



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:42 PM GMT

PDB ID : 5AKD
Title : MutS in complex with the N-terminal domain of MutL - crystal form 3
Authors : Groothuizen, F.S.; Winkler, I.; Cristovao, M.; Fish, A.; Winterwerp, H.H.K.; Reumer, A.; Marx, A.D.; Hermans, N.; Nicholls, R.A.; Murshudov, G.N.; Lebbink, J.H.G.; Friedhoff, P.; Sixma, T.K.
Deposited on : 2015-03-03
Resolution : 7.60 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

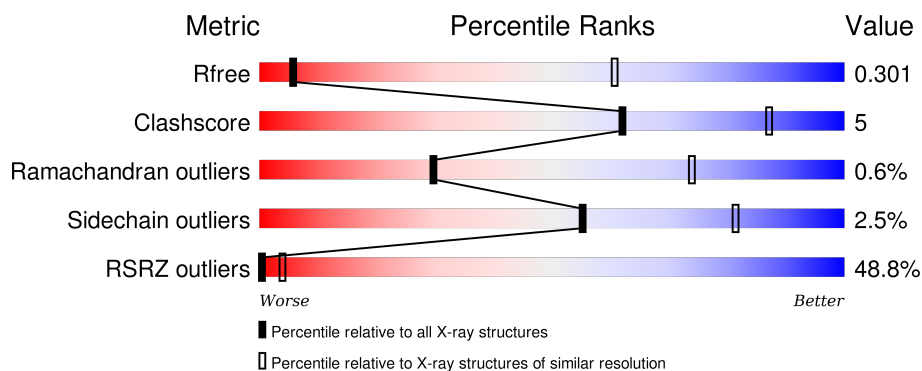
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.60 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}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	800	<div> <div>39%</div> <div>72% 10% 17%</div> </div>
1	B	800	<div> <div>36%</div> <div>73% 9% 17%</div> </div>
1	E	800	<div> <div>43%</div> <div>72% 10% 17%</div> </div>
1	F	800	<div> <div>35%</div> <div>73% 10% 17%</div> </div>
1	I	800	<div> <div>41%</div> <div>75% 7% 17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	J	800	
2	C	369	
2	D	369	
2	G	369	
2	H	369	
2	K	369	
2	L	369	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	A	1801	-	-	-	X
3	ANP	E	1801	-	-	-	X
3	ANP	I	1801	-	-	-	X
3	ANP	J	1801	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45054 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 MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	B	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	E	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	F	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	I	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	J	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ALA	CYS	ENGINEERED MUTATION	UNP P23909
A	235	SER	CYS	ENGINEERED MUTATION	UNP P23909
A	239	ALA	CYS	ENGINEERED MUTATION	UNP P23909
A	246	CYS	ASP	ENGINEERED MUTATION	UNP P23909
A	297	SER	CYS	ENGINEERED MUTATION	UNP P23909
A	569	SER	CYS	ENGINEERED MUTATION	UNP P23909
A	711	VAL	CYS	ENGINEERED MUTATION	UNP P23909
B	93	ALA	CYS	ENGINEERED MUTATION	UNP P23909
B	235	SER	CYS	ENGINEERED MUTATION	UNP P23909
B	239	ALA	CYS	ENGINEERED MUTATION	UNP P23909
B	246	CYS	ASP	ENGINEERED MUTATION	UNP P23909
B	297	SER	CYS	ENGINEERED MUTATION	UNP P23909
B	569	SER	CYS	ENGINEERED MUTATION	UNP P23909
B	711	VAL	CYS	ENGINEERED MUTATION	UNP P23909
E	93	ALA	CYS	ENGINEERED MUTATION	UNP P23909
E	235	SER	CYS	ENGINEERED MUTATION	UNP P23909
E	239	ALA	CYS	ENGINEERED MUTATION	UNP P23909

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Chain	Residue	Modelled	Actual	Comment	Reference
E	246	CYS	ASP	ENGINEERED MUTATION	UNP P23909
E	297	SER	CYS	ENGINEERED MUTATION	UNP P23909
E	569	SER	CYS	ENGINEERED MUTATION	UNP P23909
E	711	VAL	CYS	ENGINEERED MUTATION	UNP P23909
F	93	ALA	CYS	ENGINEERED MUTATION	UNP P23909
F	235	SER	CYS	ENGINEERED MUTATION	UNP P23909
F	239	ALA	CYS	ENGINEERED MUTATION	UNP P23909
F	246	CYS	ASP	ENGINEERED MUTATION	UNP P23909
F	297	SER	CYS	ENGINEERED MUTATION	UNP P23909
F	569	SER	CYS	ENGINEERED MUTATION	UNP P23909
F	711	VAL	CYS	ENGINEERED MUTATION	UNP P23909
I	93	ALA	CYS	ENGINEERED MUTATION	UNP P23909
I	235	SER	CYS	ENGINEERED MUTATION	UNP P23909
I	239	ALA	CYS	ENGINEERED MUTATION	UNP P23909
I	246	CYS	ASP	ENGINEERED MUTATION	UNP P23909
I	297	SER	CYS	ENGINEERED MUTATION	UNP P23909
I	569	SER	CYS	ENGINEERED MUTATION	UNP P23909
I	711	VAL	CYS	ENGINEERED MUTATION	UNP P23909
J	93	ALA	CYS	ENGINEERED MUTATION	UNP P23909
J	235	SER	CYS	ENGINEERED MUTATION	UNP P23909
J	239	ALA	CYS	ENGINEERED MUTATION	UNP P23909
J	246	CYS	ASP	ENGINEERED MUTATION	UNP P23909
J	297	SER	CYS	ENGINEERED MUTATION	UNP P23909
J	569	SER	CYS	ENGINEERED MUTATION	UNP P23909
J	711	VAL	CYS	ENGINEERED MUTATION	UNP P23909

- Molecule 2 is a protein called DNA MISMATCH REPAIR PROTEIN MUTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	D	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	G	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	H	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	K	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			
2	L	285	Total	C	N	O	S	0	0	0
			2252	1423	409	418	2			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	EXPRESSION TAG	UNP P23367
C	-18	GLY	-	EXPRESSION TAG	UNP P23367
C	-17	SER	-	EXPRESSION TAG	UNP P23367
C	-16	SER	-	EXPRESSION TAG	UNP P23367
C	-15	HIS	-	EXPRESSION TAG	UNP P23367
C	-14	HIS	-	EXPRESSION TAG	UNP P23367
C	-13	HIS	-	EXPRESSION TAG	UNP P23367
C	-12	HIS	-	EXPRESSION TAG	UNP P23367
C	-11	HIS	-	EXPRESSION TAG	UNP P23367
C	-10	HIS	-	EXPRESSION TAG	UNP P23367
C	-9	SER	-	EXPRESSION TAG	UNP P23367
C	-8	SER	-	EXPRESSION TAG	UNP P23367
C	-7	GLY	-	EXPRESSION TAG	UNP P23367
C	-6	LEU	-	EXPRESSION TAG	UNP P23367
C	-5	VAL	-	EXPRESSION TAG	UNP P23367
C	-4	PRO	-	EXPRESSION TAG	UNP P23367
C	-3	ARG	-	EXPRESSION TAG	UNP P23367
C	-2	GLY	-	EXPRESSION TAG	UNP P23367
C	-1	SER	-	EXPRESSION TAG	UNP P23367
C	0	HIS	-	EXPRESSION TAG	UNP P23367
C	61	SER	CYS	ENGINEERED MUTATION	UNP P23367
C	131	CYS	ASN	ENGINEERED MUTATION	UNP P23367
C	216	LEU	CYS	ENGINEERED MUTATION	UNP P23367
C	256	PHE	CYS	ENGINEERED MUTATION	UNP P23367
C	276	TYR	CYS	ENGINEERED MUTATION	UNP P23367
D	-19	MET	-	EXPRESSION TAG	UNP P23367
D	-18	GLY	-	EXPRESSION TAG	UNP P23367
D	-17	SER	-	EXPRESSION TAG	UNP P23367
D	-16	SER	-	EXPRESSION TAG	UNP P23367
D	-15	HIS	-	EXPRESSION TAG	UNP P23367
D	-14	HIS	-	EXPRESSION TAG	UNP P23367
D	-13	HIS	-	EXPRESSION TAG	UNP P23367
D	-12	HIS	-	EXPRESSION TAG	UNP P23367
D	-11	HIS	-	EXPRESSION TAG	UNP P23367
D	-10	HIS	-	EXPRESSION TAG	UNP P23367
D	-9	SER	-	EXPRESSION TAG	UNP P23367
D	-8	SER	-	EXPRESSION TAG	UNP P23367
D	-7	GLY	-	EXPRESSION TAG	UNP P23367
D	-6	LEU	-	EXPRESSION TAG	UNP P23367
D	-5	VAL	-	EXPRESSION TAG	UNP P23367
D	-4	PRO	-	EXPRESSION TAG	UNP P23367
D	-3	ARG	-	EXPRESSION TAG	UNP P23367
D	-2	GLY	-	EXPRESSION TAG	UNP P23367

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	EXPRESSION TAG	UNP P23367
D	0	HIS	-	EXPRESSION TAG	UNP P23367
D	61	SER	CYS	ENGINEERED MUTATION	UNP P23367
D	131	CYS	ASN	ENGINEERED MUTATION	UNP P23367
D	216	LEU	CYS	ENGINEERED MUTATION	UNP P23367
D	256	PHE	CYS	ENGINEERED MUTATION	UNP P23367
D	276	TYR	CYS	ENGINEERED MUTATION	UNP P23367
G	-19	MET	-	EXPRESSION TAG	UNP P23367
G	-18	GLY	-	EXPRESSION TAG	UNP P23367
G	-17	SER	-	EXPRESSION TAG	UNP P23367
G	-16	SER	-	EXPRESSION TAG	UNP P23367
G	-15	HIS	-	EXPRESSION TAG	UNP P23367
G	-14	HIS	-	EXPRESSION TAG	UNP P23367
G	-13	HIS	-	EXPRESSION TAG	UNP P23367
G	-12	HIS	-	EXPRESSION TAG	UNP P23367
G	-11	HIS	-	EXPRESSION TAG	UNP P23367
G	-10	HIS	-	EXPRESSION TAG	UNP P23367
G	-9	SER	-	EXPRESSION TAG	UNP P23367
G	-8	SER	-	EXPRESSION TAG	UNP P23367
G	-7	GLY	-	EXPRESSION TAG	UNP P23367
G	-6	LEU	-	EXPRESSION TAG	UNP P23367
G	-5	VAL	-	EXPRESSION TAG	UNP P23367
G	-4	PRO	-	EXPRESSION TAG	UNP P23367
G	-3	ARG	-	EXPRESSION TAG	UNP P23367
G	-2	GLY	-	EXPRESSION TAG	UNP P23367
G	-1	SER	-	EXPRESSION TAG	UNP P23367
G	0	HIS	-	EXPRESSION TAG	UNP P23367
G	61	SER	CYS	ENGINEERED MUTATION	UNP P23367
G	131	CYS	ASN	ENGINEERED MUTATION	UNP P23367
G	216	LEU	CYS	ENGINEERED MUTATION	UNP P23367
G	256	PHE	CYS	ENGINEERED MUTATION	UNP P23367
G	276	TYR	CYS	ENGINEERED MUTATION	UNP P23367
H	-19	MET	-	EXPRESSION TAG	UNP P23367
H	-18	GLY	-	EXPRESSION TAG	UNP P23367
H	-17	SER	-	EXPRESSION TAG	UNP P23367
H	-16	SER	-	EXPRESSION TAG	UNP P23367
H	-15	HIS	-	EXPRESSION TAG	UNP P23367
H	-14	HIS	-	EXPRESSION TAG	UNP P23367
H	-13	HIS	-	EXPRESSION TAG	UNP P23367
H	-12	HIS	-	EXPRESSION TAG	UNP P23367
H	-11	HIS	-	EXPRESSION TAG	UNP P23367
H	-10	HIS	-	EXPRESSION TAG	UNP P23367

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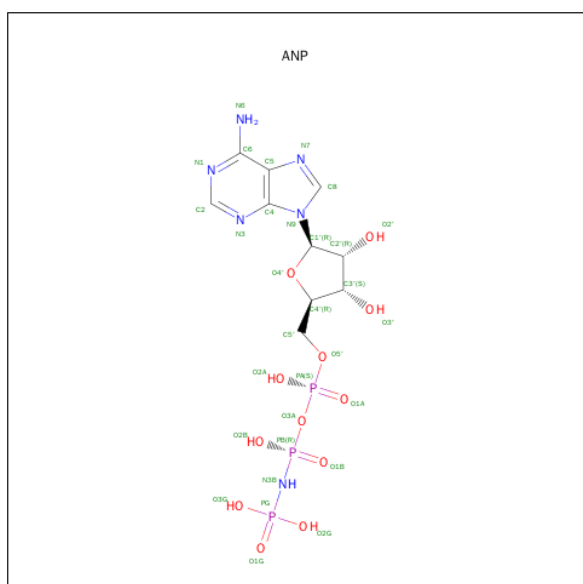
Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	SER	-	EXPRESSION TAG	UNP P23367
H	-8	SER	-	EXPRESSION TAG	UNP P23367
H	-7	GLY	-	EXPRESSION TAG	UNP P23367
H	-6	LEU	-	EXPRESSION TAG	UNP P23367
H	-5	VAL	-	EXPRESSION TAG	UNP P23367
H	-4	PRO	-	EXPRESSION TAG	UNP P23367
H	-3	ARG	-	EXPRESSION TAG	UNP P23367
H	-2	GLY	-	EXPRESSION TAG	UNP P23367
H	-1	SER	-	EXPRESSION TAG	UNP P23367
H	0	HIS	-	EXPRESSION TAG	UNP P23367
H	61	SER	CYS	ENGINEERED MUTATION	UNP P23367
H	131	CYS	ASN	ENGINEERED MUTATION	UNP P23367
H	216	LEU	CYS	ENGINEERED MUTATION	UNP P23367
H	256	PHE	CYS	ENGINEERED MUTATION	UNP P23367
H	276	TYR	CYS	ENGINEERED MUTATION	UNP P23367
K	-19	MET	-	EXPRESSION TAG	UNP P23367
K	-18	GLY	-	EXPRESSION TAG	UNP P23367
K	-17	SER	-	EXPRESSION TAG	UNP P23367
K	-16	SER	-	EXPRESSION TAG	UNP P23367
K	-15	HIS	-	EXPRESSION TAG	UNP P23367
K	-14	HIS	-	EXPRESSION TAG	UNP P23367
K	-13	HIS	-	EXPRESSION TAG	UNP P23367
K	-12	HIS	-	EXPRESSION TAG	UNP P23367
K	-11	HIS	-	EXPRESSION TAG	UNP P23367
K	-10	HIS	-	EXPRESSION TAG	UNP P23367
K	-9	SER	-	EXPRESSION TAG	UNP P23367
K	-8	SER	-	EXPRESSION TAG	UNP P23367
K	-7	GLY	-	EXPRESSION TAG	UNP P23367
K	-6	LEU	-	EXPRESSION TAG	UNP P23367
K	-5	VAL	-	EXPRESSION TAG	UNP P23367
K	-4	PRO	-	EXPRESSION TAG	UNP P23367
K	-3	ARG	-	EXPRESSION TAG	UNP P23367
K	-2	GLY	-	EXPRESSION TAG	UNP P23367
K	-1	SER	-	EXPRESSION TAG	UNP P23367
K	0	HIS	-	EXPRESSION TAG	UNP P23367
K	61	SER	CYS	ENGINEERED MUTATION	UNP P23367
K	131	CYS	ASN	ENGINEERED MUTATION	UNP P23367
K	216	LEU	CYS	ENGINEERED MUTATION	UNP P23367
K	256	PHE	CYS	ENGINEERED MUTATION	UNP P23367
K	276	TYR	CYS	ENGINEERED MUTATION	UNP P23367
L	-19	MET	-	EXPRESSION TAG	UNP P23367
L	-18	GLY	-	EXPRESSION TAG	UNP P23367

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-17	SER	-	EXPRESSION TAG	UNP P23367
L	-16	SER	-	EXPRESSION TAG	UNP P23367
L	-15	HIS	-	EXPRESSION TAG	UNP P23367
L	-14	HIS	-	EXPRESSION TAG	UNP P23367
L	-13	HIS	-	EXPRESSION TAG	UNP P23367
L	-12	HIS	-	EXPRESSION TAG	UNP P23367
L	-11	HIS	-	EXPRESSION TAG	UNP P23367
L	-10	HIS	-	EXPRESSION TAG	UNP P23367
L	-9	SER	-	EXPRESSION TAG	UNP P23367
L	-8	SER	-	EXPRESSION TAG	UNP P23367
L	-7	GLY	-	EXPRESSION TAG	UNP P23367
L	-6	LEU	-	EXPRESSION TAG	UNP P23367
L	-5	VAL	-	EXPRESSION TAG	UNP P23367
L	-4	PRO	-	EXPRESSION TAG	UNP P23367
L	-3	ARG	-	EXPRESSION TAG	UNP P23367
L	-2	GLY	-	EXPRESSION TAG	UNP P23367
L	-1	SER	-	EXPRESSION TAG	UNP P23367
L	0	HIS	-	EXPRESSION TAG	UNP P23367
L	61	SER	CYS	ENGINEERED MUTATION	UNP P23367
L	131	CYS	ASN	ENGINEERED MUTATION	UNP P23367
L	216	LEU	CYS	ENGINEERED MUTATION	UNP P23367
L	256	PHE	CYS	ENGINEERED MUTATION	UNP P23367
L	276	TYR	CYS	ENGINEERED MUTATION	UNP P23367

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

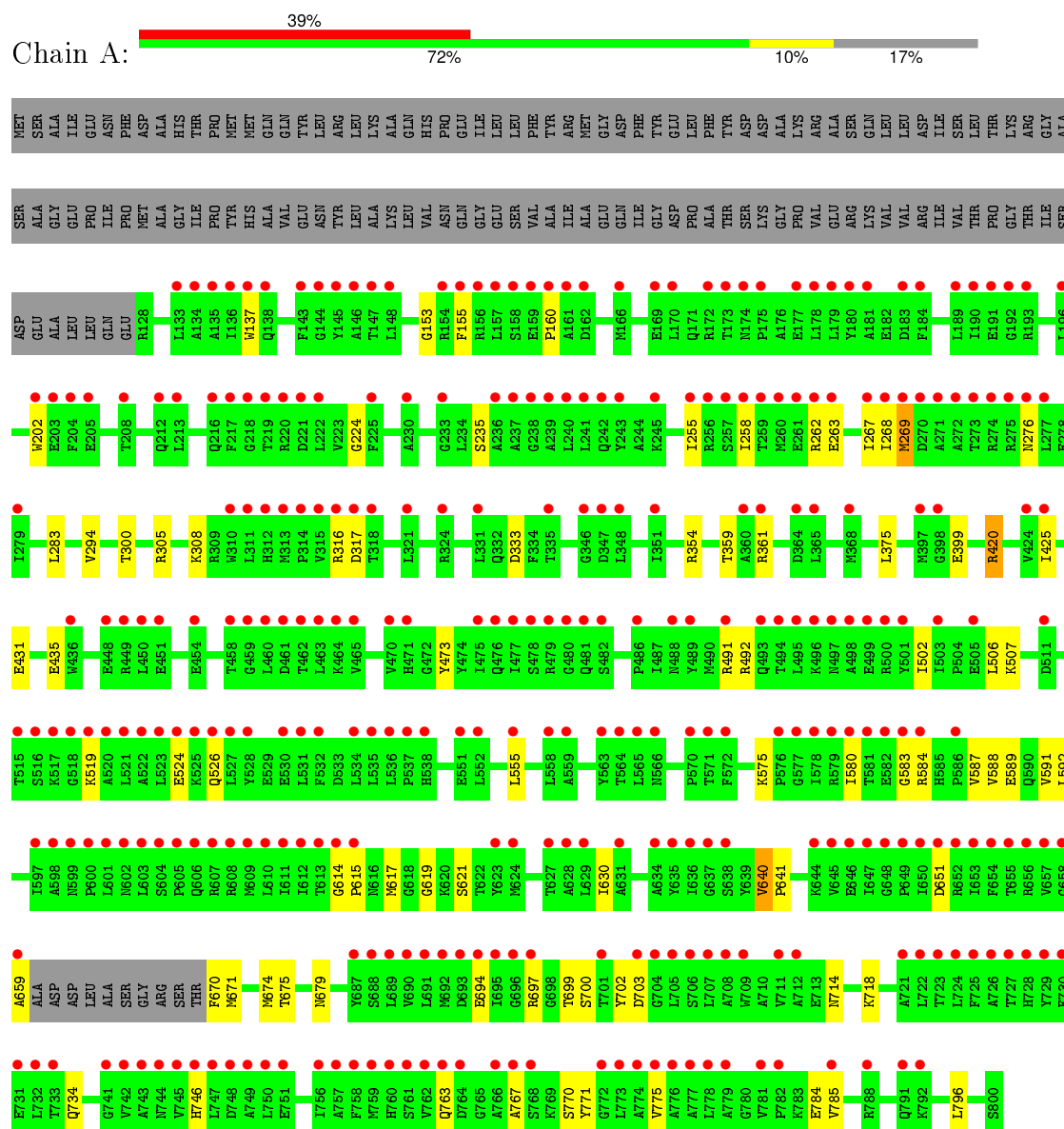


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

3 Residue-property plots

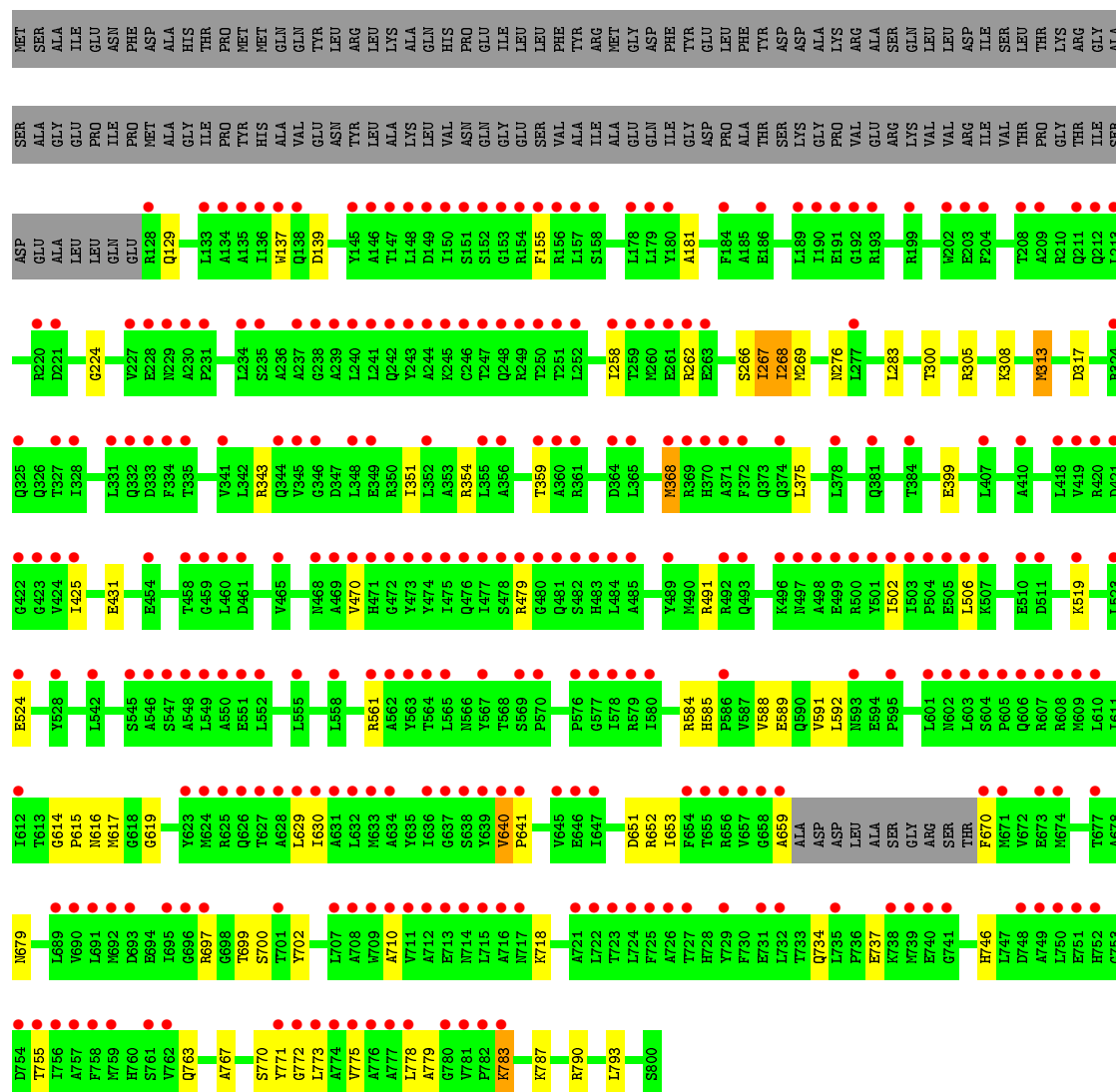
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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 MISMATCH REPAIR PROTEIN MUTS

