



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:23 am BST

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

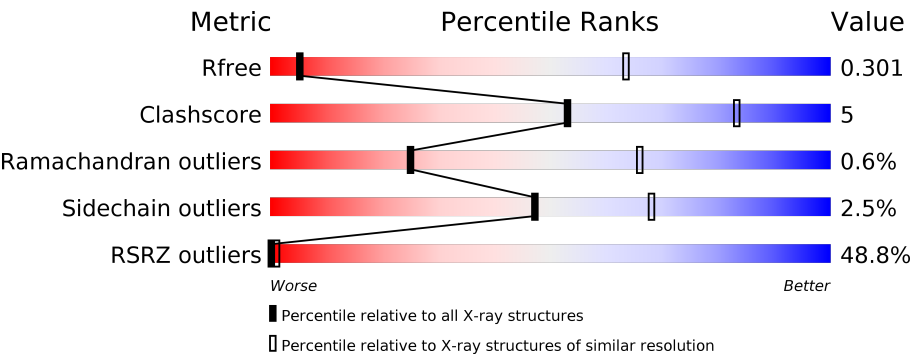
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	800	
1	B	800	
1	E	800	
1	F	800	
1	I	800	
1	J	800	

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Mol	Chain	Length	Quality of chain
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	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

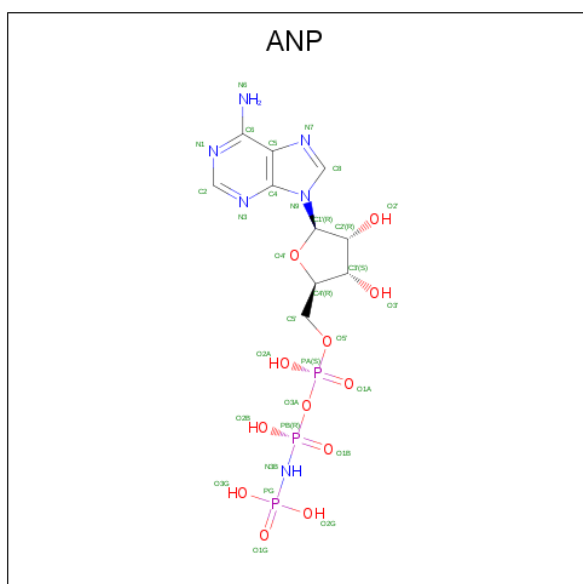
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Chain	Residue	Modelled	Actual	Comment	Reference
L	-17	SER	-	expression tag	UNP P23367
L	-16	SER	-	expression tag	UNP P23367
L	-15	HIS	-	expression tag	UNP P23367
L	-14	HIS	-	expression tag	UNP P23367
L	-13	HIS	-	expression tag	UNP P23367
L	-12	HIS	-	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:  $C_{10}H_{17}N_6O_{12}P_3$ ).

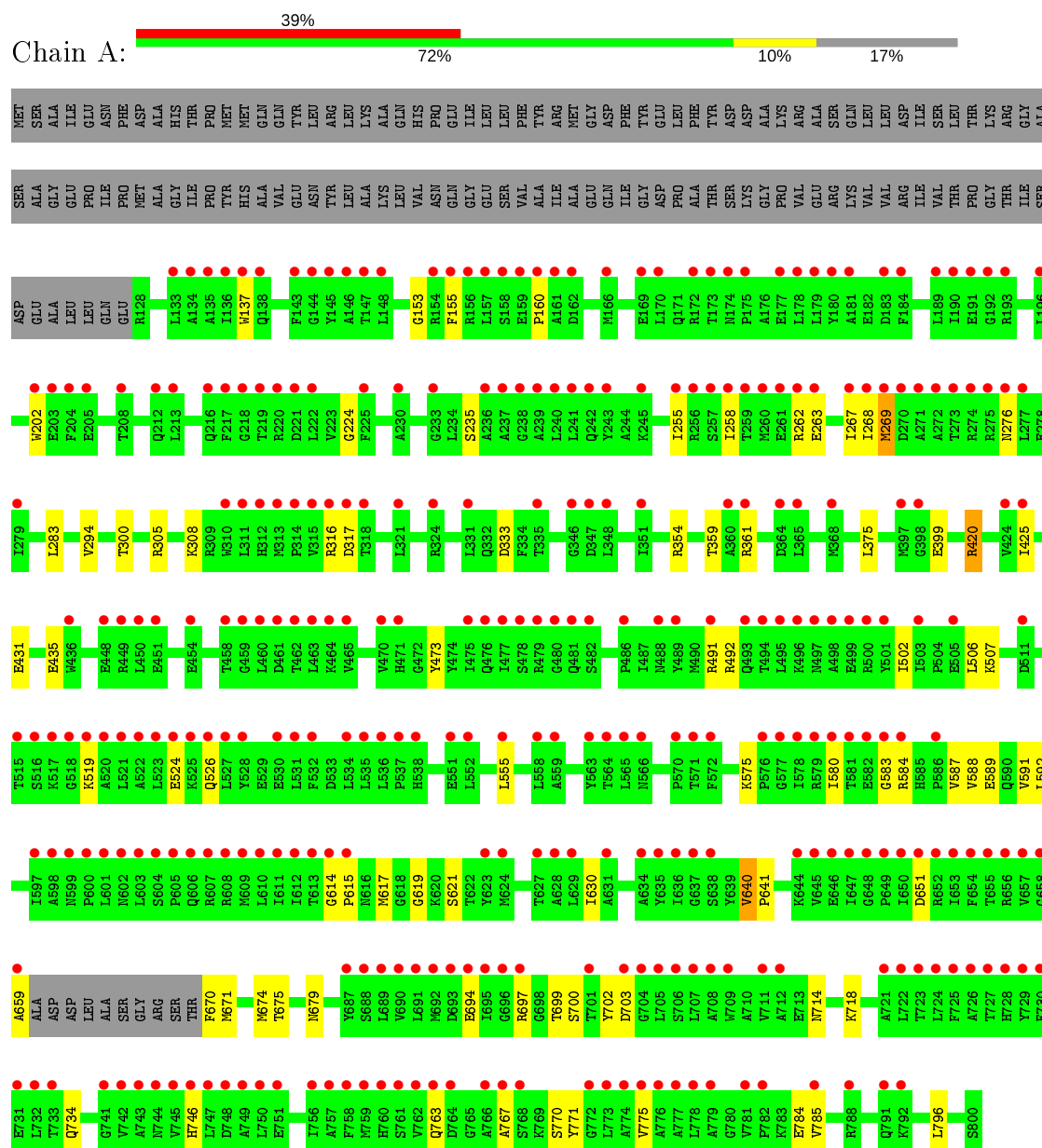


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

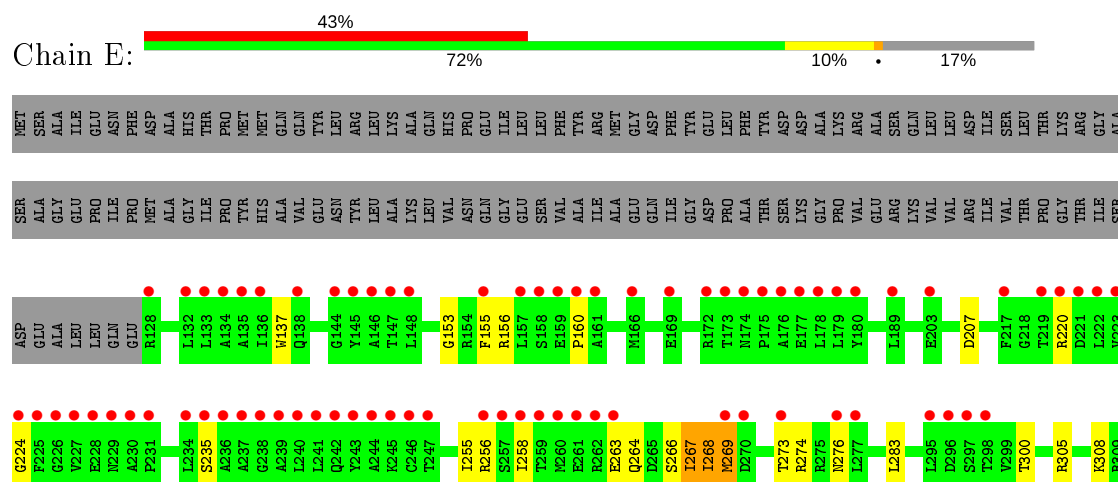
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

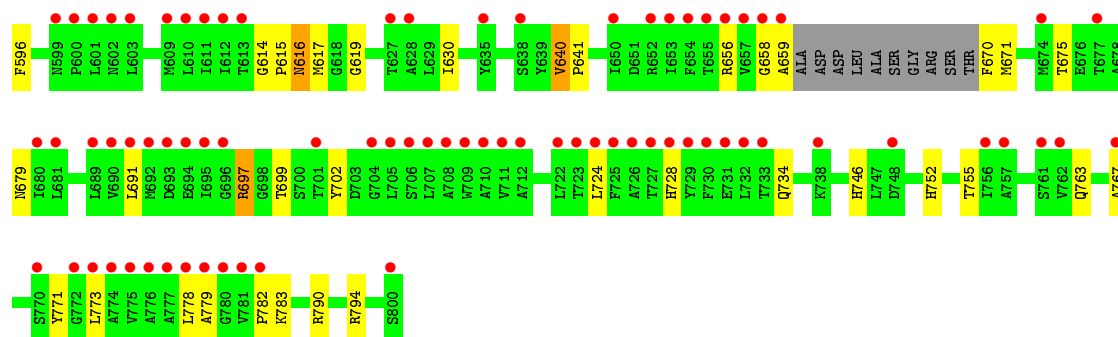
- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



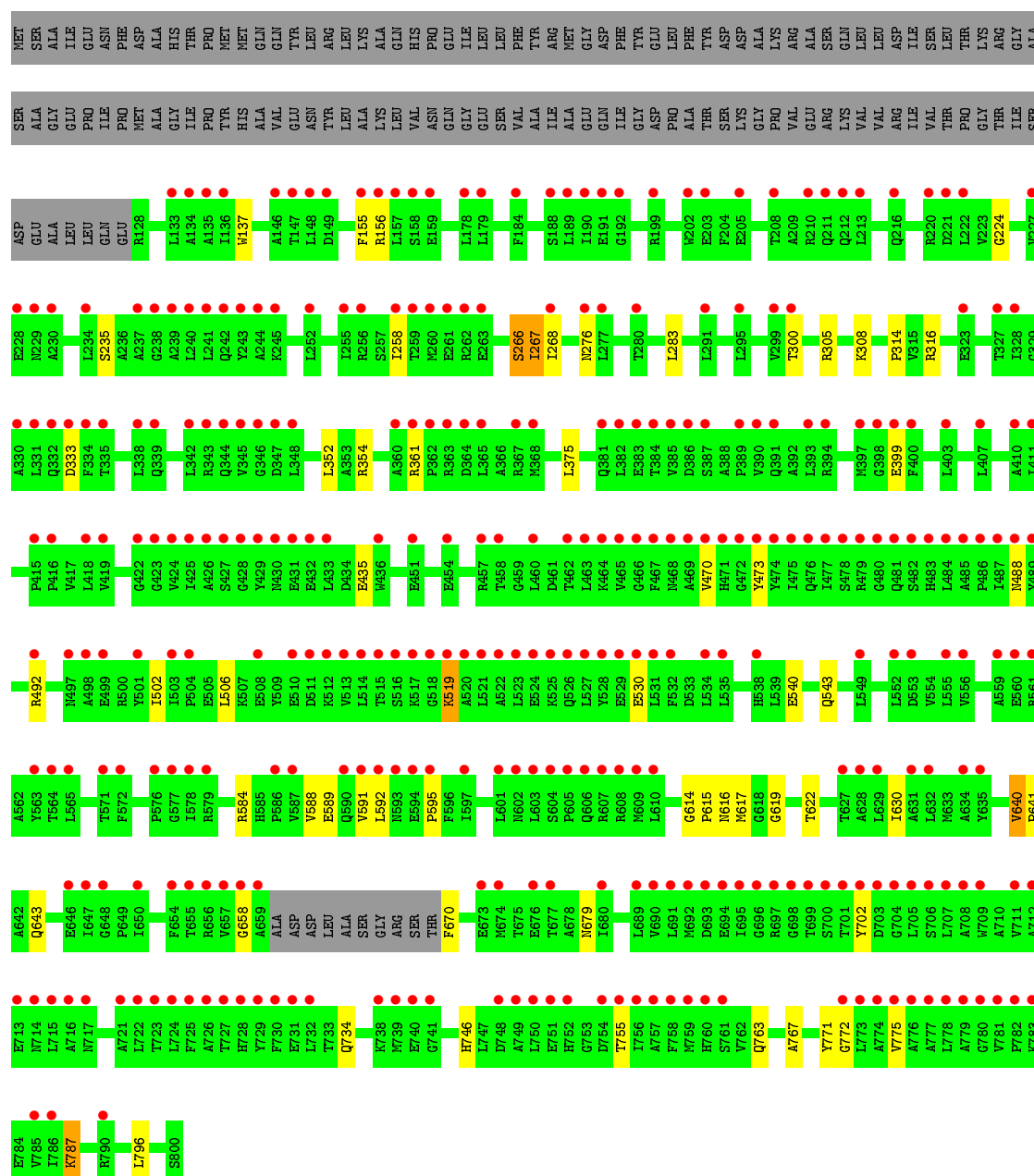
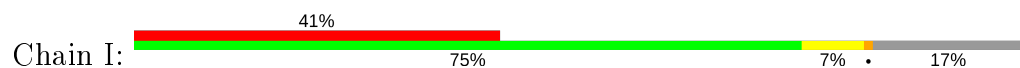
- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS





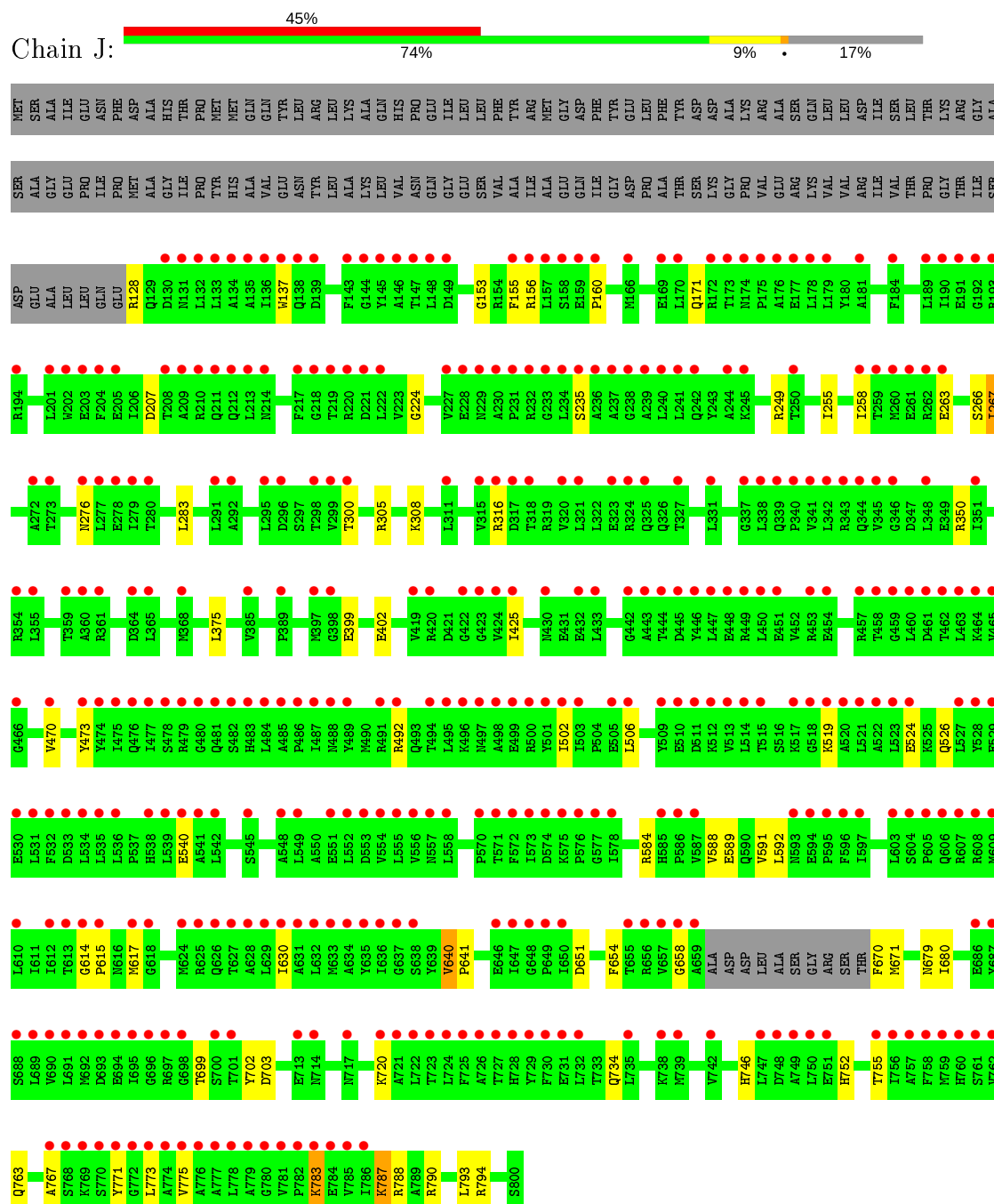


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



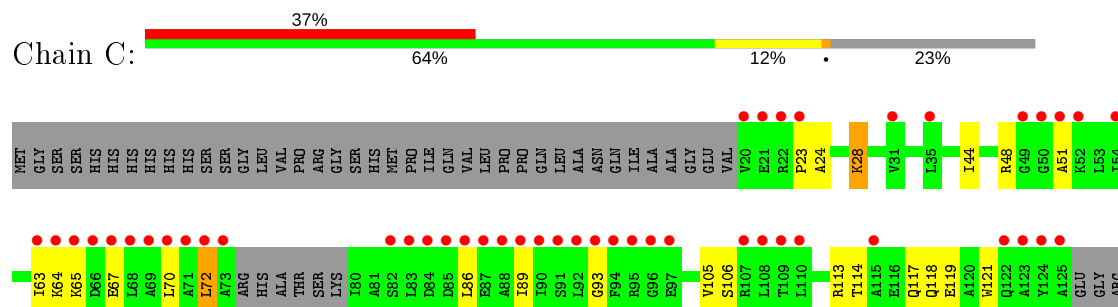
- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

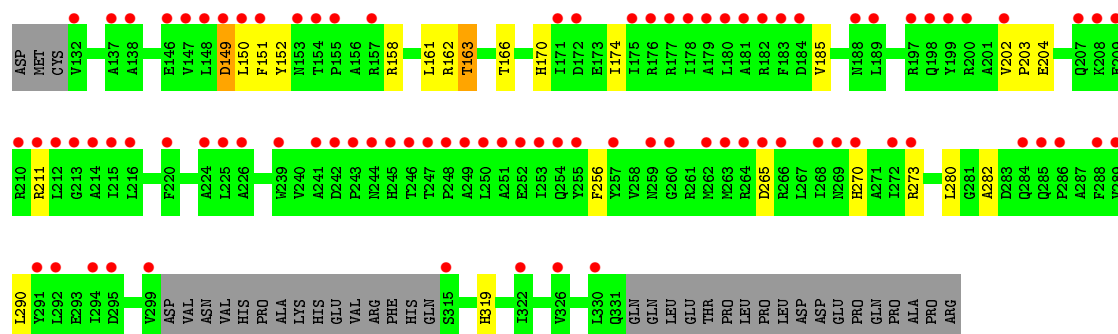
Chain J:



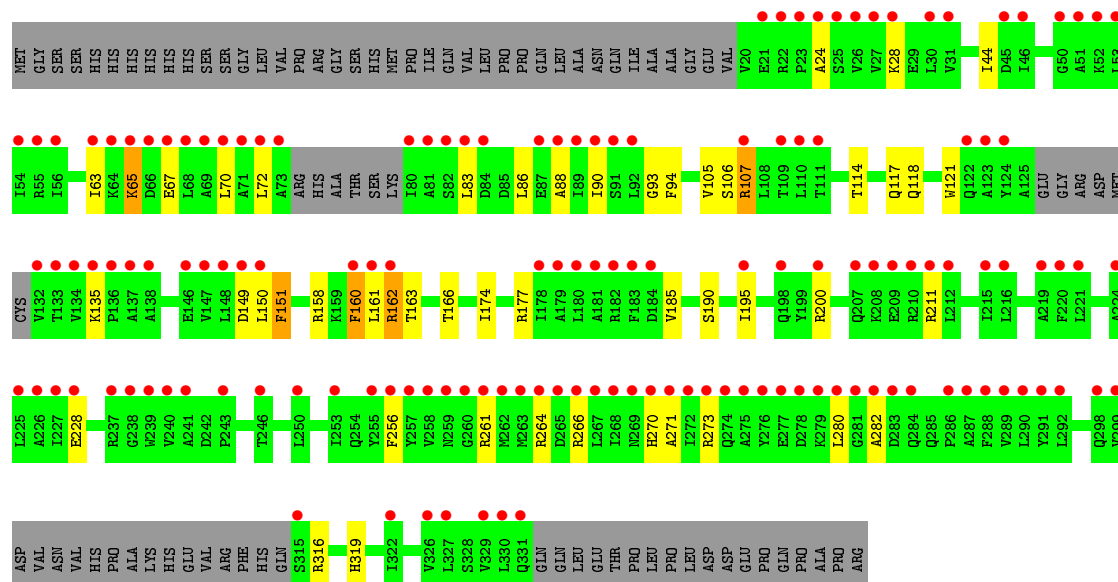
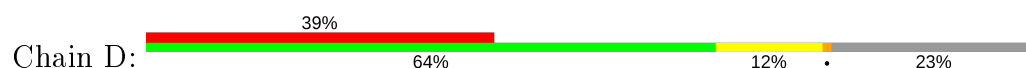
- Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

Chain C:

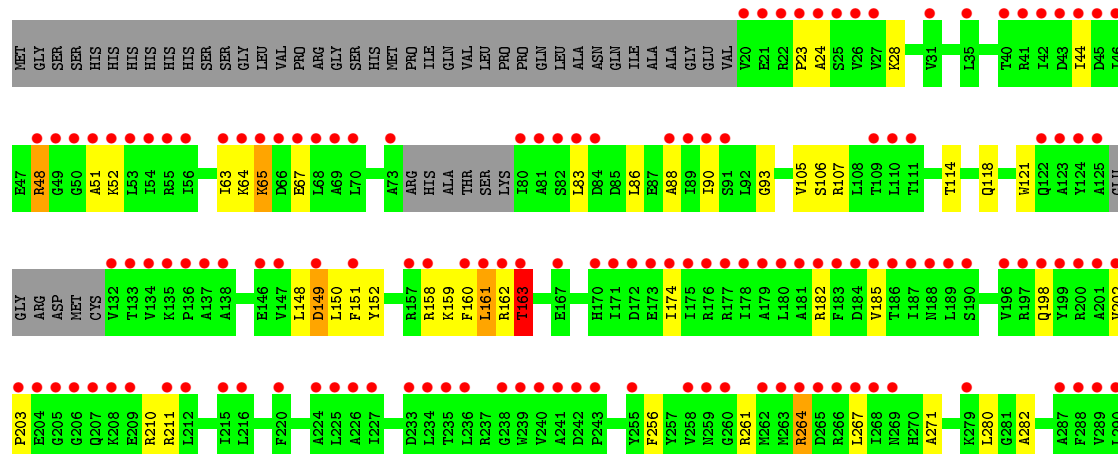
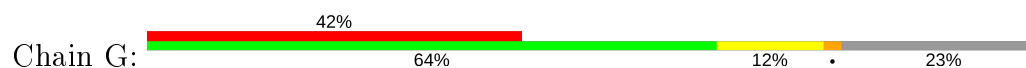




• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

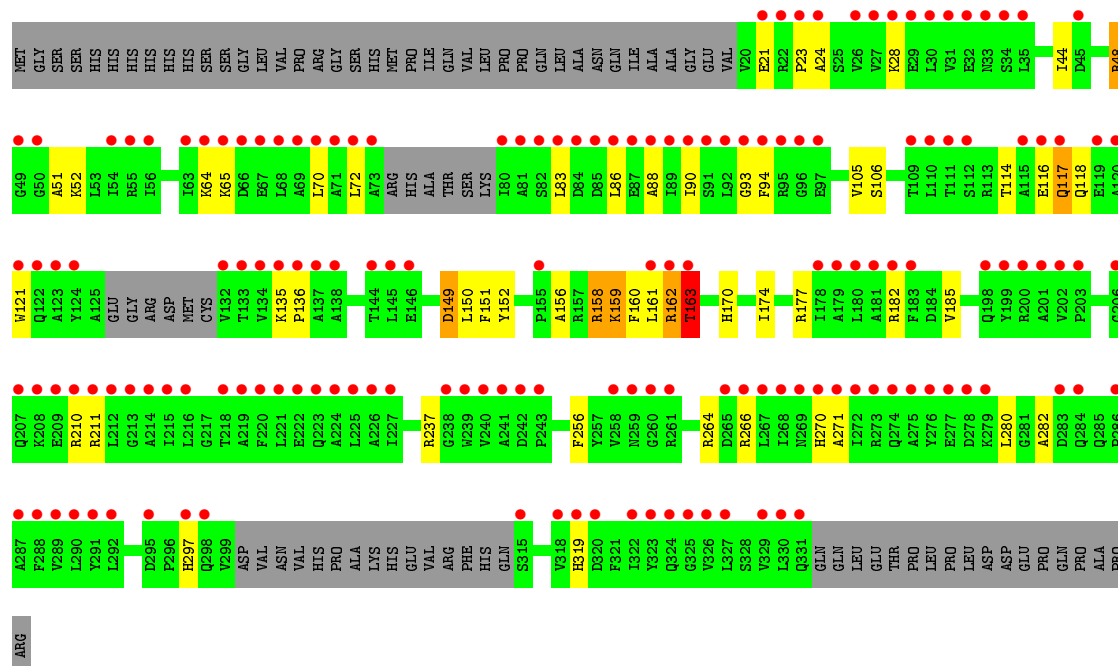
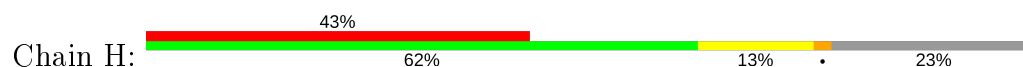


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

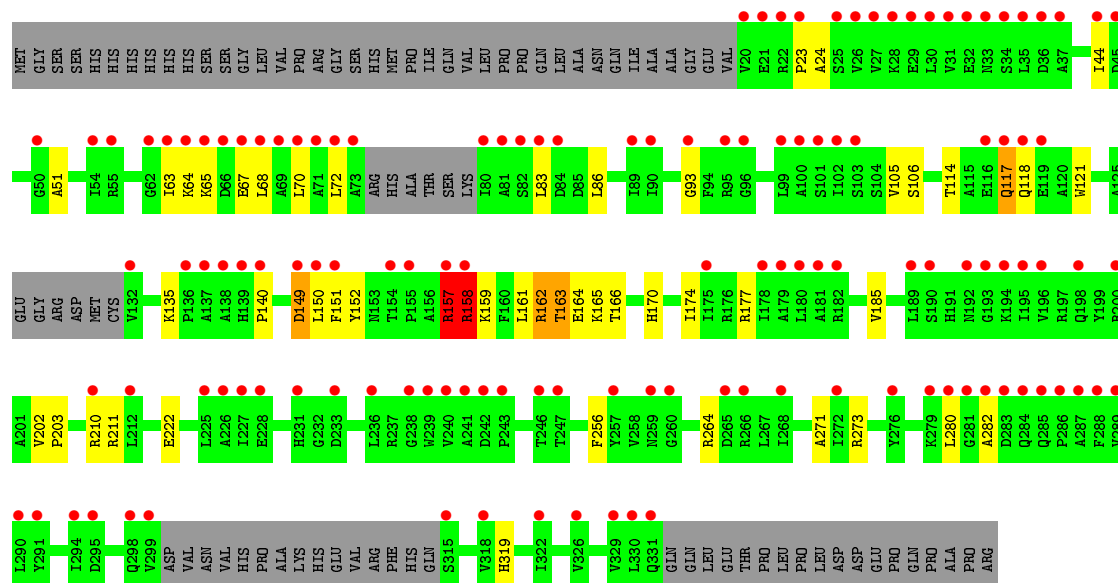




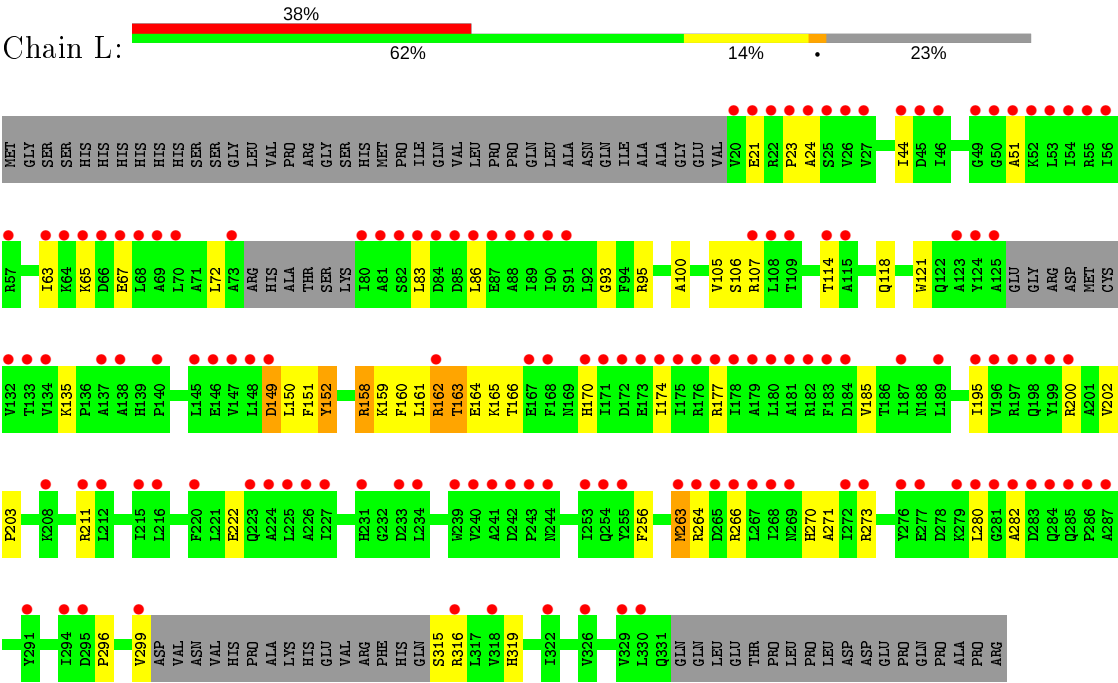
- Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



- Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



- Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	585 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	441.7	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 500.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.090 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	45054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 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:NZ	2:C:28:LYS:CE	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:H:105:VAL:O	2:H:150:LEU:O	1.99	0.80
2:K:105:VAL:O	2:K:150:LEU:O	2.00	0.80
1:A:675:THR:N	1:B:779:ALA:HB1	1.97	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
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:A:670:PHE:CD2	1:B:775:VAL:HG11	2.30	0.66
1:E:268:ILE:HG23	1:E:274:ARG:HH12	1.60	0.66
1:A:702:TYR:HB3	1:B:793:LEU:CD1	2.25	0.66
2:H:256:PHE:CZ	2:H:264:ARG:HA	2.29	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
3:A:1801:ANP:O1G	1:B:670:PHE:N	2.29	0.65
2:H:88:ALA:HB1	2:L:316:ARG:NH2	2.12	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
1:A:305:ARG:HA	1:A:308:LYS:HE3	1.84	0.59
2:C:162:ARG:O	2:C:163:THR:O	2.21	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:23:PRO:HD3	2:K:161:LEU:HD11	1.86	0.57
2:K:51:ALA:O	2:K:149:ASP:HA	2.04	0.57
1:A:703:ASP:OD2	1:B:772:GLY:HA3	2.04	0.57
1:F:773:LEU:HD13	1:F:790:ARG:HG2	1.86	0.57
2:G:83:LEU:HD13	2:G:90:ILE:CD1	2.35	0.57
1:F:305:ARG:HA	1:F:308:LYS:HE3	1.86	0.57
2:K:162:ARG:O	2:K:163:THR:O	2.20	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
2:D:83:LEU:HD22	2:D:86:LEU:HD21	1.87	0.56
1:E:269:MET:HE2	1:E:273:THR:CG2	2.36	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:B:614:GLY:HA2	1:B:767:ALA:HB2	1.86	0.56
1:E:375:LEU:HD13	1:E:399:GLU:HA	1.87	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
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
2:C:151:PHE:O	2:C:158:ARG:NH1	2.40	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:G:48:ARG:NH2	2:G:52:LYS:HG3	2.21	0.55
2:H:48:ARG:CZ	2:H:52:LYS:HG3	2.37	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
1:F:640:VAL:HG12	1:F:641:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:151:PHE:O	2:K:158:ARG:NH1	2.39	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
1:B:755:THR:HG21	2:D:135:LYS:HD3	1.88	0.55
2:G:48:ARG:CZ	2:G:52:LYS:HG3	2.37	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:E:588:VAL:O	1:E:592:LEU:HB2	2.08	0.54
1:I:640:VAL:HG12	1:I:641:PRO:HD2	1.89	0.54
1:A:614:GLY:HA2	1:A:767:ALA:HB2	1.90	0.54
1:E:269:MET:HE3	1:E:653:ILE:O	2.08	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:A:491:ARG:HB3	1:A:491:ARG:CZ	2.37	0.53
1:A:630:ILE:HG23	1:A:640:VAL:HG11	1.91	0.53
1:E:694:GLU:OE1	1:F:697:ARG:NH1	2.41	0.53
1:A:621:SER:N	3:A:1801:ANP:O1A	2.42	0.53
1:B:588:VAL:O	1:B:592:LEU:HB2	2.09	0.53
1:A:700:SER:HB2	1:B:770:SER:HB3	1.90	0.53
1:E:615:PRO:HB3	1:E:771:TYR:CD1	2.44	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:A:137:TRP:CZ2	1:A:235:SER:HB2	2.44	0.53
1:B:630:ILE:HG23	1:B:640:VAL:HG11	1.91	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:G:63:ILE:HG23	2:G:67:GLU:HB2	1.91	0.52
1:J:137:TRP:CZ2	1:J:235:SER:HB2	2.44	0.52
2:L:299:VAL:HA	2:L:315:SER:OG	2.10	0.52
2:D:271:ALA:HB2	2:D:319:HIS:CD2	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLN:HG2	1:B:470:VAL:HG21	1.92	0.52
1:E:658:GLY:O	1:F:659:ALA:CB	2.58	0.52
1:F:137:TRP:CZ2	1:F:235:SER:HB2	2.45	0.52
1:E:670:PHE:CD2	1:F:616:ASN:OD1	2.63	0.52
1:I:670:PHE:N	3:J:1801:ANP:O1G	2.43	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:A:746:HIS:CE1	1:A:763:GLN:HB2	2.45	0.52
1:J:588:VAL:O	1:J:592:LEU:HB2	2.10	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:271:ALA:HB2	2:L:319:HIS:CD2	2.46	0.51
2:L:63:ILE:HG23	2:L:67:GLU:HB2	1.93	0.51
1:E:268:ILE:HG23	1:E:269:MET:N	2.25	0.51
1:F:224:GLY:O	1:F:679:ASN:HA	2.11	0.51
2:H:23:PRO:HD3	2:H:161:LEU:HD11	1.92	0.51
1:E:771:TYR:N	1:F:699:THR:OG1	2.43	0.51
2:H:160:PHE:CE2	2:L:162:ARG:HD3	2.45	0.51
2:D:163:THR:OG1	2:D:166:THR:CG2	2.59	0.51
1:E:269:MET:CE	1:E:273:THR:HG21	2.41	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:E:746:HIS:CE1	1:E:763:GLN:HB2	2.47	0.50
1:F:630:ILE:HG23	1:F:640:VAL:HG11	1.93	0.50
1:I:519:LYS:HE3	1:J:470:VAL:O	2.11	0.50
1:I:588:VAL:O	1:I:592:LEU:HB2	2.12	0.50
1:I:702:TYR:CB	1:J:793:LEU:CD1	2.86	0.50
1:J:588:VAL:HA	1:J:591:VAL:HG12	1.94	0.50
1:J:617:MET:CE	1:J:775:VAL:HG13	2.41	0.50
2:L:105:VAL:HG12	2:L:151:PHE:HA	1.94	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:HE2	1:F:671:MET:HB2	1.94	0.50
1:E:617:MET:CE	1:F:671:MET:HB2	2.42	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:A:671:MET:CE	1:B:778:LEU:HD23	2.42	0.49
1:E:224:GLY:O	1:E:679:ASN:HA	2.13	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: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
2:G:105:VAL:HG12	2:G:151:PHE:HA	1.96	0.48
1:I:224:GLY:O	1:I:679:ASN:HA	2.12	0.48
1:B:268:ILE:HG13	1:B:268:ILE:O	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:A:276:ASN:HA	1:A:283:LEU:HD21	1.94	0.48
1:E:267:ILE:HD12	1:E:316:ARG:CD	2.07	0.48
1:J:746:HIS:CE1	1:J:763:GLN:HB2	2.48	0.48
2:H:90:ILE:HG23	2:L:266:ARG:HD3	1.95	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:A:784:GLU:HG2	1:B:718:LYS:HZ1	1.77	0.48
1:E:694:GLU:OE1	1:F:697:ARG:CZ	2.62	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
1:A:659:ALA:HB3	1:B:659:ALA:HB3	1.96	0.48
2:C:113:ARG:CG	2:C:118:GLN:OE1	2.41	0.48
2:D:163:THR:OG1	2:D:166:THR:CB	2.62	0.48
1:I:267:ILE:C	1:I:268:ILE:HG13	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:ARG:HB2	2:D:316:ARG:NH1	2.29	0.47
2:D:63:ILE:HG23	2:D:67:GLU:HB2	1.96	0.47
2:D:65:LYS:HB3	2:D:121:TRP:CD1	2.49	0.47
1:F:491:ARG:HB3	1:F:491:ARG:CZ	2.44	0.47
1:J:615:PRO:HB3	1:J:771:TYR:CD1	2.49	0.47
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:E:616:ASN:HD22	3:E:1801:ANP:HNB1	1.60	0.47
2:G:107:ARG:NH2	2:G:148:LEU:HD13	2.29	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
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
1:B:588:VAL:HA	1:B:591:VAL:HG12	1.97	0.47
2:G:83:LEU:HD22	2:G:90:ILE:HD11	1.95	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:502:ILE:HD12	1:A:506:LEU:HD23	1.97	0.47
1:A:588:VAL:HA	1:A:591:VAL:HG12	1.97	0.47
1:F:584:ARG:NE	1:F:589:GLU:OE1	2.47	0.47
1:F:153:GLY:HA2	1:F:255:ILE:HG12	1.97	0.47
1:I:267:ILE:CD1	1:I:316:ARG:HG3	2.43	0.47
2:G:106:SER:HB3	2:G:150:LEU:CD2	2.35	0.47
2:D:88:ALA:HB2	2:G:316:ARG:NH1	2.30	0.46
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: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:A:584:ARG:NE	1:A:589:GLU:OE1	2.47	0.46
1:E:333:ASP:CG	2:G:210:ARG:HH12	2.18	0.46
1:A:224:GLY:O	1:A:679:ASN:HA	2.16	0.46
3:E:1801:ANP:O1G	1:F:670:PHE:N	2.49	0.46
1:E:658:GLY:O	1:F:659:ALA:HB1	2.16	0.46
2:G:23:PRO:HD3	2:G:161:LEU:HD11	1.98	0.46
2:K:106:SER:HB3	2:K:150:LEU:CD2	2.37	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
1:I:771:TYR:N	1:J:699:THR:OG1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:ILE:HG21	1:B:368:MET:CE	2.46	0.46
2:C:113:ARG:HA	2:C:118:GLN:HE22	1.81	0.46
1:E:266:SER:O	1:E:267:ILE:HB	2.16	0.46
1:B:502:ILE:HD12	1:B:506:LEU:HD23	1.97	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:J:425:ILE:HG13	1:J:524:GLU:HG3	1.98	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:266:SER:O	1:I:267:ILE:HB	2.15	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
2:C:270:HIS:CD2	2:C:319:HIS:CE1	3.05	0.45
1:E:773:LEU:HD13	1:E:790:ARG:HG2	1.98	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: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
1:A:674:MET:CB	1:B:779:ALA:CB	2.95	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
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
2:H:83:LEU:HD13	2:H:90:ILE:CD1	2.46	0.45
1:I:470:VAL:HG21	1:J:526:GLN:HG2	1.99	0.45
1:F:402:GLU:HG3	1:F:403:LEU:N	2.31	0.44
1:I:502:ILE:HD12	1:I:506:LEU:HD23	1.99	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:B:584:ARG:NE	1:B:589:GLU:OE1	2.49	0.44
1:J:267:ILE:HG23	1:J:316:ARG:HD2	2.00	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
1:J:153:GLY:HA2	1:J:255:ILE:HG12	2.00	0.43
2:L:65:LYS:HB3	2:L:121:TRP:CD1	2.52	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:B:313:MET:HG2	1:B:313:MET:O	2.19	0.43
1:E:675:THR:HG23	1:F:779:ALA:O	2.17	0.43
2:H:65:LYS:HB3	2:H:121:TRP:CD1	2.54	0.43
1:E:473:TYR:O	1:E:492:ARG:NH1	2.52	0.43
1:F:752:HIS:CD2	1:F:755:THR:HG23	2.54	0.43
1:I:155:PHE:CE2	1:I:258:ILE:HD12	2.54	0.43
1:I:619:GLY:HA2	3:I:1801:ANP:C8	2.49	0.43
2:L:202:VAL:HG12	2:L:203:PRO:O	2.19	0.43
1:A:674:MET:HB2	1:B:779:ALA:HB2	2.00	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
2:K:280:LEU:HD13	2:K:282:ALA:HB3	2.01	0.43
2:C:51:ALA:O	2:C:149:ASP:CA	2.67	0.42
2:C:65:LYS:HB3	2:C:121:TRP:CD1	2.54	0.42
2:D:150:LEU:HD12	2:D:150:LEU:HA	1.37	0.42
1:J:502:ILE:HD12	1:J:506:LEU:HD23	2.01	0.42
1:E:699:THR:HA	1:F:728:HIS:CG	2.54	0.42
2:H:117:GLN:HG2	2:H:117:GLN:O	2.19	0.42
1:I:267:ILE:CD1	1:I:314:PRO:O	2.45	0.42
1:A:160:PRO:HA	1:A:263:GLU:OE2	2.19	0.42
1:A:714:ASN:HA	1:A:718:LYS:HD3	2.00	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:752:HIS:CD2	1:J:755:THR:HG23	2.54	0.42
1:J:584:ARG:NE	1:J:589:GLU:OE1	2.53	0.42
2:C:280:LEU:HD13	2:C:282:ALA:HB3	2.01	0.42
1:J:267:ILE:HG22	1:J:651:ASP:O	2.20	0.42
1:E:425:ILE:HG13	1:E:524:GLU:HG3	2.01	0.42
1:E:269:MET:HE1	1:E:653:ILE:HB	2.01	0.42
1:J:160:PRO:HA	1:J:263:GLU:OE2	2.20	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
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)
2:C:63:ILE:CG2	2:C:67:GLU:HB2	2.49	0.42
1:E:276:ASN:HA	1:E:283:LEU:HD21	2.00	0.42
1:E:351:ILE:HG21	1:E:368:MET:CE	2.50	0.42
1:I:622:THR:HB	3:I:1801:ANP:N7	2.34	0.42
1:E:269:MET:HE1	1:E:653:ILE:CG2	2.49	0.42
1:F:473:TYR:O	1:F:492:ARG:NH1	2.53	0.42
2:L:51:ALA:HB1	2:L:149:ASP:OD2	2.20	0.42
1:A:153:GLY:HA2	1:A:255:ILE:HG12	2.01	0.41
1:A:425:ILE:HG13	1:A:524:GLU:HG3	2.02	0.41
1:B:155:PHE:CE2	1:B:258:ILE:HD12	2.55	0.41
2:D:162:ARG:HB3	2:D:163:THR:H	1.71	0.41
2:D:160:PHE:CE1	2:G:160:PHE:HB3	2.55	0.41
2:C:51:ALA:HB1	2:C:149:ASP:OD2	2.21	0.41
2:D:280:LEU:HD13	2:D:282:ALA:HB3	2.02	0.41
2:H:271:ALA:HB2	2:H:319:HIS:ND1	2.34	0.41
2:K:64:LYS:HG2	2:K:114:THR:HG21	2.03	0.41
1:A:155:PHE:CE2	1:A:258:ILE:HD12	2.56	0.41
1:A:473:TYR:O	1:A:492:ARG:NH1	2.52	0.41
1:B:425:ILE:HG13	1:B:524:GLU:HG3	2.02	0.41
1:E:269:MET:SD	1:E:653:ILE:HD12	2.61	0.41
1:A:502:ILE:CD1	1:A:506:LEU:HD23	2.51	0.41
1:B:491:ARG:HB3	1:B:491:ARG:CZ	2.50	0.41
2:G:202:VAL:HG12	2:G:203:PRO:O	2.20	0.41
1:J:155:PHE:CE2	1:J:258:ILE:HD12	2.54	0.41
2:L:51:ALA:O	2:L:149:ASP:CA	2.68	0.41
2:L:164:GLU:CG	2:L:165:LYS:N	2.84	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
1:B:585:HIS:CE1	1:B:629:LEU:CD1	3.03	0.41
1:E:502:ILE:HD12	1:E:506:LEU:HD23	2.01	0.41
2:G:83:LEU:HD13	2:G:90:ILE:HD12	2.01	0.41
1:J:654:PHE:HB3	1:J:680:ILE:HG12	2.03	0.41
1:E:160:PRO:HA	1:E:263:GLU:OE2	2.21	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:F:752:HIS:CD2	2:H:136:PRO:HG2	2.56	0.41
2:H:156:ALA:HB1	2:H:160:PHE:CZ	2.56	0.41
1:A:267:ILE:HG22	1:A:651:ASP:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:PRO:HA	1:F:263:GLU:OE2	2.21	0.41
1:I:473:TYR:O	1:I:492:ARG:NH1	2.54	0.41
1:B:502:ILE:CD1	1:B:506:LEU:HD23	2.51	0.40
1:I:352:LEU:HD13	1:I:543:GLN:HA	2.03	0.40
1:I:616:ASN:ND2	1:J:670:PHE:CD2	2.89	0.40
1:B:491:ARG:HB3	1:B:491:ARG:NH1	2.36	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:A:784:GLU:OE2	1:B:718:LYS:NZ	2.54	0.40
1:E:659:ALA:HB3	1:F:659:ALA:CB	2.45	0.40
1:F:596:PHE:HA	3:F:1801:ANP:H2	2.03	0.40
2:H:280:LEU:HD13	2:H:282:ALA:HB3	2.02	0.40
1:E:207:ASP:HB2	2:H:52:LYS:HE2	2.03	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
2:C:202:VAL:HG12	2:C:203:PRO:O	2.21	0.40
2:D:316:ARG:HH21	2:G:88:ALA:CB	2.34	0.40
1:F:155:PHE:CE2	1:F:258:ILE:HD12	2.55	0.40
1:I:267:ILE:CG2	1:I:268:ILE:N	2.82	0.40
1:E:220:ARG:CD	1:F:778:LEU:HD11	2.51	0.40
2:H:70:LEU:HD22	2:H:86:LEU:HD22	2.03	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%)	29	69
1	F	659/800 (82%)	634 (96%)	23 (4%)	2 (0%)	41	77
1	I	659/800 (82%)	635 (96%)	22 (3%)	2 (0%)	41	77
1	J	659/800 (82%)	639 (97%)	18 (3%)	2 (0%)	41	77
2	C	277/369 (75%)	258 (93%)	15 (5%)	4 (1%)	11	46
2	D	277/369 (75%)	260 (94%)	13 (5%)	4 (1%)	11	46
2	G	277/369 (75%)	261 (94%)	13 (5%)	3 (1%)	14	52
2	H	277/369 (75%)	260 (94%)	13 (5%)	4 (1%)	11	46
2	K	277/369 (75%)	262 (95%)	11 (4%)	4 (1%)	11	46
2	L	277/369 (75%)	261 (94%)	12 (4%)	4 (1%)	11	46
All	All	5616/7014 (80%)	5376 (96%)	208 (4%)	32 (1%)	25	66

