2
2	B	1126	GLY	4.2
1	A	900	ASP	4.2
2	B	591	ARG	4.2
1	A	920	LEU	4.2
5	E	35	VAL	4.2
1	A	455	MET	4.2
1	A	207	ILE	4.2
1	A	644	LYS	4.2
1	A	44	THR	4.2
2	B	310	MET	4.2
3	C	141	GLY	4.2
1	A	631	HIS	4.1
10	J	32	GLU	4.1
2	B	694	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	271	LYS	4.1
2	B	770	GLN	4.1
13	S	173	HIS	4.1
11	K	12	LEU	4.1
3	C	104	PHE	4.1
1	A	263	THR	4.1
1	A	602	ASP	4.1
6	F	83	PRO	4.1
3	C	245	VAL	4.1
1	A	799	PHE	4.1
1	A	1094	VAL	4.1
6	F	120	ILE	4.1
2	B	1000	PRO	4.1
9	I	77	LYS	4.1
1	A	562	THR	4.1
1	A	1308	THR	4.1
1	A	1352	VAL	4.1
2	B	1095	LEU	4.1
1	A	1081	LEU	4.1
1	A	422	GLY	4.1
1	A	750	GLY	4.1
1	A	718	VAL	4.1
1	A	889	SER	4.1
2	B	44	VAL	4.1
3	C	40	GLU	4.1
6	F	100	GLN	4.1
2	B	461	LEU	4.1
2	B	572	HIS	4.1
2	B	294	ASP	4.1
1	A	1119	TYR	4.1
5	E	162	ARG	4.1
1	A	389	THR	4.1
1	A	467	THR	4.1
1	A	528	LEU	4.1
2	B	903	VAL	4.1
7	G	111	THR	4.1
1	A	737	LEU	4.1
1	A	1338	VAL	4.1
2	B	680	THR	4.1
1	A	486	GLU	4.1
6	F	99	LEU	4.1
1	A	145	LYS	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	186	LYS	4.1
7	G	2	PHE	4.0
1	A	1134	ILE	4.0
1	A	1445	ILE	4.0
11	K	78	THR	4.0
1	A	508	PRO	4.0
2	B	999	MET	4.0
1	A	598	LEU	4.0
1	A	1240	CYS	4.0
2	B	865	LYS	4.0
1	A	1227	ILE	4.0
1	A	543	LEU	4.0
2	B	893	LEU	4.0
3	C	69	LEU	4.0
2	B	511	PRO	4.0
1	A	1392	SER	4.0
2	B	915	THR	4.0
1	A	741	ASN	4.0
1	A	135	PHE	4.0
3	C	37	MET	4.0
2	B	1197	PRO	4.0
9	I	92	ARG	4.0
3	C	151	GLN	4.0
1	A	1018	PHE	4.0
1	A	1178	ASP	4.0
1	A	693	VAL	4.0
2	B	215	GLN	4.0
2	B	624	LEU	4.0
2	B	1161	HIS	4.0
1	A	295	LEU	4.0
2	B	316	PRO	4.0
2	B	507	LYS	4.0
1	A	1409	LEU	4.0
1	A	1146	VAL	4.0
2	B	872	GLU	4.0
8	H	39	THR	4.0
1	A	606	LEU	4.0
1	A	956	LEU	4.0
7	G	95	SER	4.0
2	B	410	GLY	4.0
2	B	1201	LYS	4.0
6	F	116	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1054	LEU	4.0
2	B	273	LEU	4.0
3	C	193	TYR	4.0
1	A	1029	ARG	4.0
1	A	1165	GLU	4.0
2	B	681	TRP	4.0
2	B	848	ARG	4.0
1	A	153	PRO	3.9
2	B	208	SER	3.9
2	B	1179	GLN	3.9
5	E	77	SER	3.9
12	L	60	ARG	3.9
13	S	242	LYS	3.9
5	E	206	GLY	3.9
2	B	741	CYS	3.9
8	H	27	GLU	3.9
2	B	381	MET	3.9
1	A	416	ARG	3.9
13	S	233	ALA	3.9
2	B	544	CYS	3.9
1	A	896	ARG	3.9
1	A	647	GLY	3.9
2	B	1028	GLU	3.9
3	C	263	THR	3.9
5	E	212	ARG	3.9
9	I	79	HIS	3.9
1	A	800	VAL	3.9
8	H	57	VAL	3.9
2	B	1146	PHE	3.9
2	B	1203	LEU	3.9
7	G	110	VAL	3.9
1	A	127	ALA	3.9
1	A	169	ASN	3.9
3	C	161	LYS	3.9
1	A	405	VAL	3.9
2	B	104	GLU	3.9
6	F	118	LEU	3.9
1	A	867	ILE	3.9
2	B	560	GLU	3.9
2	B	771	SER	3.9
5	E	80	VAL	3.9
2	B	1076	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
5	E	201	LYS	3.9
11	K	106	GLU	3.9
3	C	157	CYS	3.9
9	I	66	PRO	3.9
5	E	97	VAL	3.9
3	C	15	LYS	3.9
2	B	728	ARG	3.8