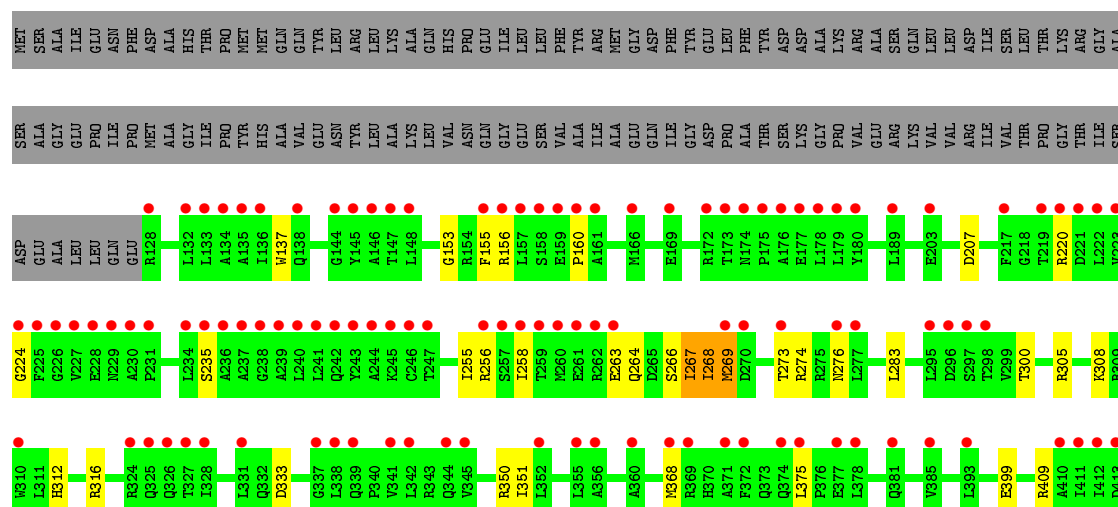


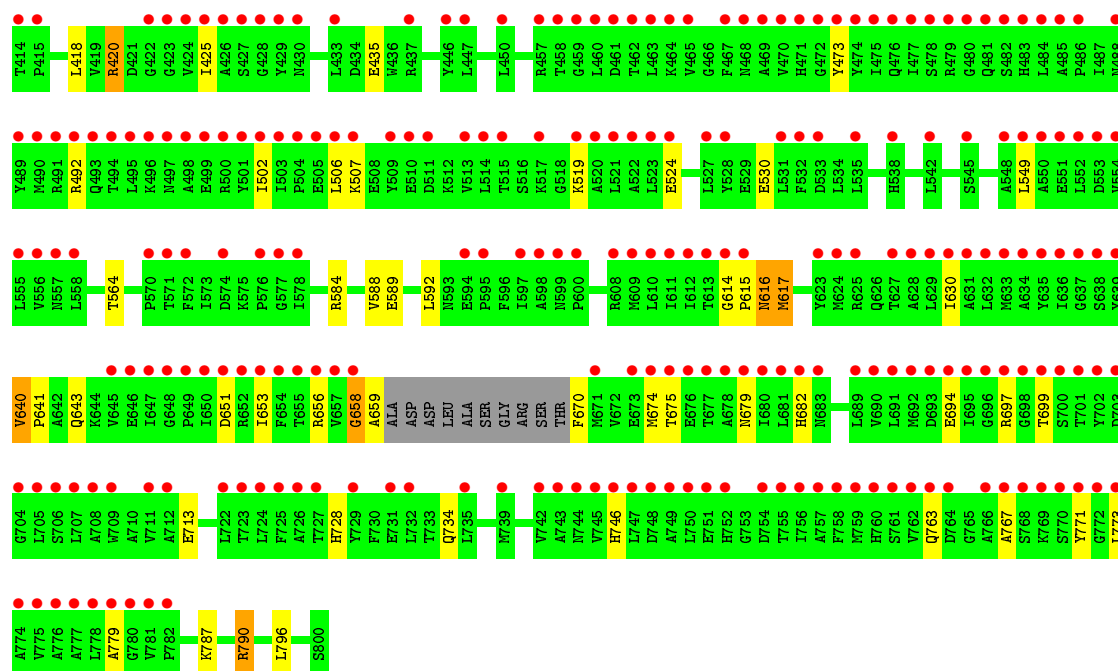
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



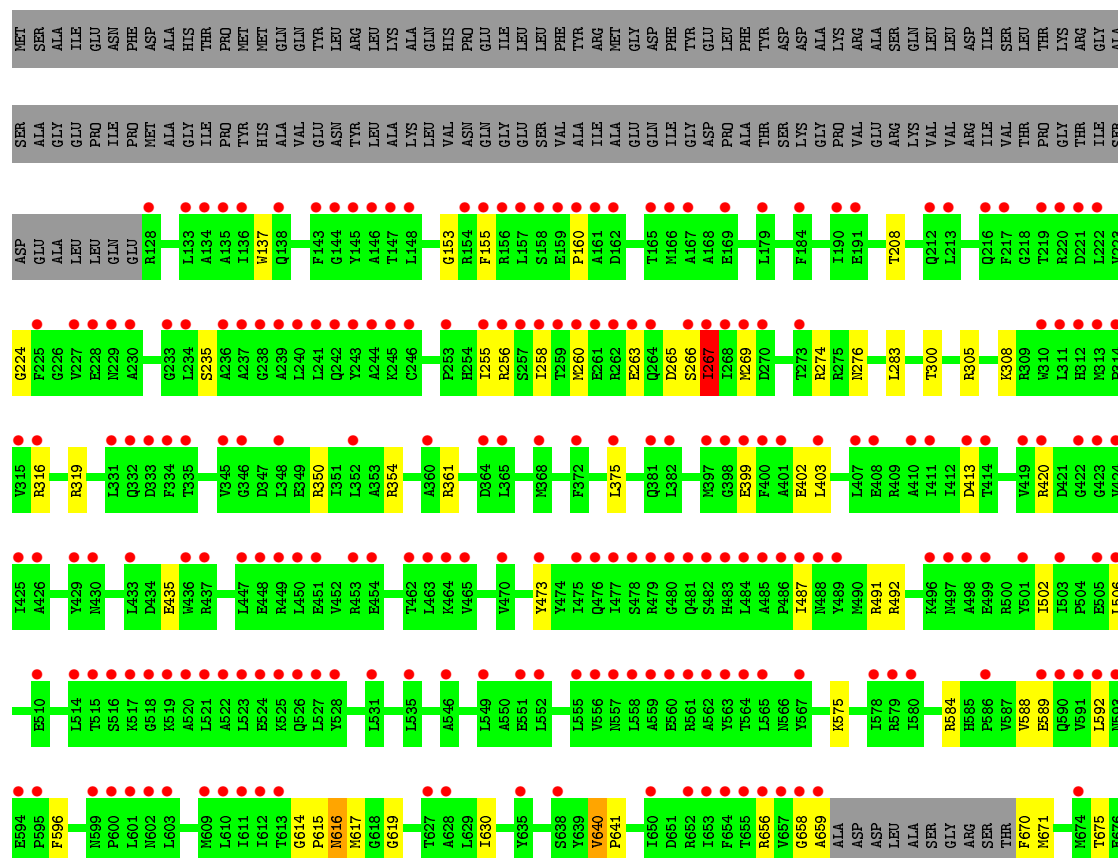


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

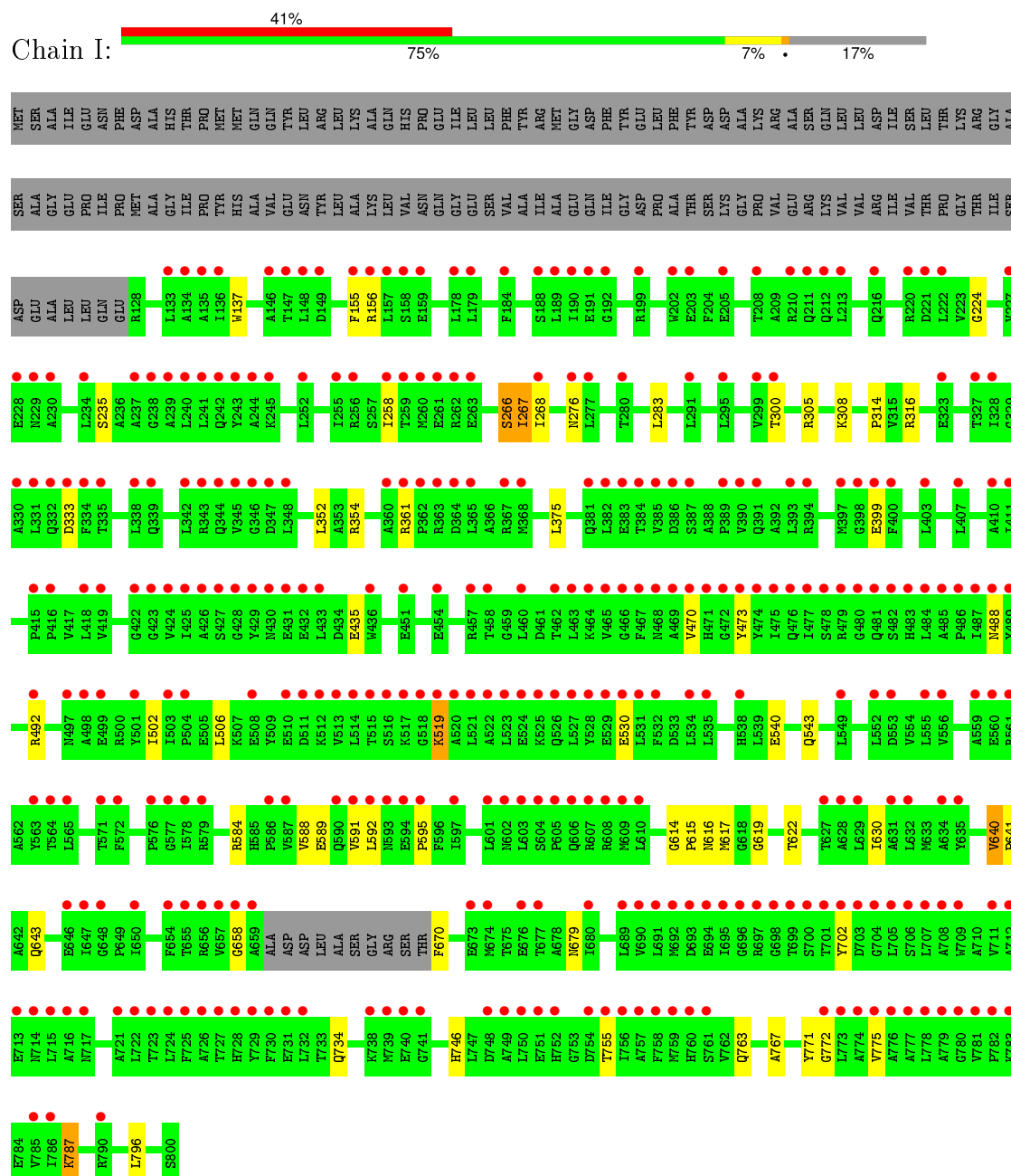




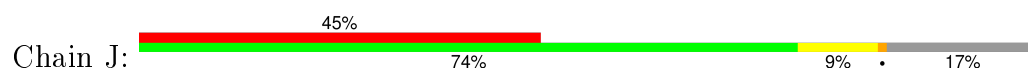
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

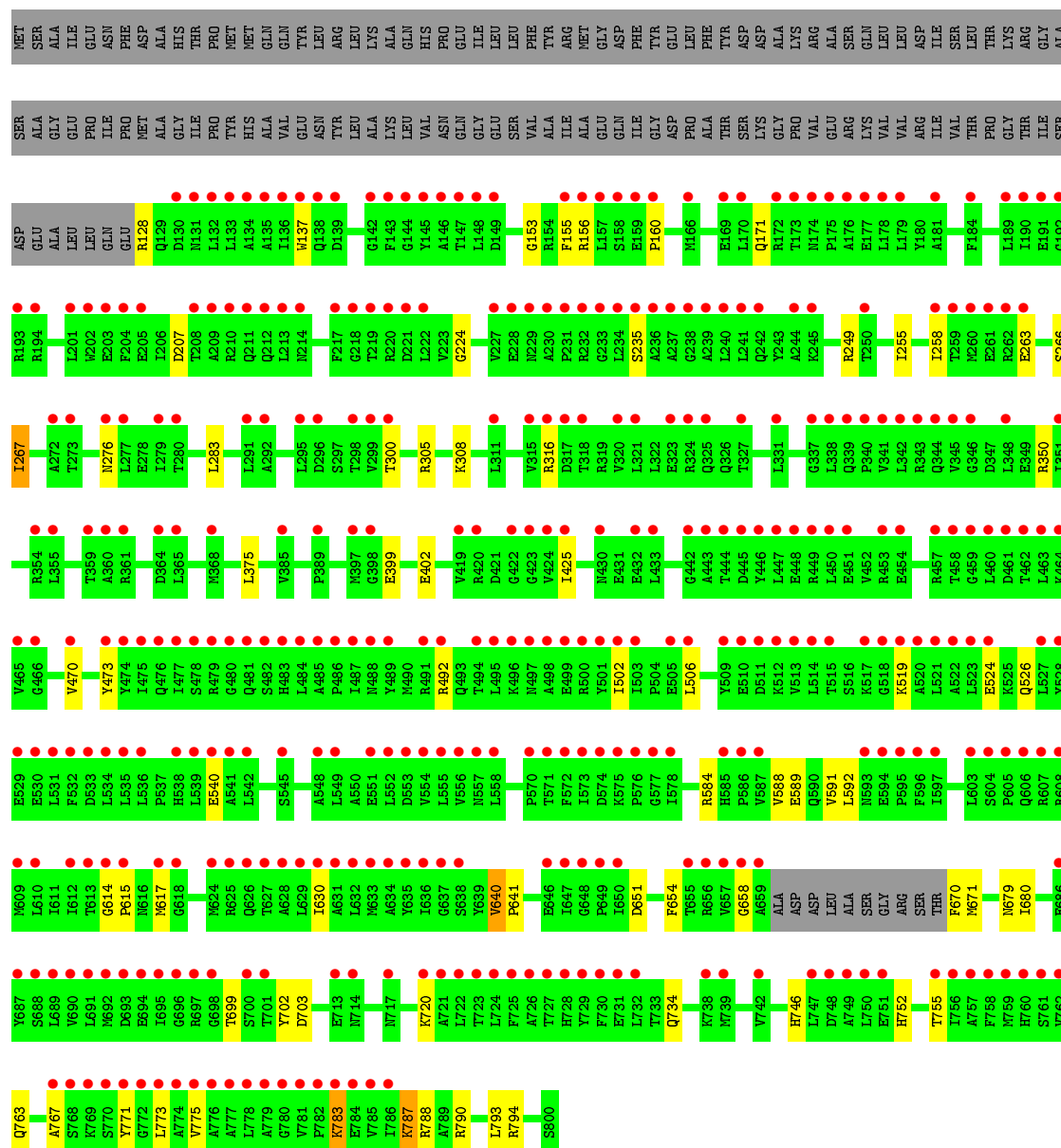


- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

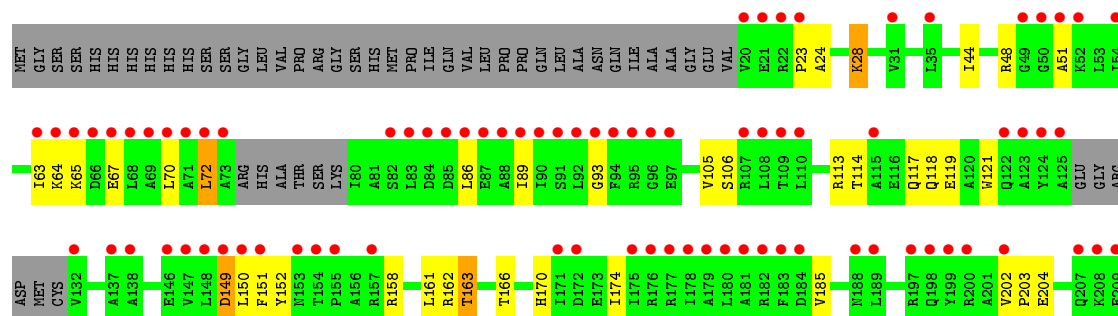


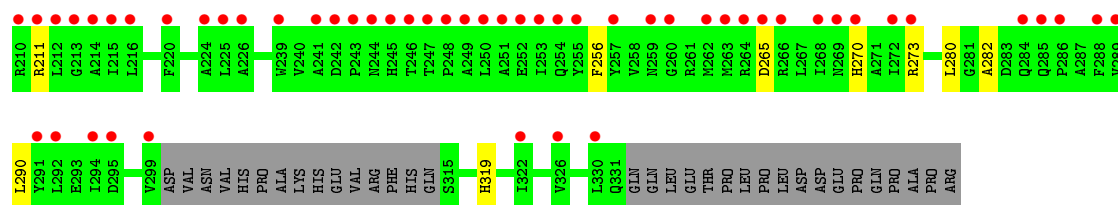
- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



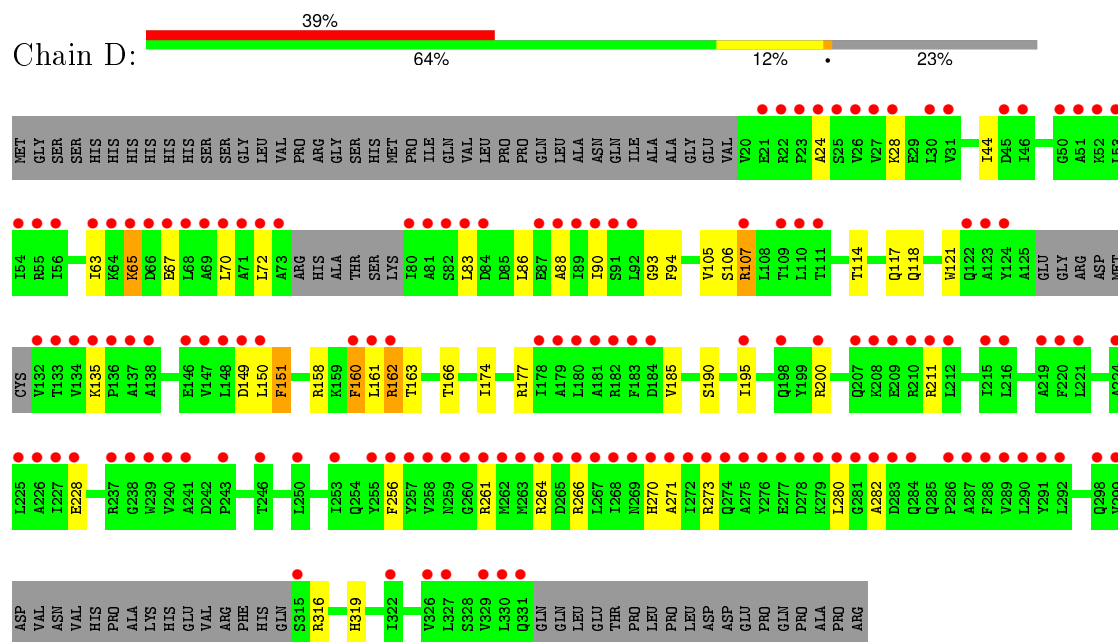


● Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

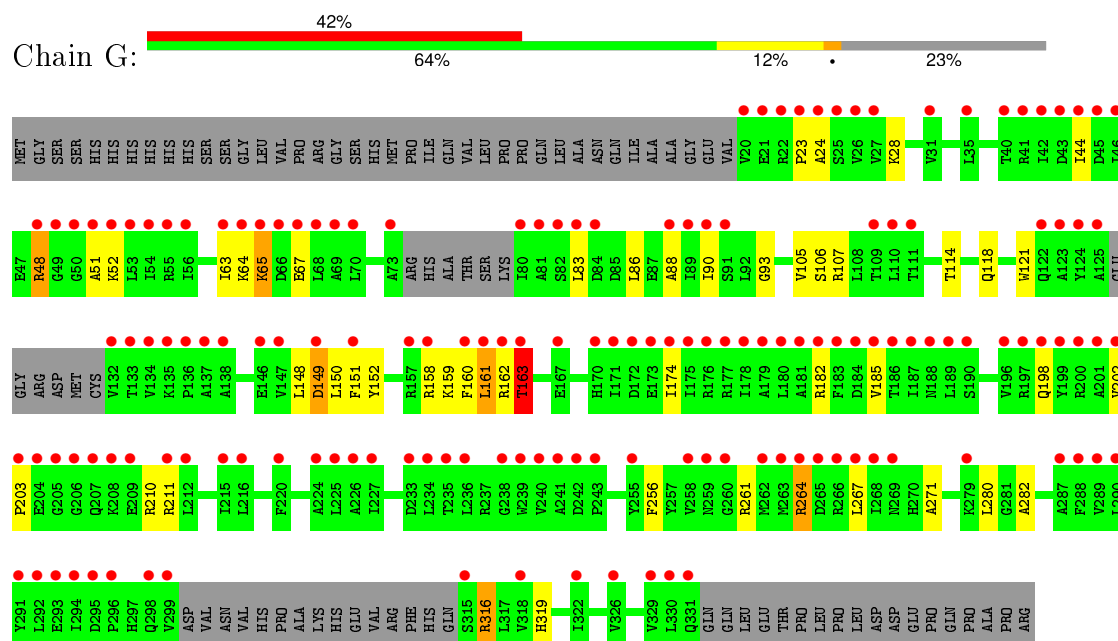




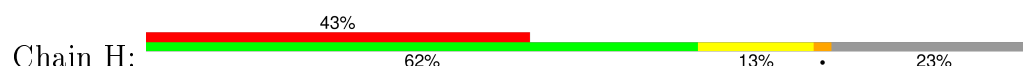
• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

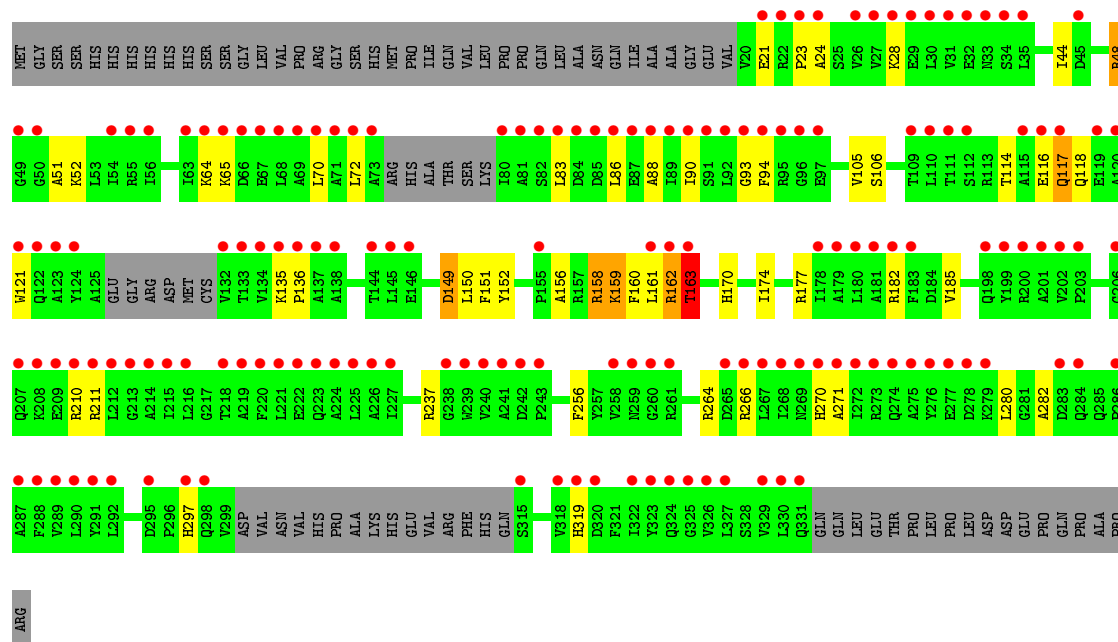


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

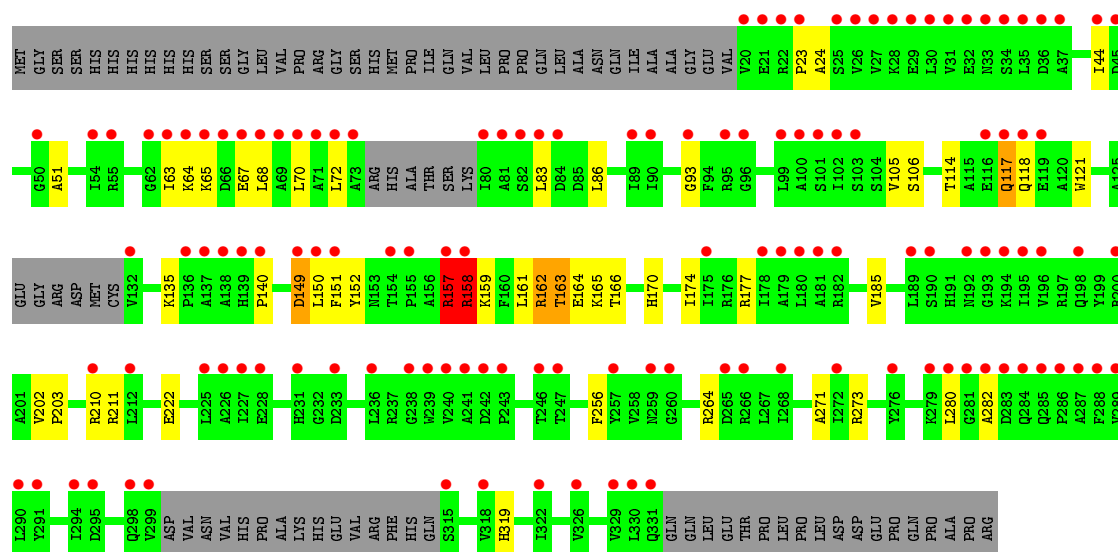


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

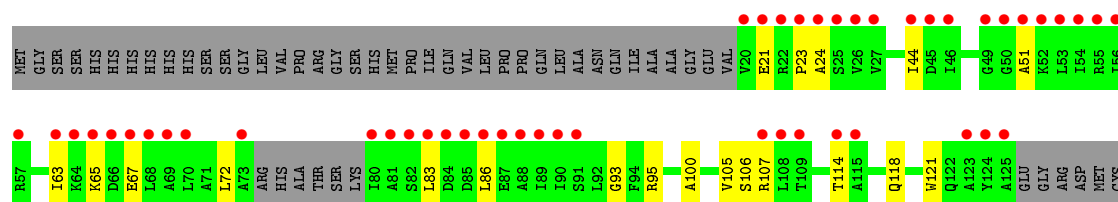


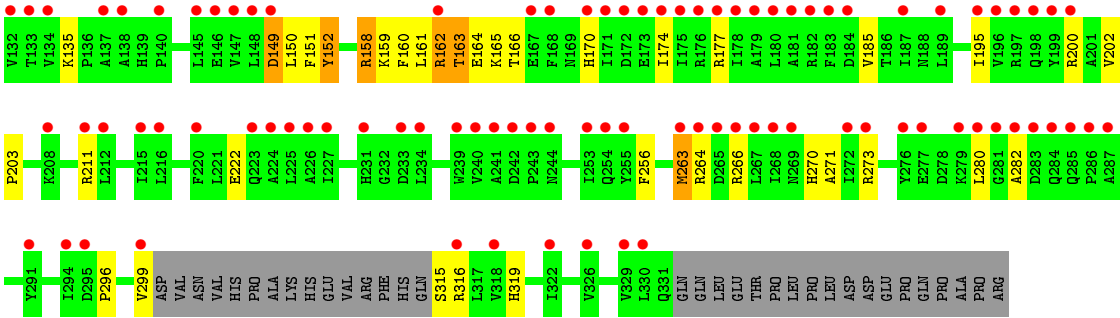


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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	193.02Å 109.76Å 275.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	275.84 – 7.60 49.30 – 7.60	Depositor EDS
% Data completeness (in resolution range)	80.1 (275.84-7.60) 80.5 (49.30-7.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 7.37Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.264 , 0.306 0.260 , 0.301	Depositor DCC
R_{free} test set	586 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	441.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 500.0	EDS
Estimated twinning fraction	0.090 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 11750 reflections	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	45054	wwPDB-VP
Average B, all atoms (Å ²)	231.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ANP