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%)	55	74
1	B	550/662 (83%)	541 (98%)	9 (2%)	62	79
1	E	550/662 (83%)	539 (98%)	11 (2%)	55	74
1	F	550/662 (83%)	541 (98%)	9 (2%)	62	79
1	I	550/662 (83%)	538 (98%)	12 (2%)	52	71
1	J	550/662 (83%)	541 (98%)	9 (2%)	62	79
2	C	235/308 (76%)	228 (97%)	7 (3%)	41	63
2	D	235/308 (76%)	225 (96%)	10 (4%)	29	53
2	G	235/308 (76%)	227 (97%)	8 (3%)	37	60
2	H	235/308 (76%)	223 (95%)	12 (5%)	24	48
2	K	235/308 (76%)	227 (97%)	8 (3%)	37	60
2	L	235/308 (76%)	224 (95%)	11 (5%)	26	51
All	All	4710/5820 (81%)	4593 (98%)	117 (2%)	47	68

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	J	1801	-	29,33,33	1.88	9 (31%)	31,52,52	1.87	7 (22%)
3	ANP	F	1801	-	29,33,33	1.75	9 (31%)	31,52,52	2.06	10 (32%)
3	ANP	E	1801	-	29,33,33	1.96	10 (34%)	31,52,52	2.09	8 (25%)
3	ANP	A	1801	-	29,33,33	1.99	7 (24%)	31,52,52	2.03	8 (25%)
3	ANP	I	1801	-	29,33,33	1.85	8 (27%)	31,52,52	1.83	7 (22%)
3	ANP	B	1801	-	29,33,33	1.80	7 (24%)	31,52,52	2.10	9 (29%)

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	J	1801	-	-	2/14/38/38	0/3/3/3
3	ANP	F	1801	-	-	5/14/38/38	0/3/3/3
3	ANP	E	1801	-	-	7/14/38/38	0/3/3/3
3	ANP	A	1801	-	-	5/14/38/38	0/3/3/3
3	ANP	I	1801	-	-	3/14/38/38	0/3/3/3
3	ANP	B	1801	-	-	8/14/38/38	0/3/3/3

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1801	ANP	PG-N3B	4.96	1.76	1.63
3	A	1801	ANP	PG-N3B	4.86	1.76	1.63
3	A	1801	ANP	PB-N3B	4.74	1.75	1.63
3	J	1801	ANP	PB-N3B	4.42	1.74	1.63
3	I	1801	ANP	PB-N3B	4.28	1.74	1.63
3	E	1801	ANP	PG-N3B	4.22	1.74	1.63
3	F	1801	ANP	PG-N3B	4.20	1.74	1.63
3	B	1801	ANP	PB-N3B	4.05	1.73	1.63
3	E	1801	ANP	PB-N3B	3.98	1.73	1.63
3	F	1801	ANP	PB-N3B	3.81	1.73	1.63
3	B	1801	ANP	PB-O1B	3.66	1.52	1.46
3	A	1801	ANP	PG-O3G	-3.58	1.47	1.56
3	I	1801	ANP	PG-N3B	3.56	1.72	1.63
3	I	1801	ANP	PG-O2G	-3.49	1.47	1.56
3	E	1801	ANP	PG-O2G	-3.29	1.47	1.56
3	I	1801	ANP	PG-O3G	-3.16	1.48	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1801	ANP	PB-O2B	-3.09	1.48	1.56
3	E	1801	ANP	C2-N3	3.09	1.37	1.32
3	A	1801	ANP	C5-C4	3.08	1.49	1.40
3	E	1801	ANP	C5-C4	3.00	1.48	1.40
3	E	1801	ANP	PB-O2B	-2.99	1.48	1.56
3	B	1801	ANP	PG-O3G	-2.87	1.49	1.56
3	I	1801	ANP	PB-O2B	-2.81	1.49	1.56
3	I	1801	ANP	C5-C4	2.78	1.48	1.40
3	B	1801	ANP	PG-N3B	2.78	1.70	1.63
3	J	1801	ANP	C5-C4	2.78	1.48	1.40
3	A	1801	ANP	PB-O2B	-2.77	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	-2.70	1.49	1.56
3	B	1801	ANP	C5-C4	2.61	1.47	1.40
3	J	1801	ANP	PG-O2G	-2.60	1.49	1.56
3	I	1801	ANP	C2-N3	2.60	1.36	1.32
3	F	1801	ANP	C2'-C1'	-2.54	1.49	1.53
3	F	1801	ANP	PG-O2G	-2.49	1.50	1.56
3	F	1801	ANP	PG-O3G	-2.47	1.50	1.56
3	F	1801	ANP	C5-C4	2.39	1.47	1.40
3	B	1801	ANP	PG-O2G	-2.38	1.50	1.56
3	E	1801	ANP	PG-O3G	-2.36	1.50	1.56
3	E	1801	ANP	PB-O1B	2.25	1.49	1.46
3	I	1801	ANP	PG-O1G	2.25	1.49	1.46
3	A	1801	ANP	O4'-C1'	2.23	1.44	1.41
3	F	1801	ANP	PB-O1B	2.17	1.49	1.46
3	J	1801	ANP	O3'-C3'	2.13	1.48	1.43
3	F	1801	ANP	PG-O1G	2.12	1.49	1.46
3	F	1801	ANP	PB-O2B	-2.09	1.51	1.56
3	E	1801	ANP	O4'-C1'	2.06	1.44	1.41
3	J	1801	ANP	PB-O1B	2.05	1.49	1.46
3	J	1801	ANP	O4'-C1'	2.05	1.43	1.41
3	E	1801	ANP	C4-N3	2.01	1.38	1.35

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1801	ANP	O1G-PG-N3B	-6.82	101.73	111.77
3	F	1801	ANP	O1G-PG-N3B	-6.64	101.99	111.77
3	J	1801	ANP	O1G-PG-N3B	-5.55	103.59	111.77
3	E	1801	ANP	O1G-PG-N3B	-5.23	104.07	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1801	ANP	C3'-C2'-C1'	5.03	108.55	100.98
3	A	1801	ANP	O1G-PG-N3B	-4.99	104.42	111.77
3	I	1801	ANP	O1G-PG-N3B	-4.40	105.29	111.77
3	A	1801	ANP	C3'-C2'-C1'	4.18	107.28	100.98
3	A	1801	ANP	N3-C2-N1	-4.12	122.24	128.68
3	B	1801	ANP	C3'-C2'-C1'	4.01	107.01	100.98
3	E	1801	ANP	C4-C5-N7	-3.90	105.34	109.40
3	F	1801	ANP	PA-O3A-PB	-3.88	118.96	132.62
3	I	1801	ANP	PA-O3A-PB	-3.83	119.12	132.62
3	F	1801	ANP	O2B-PB-O1B	3.78	117.85	109.92
3	I	1801	ANP	O2B-PB-O1B	3.76	117.81	109.92
3	E	1801	ANP	PA-O3A-PB	-3.69	119.62	132.62
3	A	1801	ANP	O2B-PB-O1B	3.55	117.36	109.92
3	I	1801	ANP	C3'-C2'-C1'	3.44	106.15	100.98
3	J	1801	ANP	C3'-C2'-C1'	3.32	105.98	100.98
3	J	1801	ANP	O2B-PB-O1B	3.30	116.85	109.92
3	B	1801	ANP	PA-O3A-PB	-3.30	120.99	132.62
3	J	1801	ANP	N3-C2-N1	-3.25	123.61	128.68
3	A	1801	ANP	PA-O3A-PB	-3.22	121.29	132.62
3	E	1801	ANP	N3-C2-N1	-3.12	123.81	128.68
3	I	1801	ANP	N3-C2-N1	-3.04	123.92	128.68
3	B	1801	ANP	N3-C2-N1	-3.03	123.94	128.68
3	B	1801	ANP	C4-C5-N7	-3.03	106.24	109.40
3	J	1801	ANP	C4-C5-N7	-2.86	106.42	109.40
3	F	1801	ANP	N3-C2-N1	-2.86	124.21	128.68
3	B	1801	ANP	O3G-PG-O2G	2.85	115.24	107.64
3	I	1801	ANP	C4-C5-N7	-2.85	106.43	109.40
3	E	1801	ANP	O2B-PB-O1B	2.83	115.84	109.92
3	B	1801	ANP	O2B-PB-O1B	2.81	115.81	109.92
3	A	1801	ANP	N6-C6-N1	2.71	124.19	118.57
3	A	1801	ANP	O5'-C5'-C4'	2.66	118.16	108.99
3	J	1801	ANP	PA-O3A-PB	-2.58	123.53	132.62
3	J	1801	ANP	O3G-PG-O2G	2.58	114.50	107.64
3	E	1801	ANP	O3G-PG-O2G	2.52	114.34	107.64
3	A	1801	ANP	C2-N1-C6	2.49	123.01	118.75
3	F	1801	ANP	C2'-C3'-C4'	2.47	107.43	102.64
3	E	1801	ANP	C1'-N9-C4	2.42	130.89	126.64
3	F	1801	ANP	O3G-PG-O2G	2.40	114.04	107.64
3	B	1801	ANP	O4'-C4'-C3'	2.26	109.58	105.11
3	B	1801	ANP	O5'-C5'-C4'	2.18	116.51	108.99
3	F	1801	ANP	N6-C6-N1	2.11	122.96	118.57
3	F	1801	ANP	C2-N1-C6	2.05	122.27	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1801	ANP	O3G-PG-O1G	2.02	118.53	113.45
3	F	1801	ANP	C4-C5-N7	-2.02	107.29	109.40
3	F	1801	ANP	O4'-C1'-C2'	2.00	109.85	106.93

There are no chirality outliers.

All (30) torsion outliers are listed below:

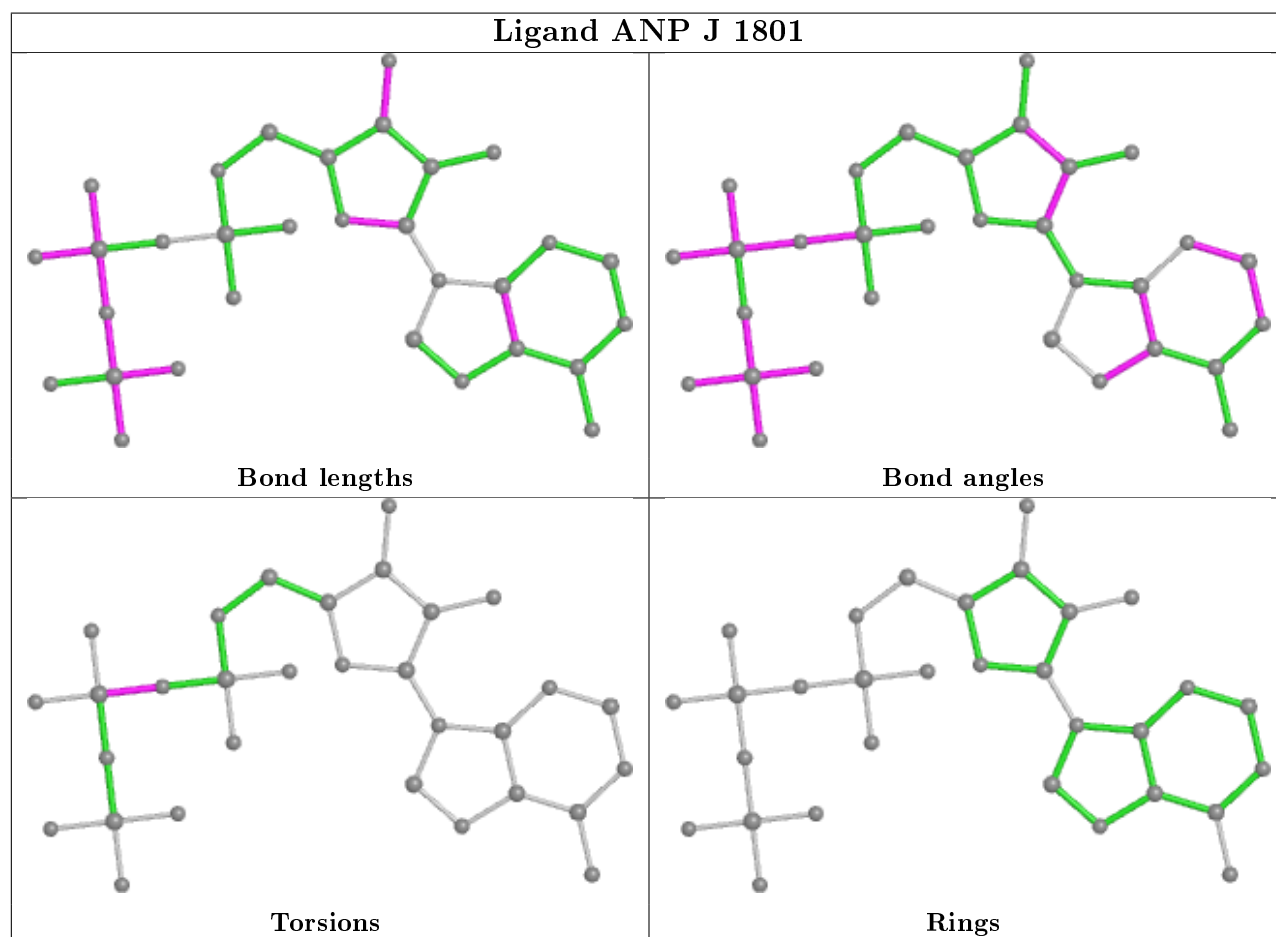
Mol	Chain	Res	Type	Atoms
3	J	1801	ANP	PA-O3A-PB-O1B
3	J	1801	ANP	PA-O3A-PB-O2B
3	F	1801	ANP	PG-N3B-PB-O1B
3	F	1801	ANP	PA-O3A-PB-O1B
3	F	1801	ANP	PA-O3A-PB-O2B
3	E	1801	ANP	PG-N3B-PB-O1B
3	E	1801	ANP	PA-O3A-PB-O1B
3	E	1801	ANP	PA-O3A-PB-O2B
3	E	1801	ANP	C5'-O5'-PA-O3A
3	E	1801	ANP	O4'-C4'-C5'-O5'
3	E	1801	ANP	C3'-C4'-C5'-O5'
3	A	1801	ANP	PA-O3A-PB-O1B
3	A	1801	ANP	PA-O3A-PB-O2B
3	A	1801	ANP	C5'-O5'-PA-O1A
3	A	1801	ANP	C5'-O5'-PA-O2A
3	A	1801	ANP	C5'-O5'-PA-O3A
3	I	1801	ANP	PB-N3B-PG-O1G
3	I	1801	ANP	PA-O3A-PB-O1B
3	I	1801	ANP	PA-O3A-PB-O2B
3	B	1801	ANP	PG-N3B-PB-O1B
3	B	1801	ANP	PA-O3A-PB-O1B
3	B	1801	ANP	PA-O3A-PB-O2B
3	B	1801	ANP	C5'-O5'-PA-O3A
3	B	1801	ANP	O4'-C4'-C5'-O5'
3	B	1801	ANP	C3'-C4'-C5'-O5'
3	E	1801	ANP	C5'-O5'-PA-O1A
3	B	1801	ANP	C5'-O5'-PA-O1A
3	B	1801	ANP	C5'-O5'-PA-O2A
3	F	1801	ANP	O4'-C4'-C5'-O5'
3	F	1801	ANP	C3'-C4'-C5'-O5'

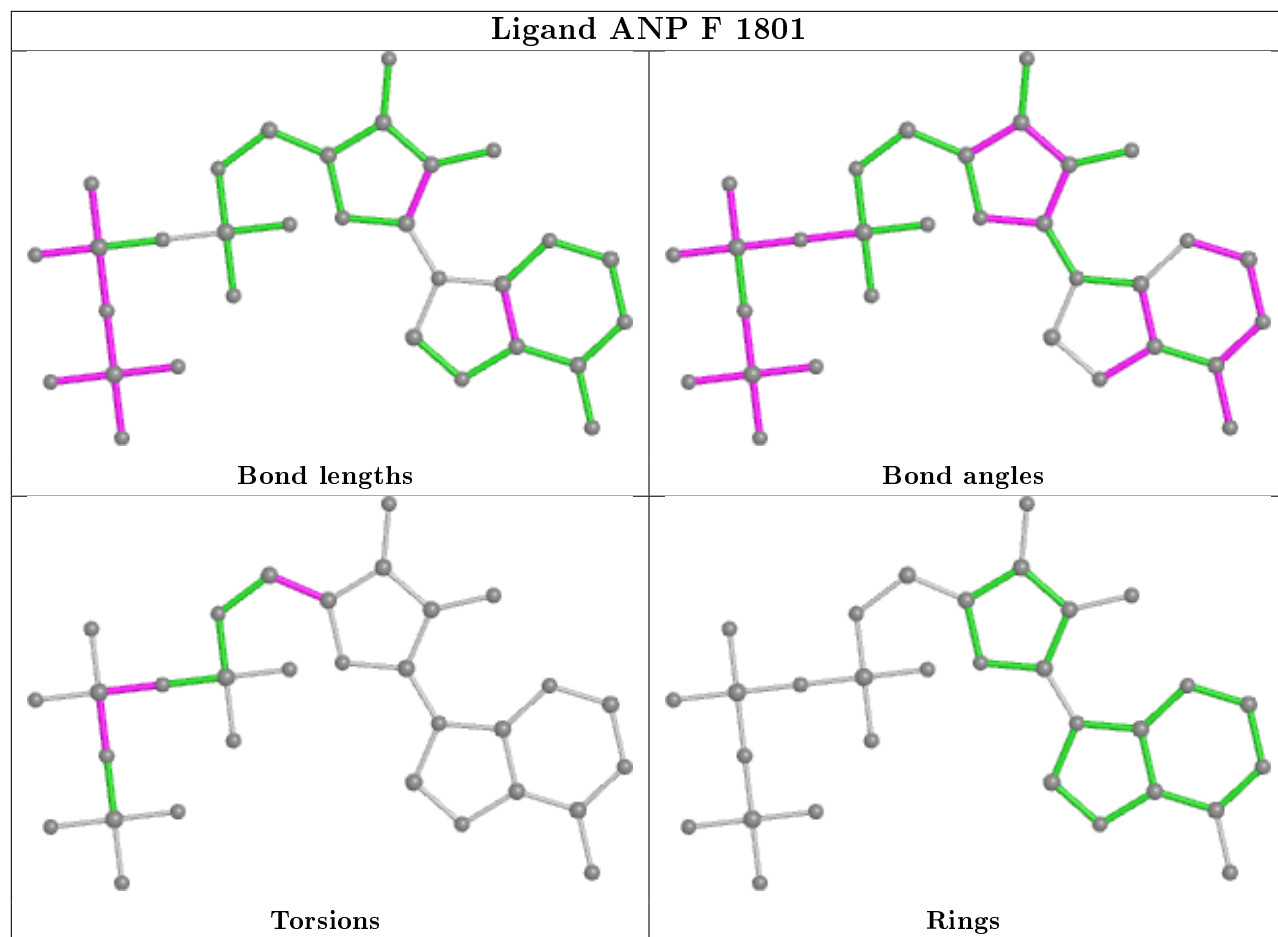
There are no ring outliers.

6 monomers are involved in 22 short contacts:

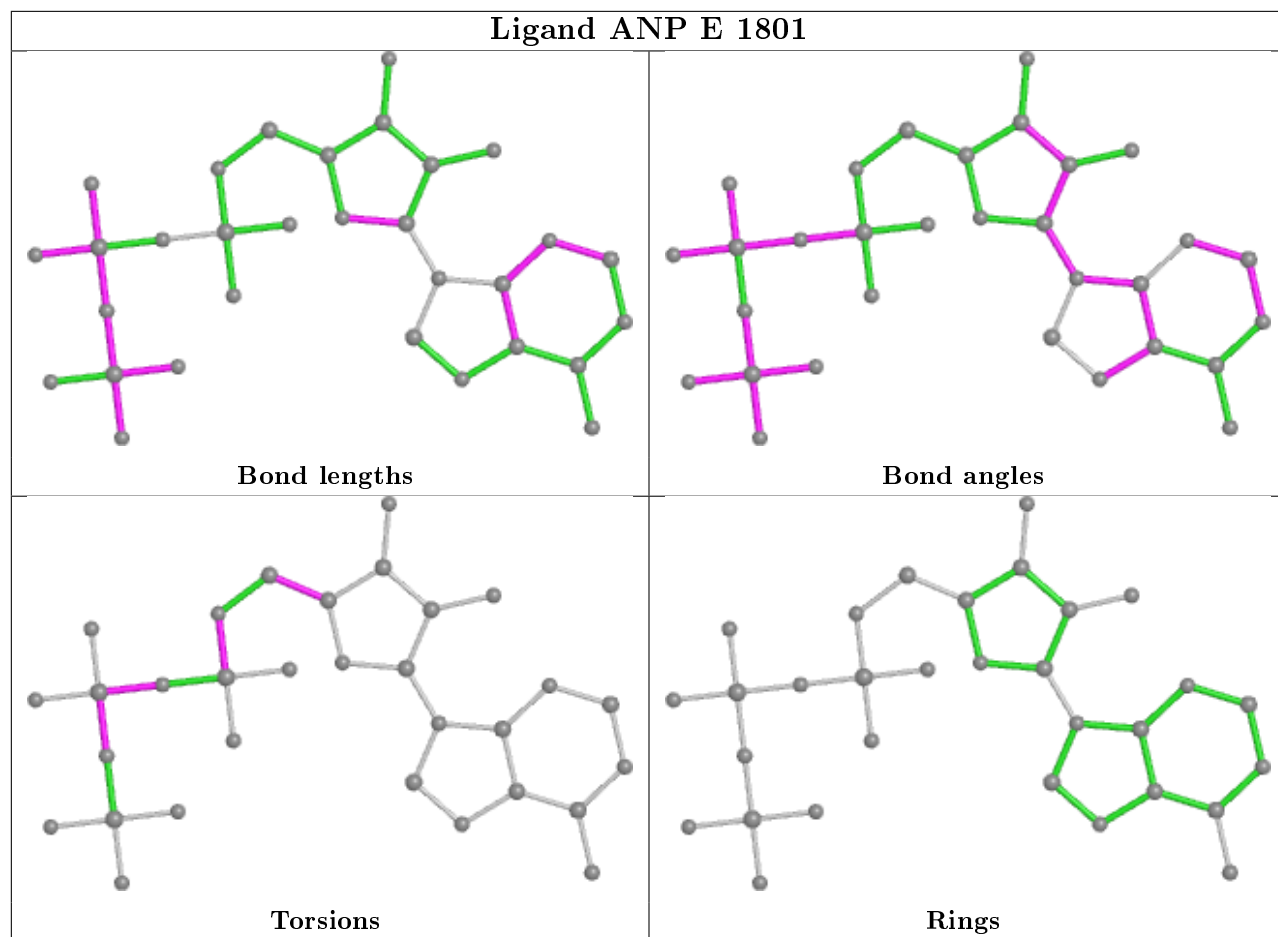
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1801	ANP	2	0
3	F	1801	ANP	3	0
3	E	1801	ANP	2	0
3	A	1801	ANP	5	0
3	I	1801	ANP	6	0
3	B	1801	ANP	4	0