2	B	1184	GLY	3.8
6	F	111	LEU	3.8
2	B	1002	THR	3.8
1	A	233	TRP	3.8
11	K	77	THR	3.8
1	A	363	GLN	3.8
1	A	11	LEU	3.8
1	A	509	LEU	3.8
1	A	534	LEU	3.8
1	A	1195	LEU	3.8
1	A	522	GLY	3.8
6	F	134	ILE	3.8
11	K	97	LYS	3.8
5	E	168	TYR	3.8
1	A	28	ARG	3.8
1	A	1417	GLU	3.8
1	A	1089	VAL	3.8
4	D	217	LEU	3.8
13	S	230	THR	3.8
1	A	619	LYS	3.8
2	B	348	ARG	3.8
2	B	1055	ILE	3.8
1	A	365	GLY	3.8
6	F	117	PRO	3.8
1	A	301	ALA	3.8
2	B	446	LEU	3.8
2	B	490	SER	3.8
2	B	535	LEU	3.8
5	E	61	GLN	3.8
2	B	767	ASN	3.8
4	D	143	ASN	3.8
13	S	274	CYS	3.8
2	B	1163	CYS	3.8
3	C	187	LYS	3.8
10	J	28	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	1105	ALA	3.8
2	B	784	ASN	3.8
1	A	242	PRO	3.8
3	C	218	PRO	3.8
2	B	54	PHE	3.8
2	B	179	CYS	3.8
1	A	1346	ALA	3.8
1	A	561	PRO	3.8
1	A	1419	ASP	3.8
2	B	1078	GLY	3.8
3	C	247	GLY	3.8
12	L	36	SER	3.8
1	A	142	CYS	3.7
1	A	1355	VAL	3.7
1	A	415	LEU	3.7
1	A	473	SER	3.7
1	A	1256	GLU	3.7
2	B	853	SER	3.7
1	A	322	VAL	3.7
1	A	548	ASN	3.7
9	I	98	VAL	3.7
10	J	14	VAL	3.7
1	A	504	LEU	3.7
1	A	1174	PHE	3.7
2	B	32	ALA	3.7
2	B	1140	ALA	3.7
1	A	490	HIS	3.7
1	A	1326	ARG	3.7
1	A	682	THR	3.7
13	S	285	GLN	3.7
4	D	189	ASP	3.7
2	B	522	VAL	3.7
7	G	133	SER	3.7
1	A	82	GLY	3.7
1	A	1296	GLY	3.7
2	B	258	LEU	3.7
2	B	550	ASP	3.7
2	B	897	GLY	3.7
2	B	1173	ALA	3.7
1	A	863	VAL	3.7
5	E	62	ALA	3.7
13	S	250	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	482	VAL	3.7
1	A	789	LYS	3.7
2	B	858	SER	3.7
2	B	908	GLU	3.6
5	E	44	ALA	3.7
5	E	213	ILE	3.6
11	K	90	ALA	3.7
13	S	229	ALA	3.7
13	S	147	LYS	3.6
12	L	52	GLY	3.6
1	A	633	VAL	3.6
13	S	286	THR	3.6
2	B	823	ALA	3.6
1	A	711	ARG	3.6
1	A	531	ILE	3.6
1	A	810	PRO	3.6
2	B	460	ALA	3.6
2	B	478	GLY	3.6
1	A	1328	TYR	3.6
2	B	822	ASN	3.6
5	E	193	GLY	3.6
1	A	259	GLU	3.6
5	E	116	ILE	3.6
11	K	17	SER	3.6
1	A	872	GLY	3.6
1	A	1440	ALA	3.6
2	B	55	VAL	3.6
2	B	549	THR	3.6
13	S	212	PRO	3.6
2	B	388	CYS	3.6
12	L	47	ARG	3.6
1	A	359	LEU	3.6
1	A	554	PRO	3.6
1	A	1303	GLU	3.6
5	E	165	LEU	3.6
9	I	101	PHE	3.6
1	A	1136	SER	3.6
5	E	30	ILE	3.6
2	B	1152	MET	3.6
2	B	1049	ASP	3.6
1	A	720	ARG	3.6
2	B	263	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
3	C	234	SER	3.6
2	B	810	GLU	3.6
3	C	48	SER	3.6
8	H	105	GLU	3.6
1	A	524	VAL	3.6
2	B	195	CYS	3.6
2	B	553	PRO	3.6
8	H	114	VAL	3.6
1	A	1384	VAL	3.6
1	A	527	THR	3.6
2	B	46	GLN	3.6
1	A	1370	LEU	3.6
2	B	415	GLN	3.5
6	F	96	THR	3.6
1	A	1180	GLU	3.5
4	D	179	GLN	3.5
11	K	107	THR	3.5
5	E	205	SER	3.5
1	A	1053	PHE	3.5
13	S	302	CYS	3.5
1	A	1389	PHE	3.5
2	B	960	GLY	3.5
2	B	686	ASN	3.5
8	H	43	ASN	3.5
13	S	197	ALA	3.5
1	A	855	THR	3.5
4	D	170	THR	3.5
1	A	743	VAL	3.5
1	A	968	GLN	3.5
11	K	58	PHE	3.5
2	B	365	THR	3.5