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	0.66	1/5311 (0.0%)	0.80	9/7186 (0.1%)
1	B	0.66	0/5311	0.80	10/7186 (0.1%)
1	E	0.65	3/5311 (0.1%)	0.84	16/7186 (0.2%)
1	F	0.64	0/5311	0.77	13/7186 (0.2%)
1	I	0.62	0/5311	0.74	2/7186 (0.0%)
1	J	0.70	3/5311 (0.1%)	0.86	11/7186 (0.2%)
2	C	0.72	1/2288 (0.0%)	0.79	2/3096 (0.1%)
2	D	0.82	2/2288 (0.1%)	0.85	6/3096 (0.2%)
2	G	0.71	0/2288	0.81	4/3096 (0.1%)
2	H	0.71	1/2288 (0.0%)	0.84	8/3096 (0.3%)
2	K	0.90	3/2288 (0.1%)	1.03	8/3096 (0.3%)
2	L	0.71	0/2288	0.82	5/3096 (0.2%)
All	All	0.69	14/45594 (0.0%)	0.82	94/61692 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
2	K	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	157	ARG	CD-NE	17.42	1.76	1.46
2	K	157	ARG	NE-CZ	17.13	1.55	1.33
1	J	787	LYS	CE-NZ	15.77	1.88	1.49
1	J	249	ARG	NE-CZ	13.73	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	228	GLU	CD-OE1	11.54	1.38	1.25
2	D	228	GLU	CD-OE2	11.16	1.38	1.25
2	C	28	LYS	CE-NZ	8.78	1.71	1.49
2	K	157	ARG	CZ-NH1	8.59	1.44	1.33
1	E	156	ARG	CZ-NH1	-7.00	1.24	1.33
2	H	28	LYS	CE-NZ	6.26	1.64	1.49
1	A	435	GLU	CD-OE2	6.25	1.32	1.25
1	J	171	GLN	CG-CD	5.16	1.62	1.51
1	E	713	GLU	CG-CD	5.04	1.59	1.51
1	E	420	ARG	CG-CD	5.02	1.64	1.51

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	157	ARG	NE-CZ-NH1	31.56	136.08	120.30
1	J	249	ARG	NE-CZ-NH1	29.02	134.81	120.30
1	J	249	ARG	NE-CZ-NH2	-20.07	110.27	120.30
1	E	156	ARG	NE-CZ-NH2	16.87	128.74	120.30
1	E	420	ARG	NE-CZ-NH1	13.33	126.97	120.30
2	K	157	ARG	CD-NE-CZ	12.09	140.52	123.60
1	E	156	ARG	NH1-CZ-NH2	-11.26	107.02	119.40
1	E	420	ARG	NE-CZ-NH2	-10.73	114.94	120.30
2	K	157	ARG	NH1-CZ-NH2	-9.99	108.41	119.40
1	A	354	ARG	NE-CZ-NH2	-9.98	115.31	120.30
2	K	157	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	A	507	LYS	CD-CE-NZ	-9.31	90.29	111.70
1	F	354	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	E	420	ARG	CD-NE-CZ	8.38	135.33	123.60
1	B	561	ARG	NE-CZ-NH2	-8.32	116.14	120.30
2	H	28	LYS	CD-CE-NZ	7.71	129.44	111.70
1	E	156	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	F	350	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	F	319	ARG	NE-CZ-NH2	-7.01	116.80	120.30
2	L	200	ARG	CG-CD-NE	6.90	126.30	111.80
1	J	350	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	317	ASP	CB-CG-OD2	6.78	124.41	118.30
1	F	256	ARG	NE-CZ-NH1	6.77	123.69	120.30
2	D	94	PHE	CB-CG-CD2	-6.75	116.08	120.80
1	B	368	MET	CG-SD-CE	6.74	110.98	100.20
1	F	361	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	J	128	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	J	783	LYS	CB-CG-CD	6.55	128.62	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	94	PHE	CB-CG-CD2	-6.47	116.27	120.80
2	C	273	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	F	265	ASP	CB-CG-OD2	6.45	124.11	118.30
1	F	269	MET	CG-SD-CE	6.33	110.32	100.20
1	B	313	MET	CB-CG-SD	6.30	131.30	112.40
2	H	159	LYS	CB-CG-CD	6.28	127.92	111.60
1	A	435	GLU	OE1-CD-OE2	-6.18	115.89	123.30
1	A	354	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	J	156	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	555	LEU	CB-CG-CD2	-6.15	100.55	111.00
1	E	350	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	317	ASP	CB-CG-OD2	6.13	123.82	118.30
2	L	263	MET	CG-SD-CE	6.13	110.01	100.20
2	K	222	GLU	CA-CB-CG	6.11	126.83	113.40
2	L	95	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	262	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	E	656	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	D	200	ARG	CG-CD-NE	5.94	124.28	111.80
1	B	354	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	E	409	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	783	LYS	CB-CG-CD	5.91	126.95	111.60
1	A	361	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	F	435	GLU	OE1-CD-OE2	-5.83	116.31	123.30
1	E	507	LYS	CD-CE-NZ	5.79	125.01	111.70
2	H	297	HIS	N-CA-C	5.78	126.60	111.00
1	A	269	MET	CG-SD-CE	5.74	109.39	100.20
1	J	783	LYS	CD-CE-NZ	5.72	124.86	111.70
1	E	549	LEU	CB-CG-CD2	-5.69	101.33	111.00
1	F	413	ASP	CB-CG-OD2	5.67	123.41	118.30
1	F	656	ARG	NE-CZ-NH1	5.67	123.13	120.30
2	K	158	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	420	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	J	720	LYS	CG-CD-CE	5.61	128.73	111.90
2	H	94	PHE	CB-CG-CD1	5.60	124.72	120.80
2	K	273	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	E	418	LEU	CB-CG-CD1	-5.54	101.58	111.00
2	D	266	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	G	264	ARG	NE-CZ-NH2	-5.49	117.55	120.30
2	L	273	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	G	65	LYS	CD-CE-NZ	5.46	124.25	111.70
2	K	210	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	J	207	ASP	CB-CG-OD2	5.41	123.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	94	PHE	CB-CG-CD1	5.40	124.58	120.80
1	B	431	GLU	OE1-CD-OE2	-5.40	116.83	123.30
1	I	354	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	D	273	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	E	269	MET	N-CA-CB	-5.35	100.98	110.60
2	H	182	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	J	128	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	E	617	MET	CG-SD-CE	5.31	108.69	100.20
2	D	151	PHE	N-CA-C	5.29	125.29	111.00
1	F	274	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	E	697	ARG	CG-CD-NE	5.24	122.81	111.80
2	H	237	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	343	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	F	260	MET	CG-SD-CE	5.20	108.51	100.20
2	L	222	GLU	CA-CB-CG	5.17	124.78	113.40
2	G	182	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	E	790	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	J	249	ARG	CD-NE-CZ	5.15	130.81	123.60
2	G	159	LYS	CD-CE-NZ	5.11	123.46	111.70
1	B	479	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	C	72	LEU	CA-CB-CG	5.07	126.95	115.30
2	H	210	ARG	CB-CG-CD	5.04	124.69	111.60
1	F	267	ILE	N-CA-CB	5.04	122.38	110.80
1	I	156	ARG	NE-CZ-NH2	5.03	122.82	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	129	GLN	Peptide
1	B	268	ILE	Peptide
2	K	157	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5226	0	5283	64	0
1	B	5226	0	5283	74	1
1	E	5226	0	5283	86	0
1	F	5226	0	5283	61	1
1	I	5226	0	5283	46	1
1	J	5226	0	5283	42	0
2	C	2252	0	2272	29	0
2	D	2252	0	2272	37	0
2	G	2252	0	2272	38	0
2	H	2252	0	2272	41	0
2	K	2252	0	2272	29	1
2	L	2252	0	2272	39	0
3	A	31	0	13	5	0
3	B	31	0	13	4	0
3	E	31	0	13	2	0
3	F	31	0	13	3	0
3	I	31	0	13	6	0
3	J	31	0	13	2	0
All	All	45054	0	45408	488	2

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 5.