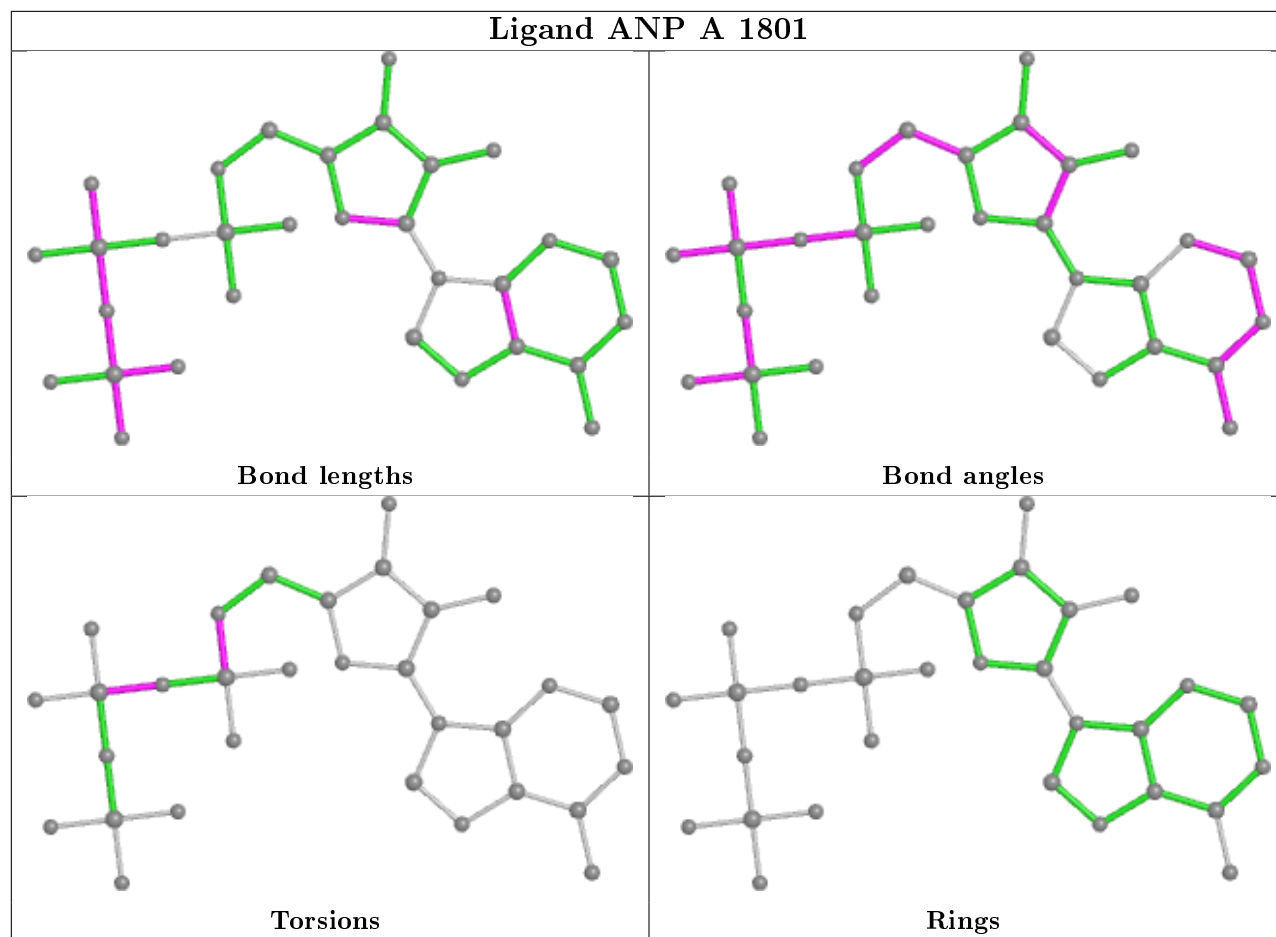
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

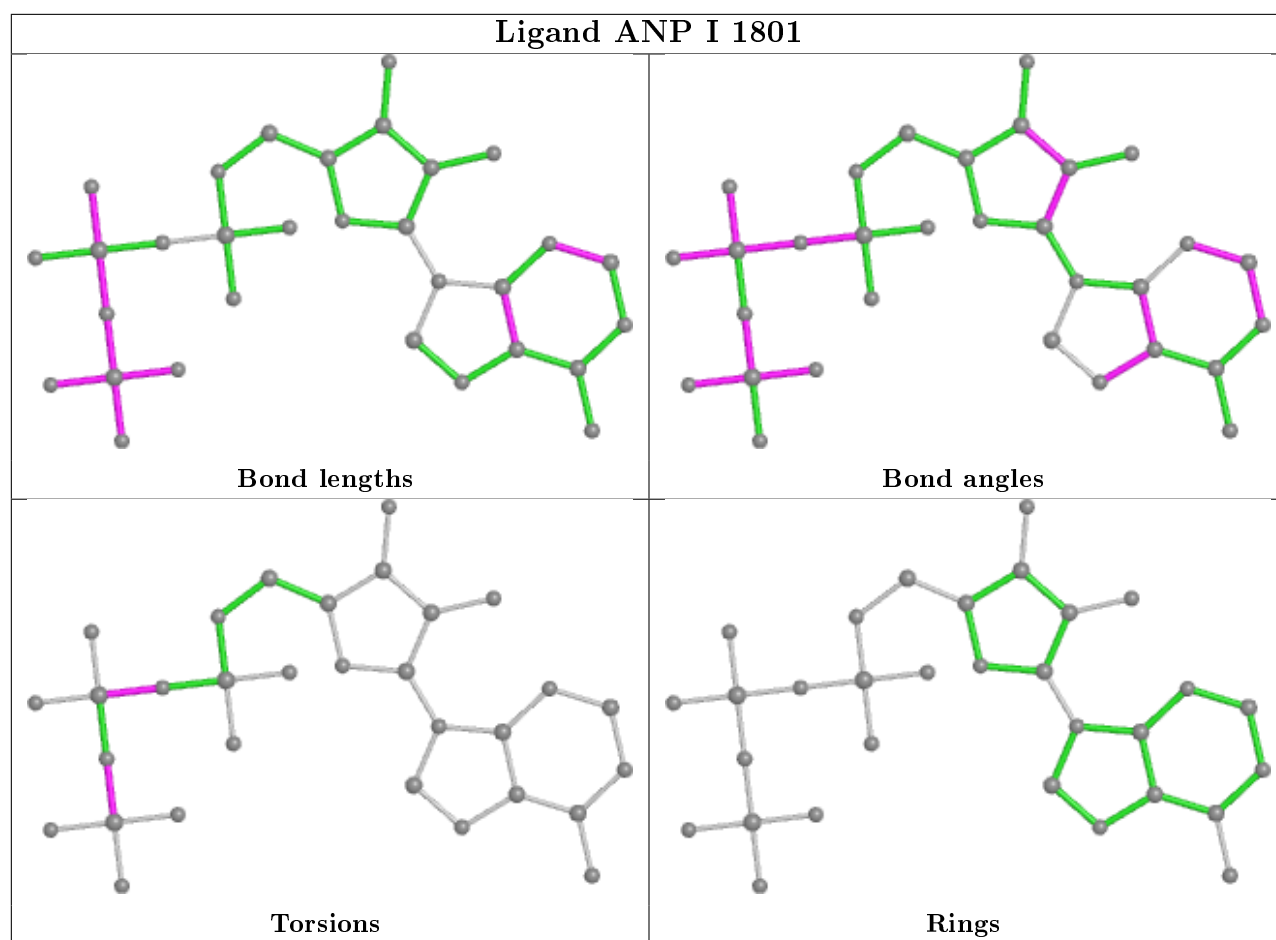


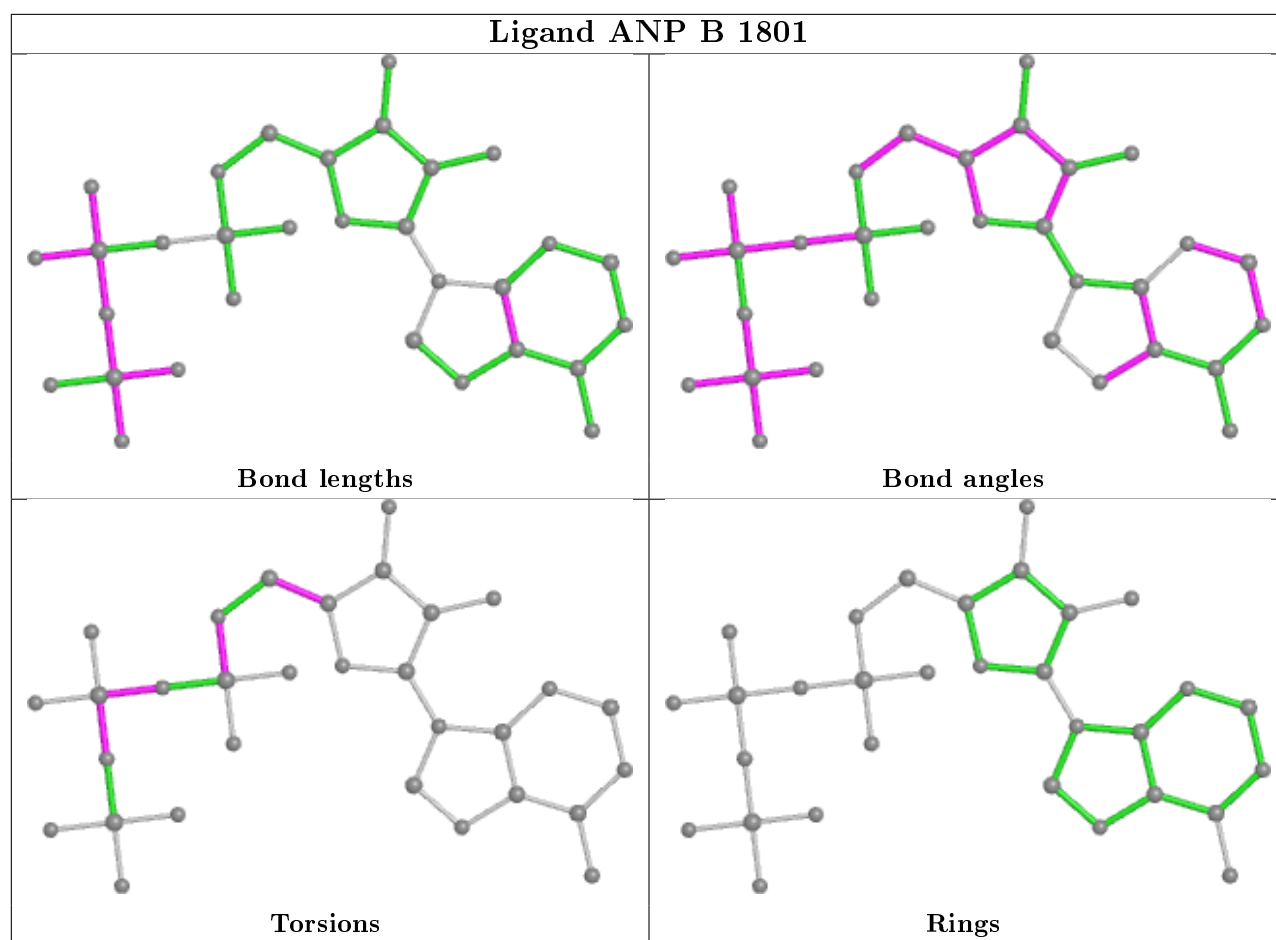












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	663/800 (82%)	2.23	315 (47%) 0 1	120, 187, 361, 469	0
1	B	663/800 (82%)	2.06	289 (43%) 0 1	125, 203, 272, 321	0
1	E	663/800 (82%)	2.67	343 (51%) 0 1	170, 262, 510, 665	0
1	F	663/800 (82%)	2.01	276 (41%) 0 1	127, 197, 351, 463	0
1	I	663/800 (82%)	2.38	325 (49%) 0 1	174, 224, 402, 487	0
1	J	663/800 (82%)	2.73	363 (54%) 0 1	172, 231, 378, 460	0
2	C	285/369 (77%)	2.04	136 (47%) 0 1	178, 213, 254, 293	0
2	D	285/369 (77%)	2.37	144 (50%) 0 1	170, 201, 273, 306	0
2	G	285/369 (77%)	2.38	155 (54%) 0 1	204, 224, 251, 265	0
2	H	285/369 (77%)	2.60	159 (55%) 0 1	154, 218, 301, 389	0
2	K	285/369 (77%)	2.12	130 (45%) 0 1	185, 220, 264, 283	0
2	L	285/369 (77%)	2.31	139 (48%) 0 1	210, 231, 253, 269	0
All	All	5688/7014 (81%)	2.33	2774 (48%) 0 1	120, 220, 361, 665	0