2	B	556	THR	3.5
10	J	9	SER	3.5
1	A	1375	MET	3.5
1	A	1073	GLY	3.5
1	A	366	VAL	3.5
1	A	414	ASP	3.5
1	A	884	ASP	3.5
13	S	270	THR	3.5
1	A	559	VAL	3.5
1	A	861	GLY	3.5
1	A	1299	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	458	LYS	3.5
1	A	994	GLN	3.5
1	A	154	SER	3.5
2	B	599	THR	3.5
11	K	16	GLU	3.5
1	A	281	HIS	3.5
1	A	926	GLN	3.5
1	A	1416	ALA	3.5
2	B	360	PHE	3.5
2	B	495	LEU	3.5
2	B	755	ILE	3.5
3	C	107	SER	3.5
10	J	18	TRP	3.5
2	B	1117	GLN	3.5
1	A	326	ARG	3.4
1	A	81	PHE	3.4
1	A	988	LEU	3.4
3	C	221	TYR	3.4
1	A	1137	ALA	3.4
1	A	642	CYS	3.4
1	A	825	ILE	3.4
1	A	1037	LEU	3.4
1	A	1446	ASP	3.4
11	K	83	PRO	3.4
1	A	65	LEU	3.4
1	A	757	ASN	3.4
7	G	67	SER	3.4
1	A	797	LYS	3.4
1	A	1044	TRP	3.4
1	A	489	LEU	3.4
8	H	16	ASP	3.4
1	A	630	ILE	3.4
1	A	966	ASN	3.4
2	B	794	ASN	3.4
1	A	492	PRO	3.4
1	A	1183	GLN	3.4
3	C	129	ILE	3.4
3	C	195	GLN	3.4
1	A	107	CYS	3.4
1	A	25	GLU	3.4
1	A	305	ASP	3.4
1	A	1282	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	834	ASN	3.4
2	B	186	GLU	3.4
1	A	332	LYS	3.4
1	A	776	ALA	3.4
2	B	40	GLU	3.4
3	C	251	LEU	3.4
2	B	818	PRO	3.4
1	A	433	GLU	3.4
1	A	553	VAL	3.4
2	B	797	TYR	3.4
1	A	341	MET	3.4
1	A	361	LEU	3.4
2	B	1128	LEU	3.4
2	B	1025	HIS	3.4
2	B	609	ILE	3.4
3	C	145	CYS	3.4
1	A	46	THR	3.4
2	B	528	PRO	3.4
11	K	6	ARG	3.4
5	E	147	HIS	3.4
1	A	39	GLU	3.4
2	B	1004	GLU	3.4
9	I	15	TYR	3.4
1	A	759	ALA	3.4
1	A	352	VAL	3.4
2	B	974	PRO	3.3
8	H	104	PHE	3.3
1	A	223	GLY	3.3
8	H	103	LYS	3.3
5	E	141	VAL	3.3
3	C	32	SER	3.3
5	E	150	VAL	3.3
1	A	1294	PRO	3.3
11	K	111	LEU	3.3
1	A	1091	SER	3.3
1	A	1369	ALA	3.3
3	C	85	ASP	3.3
1	A	699	ALA	3.3
2	B	220	GLY	3.3
1	A	770	VAL	3.3
3	C	106	GLU	3.3
2	B	584	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	1144	ALA	3.3
11	K	99	GLY	3.3
1	A	954	TRP	3.3
6	F	86	THR	3.3
2	B	261	ARG	3.3
2	B	795	ILE	3.3
2	B	957	ASN	3.3
3	C	177	GLU	3.3
2	B	205	ILE	3.3
2	B	494	HIS	3.3
3	C	103	ALA	3.3
6	F	132	LEU	3.3
2	B	34	ILE	3.3
1	A	1332	PHE	3.3
2	B	981	ALA	3.3
2	B	1079	LYS	3.3
2	B	714	GLU	3.3
10	J	35	ALA	3.3
2	B	227	LYS	3.3
4	D	139	LYS	3.3
3	C	98	VAL	3.3
3	C	61	GLU	3.3
5	E	21	GLU	3.3
2	B	664	THR	3.3
8	H	137	GLN	3.3
8	H	143	LEU	3.3
1	A	899	VAL	3.3
2	B	643	ASP	3.2
1	A	79	GLY	3.2
11	K	27	ALA	3.2
10	J	21	TYR	3.2
2	B	956	THR	3.2
7	G	137	ILE	3.2
2	B	636	PRO	3.2
3	C	138	GLU	3.2
3	C	231	ASN	3.2
4	D	145	MET	3.2
13	S	255	ASN	3.2
2	B	776	GLN	3.2
4	D	157	GLN	3.2
2	B	426	LYS	3.2
2	B	355	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	90	VAL	3.2
8	H	92	ASP	3.2
1	A	240	PRO	3.2
1	A	925	LEU	3.2
2	B	508	LEU	3.2
11	K	65	HIS	3.2
6	F	148	VAL	3.2
13	S	165	GLU	3.2
1	A	375	THR	3.2
1	A	1016	THR	3.2
13	S	150	ASP	3.2