All (488) 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)
2:C:28:LYS:CE	2:C:28:LYS:NZ	1.71	1.50
2:K:157:ARG:NE	2:K:157:ARG:CD	1.76	1.46
1:J:787:LYS:CE	1:J:787:LYS:NZ	1.88	1.35
1:E:269:MET:SD	1:E:653:ILE:HB	1.69	1.31
2:D:105:VAL:O	2:D:150:LEU:CD1	1.90	1.20
2:D:105:VAL:O	2:D:150:LEU:HD11	1.03	1.18
1:E:333:ASP:HA	2:G:210:ARG:HH22	1.00	1.16
2:C:113:ARG:HG3	2:C:118:GLN:OE1	1.47	1.14
1:E:267:ILE:HD12	1:E:316:ARG:HD2	1.12	1.11
1:I:267:ILE:HD13	1:I:314:PRO:O	1.55	1.07
1:A:770:SER:HB3	1:B:700:SER:HB2	1.41	1.00
1:E:267:ILE:HD13	1:E:651:ASP:HA	1.44	0.98
1:B:268:ILE:CD1	1:B:652:ARG:HA	1.96	0.96
1:E:333:ASP:HA	2:G:210:ARG:NH2	1.82	0.94
1:B:268:ILE:HD13	1:B:652:ARG:HA	1.50	0.93
2:H:83:LEU:HD12	2:L:270:HIS:HB2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:106:SER:HB3	2:G:150:LEU:HD22	1.52	0.91
2:K:106:SER:HB3	2:K:150:LEU:HD22	1.52	0.91
2:C:106:SER:HB3	2:C:150:LEU:HD22	1.53	0.91
1:E:267:ILE:CD1	1:E:651:ASP:HA	2.00	0.91
2:L:106:SER:HB3	2:L:150:LEU:HD22	1.53	0.90
1:F:697:ARG:O	1:F:697:ARG:HG3	1.70	0.90
1:A:670:PHE:N	3:B:1801:ANP:O1G	2.04	0.90
2:D:163:THR:OG1	2:D:166:THR:OG1	1.91	0.89
2:H:106:SER:HB3	2:H:150:LEU:HD22	1.55	0.88
1:B:617:MET:HA	3:B:1801:ANP:H5'2	1.58	0.86
2:L:163:THR:OG1	2:L:166:THR:OG1	1.92	0.86
1:E:333:ASP:CA	2:G:210:ARG:HH22	1.87	0.85
1:B:137:TRP:CH2	1:B:139:ASP:HB3	2.10	0.84
2:K:163:THR:OG1	2:K:166:THR:OG1	1.90	0.84
2:C:70:LEU:CD2	2:C:86:LEU:HD22	2.07	0.83
2:D:270:HIS:HB2	2:G:83:LEU:HD12	1.62	0.82
2:C:163:THR:OG1	2:C:166:THR:OG1	1.92	0.82
1:J:266:SER:O	1:J:267:ILE:HG12	1.80	0.82
1:F:266:SER:O	1:F:267:ILE:HG12	1.80	0.82
2:D:105:VAL:C	2:D:150:LEU:HD11	1.99	0.81
2:K:105:VAL:O	2:K:150:LEU:O	2.00	0.80
2:H:105:VAL:O	2:H:150:LEU:O	1.99	0.80
1:E:694:GLU:OE1	1:F:697:ARG:NH2	2.14	0.80
1:I:702:TYR:HB3	1:J:793:LEU:CD1	2.12	0.80
1:A:675:THR:N	1:B:779:ALA:HB1	1.97	0.80
2:C:118:GLN:NE2	2:C:119:GLU:O	2.15	0.80
2:L:105:VAL:O	2:L:150:LEU:O	1.99	0.79
1:E:267:ILE:CD1	1:E:316:ARG:HD2	2.05	0.79
2:G:114:THR:OG1	2:G:118:GLN:OE1	2.00	0.79
2:G:105:VAL:O	2:G:150:LEU:O	2.01	0.79
1:B:268:ILE:HD13	1:B:652:ARG:CA	2.13	0.79
1:I:617:MET:HE1	3:I:1801:ANP:O3G	1.81	0.78
2:C:105:VAL:O	2:C:150:LEU:O	2.00	0.78
2:D:114:THR:OG1	2:D:118:GLN:OE1	2.01	0.78
2:H:90:ILE:HG21	2:L:266:ARG:HG3	1.66	0.78
2:H:114:THR:OG1	2:H:118:GLN:OE1	2.01	0.78
2:C:70:LEU:HD21	2:C:86:LEU:HD22	1.65	0.78
1:A:770:SER:HB3	1:B:700:SER:CB	2.13	0.77
1:B:268:ILE:HD13	1:B:651:ASP:O	1.83	0.77
2:G:24:ALA:HB1	2:G:174:ILE:HD12	1.67	0.76
2:L:114:THR:OG1	2:L:118:GLN:OE1	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:114:THR:OG1	2:K:118:GLN:OE1	2.01	0.75
1:B:268:ILE:O	1:B:269:MET:CG	2.34	0.75
2:K:24:ALA:HB1	2:K:174:ILE:HD12	1.68	0.75
1:B:268:ILE:HD13	1:B:651:ASP:C	2.06	0.74
2:D:24:ALA:HB1	2:D:174:ILE:HD12	1.70	0.74
1:E:220:ARG:NE	1:F:778:LEU:HD11	2.04	0.72
2:L:24:ALA:HB1	2:L:174:ILE:HD12	1.70	0.72
1:B:268:ILE:CD1	1:B:652:ARG:CA	2.68	0.72
1:F:617:MET:HA	3:F:1801:ANP:H5'1	1.70	0.71
2:D:105:VAL:O	2:D:150:LEU:HD21	1.90	0.71
1:E:659:ALA:HB3	1:F:659:ALA:HB3	1.73	0.70
2:C:24:ALA:HB1	2:C:174:ILE:HD12	1.74	0.69
2:D:256:PHE:CZ	2:D:264:ARG:HA	2.28	0.68
1:B:137:TRP:CZ3	1:B:139:ASP:HB3	2.27	0.68
1:E:267:ILE:HD13	1:E:651:ASP:CA	2.22	0.68
2:H:24:ALA:HB1	2:H:174:ILE:HD12	1.75	0.67
2:K:256:PHE:CZ	2:K:264:ARG:HA	2.29	0.67
2:C:86:LEU:HD11	2:C:89:ILE:HB	1.76	0.67
2:G:256:PHE:CZ	2:G:264:ARG:HA	2.29	0.67
2:L:256:PHE:CZ	2:L:264:ARG:HA	2.30	0.67
1:E:268:ILE:HG23	1:E:274:ARG:HH12	1.60	0.66
1:A:670:PHE:CD2	1:B:775:VAL:HG11	2.30	0.66
2:H:256:PHE:CZ	2:H:264:ARG:HA	2.29	0.66
1:A:702:TYR:HB3	1:B:793:LEU:CD1	2.25	0.66
1:E:269:MET:SD	1:E:653:ILE:CB	2.65	0.66
1:I:267:ILE:HD11	1:I:316:ARG:HG3	1.78	0.66
1:E:617:MET:HE3	1:F:671:MET:HB3	1.78	0.66
2:C:256:PHE:CD2	2:C:290:LEU:HB2	2.31	0.65
2:L:185:VAL:O	2:L:211:ARG:NH2	2.30	0.65
1:E:269:MET:CE	1:E:653:ILE:HB	2.25	0.65
2:D:105:VAL:O	2:D:150:LEU:CG	2.44	0.65
2:G:185:VAL:O	2:G:211:ARG:NH2	2.29	0.65
1:B:268:ILE:O	1:B:269:MET:HG2	1.95	0.65
2:H:88:ALA:HB1	2:L:316:ARG:NH2	2.12	0.65
3:A:1801:ANP:O1G	1:B:670:PHE:N	2.29	0.65
1:E:269:MET:HE2	1:E:273:THR:CB	2.27	0.64
2:D:190:SER:HB3	2:D:195:ILE:HD13	1.79	0.64
1:F:619:GLY:HA2	3:F:1801:ANP:H8	1.80	0.64
2:K:185:VAL:O	2:K:211:ARG:NH2	2.30	0.64
2:D:185:VAL:O	2:D:211:ARG:NH2	2.29	0.64
2:C:63:ILE:HG23	2:C:67:GLU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:185:VAL:O	2:H:211:ARG:NH2	2.31	0.64
2:C:185:VAL:O	2:C:211:ARG:NH2	2.30	0.63
1:B:305:ARG:HA	1:B:308:LYS:HE3	1.80	0.63
1:E:564:THR:HG23	2:G:198:GLN:OE1	1.99	0.62
1:B:268:ILE:HD12	1:B:652:ARG:HA	1.78	0.62
1:I:772:GLY:HA3	1:J:703:ASP:OD2	1.99	0.62
1:F:755:THR:HG21	2:H:135:LYS:HD3	1.80	0.62
1:A:771:TYR:N	1:B:699:THR:OG1	2.32	0.62
1:B:266:SER:O	1:B:267:ILE:HD13	1.99	0.62
1:E:675:THR:N	1:F:779:ALA:HB1	2.15	0.62
1:E:617:MET:CE	1:F:671:MET:HB3	2.30	0.61
1:B:268:ILE:HD13	1:B:652:ARG:N	2.16	0.61
1:E:682:HIS:CE1	1:F:782:PRO:HG3	2.36	0.61
1:A:674:MET:C	1:B:779:ALA:HB1	2.20	0.61
1:B:773:LEU:HD13	1:B:790:ARG:HG2	1.83	0.61
1:B:268:ILE:O	1:B:269:MET:HG3	2.00	0.61
2:D:105:VAL:O	2:D:150:LEU:CD2	2.49	0.60
1:J:305:ARG:HA	1:J:308:LYS:HE3	1.82	0.60
1:E:617:MET:CE	1:F:671:MET:CB	2.80	0.60
1:E:268:ILE:HG23	1:E:269:MET:H	1.65	0.60
1:E:305:ARG:HA	1:E:308:LYS:HE3	1.83	0.60
2:D:107:ARG:NH1	2:D:107:ARG:HB3	2.16	0.60
2:D:90:ILE:HD11	2:G:267:LEU:HD13	1.83	0.60
1:E:269:MET:HE2	1:E:273:THR:HG21	1.84	0.60
2:H:48:ARG:NH2	2:H:52:LYS:HG3	2.17	0.59
2:H:83:LEU:HD22	2:H:86:LEU:HD21	1.83	0.59
1:I:305:ARG:HA	1:I:308:LYS:HE3	1.83	0.59
1:B:617:MET:HA	3:B:1801:ANP:C5'	2.28	0.59
1:A:699:THR:OG1	1:B:771:TYR:N	2.35	0.59
2:C:162:ARG:O	2:C:163:THR:O	2.21	0.59
1:A:305:ARG:HA	1:A:308:LYS:HE3	1.84	0.59
1:E:268:ILE:HD11	1:E:312:HIS:O	2.03	0.59
1:E:268:ILE:CD1	1:E:312:HIS:O	2.51	0.59
2:G:162:ARG:O	2:G:163:THR:O	2.20	0.59
2:L:162:ARG:O	2:L:163:THR:O	2.21	0.58
2:L:83:LEU:HD22	2:L:86:LEU:HD21	1.85	0.58
2:H:162:ARG:O	2:H:163:THR:O	2.21	0.58
1:E:269:MET:HE2	1:E:273:THR:HB	1.85	0.58
2:L:164:GLU:HG3	2:L:165:LYS:N	2.18	0.58
1:A:640:VAL:HG12	1:A:641:PRO:HD2	1.86	0.58
2:G:83:LEU:HD22	2:G:86:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:702:TYR:HB3	1:J:793:LEU:HD13	1.85	0.58
1:I:614:GLY:HA2	1:I:767:ALA:HB2	1.86	0.58
1:B:375:LEU:HD13	1:B:399:GLU:HA	1.86	0.58
2:H:51:ALA:O	2:H:149:ASP:HA	2.03	0.57
2:K:51:ALA:O	2:K:149:ASP:HA	2.04	0.57
2:K:23:PRO:HD3	2:K:161:LEU:HD11	1.86	0.57
2:G:83:LEU:HD13	2:G:90:ILE:CD1	2.35	0.57
1:F:773:LEU:HD13	1:F:790:ARG:HG2	1.86	0.57
1:A:703:ASP:OD2	1:B:772:GLY:HA3	2.04	0.57
2:K:162:ARG:O	2:K:163:THR:O	2.20	0.57
1:F:305:ARG:HA	1:F:308:LYS:HE3	1.86	0.57
1:A:675:THR:CA	1:B:779:ALA:HB1	2.35	0.57
1:E:614:GLY:HA2	1:E:767:ALA:HB2	1.85	0.57
2:C:118:GLN:HG2	2:C:119:GLU:N	2.19	0.57
1:E:616:ASN:OD1	1:F:670:PHE:CD2	2.58	0.57
2:G:151:PHE:O	2:G:158:ARG:NH1	2.38	0.56
2:K:83:LEU:HD22	2:K:86:LEU:HD21	1.87	0.56
1:A:784:GLU:HG2	1:B:718:LYS:NZ	2.21	0.56
2:C:64:LYS:HG2	2:C:114:THR:HG21	1.88	0.56
1:E:269:MET:HE2	1:E:273:THR:CG2	2.36	0.56
2:D:83:LEU:HD22	2:D:86:LEU:HD21	1.87	0.56
1:F:375:LEU:HD13	1:F:399:GLU:HA	1.87	0.56
2:L:51:ALA:O	2:L:149:ASP:HA	2.05	0.56
1:E:375:LEU:HD13	1:E:399:GLU:HA	1.87	0.56
1:B:614:GLY:HA2	1:B:767:ALA:HB2	1.86	0.56
1:A:262:ARG:HD2	1:A:268:ILE:HD13	1.88	0.56
1:F:614:GLY:HA2	1:F:767:ALA:HB2	1.87	0.56
2:H:151:PHE:O	2:H:158:ARG:NH1	2.39	0.56
1:J:614:GLY:HA2	1:J:767:ALA:HB2	1.87	0.56
1:A:675:THR:HG23	1:B:779:ALA:O	2.06	0.56
2:L:151:PHE:O	2:L:158:ARG:NH1	2.39	0.55
2:C:151:PHE:O	2:C:158:ARG:NH1	2.40	0.55
1:A:615:PRO:HB3	1:A:771:TYR:CD1	2.42	0.55
2:C:51:ALA:O	2:C:149:ASP:HA	2.06	0.55
1:I:375:LEU:HD13	1:I:399:GLU:HA	1.88	0.55
1:E:267:ILE:O	1:E:268:ILE:HG12	2.07	0.55
2:H:48:ARG:CZ	2:H:52:LYS:HG3	2.37	0.55
2:G:48:ARG:NH2	2:G:52:LYS:HG3	2.21	0.55
1:J:640:VAL:HG12	1:J:641:PRO:HD2	1.89	0.55
1:I:630:ILE:HG23	1:I:640:VAL:HG11	1.89	0.55
2:K:151:PHE:O	2:K:158:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:640:VAL:HG12	1:F:641:PRO:HD2	1.89	0.55
1:B:268:ILE:HG21	1:B:652:ARG:HG2	1.89	0.55
2:H:162:ARG:HD3	2:L:160:PHE:CZ	2.41	0.55
2:G:48:ARG:CZ	2:G:52:LYS:HG3	2.37	0.55
1:B:755:THR:HG21	2:D:135:LYS:HD3	1.88	0.55
1:E:267:ILE:HG12	1:E:651:ASP:O	2.07	0.54
2:H:266:ARG:HH12	2:L:100:ALA:HB2	1.72	0.54
1:A:375:LEU:HD13	1:A:399:GLU:HA	1.89	0.54
1:F:615:PRO:HB3	1:F:771:TYR:CD1	2.42	0.54
1:J:375:LEU:HD13	1:J:399:GLU:HA	1.89	0.54
2:D:107:ARG:HB3	2:D:107:ARG:HH11	1.73	0.54
1:I:640:VAL:HG12	1:I:641:PRO:HD2	1.89	0.54
1:E:588:VAL:O	1:E:592:LEU:HB2	2.08	0.54
1:E:269:MET:HE3	1:E:653:ILE:O	2.08	0.54
1:A:614:GLY:HA2	1:A:767:ALA:HB2	1.90	0.54
2:G:51:ALA:O	2:G:149:ASP:HA	2.07	0.54
2:H:64:LYS:HG2	2:H:114:THR:HG21	1.90	0.53
1:J:617:MET:HE3	1:J:775:VAL:HG13	1.89	0.53
1:E:694:GLU:OE1	1:F:697:ARG:NH1	2.41	0.53
1:A:630:ILE:HG23	1:A:640:VAL:HG11	1.91	0.53
1:A:491:ARG:HB3	1:A:491:ARG:CZ	2.37	0.53
1:A:621:SER:N	3:A:1801:ANP:O1A	2.42	0.53
1:E:615:PRO:HB3	1:E:771:TYR:CD1	2.44	0.53
1:A:700:SER:HB2	1:B:770:SER:HB3	1.90	0.53
1:B:588:VAL:O	1:B:592:LEU:HB2	2.09	0.53
2:C:23:PRO:HD3	2:C:161:LEU:HD11	1.91	0.53
1:E:269:MET:CE	1:E:653:ILE:O	2.56	0.53
1:I:137:TRP:CZ2	1:I:235:SER:HB2	2.44	0.53
1:B:630:ILE:HG23	1:B:640:VAL:HG11	1.91	0.53
1:A:137:TRP:CZ2	1:A:235:SER:HB2	2.44	0.53
1:E:137:TRP:CZ2	1:E:235:SER:HB2	2.45	0.52
1:E:630:ILE:HG23	1:E:640:VAL:HG11	1.91	0.52
1:A:617:MET:HA	3:A:1801:ANP:C5'	2.39	0.52
1:J:630:ILE:HG23	1:J:640:VAL:HG11	1.90	0.52
1:E:267:ILE:HD11	1:E:651:ASP:HA	1.86	0.52
2:L:299:VAL:HA	2:L:315:SER:OG	2.10	0.52
1:J:137:TRP:CZ2	1:J:235:SER:HB2	2.44	0.52
2:G:63:ILE:HG23	2:G:67:GLU:HB2	1.91	0.52
2:D:270:HIS:CB	2:G:83:LEU:HD12	2.37	0.52
1:I:619:GLY:HA2	3:I:1801:ANP:H8	1.91	0.52
2:D:271:ALA:HB2	2:D:319:HIS:CD2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:658:GLY:O	1:F:659:ALA:CB	2.58	0.52
1:A:526:GLN:HG2	1:B:470:VAL:HG21	1.92	0.52
1:I:670:PHE:N	3:J:1801:ANP:O1G	2.43	0.52
1:E:670:PHE:CD2	1:F:616:ASN:OD1	2.63	0.52
1:F:137:TRP:CZ2	1:F:235:SER:HB2	2.45	0.52
1:B:640:VAL:HG12	1:B:641:PRO:HD2	1.92	0.52
1:E:640:VAL:HG12	1:E:641:PRO:HD2	1.91	0.52
2:K:63:ILE:HG23	2:K:67:GLU:HB2	1.90	0.52
1:J:588:VAL:O	1:J:592:LEU:HB2	2.10	0.52
1:A:746:HIS:CE1	1:A:763:GLN:HB2	2.45	0.52
1:B:137:TRP:HD1	1:B:181:ALA:CB	2.22	0.52
2:K:271:ALA:HB2	2:K:319:HIS:CD2	2.45	0.52
1:E:796:LEU:HB3	1:F:702:TYR:CE1	2.46	0.51
2:G:64:LYS:HG3	2:G:114:THR:HG21	1.90	0.51
2:K:70:LEU:HD22	2:K:86:LEU:HD22	1.92	0.51
2:L:23:PRO:HD3	2:L:161:LEU:HD11	1.90	0.51
2:G:271:ALA:HB2	2:G:319:HIS:CD2	2.46	0.51
2:L:63:ILE:HG23	2:L:67:GLU:HB2	1.93	0.51
2:L:271:ALA:HB2	2:L:319:HIS:CD2	2.46	0.51
1:E:268:ILE:HG23	1:E:269:MET:N	2.25	0.51
2:H:23:PRO:HD3	2:H:161:LEU:HD11	1.92	0.51
1:F:224:GLY:O	1:F:679:ASN:HA	2.11	0.51
2:H:160:PHE:CE2	2:L:162:ARG:HD3	2.45	0.51
1:E:771:TYR:N	1:F:699:THR:OG1	2.43	0.51
1:E:269:MET:CE	1:E:273:THR:HG21	2.41	0.51
2:D:163:THR:OG1	2:D:166:THR:CG2	2.59	0.51
1:J:266:SER:O	1:J:267:ILE:CG1	2.57	0.51
1:F:267:ILE:HG23	1:F:316:ARG:HD2	1.93	0.51
1:F:588:VAL:O	1:F:592:LEU:HB2	2.11	0.51
1:B:615:PRO:HB3	1:B:771:TYR:CD1	2.46	0.50
1:B:268:ILE:HD12	1:B:652:ARG:CA	2.39	0.50
1:F:266:SER:O	1:F:267:ILE:CG1	2.56	0.50
2:H:105:VAL:HG12	2:H:151:PHE:HA	1.93	0.50
1:F:630:ILE:HG23	1:F:640:VAL:HG11	1.93	0.50
1:E:746:HIS:CE1	1:E:763:GLN:HB2	2.47	0.50
1:I:519:LYS:HE3	1:J:470:VAL:O	2.11	0.50
2:L:105:VAL:HG12	2:L:151:PHE:HA	1.94	0.50
1:I:702:TYR:CB	1:J:793:LEU:CD1	2.86	0.50
1:J:617:MET:CE	1:J:775:VAL:HG13	2.41	0.50
1:J:588:VAL:HA	1:J:591:VAL:HG12	1.94	0.50
1:I:588:VAL:O	1:I:592:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:MET:HA	3:A:1801:ANP:H5'1	1.93	0.50
1:I:276:ASN:HA	1:I:283:LEU:HD21	1.93	0.50
1:A:588:VAL:O	1:A:592:LEU:HB2	2.11	0.50
1:E:617:MET:CE	1:F:671:MET:HB2	2.42	0.50
1:E:617:MET:HE2	1:F:671:MET:HB2	1.94	0.50
2:D:190:SER:CB	2:D:195:ILE:HD13	2.42	0.49
1:J:617:MET:HA	3:J:1801:ANP:H5'1	1.94	0.49
2:H:160:PHE:CE1	2:L:162:ARG:NH1	2.80	0.49
2:L:316:ARG:HB2	2:L:316:ARG:NH1	2.27	0.49
1:E:617:MET:HE2	1:F:671:MET:CB	2.42	0.49
2:K:164:GLU:CG	2:K:165:LYS:N	2.75	0.49
1:E:674:MET:C	1:F:779:ALA:HB1	2.33	0.49
1:B:268:ILE:HD12	1:B:653:ILE:N	2.28	0.49
1:E:224:GLY:O	1:E:679:ASN:HA	2.13	0.49
1:A:671:MET:CE	1:B:778:LEU:HD23	2.42	0.49
1:I:796:LEU:HB3	1:J:702:TYR:CE1	2.47	0.49
2:H:90:ILE:HG21	2:L:266:ARG:CG	2.40	0.49
2:K:164:GLU:HG3	2:K:165:LYS:N	2.27	0.49
1:E:269:MET:HE1	1:E:653:ILE:HG22	1.94	0.49
1:B:746:HIS:CE1	1:B:763:GLN:HB2	2.48	0.48
2:G:105:VAL:HG12	2:G:151:PHE:HA	1.96	0.48
2:D:163:THR:OG1	2:D:166:THR:HG23	2.13	0.48
2:D:70:LEU:HD22	2:D:86:LEU:HD22	1.95	0.48
1:I:224:GLY:O	1:I:679:ASN:HA	2.12	0.48
1:B:268:ILE:O	1:B:268:ILE:HG13	2.12	0.48
2:D:162:ARG:NH1	2:D:166:THR:HG21	2.28	0.48
1:I:615:PRO:HB3	1:I:771:TYR:CD1	2.48	0.48
1:E:267:ILE:HD12	1:E:316:ARG:CD	2.07	0.48
2:H:90:ILE:HG23	2:L:266:ARG:HD3	1.95	0.48
1:A:276:ASN:HA	1:A:283:LEU:HD21	1.94	0.48
1:J:746:HIS:CE1	1:J:763:GLN:HB2	2.48	0.48
1:A:785:VAL:HG13	1:B:710:ALA:HB3	1.96	0.48
1:E:779:ALA:HB1	1:F:675:THR:HA	1.94	0.48
1:E:694:GLU:OE1	1:F:697:ARG:CZ	2.62	0.48
1:A:784:GLU:HG2	1:B:718:LYS:HZ1	1.77	0.48
2:K:202:VAL:HG12	2:K:203:PRO:O	2.13	0.48
1:B:224:GLY:O	1:B:679:ASN:HA	2.14	0.48
2:C:113:ARG:CG	2:C:118:GLN:OE1	2.41	0.48
1:I:267:ILE:C	1:I:268:ILE:HG13	2.34	0.48
2:D:163:THR:OG1	2:D:166:THR:CB	2.62	0.48
1:A:659:ALA:HB3	1:B:659:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:105:VAL:HG12	2:K:151:PHE:HA	1.95	0.47
2:H:88:ALA:CB	2:L:316:ARG:NH2	2.77	0.47
1:J:615:PRO:HB3	1:J:771:TYR:CD1	2.49	0.47
2:D:65:LYS:HB3	2:D:121:TRP:CD1	2.49	0.47
2:D:316:ARG:HB2	2:D:316:ARG:NH1	2.29	0.47
1:F:491:ARG:HB3	1:F:491:ARG:CZ	2.44	0.47
2:D:63:ILE:HG23	2:D:67:GLU:HB2	1.96	0.47
1:E:616:ASN:HD22	3:E:1801:ANP:HNB1	1.60	0.47
2:L:165:LYS:HG3	2:L:166:THR:N	2.30	0.47
2:H:88:ALA:CB	2:L:316:ARG:HH21	2.27	0.47
2:G:107:ARG:NH2	2:G:148:LEU:HD13	2.29	0.47
1:A:617:MET:CE	1:A:775:VAL:HG13	2.44	0.47
2:H:162:ARG:HD3	2:L:160:PHE:CE1	2.49	0.47
2:C:105:VAL:HG12	2:C:151:PHE:HA	1.97	0.47
2:G:83:LEU:HD22	2:G:90:ILE:HD11	1.95	0.47
1:B:588:VAL:HA	1:B:591:VAL:HG12	1.97	0.47
1:J:224:GLY:O	1:J:679:ASN:HA	2.14	0.47
1:J:276:ASN:HA	1:J:283:LEU:HD21	1.95	0.47
1:A:588:VAL:HA	1:A:591:VAL:HG12	1.97	0.47
1:A:502:ILE:HD12	1:A:506:LEU:HD23	1.97	0.47
1:F:584:ARG:NE	1:F:589:GLU:OE1	2.47	0.47
1:I:267:ILE:CD1	1:I:316:ARG:HG3	2.43	0.47
1:F:153:GLY:HA2	1:F:255:ILE:HG12	1.97	0.47
2:G:106:SER:HB3	2:G:150:LEU:CD2	2.35	0.47
1:E:268:ILE:CG2	1:E:269:MET:N	2.77	0.46
1:F:491:ARG:NH1	1:F:491:ARG:HB3	2.29	0.46
2:D:88:ALA:HB2	2:G:316:ARG:NH1	2.30	0.46
2:L:107:ARG:HD3	2:L:152:TYR:CE2	2.50	0.46
1:I:267:ILE:O	1:I:268:ILE:HG13	2.15	0.46
1:I:617:MET:HE3	1:J:671:MET:HB3	1.97	0.46
2:K:65:LYS:HB3	2:K:121:TRP:CD1	2.51	0.46
1:E:333:ASP:CG	2:G:210:ARG:HH12	2.18	0.46
1:A:584:ARG:NE	1:A:589:GLU:OE1	2.47	0.46
2:K:106:SER:HB3	2:K:150:LEU:CD2	2.37	0.46
1:E:658:GLY:O	1:F:659:ALA:HB1	2.16	0.46
3:E:1801:ANP:O1G	1:F:670:PHE:N	2.49	0.46
2:G:23:PRO:HD3	2:G:161:LEU:HD11	1.98	0.46
1:A:224:GLY:O	1:A:679:ASN:HA	2.16	0.46
1:I:771:TYR:N	1:J:699:THR:OG1	2.47	0.46
1:E:584:ARG:NE	1:E:589:GLU:OE1	2.48	0.46
1:I:746:HIS:CE1	1:I:763:GLN:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:SER:O	1:E:267:ILE:HB	2.16	0.46
2:C:113:ARG:HA	2:C:118:GLN:HE22	1.81	0.46
1:B:351:ILE:HG21	1:B:368:MET:CE	2.46	0.46
1:J:425:ILE:HG13	1:J:524:GLU:HG3	1.98	0.45
1:A:202:TRP:NE1	2:D:158:ARG:NH1	2.64	0.45
1:E:256:ARG:NH1	1:F:783:LYS:HE3	2.31	0.45
1:B:502:ILE:HD12	1:B:506:LEU:HD23	1.97	0.45
1:I:266:SER:O	1:I:267:ILE:HB	2.15	0.45
2:G:280:LEU:HD13	2:G:282:ALA:HB3	1.98	0.45
2:H:117:GLN:N	2:H:117:GLN:OE1	2.49	0.45
1:I:775:VAL:HG11	1:J:670:PHE:CE2	2.51	0.45
1:A:675:THR:HA	1:B:779:ALA:HB1	1.98	0.45
1:F:276:ASN:HA	1:F:283:LEU:HD21	1.97	0.45
1:E:773:LEU:HD13	1:E:790:ARG:HG2	1.98	0.45
2:C:270:HIS:CD2	2:C:319:HIS:CE1	3.05	0.45
1:I:755:THR:HG21	2:K:135:LYS:HD3	1.98	0.45
1:I:588:VAL:HA	1:I:591:VAL:HG12	1.99	0.45
1:J:773:LEU:HD13	1:J:790:ARG:HG2	1.98	0.45
1:A:674:MET:CB	1:B:779:ALA:CB	2.95	0.45
1:A:491:ARG:HB3	1:A:491:ARG:NH1	2.32	0.45
1:A:796:LEU:HB3	1:B:702:TYR:CE1	2.51	0.45
2:H:270:HIS:CD2	2:H:319:HIS:CE1	3.04	0.45
1:I:595:PRO:HG2	2:K:140:PRO:HD2	1.98	0.45
2:H:83:LEU:HD13	2:H:90:ILE:CD1	2.46	0.45
1:A:617:MET:HE3	1:A:775:VAL:HG13	1.98	0.45
1:F:746:HIS:CE1	1:F:763:GLN:HB2	2.52	0.45
1:I:470:VAL:HG21	1:J:526:GLN:HG2	1.99	0.45
1:I:502:ILE:HD12	1:I:506:LEU:HD23	1.99	0.44
1:F:402:GLU:HG3	1:F:403:LEU:N	2.31	0.44
1:A:267:ILE:HG23	1:A:316:ARG:HD2	1.99	0.44
1:F:691:LEU:HD21	1:F:724:LEU:HD12	1.99	0.44
1:A:671:MET:HE2	1:B:778:LEU:HD23	1.99	0.44
1:A:694:GLU:OE1	1:B:697:ARG:NH2	2.50	0.44
1:E:268:ILE:CG2	1:E:274:ARG:HH12	2.28	0.44
1:I:617:MET:HE2	3:I:1801:ANP:O1G	2.18	0.44
1:I:617:MET:SD	3:I:1801:ANP:H5'1	2.58	0.44
1:E:268:ILE:HD12	1:E:312:HIS:O	2.18	0.44
1:E:153:GLY:HA2	1:E:255:ILE:HG12	2.00	0.44
1:J:267:ILE:HG23	1:J:316:ARG:HD2	2.00	0.44
1:B:584:ARG:NE	1:B:589:GLU:OE1	2.49	0.44
1:B:276:ASN:HA	1:B:283:LEU:HD21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:GLY:HA2	3:A:1801:ANP:H8	2.00	0.43
2:L:65:LYS:HB3	2:L:121:TRP:CD1	2.52	0.43
1:J:153:GLY:HA2	1:J:255:ILE:HG12	2.00	0.43
2:G:65:LYS:HB3	2:G:121:TRP:CD1	2.53	0.43
1:I:787:LYS:HE2	1:I:787:LYS:HB2	1.86	0.43
1:A:674:MET:HB3	1:B:779:ALA:CB	2.49	0.43
1:E:675:THR:HG23	1:F:779:ALA:O	2.17	0.43
1:B:313:MET:HG2	1:B:313:MET:O	2.19	0.43
2:H:65:LYS:HB3	2:H:121:TRP:CD1	2.54	0.43
1:I:619:GLY:HA2	3:I:1801:ANP:C8	2.49	0.43
1:F:752:HIS:CD2	1:F:755:THR:HG23	2.54	0.43
1:E:473:TYR:O	1:E:492:ARG:NH1	2.52	0.43
1:I:155:PHE:CE2	1:I:258:ILE:HD12	2.54	0.43
2:L:202:VAL:HG12	2:L:203:PRO:O	2.19	0.43
1:A:770:SER:CB	1:B:700:SER:HB2	2.30	0.43
1:E:728:HIS:CD2	1:F:697:ARG:NH2	2.87	0.43
1:A:674:MET:HB2	1:B:779:ALA:HB2	2.00	0.43
2:K:280:LEU:HD13	2:K:282:ALA:HB3	2.01	0.43
2:D:150:LEU:HD12	2:D:150:LEU:HA	1.37	0.42
2:C:51:ALA:O	2:C:149:ASP:CA	2.67	0.42
1:J:502:ILE:HD12	1:J:506:LEU:HD23	2.01	0.42
2:C:65:LYS:HB3	2:C:121:TRP:CD1	2.54	0.42
1:I:267:ILE:CD1	1:I:314:PRO:O	2.45	0.42
2:H:117:GLN:HG2	2:H:117:GLN:O	2.19	0.42
1:E:699:THR:HA	1:F:728:HIS:CG	2.54	0.42
1:A:714:ASN:HA	1:A:718:LYS:HD3	2.00	0.42
1:A:160:PRO:HA	1:A:263:GLU:OE2	2.19	0.42
1:J:752:HIS:CD2	1:J:755:THR:HG23	2.54	0.42
1:E:155:PHE:CE2	1:E:258:ILE:HD12	2.54	0.42
1:F:502:ILE:HD12	1:F:506:LEU:HD23	2.00	0.42
1:I:584:ARG:NE	1:I:589:GLU:OE1	2.52	0.42
1:J:584:ARG:NE	1:J:589:GLU:OE1	2.53	0.42
1:J:267:ILE:HG22	1:J:651:ASP:O	2.20	0.42
2:C:280:LEU:HD13	2:C:282:ALA:HB3	2.01	0.42
1:E:269:MET:HE1	1:E:653:ILE:HB	2.01	0.42
2:K:51:ALA:O	2:K:149:ASP:CA	2.67	0.42
2:L:280:LEU:HD13	2:L:282:ALA:HB3	2.00	0.42
1:E:425:ILE:HG13	1:E:524:GLU:HG3	2.01	0.42
1:J:160:PRO:HA	1:J:263:GLU:OE2	2.20	0.42
2:D:106:SER:HA	2:D:150:LEU:CD1	2.50	0.42
1:J:473:TYR:O	1:J:492:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:622:THR:HB	3:I:1801:ANP:N7	2.34	0.42
2:C:63:ILE:CG2	2:C:67:GLU:HB2	2.49	0.42
1:E:351:ILE:HG21	1:E:368:MET:CE	2.50	0.42
1:E:276:ASN:HA	1:E:283:LEU:HD21	2.00	0.42
1:E:269:MET:HE1	1:E:653:ILE:CG2	2.49	0.42
2:L:51:ALA:HB1	2:L:149:ASP:OD2	2.20	0.42
1:F:473:TYR:O	1:F:492:ARG:NH1	2.53	0.42
2:D:162:ARG:HB3	2:D:163:THR:H	1.71	0.41
1:B:155:PHE:CE2	1:B:258:ILE:HD12	2.55	0.41
1:A:425:ILE:HG13	1:A:524:GLU:HG3	2.02	0.41
2:D:160:PHE:CE1	2:G:160:PHE:HB3	2.55	0.41
1:A:153:GLY:HA2	1:A:255:ILE:HG12	2.01	0.41
2:K:64:LYS:HG2	2:K:114:THR:HG21	2.03	0.41
2:C:51:ALA:HB1	2:C:149:ASP:OD2	2.21	0.41
2:H:271:ALA:HB2	2:H:319:HIS:ND1	2.34	0.41
2:D:280:LEU:HD13	2:D:282:ALA:HB3	2.02	0.41
1:E:269:MET:SD	1:E:653:ILE:HD12	2.61	0.41
1:B:425:ILE:HG13	1:B:524:GLU:HG3	2.02	0.41
1:A:473:TYR:O	1:A:492:ARG:NH1	2.52	0.41
1:A:155:PHE:CE2	1:A:258:ILE:HD12	2.56	0.41
1:A:502:ILE:CD1	1:A:506:LEU:HD23	2.51	0.41
1:B:491:ARG:CZ	1:B:491:ARG:HB3	2.50	0.41
1:J:155:PHE:CE2	1:J:258:ILE:HD12	2.54	0.41
2:G:202:VAL:HG12	2:G:203:PRO:O	2.20	0.41
2:L:164:GLU:CG	2:L:165:LYS:N	2.84	0.41
2:L:51:ALA:O	2:L:149:ASP:CA	2.68	0.41
1:A:670:PHE:CE2	1:B:775:VAL:HG11	2.56	0.41
2:H:51:ALA:HB1	2:H:149:ASP:OD2	2.20	0.41
2:H:51:ALA:O	2:H:149:ASP:CA	2.67	0.41
2:G:83:LEU:HD13	2:G:90:ILE:HD12	2.01	0.41
1:E:502:ILE:HD12	1:E:506:LEU:HD23	2.01	0.41
1:B:585:HIS:CE1	1:B:629:LEU:CD1	3.03	0.41
1:J:654:PHE:HB3	1:J:680:ILE:HG12	2.03	0.41
2:H:156:ALA:HB1	2:H:160:PHE:CZ	2.56	0.41
1:F:752:HIS:CD2	2:H:136:PRO:HG2	2.56	0.41
2:G:51:ALA:O	2:G:149:ASP:CA	2.69	0.41
2:K:68:LEU:CD1	2:K:121:TRP:HB2	2.51	0.41
1:E:160:PRO:HA	1:E:263:GLU:OE2	2.21	0.41
1:B:619:GLY:HA2	3:B:1801:ANP:H8	2.03	0.41
1:F:208:THR:HG23	2:G:107:ARG:NH2	2.35	0.41
1:A:267:ILE:HG22	1:A:651:ASP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:473:TYR:O	1:I:492:ARG:NH1	2.54	0.41
1:F:160:PRO:HA	1:F:263:GLU:OE2	2.21	0.41
1:B:502:ILE:CD1	1:B:506:LEU:HD23	2.51	0.40
1:I:616:ASN:ND2	1:J:670:PHE:CD2	2.89	0.40
1:I:352:LEU:HD13	1:I:543:GLN:HA	2.03	0.40
2:K:51:ALA:HB1	2:K:149:ASP:OD2	2.21	0.40
1:J:755:THR:HG21	2:L:135:LYS:HD3	2.02	0.40
1:B:491:ARG:NH1	1:B:491:ARG:HB3	2.36	0.40
1:F:596:PHE:HA	3:F:1801:ANP:H2	2.03	0.40
1:E:659:ALA:HB3	1:F:659:ALA:CB	2.45	0.40
1:E:207:ASP:HB2	2:H:52:LYS:HE2	2.03	0.40
1:A:784:GLU:OE2	1:B:718:LYS:NZ	2.54	0.40
2:H:280:LEU:HD13	2:H:282:ALA:HB3	2.02	0.40
1:I:267:ILE:CG2	1:I:268:ILE:N	2.82	0.40
2:D:316:ARG:HH21	2:G:88:ALA:CB	2.34	0.40
1:A:580:ILE:HG21	1:A:583:GLY:HA3	2.04	0.40
1:A:294:VAL:HG21	1:A:587:VAL:HG13	2.04	0.40
1:F:155:PHE:CE2	1:F:258:ILE:HD12	2.55	0.40
2:C:202:VAL:HG12	2:C:203:PRO:O	2.21	0.40
2:H:70:LEU:HD22	2:H:86:LEU:HD22	2.03	0.40
1:E:220:ARG:CD	1:F:778:LEU:HD11	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:GLU:OE2	1:F:491:ARG:NH1[2_544]	1.87	0.33
1:I:488:ASN:ND2	2:K:117:GLN:OE1[1_545]	1.91	0.29

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	659/800 (82%)	636 (96%)	23 (4%)	0	100	100
1	B	659/800 (82%)	638 (97%)	21 (3%)	0	100	100
1	E	659/800 (82%)	632 (96%)	24 (4%)	3 (0%)	34	77
1	F	659/800 (82%)	634 (96%)	23 (4%)	2 (0%)	46	83
1	I	659/800 (82%)	635 (96%)	22 (3%)	2 (0%)	46	83
1	J	659/800 (82%)	639 (97%)	18 (3%)	2 (0%)	46	83
2	C	277/369 (75%)	258 (93%)	15 (5%)	4 (1%)	14	58
2	D	277/369 (75%)	260 (94%)	13 (5%)	4 (1%)	14	58
2	G	277/369 (75%)	261 (94%)	13 (5%)	3 (1%)	17	63
2	H	277/369 (75%)	260 (94%)	13 (5%)	4 (1%)	14	58
2	K	277/369 (75%)	262 (95%)	11 (4%)	4 (1%)	14	58
2	L	277/369 (75%)	261 (94%)	12 (4%)	4 (1%)	14	58
All	All	5616/7014 (80%)	5376 (96%)	208 (4%)	32 (1%)	30	74

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	163	THR
2	D	151	PHE
1	F	267	ILE
2	G	163	THR
2	H	163	THR
1	J	267	ILE
2	K	163	THR
2	L	163	THR
2	C	149	ASP
2	D	149	ASP
1	E	264	GLN
1	E	267	ILE
2	G	149	ASP
2	H	149	ASP
1	I	267	ILE
2	K	149	ASP
2	L	149	ASP
2	D	117	GLN
2	C	117	GLN
2	H	117	GLN
1	I	658	GLY
2	K	117	GLN

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Mol	Chain	Res	Type
2	L	296	PRO
2	C	93	GLY
2	D	93	GLY
2	G	93	GLY
2	H	93	GLY
2	K	93	GLY
2	L	93	GLY
1	J	658	GLY
1	F	658	GLY
1	E	658	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	550/662 (83%)	539 (98%)	11 (2%)	63	85
1	B	550/662 (83%)	541 (98%)	9 (2%)	70	88
1	E	550/662 (83%)	539 (98%)	11 (2%)	63	85
1	F	550/662 (83%)	541 (98%)	9 (2%)	70	88
1	I	550/662 (83%)	538 (98%)	12 (2%)	60	83
1	J	550/662 (83%)	541 (98%)	9 (2%)	70	88
2	C	235/308 (76%)	228 (97%)	7 (3%)	48	77
2	D	235/308 (76%)	225 (96%)	10 (4%)	35	70
2	G	235/308 (76%)	227 (97%)	8 (3%)	44	75
2	H	235/308 (76%)	223 (95%)	12 (5%)	29	66
2	K	235/308 (76%)	227 (97%)	8 (3%)	44	75
2	L	235/308 (76%)	224 (95%)	11 (5%)	32	68
All	All	4710/5820 (81%)	4593 (98%)	117 (2%)	55	81