7	G	109	PHE	3.2
1	A	461	LYS	3.2
3	C	116	LYS	3.2
1	A	119	ASN	3.2
5	E	202	SER	3.2
2	B	1218	THR	3.2
4	D	187	THR	3.2
2	B	603	LEU	3.2
1	A	840	ARG	3.2
1	A	668	ASP	3.2
1	A	247	ARG	3.2
11	K	1	MET	3.2
1	A	402	ALA	3.2
11	K	24	ASP	3.2
3	C	7	GLN	3.2
11	K	31	VAL	3.2
1	A	1379	GLY	3.2
5	E	127	ILE	3.1
10	J	23	ASN	3.1
1	A	462	VAL	3.1
1	A	824	LEU	3.1
2	B	1043	ASP	3.1
5	E	58	MET	3.1
1	A	1023	ARG	3.1
2	B	375	ALA	3.1
8	H	145	ARG	3.1
1	A	355	GLY	3.1
1	A	1152	ILE	3.1
2	B	769	TYR	3.1
2	B	463	THR	3.1
1	A	1198	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	945	GLU	3.1
1	A	942	PHE	3.1
1	A	1438	THR	3.1
1	A	1049	ILE	3.1
1	A	1159	ARG	3.1
13	S	293	LEU	3.1
2	B	936	ASP	3.1
1	A	265	LYS	3.1
1	A	1279	ILE	3.1
1	A	610	GLY	3.1
2	B	871	THR	3.1
1	A	1185	PHE	3.1
8	H	61	SER	3.1
1	A	1147	THR	3.1
1	A	520	CYS	3.1
2	B	447	ALA	3.1
13	S	223	ILE	3.1
11	K	44	ASN	3.1
2	B	563	MET	3.1
2	B	1188	LYS	3.1
2	B	852	ARG	3.1
5	E	65	THR	3.1
2	B	492	LEU	3.1
1	A	1078	GLN	3.1
3	C	183	TRP	3.1
1	A	539	THR	3.1
1	A	950	GLY	3.1
2	B	403	LYS	3.1
1	A	387	ARG	3.1
2	B	846	ILE	3.1
1	A	441	PRO	3.1
1	A	100	LYS	3.1
1	A	934	LYS	3.1
1	A	857	ARG	3.1
1	A	50	ILE	3.0
1	A	848	ILE	3.0
1	A	983	ILE	3.0
2	B	826	ALA	3.0
5	E	164	LEU	3.0
2	B	225	VAL	3.0
2	B	1005	GLY	3.0
11	K	34	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	214	ALA	3.0
2	B	817	LEU	3.0
2	B	21	GLU	3.0
1	A	1313	LEU	3.0
1	A	34	LYS	3.0
3	C	9	LYS	3.0
2	B	110	HIS	3.0
2	B	319	GLU	3.0
1	A	584	ASN	3.0
11	K	88	LYS	3.0
2	B	1071	VAL	3.0
2	B	821	GLN	3.0
13	S	194	ALA	3.0
1	A	111	GLY	3.0
2	B	1096	ARG	3.0
1	A	410	GLY	3.0
1	A	535	THR	3.0
1	A	596	THR	3.0
1	A	1214	GLU	3.0
5	E	169	ARG	3.0
1	A	856	THR	3.0
1	A	1395	GLY	3.0
1	A	613	ILE	3.0
1	A	1063	MET	3.0
5	E	176	PRO	3.0
2	B	1143	ALA	3.0
1	A	59	GLY	3.0
2	B	1115	THR	3.0
1	A	746	MET	3.0
2	B	809	MET	3.0
9	I	84	VAL	3.0
8	H	82	PRO	3.0
1	A	1191	TRP	3.0
1	A	1204	ASP	3.0
3	C	28	ALA	3.0
3	C	79	GLN	3.0
3	C	158	VAL	3.0
5	E	118	PRO	3.0
2	B	259	TYR	3.0
3	C	122	SER	3.0
1	A	1274	ARG	3.0
2	B	766	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	904	ARG	3.0
3	C	99	LEU	3.0
2	B	1141	HIS	3.0
8	H	139	ASN	3.0
3	C	96	SER	3.0
8	H	9	ILE	3.0
10	J	48	ARG	3.0
5	E	121	MET	3.0
1	A	471	ASN	3.0
4	D	135	GLY	3.0
1	A	432	VAL	3.0
3	C	119	VAL	3.0
3	C	76	ASP	3.0
11	K	20	LYS	3.0
7	G	72	VAL	3.0
7	G	83	LYS	3.0
2	B	1001	PHE	2.9
1	A	89	PRO	2.9
1	A	202	LEU	2.9
1	A	740	LEU	2.9
7	G	44	TYR	2.9
3	C	162	GLY	2.9
7	G	66	GLY	2.9
8	H	99	GLY	2.9
13	S	239	ALA	2.9
1	A	505	CYS	2.9
8	H	128	ASN	2.9
2	B	600	LEU	2.9
2	B	376	PHE	2.9
1	A	246	VAL	2.9
3	C	24	ASN	2.9
13	S	259	ALA	2.9
12	L	69	ALA	2.9
1	A	961	ARG	2.9
1	A	1100	ARG	2.9
7	G	21	ARG	2.9
1	A	841	LEU	2.9
1	A	870	GLU	2.9
5	E	134	THR	2.9
2	B	610	ASN	2.9
4	D	117	GLU	2.9
9	I	35	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	1075	GLY	2.9
4	D	208	GLU	2.9
1	A	500	GLU	2.9
1	A	811	GLN	2.9
3	C	267	GLN	2.9
2	B	526	GLU	2.9
2	B	909	ASP	2.9
2	B	1074	ASN	2.9
3	C	149	LYS	2.9
5	E	46	TYR	2.9
2	B	1033	LYS	2.9
3	C	13	ALA	2.9
2	B	1011	ILE	2.9
9	I	24	ARG	2.9
2	B	1208	MET	2.9
6	F	80	ALA	2.9
13	S	188	CYS	2.9
1	A	898	ARG	2.9
1	A	1278	ASN	2.9
2	B	1219	ASP	2.9
1	A	624	SER	2.9
1	A	1226	VAL	2.8
1	A	1447	GLU	2.8
1	A	147	VAL	2.8
1	A	621	THR	2.8
1	A	1273	LEU	2.8
13	S	240	PRO	2.8
2	B	91	SER	2.8
8	H	42	ILE	2.8
1	A	893	PHE	2.8
2	B	1018	PRO	2.8
3	C	213	PRO	2.8
5	E	95	THR	2.8
1	A	604	GLY	2.8
1	A	928	LEU	2.8
2	B	1113	VAL	2.8
3	C	188	HIS	2.8
1	A	676	MET	2.8
1	A	133	LYS	2.8
1	A	846	GLU	2.8
2	B	372	SER	2.8
2	B	480	SER	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	748	ILE	2.8
1	A	662	PHE	2.8
1	A	761	MET	2.8
1	A	391	LEU	2.8
2	B	1215	ARG	2.8
5	E	188	LEU	2.8
2	B	326	ASP	2.8
2	B	385	LEU	2.8
2	B	454	THR	2.8
2	B	620	ARG	2.8
2	B	978	ASP	2.8
2	B	352	ALA	2.8
1	A	688	LYS	2.8
7	G	107	LYS	2.8
1	A	1045	VAL	2.8
4	D	123	LEU	2.8
6	F	145	ASP	2.8
1	A	139	TRP	2.8
1	A	1051	ALA	2.8
3	C	254	LYS	2.8
1	A	725	ALA	2.8
1	A	752	LYS	2.8
2	B	176	SER	2.8
2	B	958	GLN	2.8
1	A	922	ASP	2.8
2	B	1213	THR	2.8
2	B	50	SER	2.8
1	A	652	VAL	2.8
1	A	754	SER	2.8
1	A	1372	VAL	2.8
2	B	841	MET	2.8
1	A	844	ALA	2.8
1	A	1411	GLU	2.8
2	B	384	ARG	2.8
11	K	60	ALA	2.8
3	C	181	ASP	2.8
1	A	225	ASN	2.8
6	F	125	LEU	2.8
2	B	602	THR	2.8
7	G	169	GLY	2.8
2	B	994	TYR	2.8
3	C	54	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	136	ASN	2.8
10	J	60	PHE	2.8
2	B	1165	ILE	2.8
3	C	100	THR	2.8
13	S	275	LYS	2.8
1	A	782	ARG	2.7
2	B	950	ASP	2.7
3	C	128	ASN	2.7
1	A	1423	GLY	2.7
5	E	108	GLY	2.7
1	A	747	VAL	2.7
1	A	1032	LEU	2.7
2	B	1171	VAL	2.7
2	B	1060	ARG	2.7
1	A	620	LYS	2.7
1	A	1003	LYS	2.7
11	K	48	ALA	2.7
3	C	126	GLY	2.7
1	A	300	VAL	2.7
2	B	772	ALA	2.7
7	G	168	LEU	2.7
1	A	1024	SER	2.7
2	B	113	TYR	2.7
2	B	1016	ALA	2.7
13	S	181	GLU	2.7
1	A	303	TYR	2.7
1	A	350	ARG	2.7
3	C	153	LEU	2.7
6	F	138	LEU	2.7
1	A	267	ALA	2.7
1	A	517	ASN	2.7
5	E	33	GLU	2.7
5	E	160	GLU	2.7
1	A	1209	MET	2.7
3	C	55	THR	2.7
5	E	142	VAL	2.7
1	A	371	ALA	2.7
1	A	1008	GLN	2.7
3	C	36	VAL	2.7
8	H	12	VAL	2.7
2	B	1094	ARG	2.7
5	E	183	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
11	K	38	GLU	2.7
11	K	62	LYS	2.7
1	A	364	VAL	2.7
1	A	451	HIS	2.7
1	A	1300	LYS	2.7
1	A	293	GLU	2.7
7	G	68	ALA	2.7
1	A	204	THR	2.7
5	E	111	VAL	2.7
2	B	182	SER	2.7
1	A	1086	PHE	2.7
2	B	1172	ILE	2.7
3	C	175	ALA	2.7
5	E	26	ARG	2.7