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	269	MET
1	A	300	THR
1	A	333	ASP
1	A	359	THR
1	A	420	ARG
1	A	431	GLU
1	A	519	LYS
1	A	575	LYS
1	A	640	VAL
1	A	697	ARG
1	A	734	GLN
1	B	267	ILE
1	B	300	THR
1	B	359	THR
1	B	519	LYS
1	B	616	ASN
1	B	640	VAL
1	B	734	GLN
1	B	783	LYS
1	B	787	LYS
2	C	44	ILE
2	C	48	ARG
2	C	72	LEU
2	C	152	TYR
2	C	170	HIS
2	C	204	GLU
2	C	265	ASP
2	D	28	LYS
2	D	44	ILE
2	D	65	LYS
2	D	72	LEU
2	D	107	ARG
2	D	160	PHE
2	D	161	LEU
2	D	162	ARG
2	D	177	ARG
2	D	261	ARG
1	E	268	ILE
1	E	300	THR
1	E	420	ARG
1	E	435	GLU
1	E	519	LYS
1	E	530	GLU

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Mol	Chain	Res	Type
1	E	616	ASN
1	E	640	VAL
1	E	643	GLN
1	E	734	GLN
1	E	787	LYS
1	F	300	THR
1	F	420	ARG
1	F	487	ILE
1	F	575	LYS
1	F	616	ASN
1	F	640	VAL
1	F	697	ARG
1	F	734	GLN
1	F	794	ARG
2	G	28	LYS
2	G	44	ILE
2	G	48	ARG
2	G	152	TYR
2	G	161	LEU
2	G	163	THR
2	G	261	ARG
2	G	316	ARG
2	H	21	GLU
2	H	44	ILE
2	H	48	ARG
2	H	72	LEU
2	H	116	GLU
2	H	152	TYR
2	H	158	ARG
2	H	159	LYS
2	H	162	ARG
2	H	163	THR
2	H	170	HIS
2	H	177	ARG
1	I	266	SER
1	I	300	THR
1	I	333	ASP
1	I	361	ARG
1	I	435	GLU
1	I	519	LYS
1	I	530	GLU
1	I	540	GLU

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Mol	Chain	Res	Type
1	I	640	VAL
1	I	643	GLN
1	I	734	GLN
1	I	787	LYS
1	J	300	THR
1	J	402	GLU
1	J	519	LYS
1	J	540	GLU
1	J	640	VAL
1	J	734	GLN
1	J	783	LYS
1	J	788	ARG
1	J	794	ARG
2	K	44	ILE
2	K	72	LEU
2	K	152	TYR
2	K	158	ARG
2	K	159	LYS
2	K	162	ARG
2	K	170	HIS
2	K	177	ARG
2	L	21	GLU
2	L	44	ILE
2	L	72	LEU
2	L	152	TYR
2	L	158	ARG
2	L	159	LYS
2	L	162	ARG
2	L	170	HIS
2	L	177	ARG
2	L	195	ILE
2	L	263	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
1	A	585	HIS
1	A	714	ASN
1	B	264	GLN
1	B	339	GLN
1	B	526	GLN

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Mol	Chain	Res	Type
1	B	585	HIS
1	B	616	ASN
2	C	270	HIS
2	C	319	HIS
1	E	214	ASN
1	E	585	HIS
1	F	212	GLN
1	F	585	HIS
1	F	616	ASN
2	H	270	HIS
2	H	319	HIS
2	H	331	GLN
1	I	264	GLN
1	I	339	GLN
1	I	585	HIS
1	J	585	HIS

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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	A	1801	-	29,33,33	2.02	8 (27%)	26,52,52	2.29	6 (23%)
3	ANP	B	1801	-	29,33,33	1.96	7 (24%)	26,52,52	1.92	6 (23%)
3	ANP	E	1801	-	29,33,33	2.02	9 (31%)	26,52,52	2.07	6 (23%)
3	ANP	F	1801	-	29,33,33	1.85	9 (31%)	26,52,52	2.04	8 (30%)
3	ANP	I	1801	-	29,33,33	1.94	9 (31%)	26,52,52	1.95	4 (15%)
3	ANP	J	1801	-	29,33,33	1.93	8 (27%)	26,52,52	1.89	4 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	B	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	E	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	F	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	I	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	J	1801	-	-	0/13/38/38	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1801	ANP	PG-O3G	-3.59	1.47	1.56
3	I	1801	ANP	PG-O2G	-3.50	1.47	1.56
3	E	1801	ANP	PG-O2G	-3.30	1.47	1.56
3	I	1801	ANP	PG-O3G	-3.17	1.48	1.56
3	B	1801	ANP	PB-O2B	-3.10	1.48	1.56
3	E	1801	ANP	PB-O2B	-2.99	1.48	1.56
3	B	1801	ANP	PG-O3G	-2.88	1.49	1.56
3	I	1801	ANP	PB-O2B	-2.82	1.49	1.56
3	A	1801	ANP	PB-O2B	-2.78	1.49	1.56
3	A	1801	ANP	PG-O2G	-2.76	1.49	1.56
3	J	1801	ANP	PG-O3G	-2.71	1.49	1.56
3	J	1801	ANP	PB-O2B	-2.71	1.49	1.56
3	J	1801	ANP	PG-O2G	-2.61	1.49	1.56
3	F	1801	ANP	PG-O2G	-2.49	1.50	1.56
3	F	1801	ANP	PG-O3G	-2.48	1.50	1.56
3	B	1801	ANP	PG-O2G	-2.39	1.50	1.56
3	E	1801	ANP	PG-O3G	-2.37	1.50	1.56
3	F	1801	ANP	C2'-C1'	-2.35	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1801	ANP	PB-O2B	-2.10	1.51	1.56
3	A	1801	ANP	O4'-C1'	2.07	1.44	1.41
3	E	1801	ANP	PG-O1G	2.10	1.48	1.46
3	J	1801	ANP	O3'-C3'	2.14	1.48	1.43
3	I	1801	ANP	C2-N3	2.33	1.36	1.32
3	A	1801	ANP	PB-O1B	2.54	1.48	1.46
3	B	1801	ANP	PG-N3B	2.70	1.70	1.63
3	E	1801	ANP	C2-N3	2.78	1.37	1.32
3	I	1801	ANP	PB-O1B	2.89	1.49	1.46
3	F	1801	ANP	C5-C4	3.00	1.47	1.40
3	J	1801	ANP	PB-O1B	3.05	1.49	1.46
3	F	1801	ANP	PG-O1G	3.15	1.49	1.46
3	F	1801	ANP	PB-O1B	3.23	1.49	1.46
3	B	1801	ANP	C5-C4	3.25	1.47	1.40
3	I	1801	ANP	PG-O1G	3.35	1.49	1.46
3	E	1801	ANP	PB-O1B	3.35	1.49	1.46
3	I	1801	ANP	PG-N3B	3.43	1.72	1.63
3	J	1801	ANP	C5-C4	3.45	1.48	1.40
3	I	1801	ANP	C5-C4	3.45	1.48	1.40
3	F	1801	ANP	PB-N3B	3.67	1.73	1.63
3	E	1801	ANP	C5-C4	3.71	1.48	1.40
3	A	1801	ANP	C5-C4	3.80	1.49	1.40
3	E	1801	ANP	PB-N3B	3.83	1.73	1.63
3	B	1801	ANP	PB-N3B	3.89	1.73	1.63
3	F	1801	ANP	PG-N3B	4.03	1.74	1.63
3	E	1801	ANP	PG-N3B	4.05	1.74	1.63
3	I	1801	ANP	PB-N3B	4.11	1.74	1.63
3	J	1801	ANP	PB-N3B	4.23	1.74	1.63
3	A	1801	ANP	PB-N3B	4.53	1.75	1.63
3	A	1801	ANP	PG-N3B	4.65	1.76	1.63
3	J	1801	ANP	PG-N3B	4.74	1.76	1.63
3	B	1801	ANP	PB-O1B	5.42	1.52	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	ANP	N3-C2-N1	-8.44	122.24	128.87
3	J	1801	ANP	N3-C2-N1	-6.70	123.61	128.87
3	E	1801	ANP	N3-C2-N1	-6.44	123.81	128.87
3	I	1801	ANP	N3-C2-N1	-6.30	123.92	128.87
3	B	1801	ANP	N3-C2-N1	-6.27	123.94	128.87
3	F	1801	ANP	N3-C2-N1	-5.93	124.21	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1801	ANP	PA-O3A-PB	-3.79	118.96	132.71
3	I	1801	ANP	PA-O3A-PB	-3.75	119.12	132.71
3	E	1801	ANP	PA-O3A-PB	-3.61	119.62	132.71
3	B	1801	ANP	PA-O3A-PB	-3.23	120.99	132.71
3	A	1801	ANP	PA-O3A-PB	-3.15	121.29	132.71
3	J	1801	ANP	PA-O3A-PB	-2.53	123.53	132.71
3	F	1801	ANP	C1'-N9-C4	-2.46	124.06	126.81
3	F	1801	ANP	C2'-C1'-N9	-2.38	107.10	113.47
3	B	1801	ANP	O5'-C5'-C4'	2.06	116.51	109.09
3	B	1801	ANP	O4'-C4'-C3'	2.18	109.58	105.16
3	F	1801	ANP	O3G-PG-O2G	2.19	114.04	107.67
3	E	1801	ANP	O3G-PG-O2G	2.30	114.34	107.67
3	F	1801	ANP	C2'-C3'-C4'	2.34	107.43	102.64
3	J	1801	ANP	O3G-PG-O2G	2.35	114.50	107.67
3	A	1801	ANP	C2-N1-C6	2.38	123.01	118.77
3	I	1801	ANP	C4'-O4'-C1'	2.40	112.19	109.64
3	A	1801	ANP	O5'-C5'-C4'	2.51	118.16	109.09
3	B	1801	ANP	O3G-PG-O2G	2.61	115.24	107.67
3	F	1801	ANP	N6-C6-N1	2.65	122.96	118.52
3	B	1801	ANP	O2B-PB-O1B	2.94	115.81	110.02
3	E	1801	ANP	O2B-PB-O1B	2.96	115.84	110.02
3	E	1801	ANP	C4'-O4'-C1'	2.98	112.80	109.64
3	A	1801	ANP	N6-C6-N1	3.38	124.19	118.52
3	J	1801	ANP	O2B-PB-O1B	3.47	116.85	110.02
3	E	1801	ANP	C1'-N9-C4	3.66	130.89	126.81
3	A	1801	ANP	O2B-PB-O1B	3.72	117.36	110.02
3	I	1801	ANP	O2B-PB-O1B	3.95	117.81	110.02
3	F	1801	ANP	O2B-PB-O1B	3.98	117.85	110.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1801	ANP	5	0
3	B	1801	ANP	4	0
3	E	1801	ANP	2	0
3	F	1801	ANP	3	0
3	I	1801	ANP	6	0
3	J	1801	ANP	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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(Å²)	Q<0.9
1	A	663/800 (82%)	2.23	315 (47%)	0	4	120, 187, 361, 469	0
1	B	663/800 (82%)	2.06	289 (43%)	0	4	125, 203, 272, 321	0
1	E	663/800 (82%)	2.67	344 (51%)	0	4	170, 262, 510, 665	0
1	F	663/800 (82%)	2.01	278 (41%)	0	4	127, 197, 351, 463	0
1	I	663/800 (82%)	2.38	325 (49%)	0	4	174, 224, 402, 487	0
1	J	663/800 (82%)	2.73	362 (54%)	0	3	172, 231, 378, 460	0
2	C	285/369 (77%)	2.04	135 (47%)	0	4	178, 213, 254, 293	0
2	D	285/369 (77%)	2.37	144 (50%)	0	4	170, 201, 273, 306	0
2	G	285/369 (77%)	2.38	155 (54%)	0	4	204, 224, 251, 265	0
2	H	285/369 (77%)	2.60	159 (55%)	0	3	154, 218, 301, 389	0
2	K	285/369 (77%)	2.12	130 (45%)	0	4	185, 220, 264, 283	0
2	L	285/369 (77%)	2.31	139 (48%)	0	4	210, 231, 253, 269	0
All	All	5688/7014 (81%)	2.33	2775 (48%)	0	4	120, 220, 361, 665	0

All (2775) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	749	ALA	21.6
1	E	757	ALA	19.1
1	J	147	THR	16.8
1	E	134	ALA	14.9
1	A	135	ALA	14.8
1	E	749	ALA	14.6
1	B	757	ALA	14.3
1	J	748	ASP	13.9
1	A	134	ALA	13.4
1	A	147	THR	13.3
1	E	726	ALA	13.0

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Mol	Chain	Res	Type	RSRZ
1	B	723	THR	12.5
2	H	90	ILE	12.3
1	I	595	PRO	12.2
1	F	147	THR	12.1
1	J	758	PHE	11.7
1	J	146	ALA	11.6
1	E	723	THR	11.6
1	A	146	ALA	11.2
1	J	136	ILE	11.2
1	E	780	GLY	10.9
1	J	760	HIS	10.9
1	I	482	SER	10.9
2	H	123	ALA	10.8
1	A	257	SER	10.7
1	J	134	ALA	10.7
1	B	608	ARG	10.7
1	J	135	ALA	10.7
2	L	84	ASP	10.7
1	J	759	MET	10.6
1	A	136	ILE	10.4
1	E	135	ALA	10.4
1	J	576	PRO	10.4
1	A	464	LYS	10.3
1	F	482	SER	10.2
1	I	697	ARG	10.1
1	A	465	VAL	10.1
1	F	485	ALA	9.9
1	J	145	TYR	9.8
1	I	465	VAL	9.7
1	J	577	GLY	9.7
1	A	256	ARG	9.7
1	A	462	THR	9.7
1	E	462	THR	9.6
1	I	657	VAL	9.6
1	J	761	SER	9.6
1	J	757	ALA	9.6
1	E	750	LEU	9.5
1	I	696	GLY	9.5
1	B	609	MET	9.4
1	F	480	GLY	9.4
2	G	23	PRO	9.3
1	J	595	PRO	9.2

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Mol	Chain	Res	Type	RSRZ
1	E	727	THR	9.2
1	A	727	THR	9.2
2	K	226	ALA	9.2
1	F	487	ILE	9.2
1	J	634	ALA	9.2
1	A	240	LEU	9.1
1	E	503	ILE	9.1
1	F	256	ARG	9.1
1	E	775	VAL	9.1
1	F	723	THR	9.0
1	I	485	ALA	9.0
1	F	135	ALA	8.9
1	E	725	PHE	8.9
1	J	486	PRO	8.9
1	B	690	VAL	8.9
1	J	774	ALA	8.9
1	E	756	ILE	8.9
1	E	758	PHE	8.9
1	I	695	ILE	8.9
1	E	724	LEU	8.9
1	E	690	VAL	8.8
2	H	88	ALA	8.8
1	B	722	LEU	8.7
1	E	481	GLN	8.7
1	F	486	PRO	8.7
1	B	604	SER	8.6
2	H	70	LEU	8.6
1	E	776	ALA	8.5
1	E	610	LEU	8.5
1	E	655	THR	8.5
1	J	723	THR	8.5
2	L	138	ALA	8.5
1	E	423	GLY	8.5
1	J	175	PRO	8.5
1	E	502	ILE	8.4
2	L	81	ALA	8.4
1	A	613	THR	8.4
2	H	67	GLU	8.3
1	I	486	PRO	8.3
2	K	138	ALA	8.3
1	J	482	SER	8.3
2	H	68	LEU	8.3

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Mol	Chain	Res	Type	RSRZ
2	H	91	SER	8.3
2	H	69	ALA	8.3
2	H	82	SER	8.3
2	L	179	ALA	8.3
1	A	463	LEU	8.2
1	F	488	ASN	8.2
1	B	605	PRO	8.2
1	B	691	LEU	8.2
1	E	461	ASP	8.2
1	I	594	GLU	8.2
1	E	774	ALA	8.2
1	J	637	GLY	8.2
2	H	93	GLY	8.1
2	D	67	GLU	8.1
1	F	146	ALA	8.1
1	B	724	LEU	8.1
1	E	768	SER	8.1
1	J	658	GLY	8.1
1	J	657	VAL	8.0
1	I	262	ARG	8.0
1	F	257	SER	8.0
1	I	478	SER	8.0
1	I	658	GLY	8.0
1	A	749	ALA	8.0
1	F	240	LEU	8.0
2	G	24	ALA	8.0
1	E	488	ASN	8.0
1	J	133	LEU	7.9
2	H	122	GLN	7.9
1	A	461	ASP	7.9
1	A	145	TYR	7.9
1	J	638	SER	7.9
1	I	481	GLN	7.9
1	I	346	GLY	7.8
1	B	726	ALA	7.8
2	L	180	LEU	7.8
1	E	692	MET	7.8
1	E	473	TYR	7.8
1	E	506	LEU	7.8
2	H	81	ALA	7.7
1	E	781	VAL	7.7
1	B	749	ALA	7.7

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Mol	Chain	Res	Type	RSRZ
1	I	477	ILE	7.7
1	I	757	ALA	7.7
1	A	729	TYR	7.7
2	K	238	GLY	7.7
1	J	489	TYR	7.7
1	A	602	ASN	7.7
1	I	602	ASN	7.6
1	E	489	TYR	7.6
1	A	723	THR	7.6
1	J	485	ALA	7.6
1	E	226	GLY	7.6
1	J	775	VAL	7.6
1	J	780	GLY	7.6
1	J	776	ALA	7.6
1	E	179	LEU	7.5
2	D	239	TRP	7.5
1	I	480	GLY	7.5
1	J	633	MET	7.5
1	E	691	LEU	7.5
1	E	478	SER	7.5
1	I	466	GLY	7.5
1	I	476	GLN	7.5
2	C	181	ALA	7.4
1	E	227	VAL	7.4
1	E	493	GLN	7.4
1	I	524	GLU	7.4
1	F	242	GLN	7.4
2	H	73	ALA	7.4
1	J	158	SER	7.4
1	E	425	ILE	7.4
1	I	593	ASN	7.4
1	B	695	ILE	7.4
1	J	631	ALA	7.4
2	L	85	ASP	7.3
1	E	759	MET	7.3
1	J	478	SER	7.3
1	E	147	THR	7.3
1	E	471	HIS	7.3
1	E	696	GLY	7.3
2	L	21	GLU	7.3
2	H	71	ALA	7.3
1	I	729	TYR	7.3

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Mol	Chain	Res	Type	RSRZ
2	D	138	ALA	7.3
1	B	692	MET	7.3
1	B	759	MET	7.3
2	C	70	LEU	7.3
1	I	515	THR	7.2
1	B	242	GLN	7.2
1	E	477	ILE	7.2
2	H	72	LEU	7.2
2	C	69	ALA	7.2
1	E	136	ILE	7.2
1	B	656	ARG	7.2
2	H	134	VAL	7.1
1	J	605	PRO	7.1
1	B	725	PHE	7.1
1	E	492	ARG	7.1
2	D	279	LYS	7.1
1	E	228	GLU	7.1
2	K	227	ILE	7.1
2	L	284	GLN	7.1
1	F	237	ALA	7.0
1	F	524	GLU	7.0
1	I	656	ARG	7.0
1	A	133	LEU	7.0
1	I	475	ILE	7.0
1	A	726	ALA	7.0
1	J	771	TYR	7.0
2	K	283	ASP	7.0
1	E	748	ASP	7.0
1	J	193	ARG	7.0
2	C	179	ALA	7.0
1	E	609	MET	7.0
1	J	450	LEU	7.0
1	A	238	GLY	7.0
1	E	490	MET	7.0
1	F	238	GLY	6.9
2	H	133	THR	6.9
1	A	696	GLY	6.9
1	E	133	LEU	6.9
1	E	777	ALA	6.9
2	C	67	GLU	6.9
1	B	776	ALA	6.9
1	F	489	TYR	6.9

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Mol	Chain	Res	Type	RSRZ
2	H	89	ILE	6.9
1	J	501	TYR	6.9
1	A	748	ASP	6.9
1	J	693	ASP	6.9
1	A	761	SER	6.9
1	I	425	ILE	6.9
1	E	480	GLY	6.9
1	J	773	LEU	6.9
2	D	288	PHE	6.8
1	I	518	GLY	6.8
1	E	612	ILE	6.8
1	A	476	GLN	6.8
1	J	782	PRO	6.8
2	K	81	ALA	6.8
2	G	22	ARG	6.8
1	A	242	GLN	6.8
1	E	637	GLY	6.8
2	D	289	VAL	6.8
1	F	724	LEU	6.7
1	J	499	GLU	6.7
1	J	629	LEU	6.7
2	D	226	ALA	6.7
1	E	460	LEU	6.7
2	L	23	PRO	6.7
1	B	655	THR	6.7
1	I	385	VAL	6.7
1	J	722	LEU	6.7
2	L	182	ARG	6.7
1	J	604	SER	6.7
1	J	219	THR	6.7
1	E	751	GLU	6.7
1	A	609	MET	6.6
1	A	693	ASP	6.6
1	E	470	VAL	6.6
1	J	477	ILE	6.6
2	D	149	ASP	6.6
1	A	762	VAL	6.6
1	F	776	ALA	6.6
2	D	265	ASP	6.6
2	D	283	ASP	6.6
1	B	777	ALA	6.6
1	E	638	SER	6.6

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Mol	Chain	Res	Type	RSRZ
1	B	774	ALA	6.6
2	G	294	ILE	6.6
1	J	173	THR	6.6
2	C	180	LEU	6.5
2	K	239	TRP	6.5
1	F	692	MET	6.5
2	G	21	GLU	6.5
1	J	750	LEU	6.5
1	E	760	HIS	6.5
1	E	424	VAL	6.5
1	I	488	ASN	6.5
1	A	494	THR	6.5
1	E	762	VAL	6.5
1	B	471	HIS	6.5
1	J	727	THR	6.5
1	F	655	THR	6.5
1	I	260	MET	6.5
1	J	360	ALA	6.5
2	L	83	LEU	6.4
1	E	475	ILE	6.4
1	B	239	ALA	6.4
1	E	695	ILE	6.4
1	J	148	LEU	6.4
1	E	701	THR	6.4
1	I	464	LYS	6.4
2	D	272	ILE	6.4
2	K	33	ASN	6.4
2	L	82	SER	6.4
1	A	217	PHE	6.4
1	I	520	ALA	6.4
2	L	243	PRO	6.4
2	G	197	ARG	6.4
1	E	703	ASP	6.3
1	F	425	ILE	6.3
2	G	208	LYS	6.3
2	H	80	ILE	6.3
1	I	693	ASP	6.3
1	B	482	SER	6.3
1	F	690	VAL	6.3
1	I	479	ARG	6.3
1	B	147	THR	6.3
1	B	638	SER	6.3

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Mol	Chain	Res	Type	RSRZ
2	D	240	VAL	6.3
1	B	628	ALA	6.2
1	E	761	SER	6.2
2	D	238	GLY	6.2
1	E	240	LEU	6.2
1	F	691	LEU	6.2
1	E	237	ALA	6.2
1	A	219	THR	6.2
1	I	261	GLU	6.2
1	I	727	THR	6.2
1	J	594	GLU	6.2
1	I	471	HIS	6.2
1	I	519	LYS	6.2
1	A	599	ASN	6.2
2	D	276	TYR	6.2
1	I	780	GLY	6.2
2	D	66	ASP	6.2
2	D	273	ARG	6.2
1	F	465	VAL	6.2
1	I	398	GLY	6.2
1	A	694	GLU	6.1
1	B	696	GLY	6.1
2	L	215	ILE	6.1
1	J	747	LEU	6.1
2	L	282	ALA	6.1
2	H	83	LEU	6.1
2	H	209	GLU	6.1
1	I	655	THR	6.1
1	J	635	TYR	6.1
1	J	781	VAL	6.1
1	F	477	ILE	6.1
1	E	243	TYR	6.1
1	J	475	ILE	6.1
1	B	238	GLY	6.1
1	B	657	VAL	6.0
1	B	261	GLU	6.0
1	B	483	HIS	6.0
1	E	239	ALA	6.0
1	E	505	GLU	6.0
1	J	756	ILE	6.0
2	K	80	ILE	6.0
1	J	174	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	J	572	PHE	6.0
1	J	628	ALA	6.0
1	A	160	PRO	6.0
1	A	697	ARG	6.0
2	G	265	ASP	6.0
2	H	84	ASP	6.0
2	G	239	TRP	6.0
2	K	240	VAL	6.0
1	I	528	TYR	6.0
1	I	572	PHE	6.0
2	L	22	ARG	6.0
1	I	345	VAL	6.0
1	I	240	LEU	6.0
1	J	476	GLN	6.0
2	C	68	LEU	5.9
1	J	481	GLN	5.9
2	D	68	LEU	5.9
2	G	161	LEU	5.9
2	H	210	ARG	5.9
1	A	314	PRO	5.9
1	I	203	GLU	5.9
1	J	449	ARG	5.9
1	A	774	ALA	5.9
1	E	654	PHE	5.9
1	F	777	ALA	5.9
2	G	81	ALA	5.9
1	I	364	ASP	5.9
2	L	285	GLN	5.9
1	J	772	GLY	5.9
2	G	259	ASN	5.9
2	C	90	ILE	5.9
1	F	725	PHE	5.9
1	J	242	GLN	5.8
2	G	188	ASN	5.8
2	H	275	ALA	5.8
2	D	269	ASN	5.8
1	J	609	MET	5.8
1	J	729	TYR	5.8
2	H	212	LEU	5.8
2	G	172	ASP	5.8
2	H	110	LEU	5.8
1	E	146	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	630	ILE	5.8
2	G	295	ASP	5.8
1	I	740	GLU	5.8
2	K	67	GLU	5.8
1	B	473	TYR	5.8
1	F	475	ILE	5.8
1	F	594	GLU	5.7
1	J	496	LYS	5.7
2	L	283	ASP	5.7
2	G	240	VAL	5.7
1	B	610	LEU	5.7
1	B	603	LEU	5.7
1	E	634	ALA	5.7
1	J	446	TYR	5.7
1	A	148	LEU	5.7
1	I	335	THR	5.7
2	G	176	ARG	5.7
1	E	779	ALA	5.7
1	E	476	GLN	5.7
1	A	315	VAL	5.7
1	J	777	ALA	5.7
2	L	181	ALA	5.7
1	F	775	VAL	5.7
2	K	196	VAL	5.7
1	I	781	VAL	5.7
1	F	399	GLU	5.7
1	J	632	LEU	5.7
2	K	181	ALA	5.7
1	A	179	LEU	5.7
1	F	483	HIS	5.6
1	J	221	ASP	5.6
1	F	729	TYR	5.6
1	J	555	LEU	5.6
2	H	135	LYS	5.6
1	E	743	ALA	5.6
1	F	610	LEU	5.6
1	J	454	GLU	5.6
1	J	524	GLU	5.6
2	L	80	ILE	5.6
1	I	242	GLN	5.6
1	F	145	TYR	5.6
2	H	111	THR	5.6