5	E	181	ALA	2.7
1	A	429	GLY	2.7
2	B	479	VAL	2.7
2	B	363	HIS	2.7
1	A	980	ASP	2.7
9	I	6	PHE	2.7
5	E	137	GLU	2.6
1	A	357	PRO	2.6
2	B	264	SER	2.6
2	B	1008	PRO	2.6
7	G	15	PRO	2.6
1	A	571	LEU	2.6
1	A	772	GLY	2.6
10	J	29	GLU	2.6
2	B	1021	MET	2.6
2	B	788	ARG	2.6
3	C	71	PRO	2.6
3	C	111	THR	2.6
4	D	132	GLN	2.6
1	A	97	ALA	2.6
2	B	965	LYS	2.6
1	A	802	ASN	2.6
13	S	211	ASN	2.6
1	A	875	ALA	2.6
2	B	685	LEU	2.6
8	H	63	LEU	2.6
1	A	590	ARG	2.6
1	A	296	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	516	SER	2.6
2	B	1167	GLY	2.6
3	C	19	ASP	2.6
5	E	57	MET	2.6
11	K	61	TYR	2.6
2	B	234	ILE	2.6
1	A	1415	SER	2.6
2	B	982	SER	2.6
2	B	959	ASP	2.6
6	F	87	LYS	2.6
1	A	32	VAL	2.6
1	A	488	ASN	2.6
1	A	385	ILE	2.6
2	B	1037	LEU	2.6
2	B	407	ASP	2.6
12	L	45	ALA	2.6
13	S	288	SER	2.6
2	B	243	ALA	2.6
2	B	303	TYR	2.6
2	B	805	THR	2.6
1	A	921	GLY	2.6
1	A	1047	SER	2.6
3	C	35	ARG	2.6
1	A	1092	LYS	2.6
1	A	719	VAL	2.6
1	A	131	SER	2.6
1	A	122	MET	2.6
5	E	175	LEU	2.6
2	B	115	GLN	2.6
1	A	1285	MET	2.5
6	F	81	THR	2.5
8	H	133	ASN	2.5
1	A	177	ASP	2.5
1	A	552	TRP	2.5
7	G	159	ALA	2.5
2	B	48	LEU	2.5
2	B	543	SER	2.5
4	D	206	GLU	2.5
2	B	1150	ARG	2.5
1	A	1125	ALA	2.5
2	B	1072	MET	2.5
2	B	185	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	545	ILE	2.5
7	G	157	ILE	2.5
1	A	751	SER	2.5
2	B	506	GLY	2.5
1	A	299	HIS	2.5
2	B	1024	ALA	2.5
1	A	14	VAL	2.5
3	C	18	VAL	2.5
2	B	726	ALA	2.5
3	C	64	ALA	2.5
1	A	593	GLU	2.5
2	B	558	LEU	2.5
1	A	466	SER	2.5
2	B	687	GLU	2.5
2	B	361	LEU	2.5
2	B	1051	THR	2.5
1	A	532	ARG	2.5
1	A	952	ALA	2.5
11	K	100	ALA	2.5
1	A	990	VAL	2.5
2	B	33	VAL	2.5
5	E	64	PRO	2.5
1	A	232	GLU	2.5
1	A	712	GLU	2.5
13	S	264	SER	2.5
1	A	368	LYS	2.5
2	B	477	ALA	2.5
2	B	378	LEU	2.5
2	B	498	THR	2.5
2	B	63	ILE	2.5
7	G	84	GLY	2.5
1	A	614	PHE	2.5
1	A	550	LEU	2.5
6	F	137	TYR	2.5
2	B	877	PRO	2.5
1	A	372	LYS	2.5
1	A	384	ASN	2.5
2	B	1090	THR	2.4
3	C	27	LEU	2.4
7	G	163	ILE	2.4
1	A	507	VAL	2.4
1	A	1206	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	238	ALA	2.4
12	L	59	ALA	2.4
13	S	304	ASN	2.4
1	A	329	LEU	2.4
2	B	997	GLU	2.4
2	B	1148	LYS	2.4
5	E	98	ILE	2.4
12	L	68	GLU	2.4
2	B	839	MET	2.4
1	A	812	GLU	2.4
2	B	976	ILE	2.4
2	B	513	GLN	2.4
2	B	244	LEU	2.4
1	A	586	ILE	2.4
1	A	648	ASN	2.4
1	A	679	ILE	2.4
9	I	11	ASN	2.4
2	B	1010	LEU	2.4
1	A	1238	ILE	2.4
1	A	1340	GLY	2.4
7	G	69	GLU	2.4
1	A	1027	ALA	2.4
2	B	287	ARG	2.4
2	B	596	LEU	2.4
7	G	79	PHE	2.4
1	A	700	ASN	2.4
2	B	764	SER	2.4
2	B	838	SER	2.4
2	B	1119	VAL	2.4
1	A	902	LEU	2.4
2	B	551	PRO	2.4
2	B	706	GLN	2.4
10	J	1	MET	2.4
8	H	10	PHE	2.4
2	B	995	ARG	2.4
2	B	1088	GLY	2.4
11	K	57	LEU	2.4
1	A	230	ARG	2.4
11	K	72	LYS	2.4
1	A	21	LEU	2.4