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Mol	Chain	Res	Type	RSRZ
2	H	132	VAL	5.6
1	B	576	PRO	5.6
1	I	136	ILE	5.6
2	C	89	ILE	5.6
2	L	67	GLU	5.6
1	I	470	VAL	5.6
1	B	240	LEU	5.6
1	I	424	VAL	5.6
2	G	80	ILE	5.6
1	J	553	ASP	5.6
1	I	522	ALA	5.6
1	F	239	ALA	5.6
1	I	468	ASN	5.6
1	J	324	ARG	5.6
1	E	631	ALA	5.6
2	K	117	GLN	5.6
1	I	361	ARG	5.6
1	J	610	LEU	5.6
2	G	133	THR	5.6
1	F	519	LYS	5.6
1	B	756	ILE	5.5
1	F	136	ILE	5.5
2	H	180	LEU	5.5
1	J	627	THR	5.5
1	A	237	ALA	5.5
1	A	747	LEU	5.5
2	D	209	GLU	5.5
1	F	134	ALA	5.5
1	J	137	TRP	5.5
1	A	166	MET	5.5
1	J	261	GLU	5.5
1	E	689	LEU	5.5
1	E	225	PHE	5.5
1	E	551	GLU	5.5
2	D	282	ALA	5.5
1	I	750	LEU	5.5
1	I	179	LEU	5.5
2	C	182	ARG	5.5
1	B	136	ILE	5.5
1	I	523	LEU	5.5
1	B	727	THR	5.5
1	I	577	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
2	C	149	ASP	5.5
1	A	695	ILE	5.5
1	I	777	ALA	5.5
1	I	692	MET	5.5
1	I	592	LEU	5.5
1	J	448	GLU	5.4
1	F	221	ASP	5.4
2	H	66	ASP	5.4
1	J	505	GLU	5.4
2	D	287	ALA	5.4
1	B	780	GLY	5.4
1	J	724	LEU	5.4
1	E	501	TYR	5.4
1	B	758	PHE	5.4
1	E	158	SER	5.4
1	I	332	GLN	5.4
1	J	697	ARG	5.4
1	J	157	LEU	5.4
1	I	756	ILE	5.4
1	J	480	GLY	5.4
1	J	721	ALA	5.4
2	H	330	LEU	5.4
1	A	612	ILE	5.4
1	B	631	ALA	5.4
1	F	726	ALA	5.4
2	H	124	TYR	5.4
2	K	330	LEU	5.4
1	I	516	SER	5.4
2	H	211	ARG	5.4
2	D	241	ALA	5.4
1	E	257	SER	5.4
1	E	426	ALA	5.4
1	E	494	THR	5.4
2	C	86	LEU	5.4
2	D	278	ASP	5.4
1	A	155	PHE	5.3
1	A	477	ILE	5.3
1	E	722	LEU	5.3
1	A	258	ILE	5.3
1	B	546	ALA	5.3
1	E	241	LEU	5.3
2	C	82	SER	5.3

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Mol	Chain	Res	Type	RSRZ
2	K	71	ALA	5.3
2	H	241	ALA	5.3
1	J	425	ILE	5.3
1	J	276	ASN	5.3
1	J	346	GLY	5.3
2	H	181	ALA	5.3
2	C	66	ASP	5.3
1	A	722	LEU	5.3
2	C	285	GLN	5.3
1	B	607	ARG	5.3
2	D	80	ILE	5.3
1	E	486	PRO	5.3
2	G	293	GLU	5.3
1	I	776	ALA	5.3
1	B	627	THR	5.3
1	E	708	ALA	5.3
2	L	20	VAL	5.3
2	G	189	LEU	5.3
1	B	244	ALA	5.3
2	D	207	GLN	5.3
1	F	774	ALA	5.3
1	A	725	PHE	5.2
2	H	136	PRO	5.2
1	B	781	VAL	5.2
2	L	178	ILE	5.2
1	E	677	THR	5.2
1	J	498	ALA	5.2
1	B	755	THR	5.2
1	E	160	PRO	5.2
2	H	137	ALA	5.2
2	H	208	LYS	5.2
1	A	773	LEU	5.2
1	I	239	ALA	5.2
1	J	725	PHE	5.2
2	K	180	LEU	5.2
1	E	782	PRO	5.2
1	F	241	LEU	5.2
2	C	71	ALA	5.2
1	J	659	ALA	5.2
2	G	179	ALA	5.2
1	J	465	VAL	5.2
1	F	481	GLN	5.2

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Mol	Chain	Res	Type	RSRZ
1	I	514	LEU	5.2
1	I	691	LEU	5.2
2	K	284	GLN	5.2
2	L	172	ASP	5.2
1	I	458	THR	5.2
1	J	359	THR	5.2
2	G	55	ARG	5.2
1	F	335	THR	5.2
1	J	240	LEU	5.2
2	D	208	LYS	5.2
2	L	220	PHE	5.2
1	E	261	GLU	5.2
1	J	159	GLU	5.2
1	B	709	TRP	5.2
1	B	570	PRO	5.2
1	I	221	ASP	5.1
1	I	782	PRO	5.1
1	J	479	ARG	5.1
2	G	90	ILE	5.1
1	A	760	HIS	5.1
1	A	158	SER	5.1
1	E	145	TYR	5.1
1	F	155	PHE	5.1
2	L	148	LEU	5.1
1	I	469	ALA	5.1
1	B	778	LEU	5.1
1	J	483	HIS	5.1
2	G	20	VAL	5.1
1	E	771	TYR	5.1
2	L	125	ALA	5.1
2	D	286	PRO	5.1
2	G	199	TYR	5.1
1	A	276	ASN	5.1
1	A	579	ARG	5.1
1	I	422	GLY	5.1
2	H	298	GLN	5.1
2	D	291	TYR	5.1
2	D	277	GLU	5.1
1	E	570	PRO	5.1
2	H	55	ARG	5.1
1	E	507	LYS	5.1
1	A	756	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	F	730	PHE	5.1
1	I	521	LEU	5.1
2	G	180	LEU	5.1
1	J	239	ALA	5.1
2	C	88	ALA	5.1
2	D	266	ARG	5.1
1	J	419	VAL	5.1
1	J	339	GLN	5.1
2	L	86	LEU	5.1
1	I	473	TYR	5.1
1	I	778	LEU	5.1
2	H	239	TRP	5.1
2	K	119	GLU	5.1
1	J	342	LEU	5.1
1	A	750	LEU	5.1
1	E	229	ASN	5.1
1	E	510	GLU	5.1
1	F	450	LEU	5.1
1	F	762	VAL	5.1
2	C	51	ALA	5.1
2	D	64	LYS	5.1
1	F	523	LEU	5.0
1	J	237	ALA	5.0
1	I	212	GLN	5.0
2	D	280	LEU	5.0
2	G	207	GLN	5.0
1	E	242	GLN	5.0
1	I	189	LEU	5.0
1	B	189	LEU	5.0
1	B	633	MET	5.0
1	I	723	THR	5.0
1	J	528	TYR	5.0
1	B	693	ASP	5.0
2	H	326	VAL	5.0
2	G	67	GLU	5.0
2	G	45	ASP	5.0
1	I	527	LEU	5.0
2	D	180	LEU	5.0
2	G	175	ILE	5.0
1	B	750	LEU	5.0
1	E	633	MET	5.0
1	F	156	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	595	PRO	5.0
2	G	292	LEU	5.0
1	F	332	GLN	5.0
1	E	482	SER	5.0
1	I	759	MET	5.0
2	L	124	TYR	5.0
2	H	327	LEU	5.0
1	E	500	ARG	5.0
2	C	21	GLU	4.9
1	J	770	SER	4.9
2	D	181	ALA	4.9
2	H	109	THR	4.9
1	I	659	ALA	4.9
2	D	225	LEU	4.9
2	K	195	ILE	4.9
2	G	40	THR	4.9
2	K	73	ALA	4.9
1	A	728	HIS	4.9
1	I	484	LEU	4.9
2	G	241	ALA	4.9
1	E	427	SER	4.9
1	J	630	ILE	4.9
2	C	198	GLN	4.9
2	G	138	ALA	4.9
1	I	646	GLU	4.9
1	B	577	GLY	4.9
1	I	382	LEU	4.9
2	D	290	LEU	4.9
1	I	147	THR	4.9
1	I	386	ASP	4.9
1	I	517	LYS	4.9
2	C	93	GLY	4.9
1	E	635	TYR	4.9
1	I	474	TYR	4.9
1	J	778	LEU	4.9
1	E	504	PRO	4.9
1	J	636	ILE	4.9
2	G	266	ARG	4.9
2	L	330	LEU	4.9
1	B	629	LEU	4.9
1	E	729	TYR	4.9
2	D	63	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	260	MET	4.8
1	B	782	PRO	4.8
1	I	603	LEU	4.8
2	K	23	PRO	4.8
1	B	472	GLY	4.8
1	J	648	GLY	4.8
1	E	491	ARG	4.8
2	G	330	LEU	4.8
1	B	149	ASP	4.8
1	A	239	ALA	4.8
1	I	135	ALA	4.8
1	I	333	ASP	4.8
1	J	686	GLU	4.8
2	D	137	ALA	4.8
1	F	478	SER	4.8
1	A	364	ASP	4.8
1	B	772	GLY	4.8
1	E	497	ASN	4.8
2	L	171	ILE	4.8
1	B	773	LEU	4.8
1	J	447	LEU	4.8
2	H	92	LEU	4.8
1	F	314	PRO	4.8
1	I	419	VAL	4.8
2	H	138	ALA	4.8
1	A	470	VAL	4.8
1	B	245	LYS	4.8
1	J	341	VAL	4.8
1	B	260	MET	4.8
1	F	259	THR	4.8
1	I	362	PRO	4.8
1	J	695	ILE	4.8
2	C	215	ILE	4.8
2	D	268	ILE	4.8
1	J	608	ARG	4.8
1	B	485	ALA	4.8
2	G	54	ILE	4.8
1	E	262	ARG	4.7
2	L	226	ALA	4.7
1	I	698	GLY	4.7
1	J	497	ASN	4.7
1	B	237	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	607	ARG	4.7
1	B	748	ASP	4.7
1	A	775	VAL	4.7
1	F	773	LEU	4.7
2	D	90	ILE	4.7
1	B	775	VAL	4.7
2	D	224	ALA	4.7
1	F	600	PRO	4.7
1	J	238	GLY	4.7
2	G	171	ILE	4.7
2	K	140	PRO	4.7
1	J	692	MET	4.7
1	F	160	PRO	4.7
1	I	497	ASN	4.7
1	A	489	TYR	4.7
2	C	212	LEU	4.7
1	F	424	VAL	4.7
1	F	708	ALA	4.7
1	I	472	GLY	4.7
1	F	656	ARG	4.7
1	E	458	THR	4.7
1	I	774	ALA	4.7
2	K	72	LEU	4.7
1	J	423	GLY	4.7
1	E	615	PRO	4.7
1	E	675	THR	4.7
1	J	132	LEU	4.7
1	E	422	GLY	4.7
2	D	23	PRO	4.7
1	A	690	VAL	4.7
1	F	609	MET	4.7
1	J	538	HIS	4.7
1	F	166	MET	4.7
1	J	655	THR	4.7
2	L	132	VAL	4.7
1	E	700	SER	4.7
1	F	258	ILE	4.7
2	D	65	LYS	4.7
1	F	476	GLN	4.7
1	B	741	GLY	4.6
1	B	761	SER	4.6
2	G	226	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	190	ILE	4.6
1	J	212	GLN	4.6
1	I	701	THR	4.6
1	B	634	ALA	4.6
1	F	781	VAL	4.6
1	J	762	VAL	4.6
1	B	470	VAL	4.6
1	I	525	LYS	4.6
1	F	727	THR	4.6
1	I	564	THR	4.6
2	K	241	ALA	4.6
1	I	387	SER	4.6
2	K	30	LEU	4.6
1	F	179	LEU	4.6
2	D	330	LEU	4.6
1	E	223	VAL	4.6
1	E	469	ALA	4.6
1	J	144	GLY	4.6
2	G	184	ASP	4.6
1	F	593	ASN	4.6
2	G	203	PRO	4.6
1	J	751	GLU	4.6
1	B	484	LEU	4.6
1	E	653	ILE	4.6
1	E	430	ASN	4.6
1	J	170	LEU	4.6
1	J	625	ARG	4.6
2	L	224	ALA	4.6
1	E	148	LEU	4.6
1	I	605	PRO	4.6
1	B	689	LEU	4.6
1	B	481	GLN	4.6
1	J	696	GLY	4.6
1	E	463	LEU	4.6
1	A	524	GLU	4.6
1	J	260	MET	4.6
2	H	21	GLU	4.6
1	I	467	PHE	4.6
1	I	647	ILE	4.6
1	A	600	PRO	4.5
1	E	636	ILE	4.5
2	L	265	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	655	THR	4.5
1	A	657	VAL	4.5
1	A	724	LEU	4.5
2	C	87	GLU	4.5
1	E	238	GLY	4.5
2	C	183	PHE	4.5
2	L	176	ARG	4.5
1	A	601	LEU	4.5
1	I	748	ASP	4.5
1	E	244	ALA	4.5
1	E	381	GLN	4.5
1	E	429	TYR	4.5
2	K	95	ARG	4.5
2	K	228	GLU	4.5
1	A	460	LEU	4.5
1	I	511	ASP	4.5
1	F	772	GLY	4.5
2	H	240	VAL	4.5
2	D	122	GLN	4.5
1	A	178	LEU	4.5
1	A	603	LEU	4.5
1	I	241	LEU	4.5
2	G	267	LEU	4.5
2	K	66	ASP	4.5
1	A	578	ILE	4.5
2	H	323	TYR	4.5
1	E	693	ASP	4.5
2	H	243	PRO	4.5
1	F	158	SER	4.5
2	C	85	ASP	4.5
2	H	220	PHE	4.5
1	A	481	GLN	4.5
2	H	224	ALA	4.5
1	B	595	PRO	4.5
1	E	778	LEU	4.5
1	F	695	ILE	4.5
2	L	175	ILE	4.5
1	F	423	GLY	4.5
2	D	73	ALA	4.5
1	B	179	LEU	4.5
1	E	702	TYR	4.5
2	H	121	TRP	4.5

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Mol	Chain	Res	Type	RSRZ
1	I	749	ALA	4.5
1	J	176	ALA	4.5
1	E	498	ALA	4.5
1	F	654	PHE	4.5
1	J	515	THR	4.5
1	I	463	LEU	4.5
1	I	578	ILE	4.5
1	A	692	MET	4.5
1	F	522	ALA	4.5
1	I	384	THR	4.5
2	H	23	PRO	4.5
2	D	69	ALA	4.4
2	H	179	ALA	4.4
1	J	647	ILE	4.4
2	D	123	ALA	4.4
2	K	82	SER	4.4
2	D	136	PRO	4.4
2	K	282	ALA	4.4
1	B	148	LEU	4.4
1	F	484	LEU	4.4
2	L	183	PHE	4.4
1	B	602	ASN	4.4
2	H	215	ILE	4.4
1	I	690	VAL	4.4
1	I	430	ASN	4.4
1	J	345	VAL	4.4
1	J	552	LEU	4.4
2	D	212	LEU	4.4
2	K	289	VAL	4.4
1	J	503	ILE	4.4
1	A	241	LEU	4.4
1	B	241	LEU	4.4
1	F	269	MET	4.4
1	B	247	THR	4.4
1	B	460	LEU	4.4
1	I	590	GLN	4.4
2	G	198	GLN	4.4
1	E	410	ALA	4.4
2	D	24	ALA	4.4
1	E	177	GLU	4.4
2	G	167	GLU	4.4
2	G	215	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
2	L	87	GLU	4.4
2	L	197	ARG	4.4
2	D	281	GLY	4.4
2	L	50	GLY	4.4
1	I	403	LEU	4.4
2	C	72	LEU	4.4
2	G	82	SER	4.4
2	D	275	ALA	4.4
1	B	578	ILE	4.4
1	J	691	LEU	4.4
1	A	522	ALA	4.4
1	A	635	TYR	4.4
1	I	347	ASP	4.4
1	J	241	LEU	4.4
1	I	134	ALA	4.4
1	E	178	LEU	4.4
2	H	223	GLN	4.4
1	I	331	LEU	4.4
1	F	780	GLY	4.4
1	B	458	THR	4.4
1	F	612	ILE	4.4
1	A	451	GLU	4.3
1	I	423	GLY	4.3
1	J	202	TRP	4.3
1	J	204	PHE	4.3
1	E	472	GLY	4.3
1	E	773	LEU	4.3
1	B	551	GLU	4.3
1	E	769	LYS	4.3
1	E	495	LEU	4.3
2	D	70	LEU	4.3
1	A	360	ALA	4.3
2	H	289	VAL	4.3
1	A	269	MET	4.3
1	I	648	GLY	4.3
1	J	607	ARG	4.3
1	I	157	LEU	4.3
1	I	717	ASN	4.3
1	A	495	LEU	4.3
1	A	708	ALA	4.3
1	I	487	ILE	4.3
2	D	81	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
2	L	24	ALA	4.3
1	B	549	LEU	4.3
2	L	212	LEU	4.3
1	A	312	HIS	4.3
1	E	652	ARG	4.3
1	B	381	GLN	4.3
1	E	704	GLY	4.3
2	G	209	GLU	4.3
2	H	146	GLU	4.3
1	A	652	ARG	4.3
2	K	276	TYR	4.3
1	B	134	ALA	4.3
1	B	712	ALA	4.3
1	A	580	ILE	4.3
2	K	118	GLN	4.3
1	F	525	LYS	4.3
1	J	726	ALA	4.3
2	G	233	ASP	4.3
1	J	424	VAL	4.3
1	J	511	ASP	4.3
1	E	459	GLY	4.3
2	C	50	GLY	4.3
1	F	157	LEU	4.3
1	E	324	ARG	4.3
1	E	499	GLU	4.3
1	B	135	ALA	4.3
2	L	108	LEU	4.3
2	G	202	VAL	4.3
1	J	234	LEU	4.2
1	F	148	LEU	4.2
1	A	776	ALA	4.2
2	C	124	TYR	4.2
1	B	151	SER	4.2
1	J	227	VAL	4.2
1	E	755	THR	4.2
1	B	716	ALA	4.2
1	B	192	GLY	4.2
1	B	762	VAL	4.2
1	J	233	GLY	4.2
2	K	225	LEU	4.2
1	A	763	GLN	4.2
1	B	754	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	755	THR	4.2
1	A	144	GLY	4.2
1	E	468	ASN	4.2
2	C	243	PRO	4.2
2	G	177	ARG	4.2
1	I	483	HIS	4.2
1	F	243	TYR	4.2
1	J	236	ALA	4.2
1	J	597	ILE	4.2
1	E	628	ALA	4.2
1	I	334	PHE	4.2
1	B	203	GLU	4.2
2	K	29	GLU	4.2
1	F	410	ALA	4.2
2	D	256	PHE	4.2
1	I	263	GLU	4.2
1	J	327	THR	4.2
2	G	63	ILE	4.2
2	G	162	ARG	4.2
2	H	95	ARG	4.2
1	I	243	TYR	4.2
2	H	276	TYR	4.2
1	J	506	LEU	4.2
2	H	225	LEU	4.2
1	I	397	MET	4.2
1	A	270	ASP	4.2
1	F	463	LEU	4.2
2	H	94	PHE	4.2
1	E	230	ALA	4.2
2	L	266	ARG	4.1
2	L	149	ASP	4.1
1	J	190	ILE	4.1
1	J	551	GLU	4.1
1	B	248	GLN	4.1
1	E	676	GLU	4.1
1	E	707	LEU	4.1
1	J	519	LYS	4.1
1	B	477	ILE	4.1
1	E	752	HIS	4.1
1	I	758	PHE	4.1
1	F	778	LEU	4.1
1	A	203	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	I	400	PHE	4.1
1	A	475	ILE	4.1
1	E	706	SER	4.1
1	E	411	ILE	4.1
1	A	478	SER	4.1
1	I	230	ALA	4.1
1	E	632	LEU	4.1
1	E	524	GLU	4.1
1	E	128	ARG	4.1
1	B	501	TYR	4.1
1	J	484	LEU	4.1
1	B	155	PHE	4.1
1	I	604	SER	4.1
1	B	751	GLU	4.1
1	J	279	ILE	4.1
2	C	92	LEU	4.1
1	E	221	ASP	4.1
2	L	276	TYR	4.1
1	F	451	GLU	4.1
1	I	327	THR	4.1
1	I	726	ALA	4.1
2	G	182	ARG	4.1
1	B	332	GLN	4.1
1	E	767	ALA	4.1
2	L	107	ARG	4.1
2	H	272	ILE	4.1
1	A	610	LEU	4.1
1	A	746	HIS	4.1
1	B	212	GLN	4.1
1	F	262	ARG	4.1
1	F	501	TYR	4.1
1	J	575	LYS	4.1
2	H	242	ASP	4.1
2	K	27	VAL	4.1
1	A	757	ALA	4.1
2	K	329	VAL	4.1
1	A	499	GLU	4.1
1	B	243	TYR	4.1
1	A	577	GLY	4.1
2	H	226	ALA	4.1
1	B	658	GLY	4.0
1	E	697	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	210	ARG	4.0
1	B	563	TYR	4.0
1	E	772	GLY	4.0
2	G	44	ILE	4.0
2	G	289	VAL	4.0
2	K	31	VAL	4.0
1	J	769	LYS	4.0
1	E	595	PRO	4.0
1	A	169	GLU	4.0
1	J	694	GLU	4.0
1	B	480	GLY	4.0
1	F	559	ALA	4.0
1	E	159	GLU	4.0
2	C	91	SER	4.0
1	J	615	PRO	4.0
1	A	701	THR	4.0
1	E	674	MET	4.0
1	B	158	SER	4.0
1	I	531	LEU	4.0
2	D	83	LEU	4.0
2	K	70	LEU	4.0
1	B	738	LYS	4.0
2	H	279	LYS	4.0
2	K	21	GLU	4.0
1	J	422	GLY	4.0
1	B	345	VAL	4.0
1	B	190	ILE	4.0
1	E	245	LYS	4.0
1	I	724	LEU	4.0
2	H	207	GLN	4.0
2	D	220	PHE	4.0
2	H	213	GLY	4.0
2	L	55	ARG	4.0
1	B	492	ARG	4.0
1	A	496	LYS	4.0
1	A	519	LYS	4.0
1	B	150	ILE	4.0
1	F	696	GLY	4.0
2	H	96	GLY	4.0
1	I	202	TRP	4.0
2	C	109	THR	4.0
1	A	498	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
2	L	216	LEU	4.0
1	A	471	HIS	4.0
1	J	656	ARG	4.0
1	A	273	THR	4.0
2	L	241	ALA	4.0
1	E	630	ILE	4.0
2	K	83	LEU	4.0
1	J	220	ARG	4.0
2	D	299	VAL	4.0
1	A	751	GLU	4.0
1	E	629	LEU	4.0
1	J	495	LEU	4.0
1	J	510	GLU	4.0
1	J	731	GLU	4.0
2	K	299	VAL	4.0
1	B	739	MET	3.9
1	E	263	GLU	3.9
1	I	489	TYR	3.9
2	K	34	SER	3.9
1	A	758	PHE	3.9
1	E	656	ARG	3.9
1	B	246	CYS	3.9
1	E	327	THR	3.9
1	F	217	PHE	3.9
1	E	328	ILE	3.9
1	J	445	ASP	3.9
1	I	360	ALA	3.9
1	J	451	GLU	3.9
2	H	214	ALA	3.9
2	L	54	ILE	3.9
1	F	564	THR	3.9
1	J	325	GLN	3.9
2	G	315	SER	3.9
1	F	346	GLY	3.9
1	I	190	ILE	3.9
1	J	262	ARG	3.9
1	J	453	ARG	3.9
2	G	183	PHE	3.9
2	K	182	ARG	3.9
1	B	459	GLY	3.9
1	F	613	THR	3.9
1	J	494	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	G	201	ALA	3.9
2	C	216	LEU	3.9
2	L	66	ASP	3.9
1	J	156	ARG	3.9
2	H	183	PHE	3.9
1	I	365	LEU	3.9
2	K	137	ALA	3.9
1	A	156	ARG	3.9
1	A	202	TRP	3.9
1	J	155	PHE	3.9
2	C	330	LEU	3.9
1	I	635	TYR	3.9
1	B	646	GLU	3.9
1	E	479	ARG	3.9
2	D	22	ARG	3.9
1	J	603	LEU	3.9
2	H	322	ILE	3.9
1	E	742	VAL	3.9
1	F	245	LYS	3.9
1	J	462	THR	3.9
1	A	653	ILE	3.9
1	E	258	ILE	3.9
1	F	261	GLU	3.9
2	D	267	LEU	3.9
1	E	550	ALA	3.9
2	D	274	GLN	3.9
2	K	190	SER	3.9
1	E	552	LEU	3.8
1	I	563	TYR	3.8
2	G	123	ALA	3.8
1	I	694	GLU	3.8
2	D	243	PRO	3.8
2	G	134	VAL	3.8
2	L	147	VAL	3.8
1	A	528	TYR	3.8
1	E	597	ILE	3.8
1	J	614	GLY	3.8
1	J	203	GLU	3.8
1	J	586	PRO	3.8
2	K	198	GLN	3.8
1	A	268	ILE	3.8
1	J	531	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	333	ASP	3.8
1	J	556	VAL	3.8
2	L	273	ARG	3.8
1	A	503	ILE	3.8
1	F	222	LEU	3.8
2	G	178	ILE	3.8
1	F	315	VAL	3.8
2	C	242	ASP	3.8
2	L	264	ARG	3.8
1	B	708	ALA	3.8
2	L	49	GLY	3.8
1	J	571	THR	3.8
1	F	590	GLN	3.8
1	J	138	GLN	3.8
1	J	222	LEU	3.8
1	B	250	THR	3.8
2	L	199	TYR	3.8
1	F	731	GLU	3.8
2	G	26	VAL	3.8
2	L	173	GLU	3.8
2	G	42	ILE	3.8
1	E	627	THR	3.8
1	E	657	VAL	3.8
1	F	599	ASN	3.8
2	G	50	GLY	3.8
1	B	639	TYR	3.8
1	E	485	ALA	3.8
1	A	180	TYR	3.8
1	I	460	LEU	3.8
1	A	658	GLY	3.8
2	C	178	ILE	3.8
1	F	216	GLN	3.8
1	B	510	GLU	3.8
1	B	673	GLU	3.8
2	K	90	ILE	3.8
2	C	107	ARG	3.8
2	H	145	LEU	3.8
1	B	360	ALA	3.8
1	I	276	ASN	3.8
2	C	125	ALA	3.8
2	D	284	GLN	3.8
1	B	156	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	212	GLN	3.8
1	B	721	ALA	3.8
2	C	175	ILE	3.8
2	G	124	TYR	3.8
2	G	173	GLU	3.8
2	G	174	ILE	3.8
1	A	450	LEU	3.8
1	A	732	LEU	3.8
1	A	731	GLU	3.8
1	A	479	ARG	3.8
1	F	267	ILE	3.8
1	I	158	SER	3.8
2	D	329	VAL	3.8
1	E	705	LEU	3.8
1	A	572	PHE	3.8
1	J	578	ILE	3.8
1	I	607	ARG	3.8
2	C	197	ARG	3.8
2	K	326	VAL	3.8
1	F	689	LEU	3.8
2	H	221	LEU	3.8
1	B	640	VAL	3.7
1	I	498	ALA	3.7
2	C	286	PRO	3.7
1	J	690	VAL	3.7
2	L	279	LYS	3.7
1	E	433	LEU	3.7
1	E	648	GLY	3.7
2	G	68	LEU	3.7
1	I	432	GLU	3.7
1	I	330	ALA	3.7
1	F	227	VAL	3.7
1	F	707	LEU	3.7
2	K	194	LYS	3.7
1	B	697	ARG	3.7
1	A	745	VAL	3.7
1	B	157	LEU	3.7
1	E	509	TYR	3.7
1	I	731	GLU	3.7
1	F	398	GLY	3.7
2	K	286	PRO	3.7
1	A	764	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	193	ARG	3.7
1	I	556	VAL	3.7
1	J	701	THR	3.7
2	C	151	PHE	3.7
1	J	277	LEU	3.7
2	G	146	GLU	3.7
1	E	519	LYS	3.7
1	I	708	ALA	3.7
2	G	149	ASP	3.7
2	G	212	LEU	3.7
2	H	182	ARG	3.7
1	F	133	LEU	3.7
2	D	315	SER	3.7
2	G	268	ILE	3.7
1	A	538	HIS	3.7
1	A	759	MET	3.7
1	B	475	ILE	3.7
2	K	179	ALA	3.7
2	K	20	VAL	3.7
1	F	712	ALA	3.7
1	I	238	GLY	3.7
2	K	84	ASP	3.7
1	I	526	GLN	3.7
2	D	255	TYR	3.7
1	B	711	VAL	3.7
1	F	419	VAL	3.7
2	C	20	VAL	3.7
2	G	43	ASP	3.7
1	A	597	ILE	3.7
1	E	341	VAL	3.7
1	B	334	PHE	3.7
1	I	555	LEU	3.7
2	K	178	ILE	3.7
1	F	563	TYR	3.7
1	B	262	ARG	3.7
1	I	730	PHE	3.7
1	J	458	THR	3.7
1	J	218	GLY	3.7
1	F	565	LEU	3.7
1	I	725	PHE	3.7
1	A	611	ILE	3.7
1	E	446	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	259	ASN	3.6
2	G	49	GLY	3.6
1	F	611	ILE	3.6
1	B	729	TYR	3.6
1	J	160	PRO	3.6
1	A	170	LEU	3.6
1	A	535	LEU	3.6
1	A	705	LEU	3.6
1	E	549	LEU	3.6
1	F	528	TYR	3.6
1	I	228	GLU	3.6
1	E	413	ASP	3.6
1	I	156	ARG	3.6
2	G	264	ARG	3.6
1	E	173	THR	3.6
2	D	260	GLY	3.6
2	G	51	ALA	3.6
2	G	299	VAL	3.6
1	A	608	ARG	3.6
1	F	348	LEU	3.6
2	G	170	HIS	3.6
1	F	268	ILE	3.6
1	J	612	ILE	3.6
1	A	316	ARG	3.6
1	A	523	LEU	3.6
2	C	153	ASN	3.6
2	D	162	ARG	3.6
2	K	45	ASP	3.6
1	A	261	GLU	3.6
1	B	552	LEU	3.6
2	D	264	ARG	3.6
1	I	510	GLU	3.6
2	L	239	TRP	3.6
1	F	520	ALA	3.6
2	D	71	ALA	3.6
1	A	183	ASP	3.6
2	D	253	ILE	3.6
1	A	743	ALA	3.6
1	A	772	GLY	3.6
1	E	553	ASP	3.6
2	C	246	THR	3.6
2	G	66	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	236	ALA	3.6
1	F	479	ARG	3.6
2	G	64	LYS	3.6
1	A	527	LEU	3.6
1	I	722	LEU	3.6
2	H	325	GLY	3.6
1	E	572	PHE	3.6
1	J	509	TYR	3.6
2	D	91	SER	3.6
2	C	189	LEU	3.6
1	I	499	GLU	3.6
2	L	90	ILE	3.6
1	J	143	PHE	3.6
1	F	228	GLU	3.6
2	K	116	GLU	3.6
2	K	136	PRO	3.6
1	E	520	ALA	3.6
1	J	491	ARG	3.6
2	K	193	GLY	3.6
1	E	338	LEU	3.6
2	D	263	MET	3.6
1	J	488	ASN	3.6
1	A	310	TRP	3.6
1	E	412	ILE	3.6
1	I	535	LEU	3.6
2	G	187	ILE	3.6
1	F	499	GLU	3.6
1	F	779	ALA	3.6
1	A	614	GLY	3.6
2	K	35	LEU	3.6
2	L	280	LEU	3.6
1	B	505	GLU	3.6
1	I	728	HIS	3.6
2	C	138	ALA	3.6
2	K	287	ALA	3.6
2	C	210	ARG	3.6
1	F	515	THR	3.6
1	F	498	ALA	3.5
1	F	518	GLY	3.5
1	I	579	ARG	3.5
1	I	608	ARG	3.5
2	D	55	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	777	ALA	3.5
1	E	450	LEU	3.5
1	F	560	GLU	3.5
1	A	707	LEU	3.5
1	E	747	LEU	3.5
1	A	193	ARG	3.5
1	B	550	ALA	3.5
1	F	653	ILE	3.5
1	J	606	GLN	3.5
1	A	324	ARG	3.5
1	I	703	ASP	3.5
1	A	216	GLN	3.5
1	A	267	ILE	3.5
1	E	709	TRP	3.5
2	H	31	VAL	3.5
1	F	657	VAL	3.5
1	I	390	VAL	3.5
1	A	709	TRP	3.5
2	C	123	ALA	3.5
1	J	192	GLY	3.5
2	C	155	PRO	3.5
1	A	236	ALA	3.5
1	A	598	ALA	3.5
1	E	246	CYS	3.5
1	A	627	THR	3.5
2	H	331	GLN	3.5
1	B	227	VAL	3.5
1	I	732	LEU	3.5
1	I	779	ALA	3.5
2	D	257	TYR	3.5
1	A	730	PHE	3.5
1	J	149	ASP	3.5
1	A	781	VAL	3.5
1	I	429	TYR	3.5
1	I	752	HIS	3.5
1	J	554	VAL	3.5
2	D	178	ILE	3.5
2	L	63	ILE	3.5
1	J	230	ALA	3.5
2	L	170	HIS	3.5
1	E	650	ILE	3.5
2	G	206	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	220	ARG	3.5
1	A	636	ILE	3.5
1	J	728	HIS	3.5
1	I	673	GLU	3.5
1	A	173	THR	3.5
1	B	424	VAL	3.5
1	B	497	ASN	3.5
1	F	255	ILE	3.5
1	F	260	MET	3.5
1	F	514	LEU	3.5
1	I	559	ALA	3.5
2	C	64	LYS	3.5
1	F	601	LEU	3.5
2	K	189	LEU	3.5
2	L	211	ARG	3.4
1	F	454	GLU	3.4
1	A	576	PRO	3.4
1	E	157	LEU	3.4
1	F	331	LEU	3.4
1	I	210	ARG	3.4
2	K	55	ARG	3.4
1	F	263	GLU	3.4
1	I	342	LEU	3.4
2	H	87	GLU	3.4
1	A	488	ASN	3.4
2	H	56	ILE	3.4
2	H	86	LEU	3.4
1	J	208	THR	3.4
1	I	148	LEU	3.4
2	D	72	LEU	3.4
2	D	134	VAL	3.4
2	H	49	GLY	3.4
1	I	416	PRO	3.4
1	I	677	THR	3.4
1	A	493	GLN	3.4
1	B	564	THR	3.4
1	A	317	ASP	3.4
1	F	693	ASP	3.4
1	A	691	LEU	3.4
1	B	606	GLN	3.4
1	I	410	ALA	3.4
1	F	592	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	473	TYR	3.4
2	H	54	ILE	3.4
2	K	243	PRO	3.4
1	F	562	ALA	3.4
1	I	146	ALA	3.4
1	I	383	GLU	3.4
2	G	291	TYR	3.4
1	E	175	PRO	3.4
1	F	555	LEU	3.4
1	J	549	LEU	3.4
1	E	680	ILE	3.4
1	A	628	ALA	3.4
1	J	235	SER	3.4
1	I	631	ALA	3.4
2	K	26	VAL	3.4
1	F	447	LEU	3.4
1	E	465	VAL	3.4
1	E	613	THR	3.4
1	J	626	GLN	3.4
2	C	23	PRO	3.4
2	L	140	PRO	3.4
2	G	186	THR	3.4
1	F	722	LEU	3.4
2	L	272	ILE	3.4
1	A	778	LEU	3.4
1	J	299	VAL	3.4
1	B	469	ALA	3.4
1	F	169	GLU	3.4
1	B	202	TRP	3.4
1	A	143	PHE	3.4
1	E	611	ILE	3.4
2	C	260	GLY	3.4
2	K	96	GLY	3.4
2	G	122	GLN	3.4
2	D	52	LYS	3.4
2	G	205	GLY	3.4
1	J	618	GLY	3.4
2	D	27	VAL	3.4
1	B	545	SER	3.4
1	J	768	SER	3.4
2	D	227	ILE	3.4
1	A	741	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	263	GLU	3.4
1	J	344	GLN	3.4
1	B	208	THR	3.3
1	J	179	LEU	3.3
2	D	124	TYR	3.3
1	J	783	LYS	3.3
1	F	549	LEU	3.3
1	A	157	LEU	3.3
1	A	348	LEU	3.3
1	I	739	MET	3.3
1	J	527	LEU	3.3
2	D	54	ILE	3.3
2	G	242	ASP	3.3
2	H	324	GLN	3.3
1	B	632	LEU	3.3
2	L	233	ASP	3.3
1	A	604	SER	3.3
2	D	82	SER	3.3
1	A	255	ILE	3.3
1	A	454	GLU	3.3
1	J	720	LYS	3.3
1	I	512	LYS	3.3
1	I	760	HIS	3.3
2	G	136	PRO	3.3
2	G	225	LEU	3.3
2	K	280	LEU	3.3
1	B	625	ARG	3.3
2	H	283	ASP	3.3
2	L	242	ASP	3.3
1	B	506	LEU	3.3
1	I	714	ASN	3.3
1	B	344	GLN	3.3
1	E	576	PRO	3.3
2	C	73	ALA	3.3
2	C	209	GLU	3.3
1	E	166	MET	3.3
1	J	272	ALA	3.3
2	H	64	LYS	3.3
1	F	561	ARG	3.3
1	F	411	ILE	3.3
1	J	557	ASN	3.3
2	C	266	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	177	ARG	3.3
1	A	221	ASP	3.3
1	F	154	ARG	3.3
1	F	372	PHE	3.3
2	D	51	ALA	3.3
1	E	614	GLY	3.3
2	G	200	ARG	3.3
1	B	468	ASN	3.3
2	H	267	LEU	3.3
1	F	709	TRP	3.3
2	C	211	ARG	3.3
1	A	638	SER	3.3
1	E	447	LEU	3.3
1	A	520	ALA	3.3
1	J	214	ASN	3.3
2	H	290	LEU	3.3
2	L	70	LEU	3.3
2	D	182	ARG	3.3
2	K	32	GLU	3.3
1	J	541	ALA	3.3
2	D	331	GLN	3.3
1	B	251	THR	3.3
2	C	177	ARG	3.3
2	L	225	LEU	3.3
2	C	241	ALA	3.3
2	H	274	GLN	3.3
1	A	486	PRO	3.3
2	D	326	VAL	3.3
2	L	168	PHE	3.3
1	A	651	ASP	3.3
1	B	636	ILE	3.3
1	E	496	LYS	3.3
1	I	381	GLN	3.3
1	I	738	LYS	3.3
1	A	637	GLY	3.3
1	J	646	GLU	3.3
2	L	268	ILE	3.3
1	A	654	PHE	3.2
2	G	220	PHE	3.2
2	H	63	ILE	3.2
1	A	704	GLY	3.2
2	H	216	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	470	VAL	3.2
2	G	89	ILE	3.2
2	H	268	ILE	3.2
1	A	311	LEU	3.2
1	I	208	THR	3.2
1	I	571	THR	3.2
1	B	659	ALA	3.2
1	B	731	GLU	3.2
1	J	177	GLU	3.2
1	J	323	GLU	3.2
2	D	161	LEU	3.2
1	J	786	ILE	3.2
2	D	215	ILE	3.2
1	A	480	GLY	3.2
1	B	710	ALA	3.2
1	I	773	LEU	3.2
1	I	399	GLU	3.2
1	F	701	THR	3.2
1	J	397	MET	3.2
2	G	147	VAL	3.2
2	D	327	LEU	3.2
2	G	269	ASN	3.2
2	H	30	LEU	3.2
1	E	555	LEU	3.2
1	I	277	LEU	3.2
2	H	65	LYS	3.2
2	L	64	LYS	3.2
1	A	351	ILE	3.2
1	A	159	GLU	3.2
2	G	135	LYS	3.2
1	A	650	ILE	3.2
1	E	464	LYS	3.2
1	E	484	LEU	3.2
1	J	785	VAL	3.2
2	C	202	VAL	3.2
1	A	515	THR	3.2
1	E	531	LEU	3.2
1	F	407	LEU	3.2
1	I	229	ASN	3.2
1	J	500	ARG	3.2
1	I	721	ALA	3.2
2	G	185	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	570	PRO	3.2
2	C	176	ARG	3.2
2	C	264	ARG	3.2
2	L	198	GLN	3.2
2	L	167	GLU	3.2
1	B	645	VAL	3.2
1	E	222	LEU	3.2
1	I	227	VAL	3.2
2	G	132	VAL	3.2
2	L	240	VAL	3.2
1	J	514	LEU	3.2
2	C	154	THR	3.2
1	B	374	GLN	3.2
1	B	478	SER	3.2
1	B	348	LEU	3.2
2	C	157	ARG	3.2
2	H	297	HIS	3.2
1	J	444	THR	3.2
2	H	119	GLU	3.2
2	G	211	ARG	3.2
2	L	123	ALA	3.2
1	E	474	TYR	3.2
2	C	95	ARG	3.2
2	D	135	LYS	3.2
1	B	133	LEU	3.2
1	I	601	LEU	3.2
1	B	128	ARG	3.2
2	D	110	LEU	3.2
1	E	231	PRO	3.2
1	F	635	TYR	3.2
2	C	184	ASP	3.2
2	D	183	PHE	3.2
1	B	647	ILE	3.1
1	I	786	ILE	3.1
2	G	83	LEU	3.1
1	J	512	LYS	3.1
2	D	132	VAL	3.1
2	D	271	ALA	3.1
1	E	325	GLN	3.1
1	E	378	LEU	3.1
1	A	646	GLU	3.1
1	B	419	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	464	LYS	3.1
2	H	265	ASP	3.1
2	C	96	GLY	3.1
1	I	368	MET	3.1
2	C	148	LEU	3.1
1	A	181	ALA	3.1
1	A	689	LEU	3.1
1	E	295	LEU	3.1
1	F	473	TYR	3.1
1	J	315	VAL	3.1
1	F	705	LEU	3.1
1	J	779	ALA	3.1
1	E	224	GLY	3.1
2	C	49	GLY	3.1
2	C	84	ASP	3.1
1	E	483	HIS	3.1
1	A	659	ALA	3.1
1	I	211	GLN	3.1
1	J	532	PHE	3.1
1	E	169	GLU	3.1
2	G	329	VAL	3.1
1	A	279	ILE	3.1
1	E	712	ALA	3.1
2	C	247	THR	3.1
1	I	709	TRP	3.1
1	E	681	LEU	3.1
1	J	755	THR	3.1
1	B	191	GLU	3.1
1	E	763	GLN	3.1
1	E	155	PHE	3.1
1	E	437	ARG	3.1
1	F	400	PHE	3.1
2	G	238	GLY	3.1
1	F	270	ASP	3.1
1	A	649	PRO	3.1
1	B	368	MET	3.1
1	I	411	ILE	3.1
1	F	128	ARG	3.1
1	F	316	ARG	3.1
1	J	389	PRO	3.1
1	A	688	SER	3.1
1	F	558	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	558	LEU	3.1
1	I	606	GLN	3.1
1	I	237	ALA	3.1
2	D	133	THR	3.1
2	G	109	THR	3.1
1	J	539	LEU	3.1
2	G	318	VAL	3.1
2	K	315	SER	3.1
1	I	560	GLU	3.1
1	A	564	THR	3.1
2	G	227	ILE	3.1
1	A	531	LEU	3.1
1	F	437	ARG	3.1
1	F	521	LEU	3.1
2	H	22	ARG	3.1
1	A	703	ASP	3.1
2	D	45	ASP	3.1
2	D	270	HIS	3.1
1	I	222	LEU	3.1
2	D	216	LEU	3.1
2	L	294	ILE	3.1
1	A	262	ARG	3.1
2	H	117	GLN	3.1
2	G	163	THR	3.1
2	G	258	VAL	3.1
1	A	706	SER	3.1
2	C	250	LEU	3.1
1	I	258	ILE	3.1
2	C	272	ILE	3.1
1	E	557	ASN	3.1
2	C	220	PHE	3.1
2	L	189	LEU	3.1
1	E	649	PRO	3.1
1	J	263	GLU	3.1
1	J	213	LEU	3.1
2	D	292	LEU	3.1
2	G	263	MET	3.1
1	B	499	GLU	3.0
1	E	339	GLN	3.0
1	B	204	PHE	3.0
2	L	299	VAL	3.0
1	A	213	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	361	ARG	3.0
1	E	528	TYR	3.0
1	I	216	GLN	3.0
1	J	321	LEU	3.0
2	D	92	LEU	3.0
2	D	179	ALA	3.0
2	H	112	SER	3.0
2	H	115	ALA	3.0
2	L	51	ALA	3.0
1	B	154	ARG	3.0
1	B	677	THR	3.0
1	F	161	ALA	3.0
2	H	291	TYR	3.0
1	I	751	GLU	3.0
2	H	116	GLU	3.0
1	A	208	THR	3.0
2	G	224	ALA	3.0
1	E	523	LEU	3.0
1	I	591	VAL	3.0
1	J	189	LEU	3.0
1	J	535	LEU	3.0
2	C	83	LEU	3.0
1	B	771	TYR	3.0
1	J	298	THR	3.0
1	J	502	ILE	3.0
1	J	523	LEU	3.0
1	F	244	ALA	3.0
2	L	25	SER	3.0
2	C	122	GLN	3.0
2	G	322	ILE	3.0
1	E	276	ASN	3.0
1	E	698	GLY	3.0
1	F	659	ALA	3.0
1	A	335	THR	3.0
1	E	699	THR	3.0
1	F	220	ARG	3.0
1	E	532	PHE	3.0
1	E	678	ALA	3.0
1	I	389	PRO	3.0
1	B	637	GLY	3.0
2	C	273	ARG	3.0
2	G	326	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	45	ASP	3.0
2	H	278	ASP	3.0
2	K	22	ARG	3.0
2	G	65	LYS	3.0
2	L	254	GLN	3.0
1	B	528	TYR	3.0
1	J	529	GLU	3.0