1	A	734	GLU	2.4
2	B	644	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	233	GLU	2.4
1	A	427	GLN	2.4
1	A	454	SER	2.4
1	A	1365	TYR	2.4
3	C	248	ILE	2.4
5	E	178	ILE	2.4
13	S	232	ASP	2.4
1	A	17	VAL	2.4
2	B	1068	GLY	2.4
3	C	179	GLU	2.4
1	A	763	ALA	2.4
1	A	1033	GLN	2.4
1	A	638	GLY	2.4
1	A	764	CYS	2.4
2	B	483	LEU	2.4
2	B	883	LEU	2.4
4	D	129	LEU	2.4
6	F	155	LEU	2.4
13	S	190	THR	2.4
2	B	41	LYS	2.4
5	E	20	LYS	2.4
1	A	1360	GLY	2.4
2	B	829	CYS	2.4
1	A	66	LYS	2.4
1	A	963	ILE	2.4
2	B	813	LYS	2.4
4	D	151	PHE	2.4
2	B	612	GLU	2.4
2	B	697	GLU	2.4
3	C	173	ALA	2.4
7	G	122	ASN	2.4
1	A	547	LEU	2.4
2	B	119	LEU	2.4
1	A	769	SER	2.4
11	K	70	ARG	2.4
13	S	200	ARG	2.4
7	G	92	VAL	2.4
1	A	165	GLY	2.3
13	S	305	ARG	2.3
5	E	47	CYS	2.3
8	H	21	ASN	2.3
1	A	498	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1345	ARG	2.3
2	B	691	GLU	2.3
2	B	1194	ILE	2.3
5	E	25	ASP	2.3
2	B	1158	PHE	2.3
2	B	536	VAL	2.3
8	H	123	MET	2.3
2	B	1006	ILE	2.3
6	F	91	ALA	2.3
13	S	184	LYS	2.3
5	E	107	THR	2.3
1	A	137	ALA	2.3
1	A	1259	MET	2.3
1	A	851	HIS	2.3
1	A	686	ALA	2.3
1	A	84	ILE	2.3
1	A	911	SER	2.3
2	B	874	PHE	2.3
1	A	98	LYS	2.3
7	G	90	THR	2.3
2	B	762	ASN	2.3
1	A	143	LYS	2.3
1	A	599	SER	2.3
2	B	825	VAL	2.3
1	A	523	ILE	2.3
2	B	827	ILE	2.3
1	A	587	HIS	2.3
1	A	1190	PRO	2.3
2	B	541	LEU	2.3
2	B	111	ALA	2.3
13	S	247	GLU	2.3
1	A	544	ASP	2.3
2	B	260	GLY	2.3
4	D	205	ASP	2.3
2	B	964	VAL	2.3
10	J	59	LYS	2.3
1	A	1096	SER	2.3
2	B	242	SER	2.3
2	B	400	HIS	2.3
2	B	1192	TYR	2.3
3	C	87	PHE	2.3
5	E	117	THR	2.3

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Mol	Chain	Res	Type	RSRZ
11	K	47	ARG	2.3
2	B	459	TYR	2.3
12	L	29	TYR	2.3
2	B	589	VAL	2.3
2	B	307	ASP	2.3
1	A	83	HIS	2.3
1	A	304	MET	2.3
1	A	1170	ILE	2.3
1	A	1284	MET	2.3
1	A	982	THR	2.3
1	A	1297	GLU	2.3
7	G	5	LYS	2.3
1	A	354	SER	2.3
6	F	101	ILE	2.3
1	A	217	LYS	2.3
2	B	979	LYS	2.3
13	S	235	ASP	2.3
1	A	237	THR	2.2
1	A	443	LEU	2.2
2	B	1093	GLN	2.2
3	C	154	LYS	2.2
11	K	104	ASN	2.2
4	D	209	ARG	2.2
1	A	342	GLY	2.2
1	A	208	LEU	2.2
13	S	215	LYS	2.2
2	B	842	ASN	2.2
4	D	175	PHE	2.2
13	S	227	PHE	2.2
1	A	469	ARG	2.2
1	A	1318	THR	2.2
7	G	131	GLN	2.2
1	A	339	ASN	2.2
1	A	635	ARG	2.2
3	C	81	GLU	2.2
5	E	102	GLU	2.2
7	G	162	SER	2.2
1	A	1398	MET	2.2
2	B	423	LYS	2.2
1	A	639	PRO	2.2
13	S	213	ASP	2.2
1	A	661	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1071	SER	2.2
2	B	777	ALA	2.2
2	B	850	LEU	2.2
5	E	70	SER	2.2
1	A	813	PHE	2.2
1	A	888	GLY	2.2
2	B	750	GLY	2.2
1	A	818	MET	2.2
1	A	56	PRO	2.2
1	A	651	LYS	2.2
1	A	1335	ILE	2.2
2	B	1003	ALA	2.2
3	C	178	PHE	2.2
2	B	876	LYS	2.2
3	C	169	LYS	2.2
3	C	260	LEU	2.2
4	D	138	ASN	2.2