2	H	238	GLY	3.0
1	J	194	ARG	3.0
1	B	328	ILE	3.0
2	L	89	ILE	3.0
1	I	628	ALA	3.0
1	A	175	PRO	3.0
1	A	346	GLY	3.0
1	B	327	THR	3.0
1	E	247	THR	3.0
1	I	300	THR	3.0
1	B	425	ILE	3.0
1	J	210	ARG	3.0
1	J	178	LEU	3.0
1	J	338	LEU	3.0
2	L	269	ASN	3.0
2	C	239	TRP	3.0
2	D	198	GLN	3.0
1	B	331	LEU	3.0
1	I	178	LEU	3.0
1	J	337	GLY	3.0
1	B	324	ARG	3.0
2	C	63	ILE	3.0
1	E	355	LEU	3.0
2	H	155	PRO	3.0
2	K	36	ASP	3.0
1	B	230	ALA	3.0
1	J	520	ALA	3.0
2	L	267	LEU	2.9
1	B	555	LEU	2.9
1	F	144	GLY	2.9
1	I	188	SER	2.9
1	A	272	ALA	2.9
1	J	205	GLU	2.9
1	A	526	GLN	2.9
2	L	65	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	649	PRO	2.9
1	A	196	LEU	2.9
1	E	639	TYR	2.9
1	J	624	MET	2.9
2	C	199	TYR	2.9
2	H	50	GLY	2.9
1	I	761	SER	2.9
2	L	56	ILE	2.9
2	L	68	LEU	2.9
1	I	415	PRO	2.9
1	A	448	GLU	2.9
1	B	152	SER	2.9
2	G	190	SER	2.9
2	K	288	PHE	2.9
1	J	209	ALA	2.9
2	L	318	VAL	2.9
1	E	624	MET	2.9
1	A	189	LEU	2.9
2	C	244	ASN	2.9
2	H	198	GLN	2.9
1	I	553	ASP	2.9
2	L	174	ILE	2.9
1	I	576	PRO	2.9
1	I	513	VAL	2.9
1	F	526	GLN	2.9
1	I	393	LEU	2.9
2	C	291	TYR	2.9
2	D	89	ILE	2.9
1	E	754	ASP	2.9
2	C	245	HIS	2.9
1	J	530	GLU	2.9
2	D	21	GLU	2.9
2	L	286	PRO	2.9
1	B	740	GLU	2.9
1	I	775	VAL	2.9
2	D	211	ARG	2.9
2	D	195	ILE	2.9
1	E	571	THR	2.9
1	B	146	ALA	2.9
1	F	506	LEU	2.9
2	C	253	ILE	2.9
1	A	570	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	274	ARG	2.9
2	H	222	GLU	2.9
1	A	605	PRO	2.9
1	I	367	ARG	2.9
2	C	208	LYS	2.9
2	K	265	ASP	2.9
2	K	294	ILE	2.9
2	L	281	GLY	2.9
1	A	260	MET	2.9
1	J	492	ARG	2.9
1	I	707	LEU	2.9
1	B	503	ILE	2.9
2	G	56	ILE	2.9
1	E	352	LEU	2.9
1	F	527	LEU	2.9
1	I	155	PHE	2.9
1	J	474	TYR	2.8
1	I	394	ARG	2.8
2	L	326	VAL	2.8
1	E	599	ASN	2.8
1	J	245	LYS	2.8
1	F	234	LEU	2.8
1	F	552	LEU	2.8
1	A	177	GLU	2.8
1	B	713	GLU	2.8
1	A	742	VAL	2.8
2	K	139	HIS	2.8
2	K	266	ARG	2.8
2	G	181	ALA	2.8
2	L	295	ASP	2.8
1	E	428	GLY	2.8
1	E	556	VAL	2.8
1	J	542	LEU	2.8
1	B	259	THR	2.8
1	F	677	THR	2.8
1	B	235	SER	2.8
1	J	181	ALA	2.8
2	C	108	LEU	2.8
2	K	272	ILE	2.8
1	I	705	LEU	2.8
1	J	463	LEU	2.8
2	G	84	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	711	VAL	2.8
1	J	587	VAL	2.8
2	H	200	ARG	2.8
1	B	249	ARG	2.8
1	I	785	VAL	2.8
2	H	178	ILE	2.8
2	C	265	ASP	2.8
1	A	271	ALA	2.8
1	A	766	ALA	2.8
2	L	26	VAL	2.8
1	A	482	SER	2.8
1	E	234	LEU	2.8
1	I	676	GLU	2.8
1	J	231	PRO	2.8
2	G	234	LEU	2.8
1	B	370	HIS	2.8
1	A	497	ASN	2.8
1	B	371	ALA	2.8
1	B	624	MET	2.8
1	B	359	THR	2.8
1	E	298	THR	2.8
1	E	647	ILE	2.8
1	I	159	GLU	2.8
1	I	462	THR	2.8
2	G	235	THR	2.8
2	K	154	THR	2.8
1	B	234	LEU	2.8
1	F	368	MET	2.8
1	F	578	ILE	2.8
1	I	323	GLU	2.8
1	J	211	GLN	2.8
1	F	652	ARG	2.8
1	I	433	LEU	2.8
1	E	273	THR	2.8
2	D	258	VAL	2.8
1	A	744	ASN	2.8
1	E	220	ARG	2.8
1	E	414	THR	2.8
1	E	673	GLU	2.8
1	I	133	LEU	2.8
1	B	465	VAL	2.8
2	H	269	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	535	LEU	2.8
1	J	460	LEU	2.8
2	G	262	MET	2.8
1	J	461	ASP	2.8
2	K	68	LEU	2.8
1	A	137	TRP	2.8
2	D	237	ARG	2.8
2	H	260	GLY	2.8
1	A	768	SER	2.8
1	B	186	GLU	2.8
1	I	436	TRP	2.8
1	F	738	LYS	2.8
1	A	398	GLY	2.7
1	A	623	TYR	2.7
1	B	502	ILE	2.7
1	E	331	LEU	2.7
1	F	732	LEU	2.7
1	J	191	GLU	2.7
2	C	249	ALA	2.7
2	C	269	ASN	2.7
2	K	69	ALA	2.7
1	A	347	ASP	2.7
1	B	707	LEU	2.7
1	I	503	ILE	2.7
1	F	551	GLU	2.7
1	J	650	ILE	2.7
1	E	256	ARG	2.7
1	B	378	LEU	2.7
2	C	137	ALA	2.7
1	E	574	ASP	2.7
1	F	381	GLN	2.7
2	H	227	ILE	2.7
1	A	275	ARG	2.7
2	G	160	PHE	2.7
1	J	688	SER	2.7
2	D	84	ASP	2.7
1	J	217	PHE	2.7
1	F	333	ASP	2.7
1	F	453	ARG	2.7
1	I	711	VAL	2.7
1	A	259	THR	2.7
1	F	586	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	196	VAL	2.7
1	B	586	PRO	2.7
1	E	514	LEU	2.7
2	G	110	LEU	2.7
1	B	783	LYS	2.7
2	K	63	ILE	2.7
1	B	569	SER	2.7
1	B	701	THR	2.7
1	E	739	MET	2.7
1	I	741	GLY	2.7
2	C	251	ALA	2.7
2	G	216	LEU	2.7
2	G	25	SER	2.7
1	B	479	ARG	2.7
2	G	279	LYS	2.7
2	K	291	TYR	2.7
1	A	624	MET	2.7
1	F	602	ASN	2.7
1	I	552	LEU	2.7
1	I	244	ALA	2.7
1	J	784	GLU	2.7
2	G	125	ALA	2.7
1	B	670	PHE	2.7
1	J	596	PHE	2.7
2	C	150	LEU	2.7
1	E	679	ASN	2.7
2	H	33	ASN	2.7
1	I	587	VAL	2.7
2	L	253	ILE	2.7
1	A	172	ARG	2.7
1	J	295	LEU	2.7
2	L	52	LYS	2.7
1	I	704	GLY	2.7
1	A	792	LYS	2.7
1	A	313	MET	2.7
2	H	206	GLY	2.7
2	D	53	LEU	2.7
2	K	150	LEU	2.7
2	K	155	PRO	2.7
1	F	497	ASN	2.7
2	K	212	LEU	2.7
1	I	391	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	254	GLN	2.7
1	A	318	THR	2.7
1	B	511	ASP	2.7
1	F	360	ALA	2.7
1	J	355	LEU	2.7
2	C	94	PHE	2.7
2	H	266	ARG	2.7
2	D	50	GLY	2.7
1	B	752	HIS	2.7
1	J	296	ASP	2.7
2	C	259	ASN	2.7
1	A	518	GLY	2.7
1	A	712	ALA	2.7
1	F	556	VAL	2.7
2	H	202	VAL	2.7
2	K	99	LEU	2.7
1	A	204	PHE	2.7
1	A	571	THR	2.7
1	E	342	LEU	2.7
1	I	597	ILE	2.7
2	C	200	ARG	2.7
1	I	634	ALA	2.7
1	E	269	MET	2.7
2	C	268	ILE	2.6
1	A	218	GLY	2.6
1	B	184	PHE	2.6
1	J	700	SER	2.6
2	L	329	VAL	2.6
1	B	461	ASP	2.6
2	H	144	THR	2.6
1	B	258	ILE	2.6
1	I	339	GLN	2.6
1	J	131	ASN	2.6
1	A	711	VAL	2.6
1	E	345	VAL	2.6
1	E	745	VAL	2.6
2	C	65	LYS	2.6
2	L	27	VAL	2.6
2	L	263	MET	2.6
1	I	713	GLU	2.6
1	A	192	GLY	2.6
2	K	157	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	221	ASP	2.6
1	B	732	LEU	2.6
1	F	213	LEU	2.6
1	F	397	MET	2.6
1	J	291	LEU	2.6
2	C	207	GLN	2.6
2	H	329	VAL	2.6
1	F	401	ALA	2.6
1	F	680	ILE	2.6
1	I	280	THR	2.6
1	I	700	SER	2.6
2	K	175	ILE	2.6
1	I	504	PRO	2.6
2	K	298	GLN	2.6
1	E	521	LEU	2.6
1	J	361	ARG	2.6
2	G	243	PRO	2.6
1	B	579	ARG	2.6
1	B	714	ASN	2.6
1	F	230	ALA	2.6
1	F	433	LEU	2.6
1	F	589	GLU	2.6
2	G	137	ALA	2.6
1	E	558	LEU	2.6
1	I	338	LEU	2.6
1	I	426	ALA	2.6
2	L	45	ASP	2.6
1	I	715	LEU	2.6
1	B	361	ARG	2.6
1	E	176	ALA	2.6
1	E	189	LEU	2.6
1	E	545	SER	2.6
2	K	28	LYS	2.6
2	C	289	VAL	2.6
1	A	365	LEU	2.6
1	E	259	THR	2.6
1	I	234	LEU	2.6
2	L	234	LEU	2.6
1	F	503	ILE	2.6
2	K	89	ILE	2.6
1	E	270	ASP	2.6
1	B	547	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	613	THR	2.6
2	D	109	THR	2.6
1	A	449	ARG	2.6
1	J	343	ARG	2.6
1	J	518	GLY	2.6
1	J	280	THR	2.6
1	J	487	ILE	2.6
2	K	268	ILE	2.6
1	A	648	GLY	2.6
1	F	190	ILE	2.6
1	F	567	TYR	2.6
1	F	266	SER	2.6
1	F	650	ILE	2.6
2	C	146	GLU	2.6
1	I	712	ALA	2.6
2	K	279	LYS	2.6
1	E	608	ARG	2.6
1	F	579	ARG	2.6
1	I	501	TYR	2.6
1	B	418	LEU	2.6
1	I	699	THR	2.6
1	J	340	PRO	2.6
1	B	211	GLN	2.6
1	J	573	ILE	2.6
1	F	706	SER	2.6
1	J	548	ALA	2.6
2	C	224	ALA	2.6
2	C	255	TYR	2.6
1	A	263	GLU	2.6
1	B	178	LEU	2.6
2	C	288	PHE	2.6
2	D	200	ARG	2.6
2	H	284	GLN	2.6
1	F	505	GLU	2.6
2	G	204	GLU	2.6
1	F	580	ILE	2.6
2	C	213	GLY	2.6
2	L	44	ILE	2.6
1	I	348	LEU	2.6
2	C	110	LEU	2.6
2	G	298	GLN	2.6
2	H	162	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	522	ALA	2.6
1	J	585	HIS	2.6
1	E	297	SER	2.6
2	K	102	ILE	2.6
2	K	322	ILE	2.6
1	A	721	ALA	2.6
1	F	557	ASN	2.6
1	J	742	VAL	2.6
2	L	316	ARG	2.6
1	A	563	TYR	2.6
1	A	537	PRO	2.6
2	D	148	LEU	2.6
1	B	498	ALA	2.5
2	K	64	LYS	2.5
1	B	504	PRO	2.5
2	G	53	LEU	2.5
2	H	163	THR	2.5
1	A	191	GLU	2.5
1	J	443	ALA	2.5
1	B	524	GLU	2.5
1	E	217	PHE	2.5
1	E	374	GLN	2.5
1	E	467	PHE	2.5
1	F	229	ASN	2.5
2	D	146	GLU	2.5
2	K	331	GLN	2.5
2	L	146	GLU	2.5
1	A	458	THR	2.5
1	A	565	LEU	2.5
1	B	420	ARG	2.5
1	E	542	LEU	2.5
2	G	236	LEU	2.5
2	H	320	ASP	2.5
1	F	191	GLU	2.5
1	F	603	LEU	2.5
1	E	277	LEU	2.5
1	I	610	LEU	2.5
1	J	351	ILE	2.5
2	G	41	ARG	2.5
1	B	423	GLY	2.5
1	B	355	LEU	2.5
1	B	565	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	433	LEU	2.5
1	J	732	LEU	2.5
1	F	733	THR	2.5
2	L	133	THR	2.5
1	A	331	LEU	2.5
1	B	352	LEU	2.5
1	B	715	LEU	2.5
2	C	97	GLU	2.5
1	J	300	THR	2.5
1	A	555	LEU	2.5
1	A	368	MET	2.5
1	B	626	GLN	2.5
1	F	143	PHE	2.5
1	F	312	HIS	2.5
2	G	290	LEU	2.5
1	I	609	MET	2.5
2	K	151	PHE	2.5
1	F	761	SER	2.5
1	F	782	PRO	2.5
1	J	689	LEU	2.5
2	G	27	VAL	2.5
1	B	228	GLU	2.5
1	E	694	GLU	2.5
1	F	212	GLN	2.5
1	J	228	GLU	2.5
1	A	581	THR	2.5
1	B	558	LEU	2.5
1	J	466	GLY	2.5
1	A	530	GLU	2.5
1	E	548	ALA	2.5
1	F	728	HIS	2.5
2	H	219	ALA	2.5
1	E	527	LEU	2.5
1	I	454	GLU	2.5
1	B	346	GLY	2.5
1	E	161	ALA	2.5
1	J	739	MET	2.5
1	E	731	GLU	2.5
1	I	754	ASP	2.5
2	C	284	GLN	2.5
2	K	318	VAL	2.5
1	B	519	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	531	LEU	2.5
2	D	31	VAL	2.5
2	H	318	VAL	2.5
1	E	577	GLY	2.5
1	I	716	ALA	2.5
1	J	250	THR	2.5
2	D	246	THR	2.5
1	J	470	VAL	2.5
1	E	683	ASN	2.5
2	C	188	ASN	2.5
2	H	270	HIS	2.5
1	B	220	ARG	2.5
1	I	632	LEU	2.5
2	G	52	LYS	2.5
1	J	320	VAL	2.5
2	G	73	ALA	2.5
2	L	73	ALA	2.5
2	L	227	ILE	2.5
1	B	717	ASN	2.5
2	L	57	ARG	2.5
1	J	201	LEU	2.5
2	K	65	LYS	2.5
2	K	281	GLY	2.5
1	E	623	TYR	2.4
1	F	535	LEU	2.5
2	H	319	HIS	2.4
1	E	513	VAL	2.4
1	F	334	PHE	2.4
2	D	147	VAL	2.4
1	B	372	PHE	2.4
1	B	674	MET	2.4
1	A	230	ALA	2.4
1	E	344	GLN	2.4
1	J	717	ASN	2.4
2	K	259	ASN	2.4
1	E	511	ASP	2.4
1	F	591	VAL	2.4
1	I	783	LYS	2.4
2	D	26	VAL	2.4
1	F	681	LEU	2.4
1	J	169	GLU	2.4
2	H	288	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	521	LEU	2.4
1	A	634	ALA	2.4
1	E	646	GLU	2.4
1	J	767	ALA	2.4
2	K	149	ASP	2.4
1	A	501	TYR	2.4
1	F	436	TRP	2.4
2	C	52	LYS	2.4
2	D	262	MET	2.4
2	H	27	VAL	2.4
1	J	259	THR	2.4
1	B	421	ASP	2.4
1	I	213	LEU	2.4
1	J	459	GLY	2.4
1	J	232	ARG	2.4
2	G	296	PRO	2.4
2	L	134	VAL	2.4
2	L	322	ILE	2.4
1	A	767	ALA	2.4
2	H	287	ALA	2.4
2	L	223	GLN	2.4
1	E	372	PHE	2.4
1	J	457	ARG	2.4
1	J	513	VAL	2.4
2	D	56	ILE	2.4
1	E	594	GLU	2.4
1	F	408	GLU	2.4
2	G	255	TYR	2.4
1	E	522	ALA	2.4
1	F	426	ALA	2.4
1	E	578	ILE	2.4
1	F	430	ASN	2.4
1	A	161	ALA	2.4
2	C	225	LEU	2.4
1	J	574	ASP	2.4
2	G	46	ILE	2.4
2	H	35	LEU	2.4
1	B	671	MET	2.4
1	B	341	VAL	2.4
2	C	326	VAL	2.4
1	I	538	HIS	2.4
1	A	425	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	337	GLY	2.4
1	J	533	ASP	2.4
1	E	236	ALA	2.4
2	G	70	LEU	2.4
2	K	54	ILE	2.4
2	K	200	ARG	2.4
2	L	53	LEU	2.4
1	A	516	SER	2.4
2	C	263	MET	2.4
1	A	534	LEU	2.4
1	A	656	ARG	2.4
1	E	651	ASP	2.4
1	E	746	HIS	2.4
2	H	277	GLU	2.4
1	J	166	MET	2.4
1	F	225	PHE	2.4
1	A	233	GLY	2.4
2	K	103	SER	2.4
1	F	246	CYS	2.4
1	I	492	ARG	2.4
1	J	364	ASP	2.4
1	J	420	ARG	2.4
1	F	674	MET	2.4
1	E	598	ALA	2.3
1	I	427	SER	2.3
1	F	345	VAL	2.3
1	I	586	PRO	2.3
2	L	287	ALA	2.3
1	J	593	ASN	2.3
1	A	582	GLU	2.3
2	D	150	LEU	2.3
2	D	228	GLU	2.3
2	H	161	LEU	2.3
2	C	294	ILE	2.3
2	L	115	ALA	2.3
1	B	252	LEU	2.3
1	E	174	ASN	2.3
1	E	310	TRP	2.3
1	F	800	SER	2.3
1	A	277	LEU	2.3
1	A	536	LEU	2.3
1	B	476	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	203	GLU	2.3
1	I	508	GLU	2.3
1	I	530	GLU	2.3
2	C	322	ILE	2.3
2	D	46	ILE	2.3
1	A	505	GLU	2.3
2	H	29	GLU	2.3
1	B	601	LEU	2.3
1	E	554	VAL	2.3
2	C	147	VAL	2.3
1	I	457	ARG	2.3
1	A	645	VAL	2.3
1	F	375	LEU	2.3
2	C	214	ALA	2.3
2	G	287	ALA	2.3
2	L	46	ILE	2.3
1	F	448	GLU	2.3
1	I	245	LYS	2.3
2	K	93	GLY	2.3
2	D	111	THR	2.3
2	L	277	GLU	2.3
1	E	671	MET	2.3
1	F	364	ASP	2.3
1	I	706	SER	2.3
2	H	199	TYR	2.3
2	L	109	THR	2.3
2	C	132	VAL	2.3
2	K	290	LEU	2.3
2	L	195	ILE	2.3
1	E	744	ASN	2.3
2	H	34	SER	2.3
2	H	261	ARG	2.3
1	E	711	VAL	2.3
1	J	172	ARG	2.3
2	H	85	ASP	2.3
1	A	138	GLN	2.3
1	A	558	LEU	2.3
1	I	191	GLU	2.3
1	J	273	THR	2.3
1	A	184	PHE	2.3
1	E	645	VAL	2.3
1	I	199	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	343	ARG	2.3
2	D	88	ALA	2.3
1	J	698	GLY	2.3
2	H	258	VAL	2.3
1	B	137	TRP	2.3
1	A	162	ASP	2.3
2	C	115	ALA	2.3
2	D	261	ARG	2.3
1	J	184	PHE	2.3
1	B	612	ILE	2.3
2	K	210	ARG	2.3
1	E	132	LEU	2.3
1	J	139	ASP	2.3
1	E	144	GLY	2.3
1	B	496	LYS	2.3
1	B	507	LYS	2.3
1	E	770	SER	2.3
1	F	546	ALA	2.3
1	I	674	MET	2.3
2	H	120	ALA	2.3
2	H	295	ASP	2.3
1	A	733	THR	2.3
1	B	335	THR	2.3
1	E	180	TYR	2.3
2	K	247	THR	2.3
1	J	617	MET	2.3
1	F	382	LEU	2.3
1	I	255	ILE	2.3
1	I	431	GLU	2.3
1	I	627	THR	2.3
1	J	540	GLU	2.3
2	K	285	GLN	2.3
1	B	138	GLN	2.3
1	I	451	GLU	2.3
1	I	689	LEU	2.3
1	F	429	TYR	2.3
1	B	153	GLY	2.3
1	B	422	GLY	2.3
2	H	292	LEU	2.3
1	E	219	THR	2.3
1	E	377	GLU	2.3
1	A	586	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	199	ARG	2.3
1	B	349	GLU	2.2
1	F	165	THR	2.2
1	F	413	ASP	2.2
1	I	772	GLY	2.2
2	G	260	GLY	2.2
1	F	162	ASP	2.2
2	L	69	ALA	2.2
1	I	295	LEU	2.2
1	J	354	ARG	2.2
2	C	22	ARG	2.2
2	C	257	TYR	2.2
1	J	545	SER	2.2
1	E	658	GLY	2.2
2	D	219	ALA	2.2
2	K	50	GLY	2.2
1	A	525	LYS	2.2
1	B	580	ILE	2.2
1	I	532	PHE	2.2
1	J	368	MET	2.2
2	H	26	VAL	2.2
2	D	107	ARG	2.2
2	H	32	GLU	2.2
1	B	548	ALA	2.2
1	A	500	ARG	2.2
1	B	474	TYR	2.2
1	E	172	ARG	2.2
1	F	694	GLU	2.2
1	I	529	GLU	2.2
2	D	298	GLN	2.2
2	H	28	LYS	2.2
2	G	288	PHE	2.2
1	A	779	ALA	2.2
1	B	209	ALA	2.2
1	B	384	THR	2.2
1	A	644	LYS	2.2
1	F	273	THR	2.2
1	B	562	ALA	2.2
1	F	710	ALA	2.2
1	J	318	THR	2.2
2	D	250	LEU	2.2
1	F	638	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	704	GLY	2.2
1	I	184	PHE	2.2
1	J	730	PHE	2.2
1	B	493	GLN	2.2
1	E	369	ARG	2.2
2	L	208	LYS	2.2
2	H	271	ALA	2.2
2	D	30	LEU	2.2
1	A	631	ALA	2.2
1	B	325	GLN	2.2
1	E	371	ALA	2.2
1	F	767	ALA	2.2
1	I	328	ILE	2.2
1	J	713	GLU	2.2
2	C	226	ALA	2.2
2	G	151	PHE	2.2
1	E	732	LEU	2.2
1	A	551	GLU	2.2
1	E	515	THR	2.2
1	F	138	GLN	2.2
2	D	87	GLU	2.2
2	H	286	PRO	2.2
2	K	37	ALA	2.2
1	A	225	PHE	2.2
2	C	35	LEU	2.2
1	A	459	GLY	2.2
1	I	205	GLU	2.2
1	J	244	ALA	2.2
2	L	88	ALA	2.2
1	A	629	LEU	2.2
1	B	213	LEU	2.2
1	A	788	ARG	2.2
1	B	623	TYR	2.2
1	E	360	ALA	2.2
2	K	233	ASP	2.2
1	I	192	GLY	2.2
1	J	430	ASN	2.2
1	J	714	ASN	2.2
2	C	248	PRO	2.2
2	H	273	ARG	2.2
1	A	647	ILE	2.2
2	G	31	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	252	LEU	2.2
2	K	158	ARG	2.2
2	L	255	TYR	2.2
1	I	418	LEU	2.2
1	J	432	GLU	2.2
2	C	295	ASP	2.2
2	G	48	ARG	2.2
2	K	295	ASP	2.2
1	A	222	LEU	2.2
1	F	770	SER	2.2
1	B	500	ARG	2.2
1	F	253	PRO	2.2
1	F	449	ARG	2.2
2	C	31	VAL	2.2
1	E	682	HIS	2.2
1	F	516	SER	2.2
2	H	315	SER	2.2
2	K	25	SER	2.2
1	F	159	GLU	2.2
1	F	420	ARG	2.2
1	F	414	THR	2.2
2	D	322	ILE	2.2
1	I	344	GLN	2.2
2	D	25	SER	2.2
1	B	654	PHE	2.2
1	J	317	ASP	2.2
2	C	172	ASP	2.2
2	G	331	GLN	2.2
1	A	517	LYS	2.2
1	A	566	ASN	2.2
1	J	517	LYS	2.2
1	A	436	TRP	2.2
1	J	534	LEU	2.1
2	L	114	THR	2.1
2	L	187	ILE	2.1
1	E	735	LEU	2.1
1	E	326	GLN	2.1
1	F	658	GLY	2.1
1	I	299	VAL	2.1
1	J	229	ASN	2.1
1	E	296	ASP	2.1
1	E	375	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	233	GLY	2.1
2	C	292	LEU	2.1
2	K	101	SER	2.1
1	E	368	MET	2.1
2	K	257	TYR	2.1
1	F	517	LYS	2.1
1	I	629	LEU	2.1
2	C	171	ILE	2.1
2	G	196	VAL	2.1
1	A	584	ARG	2.1
1	A	615	PRO	2.1
1	A	782	PRO	2.1
1	B	561	ARG	2.1
2	G	157	ARG	2.1
2	K	260	GLY	2.1
1	J	292	ALA	2.1
1	E	517	LYS	2.1
2	K	242	ASP	2.1
1	A	243	TYR	2.1
1	B	489	TYR	2.1
1	B	567	TYR	2.1
2	L	91	SER	2.1
1	F	757	ALA	2.1
1	I	149	ASP	2.1
1	I	790	ARG	2.1
1	F	352	LEU	2.1
1	B	593	ASN	2.1
1	A	491	ARG	2.1
2	H	203	PRO	2.1
1	B	454	GLU	2.1
1	A	397	MET	2.1
1	F	462	THR	2.1
1	I	549	LEU	2.1
1	I	565	LEU	2.1
1	I	650	ILE	2.1
1	F	310	TRP	2.1
2	D	28	LYS	2.1
1	A	583	GLY	2.1
1	B	542	LEU	2.1
2	G	111	THR	2.1
1	E	415	PRO	2.1
1	J	398	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	442	GLY	2.1
1	J	687	TYR	2.1
2	C	262	MET	2.1
1	J	385	VAL	2.1
2	K	100	ALA	2.1
2	L	137	ALA	2.1
1	B	735	LEU	2.1
1	A	424	VAL	2.1
1	F	167	ALA	2.1
1	I	256	ARG	2.1
2	H	259	ASN	2.1
2	L	244	ASN	2.1
1	J	536	LEU	2.1
2	H	201	ALA	2.1
2	L	200	ARG	2.1
1	F	313	MET	2.1
1	F	464	LYS	2.1
1	F	748	ASP	2.1
1	A	559	ALA	2.1
1	B	407	LEU	2.1
1	E	457	ARG	2.1
1	J	316	ARG	2.1
2	K	246	THR	2.1
1	J	348	LEU	2.1
2	C	54	ILE	2.1
2	G	35	LEU	2.1
1	B	364	ASP	2.1
1	E	385	VAL	2.1
1	E	764	ASP	2.1
1	J	365	LEU	2.1
1	A	245	LYS	2.1
1	B	641	PRO	2.1
1	I	268	ILE	2.1
2	K	192	ASN	2.1
2	C	270	HIS	2.1
2	L	184	ASP	2.1
1	B	369	ARG	2.1
1	I	363	ARG	2.1
1	I	702	TYR	2.1
1	B	365	LEU	2.1
2	C	299	VAL	2.1
2	C	252	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	174	ASN	2.1
1	I	428	GLY	2.1
1	J	311	LEU	2.1
1	B	145	TYR	2.1
1	E	625	ARG	2.1
2	D	160	PHE	2.1
1	F	756	ILE	2.1
2	D	221	LEU	2.0
1	E	235	SER	2.0
1	A	205	GLU	2.0
1	B	180	TYR	2.0
1	I	654	PHE	2.0
1	A	785	VAL	2.0
1	B	277	LEU	2.0
1	E	393	LEU	2.0
1	F	403	LEU	2.0
1	I	534	LEU	2.0
2	D	184	ASP	2.0
2	L	145	LEU	2.0
2	K	231	HIS	2.0
2	G	88	ALA	2.0
1	J	521	LEU	2.0
1	E	766	ALA	2.0
1	J	258	ILE	2.0
1	B	356	ALA	2.0
1	F	184	PHE	2.0
1	F	422	GLY	2.0
2	H	218	THR	2.0
1	B	523	LEU	2.0
1	E	138	GLN	2.0
1	B	231	PRO	2.0
1	E	538	HIS	2.0
2	G	91	SER	2.0
2	H	97	GLU	2.0
1	B	410	ALA	2.0
1	F	365	LEU	2.0
1	F	628	ALA	2.0
1	I	220	ARG	2.0
2	L	162	ARG	2.0
1	I	259	THR	2.0
1	I	407	LEU	2.0
1	A	606	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	791	GLN	2.0
1	A	154	ARG	2.0
2	G	69	ALA	2.0
2	H	24	ALA	2.0
1	E	600	PRO	2.0
1	F	219	THR	2.0
1	F	627	THR	2.0
2	L	231	HIS	2.0
2	L	291	TYR	2.0
1	A	532	PHE	2.0
2	K	44	ILE	2.0
1	F	311	LEU	2.0
1	I	291	LEU	2.0
1	J	331	LEU	2.0
1	J	738	LYS	2.0
2	K	62	GLY	2.0
1	A	321	LEU	2.0
1	A	511	ASP	2.0
1	A	552	LEU	2.0
1	E	533	ASP	2.0
1	I	680	ILE	2.0
1	F	496	LYS	2.0
1	I	561	ARG	2.0
1	B	229	ASN	2.0
1	F	264	GLN	2.0
1	J	130	ASP	2.0
2	K	236	LEU	2.0
1	A	687	TYR	2.0
1	E	156	ARG	2.0
1	E	356	ALA	2.0
1	F	510	GLU	2.0
1	J	142	GLY	2.0
2	G	158	ARG	2.0
2	K	132	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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
3	ANP	I	1801	31/31	0.70	0.41	-0.52	177,180,186,187	0
3	ANP	E	1801	31/31	0.70	0.51	-0.72	204,216,227,232	0
3	ANP	A	1801	31/31	0.81	0.51	-0.74	156,164,170,171	0
3	ANP	J	1801	31/31	0.64	0.49	-0.83	193,199,212,213	0
3	ANP	B	1801	31/31	0.72	0.31	-0.87	165,174,179,181	0
3	ANP	F	1801	31/31	0.85	0.30	-1.06	154,162,169,174	0

6.5 Other polymers [i](#)

There are no such residues in this entry.