13	S	210	ASN	2.2
13	S	278	LYS	2.2
1	A	929	LEU	2.2
1	A	1266	THR	2.2
11	K	108	GLU	2.2
4	D	121	LYS	2.2
8	H	30	SER	2.2
3	C	147	LEU	2.2
5	E	9	ILE	2.2
13	S	306	TRP	2.2
1	A	47	ARG	2.2
2	B	194	GLU	2.2
2	B	695	ALA	2.2
10	J	34	THR	2.2
13	S	174	THR	2.2
2	B	765	PRO	2.2
2	B	641	GLU	2.2
2	B	629	ASP	2.2
13	S	195	TYR	2.2
1	A	18	GLN	2.2
1	A	1164	PRO	2.2
11	K	32	VAL	2.2
2	B	1059	LEU	2.2
2	B	1196	ILE	2.2
5	E	186	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	19	PHE	2.2
1	A	546	VAL	2.2
2	B	53	GLN	2.2
8	H	26	ILE	2.2
1	A	1097	GLY	2.2
2	B	906	SER	2.2
1	A	907	THR	2.1
2	B	1176	ASN	2.1
1	A	869	GLY	2.1
1	A	536	LEU	2.1
1	A	814	PHE	2.1
1	A	1354	ASN	2.1
1	A	943	LEU	2.1
9	I	25	LEU	2.1
2	B	757	PRO	2.1
9	I	20	LYS	2.1
1	A	1080	THR	2.1
1	A	1194	ARG	2.1
2	B	659	ALA	2.1
2	B	828	ALA	2.1
5	E	207	ARG	2.1
3	C	226	ASP	2.1
4	D	169	SER	2.1
1	A	521	MET	2.1
1	A	1270	ASN	2.1
1	A	376	TYR	2.1
1	A	512	VAL	2.1
1	A	1177	LEU	2.1
2	B	532	ALA	2.1
2	B	231	PRO	2.1
1	A	819	GLY	2.1
6	F	141	GLY	2.1
1	A	612	ILE	2.1
7	G	17	PHE	2.1
9	I	16	PRO	2.1
10	J	54	VAL	2.1
1	A	327	ALA	2.1
13	S	299	CYS	2.1
2	B	94	LYS	2.1
2	B	833	TYR	2.1
11	K	75	ILE	2.1
1	A	78	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	947	GLY	2.1
2	B	1164	GLY	2.1
2	B	408	LEU	2.1
1	A	456	MET	2.1
1	A	579	SER	2.1
2	B	512	ARG	2.1
2	B	991	GLY	2.1
1	A	292	ALA	2.1
2	B	500	THR	2.1
1	A	93	VAL	2.1
11	K	18	LYS	2.1
4	D	221	TYR	2.1
1	A	87	ALA	2.1
4	D	192	LYS	2.1
3	C	220	ASP	2.1
8	H	94	ASP	2.1
2	B	1041	GLU	2.1
13	S	291	GLU	2.1
1	A	1201	ALA	2.1
2	B	1083	ALA	2.1
3	C	11	ARG	2.1
3	C	239	PRO	2.1
10	J	47	ARG	2.0
12	L	67	PHE	2.0
1	A	236	LEU	2.0
1	A	947	PHE	2.0
2	B	191	LYS	2.0
9	I	108	HIS	2.0
3	C	39	ALA	2.0
4	D	188	ALA	2.0
4	D	155	ARG	2.0
11	K	23	PRO	2.0
4	D	124	GLU	2.0
1	A	566	ILE	2.0
9	I	85	PHE	2.0
9	I	111	THR	2.0
1	A	1107	VAL	2.0
1	A	1380	GLY	2.0
2	B	357	GLN	2.0
5	E	187	TYR	2.0
5	E	8	ASN	2.0
13	S	191	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	180	LYS	2.0
2	B	1222	ARG	2.0
8	H	97	MET	2.0
1	A	377	PRO	2.0
1	A	229	SER	2.0
1	A	607	ILE	2.0
8	H	127	GLY	2.0
2	B	172	ILE	2.0
5	E	214	CYS	2.0
8	H	144	ILE	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
15	ZN	J	100	1/1	0.98	0.20	-	30,30,30,30	0
15	ZN	C	319	1/1	0.98	0.20	-	30,30,30,30	0
15	ZN	A	1736	1/1	0.97	0.20	-	30,30,30,30	0
15	ZN	B	1300	1/1	0.97	0.23	-	30,30,30,30	0
15	ZN	S	400	1/1	0.94	0.18	-	30,30,30,30	0
15	ZN	I	201	1/1	0.96	0.15	-	30,30,30,30	0
15	ZN	I	200	1/1	0.98	0.22	-	30,30,30,30	0
15	ZN	A	1735	1/1	0.95	0.18	-	30,30,30,30	0
14	MG	A	1734	1/1	0.63	0.24	-	61,61,61,61	0
15	ZN	L	100	1/1	0.96	0.13	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.