All (2774) 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	14.7
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	723	THR	12.5
2	H	90	ILE	12.2
1	I	595	PRO	12.1
1	F	147	THR	12.1
1	J	758	PHE	11.7
1	J	146	ALA	11.7
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	J	135	ALA	10.7
1	B	608	ARG	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	J	577	GLY	9.7
1	I	465	VAL	9.7
1	A	462	THR	9.7
1	E	462	THR	9.7
1	A	256	ARG	9.7
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	F	480	GLY	9.4
1	B	609	MET	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	F	487	ILE	9.2
2	K	226	ALA	9.2
1	A	727	THR	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	F	135	ALA	8.9
1	I	485	ALA	8.9
1	E	725	PHE	8.9
1	B	690	VAL	8.9
1	J	486	PRO	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	J	723	THR	8.5
1	E	655	THR	8.5
1	E	610	LEU	8.5
2	L	138	ALA	8.5
1	E	423	GLY	8.5
1	J	175	PRO	8.5
2	L	81	ALA	8.4
1	E	502	ILE	8.4
2	H	67	GLU	8.3
1	A	613	THR	8.3
1	I	486	PRO	8.3
2	K	138	ALA	8.3
2	H	68	LEU	8.3
1	J	482	SER	8.3

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Mol	Chain	Res	Type	RSRZ
2	L	179	ALA	8.3
2	H	91	SER	8.3
2	H	69	ALA	8.3
1	A	463	LEU	8.2
2	H	82	SER	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	J	637	GLY	8.2
1	I	594	GLU	8.2
1	E	774	ALA	8.2
1	F	146	ALA	8.1
2	D	67	GLU	8.1
2	H	93	GLY	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	240	LEU	8.0
1	A	749	ALA	8.0
1	I	478	SER	8.0
1	I	658	GLY	8.0
1	F	257	SER	8.0
2	G	24	ALA	8.0
1	E	488	ASN	8.0
1	J	133	LEU	7.9
1	A	461	ASP	7.9
2	H	122	GLN	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
1	E	781	VAL	7.7
2	H	81	ALA	7.7
1	B	749	ALA	7.7

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Mol	Chain	Res	Type	RSRZ
1	I	757	ALA	7.7
1	I	477	ILE	7.7
1	A	729	TYR	7.7
2	K	238	GLY	7.7
1	A	602	ASN	7.7
1	J	489	TYR	7.7
1	I	602	ASN	7.6
1	J	485	ALA	7.6
1	A	723	THR	7.6
1	E	226	GLY	7.6
1	E	489	TYR	7.6
1	J	775	VAL	7.6
1	J	776	ALA	7.5
1	E	179	LEU	7.5
1	J	780	GLY	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
1	E	227	VAL	7.4
2	C	181	ALA	7.4
1	F	242	GLN	7.4
1	I	524	GLU	7.4
1	E	493	GLN	7.4
2	H	73	ALA	7.4
1	E	425	ILE	7.4
1	J	158	SER	7.4
1	B	695	ILE	7.4
1	J	631	ALA	7.4
1	I	593	ASN	7.4
2	L	85	ASP	7.3
1	E	759	MET	7.3
1	E	471	HIS	7.3
1	E	147	THR	7.3
2	L	21	GLU	7.3
1	E	696	GLY	7.3
1	J	478	SER	7.3
2	D	138	ALA	7.3
2	H	71	ALA	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	692	MET	7.3
1	I	729	TYR	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
2	C	69	ALA	7.2
1	E	477	ILE	7.2
2	H	72	LEU	7.2
1	B	656	ARG	7.2
1	E	136	ILE	7.2
2	H	134	VAL	7.1
1	J	605	PRO	7.1
1	B	725	PHE	7.1
2	K	227	ILE	7.1
1	E	228	GLU	7.1
2	D	279	LYS	7.1
1	E	492	ARG	7.1
1	F	524	GLU	7.1
1	F	237	ALA	7.0
1	I	656	ARG	7.0
2	L	284	GLN	7.0
1	A	133	LEU	7.0
1	I	475	ILE	7.0
2	K	283	ASP	7.0
1	A	726	ALA	7.0
1	J	771	TYR	7.0
2	C	179	ALA	7.0
1	J	193	ARG	7.0
1	E	748	ASP	7.0
1	E	609	MET	7.0
2	H	133	THR	7.0
1	J	450	LEU	7.0
1	A	696	GLY	7.0
1	E	133	LEU	6.9
1	E	490	MET	6.9
1	A	238	GLY	6.9
1	F	238	GLY	6.9
1	E	777	ALA	6.9
2	C	67	GLU	6.9
1	F	489	TYR	6.9
2	H	89	ILE	6.9

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Mol	Chain	Res	Type	RSRZ
1	B	776	ALA	6.9
1	A	748	ASP	6.9
1	A	761	SER	6.9
1	J	501	TYR	6.9
1	J	693	ASP	6.9
1	E	480	GLY	6.9
1	I	425	ILE	6.9
1	J	773	LEU	6.9
2	D	288	PHE	6.8
1	E	612	ILE	6.8
1	I	518	GLY	6.8
1	J	782	PRO	6.8
2	G	22	ARG	6.8
1	A	476	GLN	6.8
1	A	242	GLN	6.8
2	K	81	ALA	6.8
2	D	289	VAL	6.8
1	E	637	GLY	6.8
1	J	629	LEU	6.8
1	F	724	LEU	6.7
1	J	499	GLU	6.7
2	D	226	ALA	6.7
1	E	460	LEU	6.7
1	I	385	VAL	6.7
1	B	655	THR	6.7
2	L	23	PRO	6.7
1	J	722	LEU	6.7
2	L	182	ARG	6.7
1	J	219	THR	6.7
1	E	751	GLU	6.7
1	E	470	VAL	6.7
1	J	604	SER	6.7
1	A	693	ASP	6.6
1	A	609	MET	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
2	G	294	ILE	6.6

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	240	VAL	6.3
1	B	628	ALA	6.2
1	E	240	LEU	6.2
2	D	238	GLY	6.2
1	E	761	SER	6.2
1	F	691	LEU	6.2
1	E	237	ALA	6.2
1	I	261	GLU	6.2
1	A	219	THR	6.2
1	J	594	GLU	6.2
2	D	273	ARG	6.2
1	A	599	ASN	6.2
2	D	276	TYR	6.2
1	I	471	HIS	6.2
1	I	780	GLY	6.2
1	I	727	THR	6.2
1	I	519	LYS	6.2
1	F	465	VAL	6.2
1	I	398	GLY	6.2
2	D	66	ASP	6.2
2	L	215	ILE	6.2
1	A	694	GLU	6.2
1	B	696	GLY	6.2
2	H	209	GLU	6.1
1	I	655	THR	6.1
2	H	83	LEU	6.1
1	J	635	TYR	6.1
2	L	282	ALA	6.1
1	F	477	ILE	6.1
1	J	747	LEU	6.1
1	E	243	TYR	6.1
1	J	781	VAL	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	E	505	GLU	6.0
1	B	483	HIS	6.0
1	E	239	ALA	6.0
1	J	756	ILE	6.0
1	J	174	ASN	6.0
1	J	572	PHE	6.0

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Mol	Chain	Res	Type	RSRZ
2	K	80	ILE	6.0
1	J	628	ALA	6.0
1	A	697	ARG	6.0
2	G	265	ASP	6.0
2	H	84	ASP	6.0
1	A	160	PRO	6.0
2	K	240	VAL	6.0
1	I	528	TYR	6.0
1	I	572	PHE	6.0
2	G	239	TRP	6.0
2	L	22	ARG	6.0
1	I	345	VAL	6.0
1	I	240	LEU	6.0
2	C	68	LEU	5.9
1	J	476	GLN	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	J	449	ARG	5.9
1	A	774	ALA	5.9
1	I	203	GLU	5.9
1	F	777	ALA	5.9
1	E	654	PHE	5.9
2	G	81	ALA	5.9
2	L	285	GLN	5.9
1	I	364	ASP	5.9
2	G	259	ASN	5.9
1	J	772	GLY	5.9
2	C	90	ILE	5.9
1	F	725	PHE	5.8
1	J	242	GLN	5.8
2	D	269	ASN	5.8
2	G	188	ASN	5.8
2	H	275	ALA	5.8
2	G	172	ASP	5.8
1	J	609	MET	5.8
2	H	212	LEU	5.8
1	J	729	TYR	5.8
2	H	110	LEU	5.8
1	E	146	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
2	G	295	ASP	5.8
1	B	630	ILE	5.8
1	I	740	GLU	5.8
2	K	67	GLU	5.8
1	B	473	TYR	5.8
1	F	594	GLU	5.8
1	F	475	ILE	5.8
1	J	496	LYS	5.7
2	G	240	VAL	5.7
2	L	283	ASP	5.7
2	G	176	ARG	5.7
1	B	610	LEU	5.7
1	A	148	LEU	5.7
1	B	603	LEU	5.7
1	E	634	ALA	5.7
1	J	446	TYR	5.7
2	L	181	ALA	5.7
1	I	335	THR	5.7
1	E	779	ALA	5.7
1	A	315	VAL	5.7
1	E	476	GLN	5.7
1	J	777	ALA	5.7
1	F	775	VAL	5.7
2	K	196	VAL	5.7
1	F	399	GLU	5.7
1	J	632	LEU	5.7
1	I	781	VAL	5.7
2	K	181	ALA	5.6
1	F	483	HIS	5.6
1	F	729	TYR	5.6
1	F	610	LEU	5.6
1	E	743	ALA	5.6
1	A	179	LEU	5.6
1	J	555	LEU	5.6
2	H	135	LYS	5.6
2	H	132	VAL	5.6
1	J	221	ASP	5.6
1	J	454	GLU	5.6
1	J	524	GLU	5.6
2	L	80	ILE	5.6
1	F	145	TYR	5.6
1	I	242	GLN	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	111	THR	5.6
2	C	89	ILE	5.6
1	B	576	PRO	5.6
1	I	136	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	I	468	ASN	5.6
1	J	324	ARG	5.6
1	F	239	ALA	5.6
1	J	553	ASP	5.6
1	E	631	ALA	5.6
1	J	610	LEU	5.6
2	K	117	GLN	5.6
1	I	522	ALA	5.6
1	I	361	ARG	5.6
1	F	519	LYS	5.6
2	G	133	THR	5.6
1	F	136	ILE	5.5
2	H	180	LEU	5.5
1	J	627	THR	5.5
1	B	756	ILE	5.5
2	D	209	GLU	5.5
1	A	237	ALA	5.5
1	A	747	LEU	5.5
1	A	166	MET	5.5
1	F	134	ALA	5.5
1	J	137	TRP	5.5
1	E	225	PHE	5.5
1	E	689	LEU	5.5
1	J	261	GLU	5.5
1	I	750	LEU	5.5
1	E	551	GLU	5.5
2	D	282	ALA	5.5
2	C	182	ARG	5.5
1	B	727	THR	5.5
1	B	136	ILE	5.5
1	I	179	LEU	5.5
1	A	695	ILE	5.5
1	I	577	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	I	777	ALA	5.5
2	C	149	ASP	5.5
1	I	523	LEU	5.5
1	I	692	MET	5.5
1	I	592	LEU	5.4
1	J	505	GLU	5.4
2	D	287	ALA	5.4
1	J	724	LEU	5.4
2	H	66	ASP	5.4
1	J	448	GLU	5.4
1	B	780	GLY	5.4
1	F	221	ASP	5.4
1	E	158	SER	5.4
1	J	697	ARG	5.4
1	B	758	PHE	5.4
1	I	332	GLN	5.4
1	I	756	ILE	5.4
1	J	157	LEU	5.4
1	E	501	TYR	5.4
1	J	480	GLY	5.4
2	H	330	LEU	5.4
2	H	124	TYR	5.4
1	A	612	ILE	5.4
1	B	631	ALA	5.4
1	F	726	ALA	5.4
1	J	721	ALA	5.4
1	I	516	SER	5.4
2	K	330	LEU	5.4
2	H	211	ARG	5.4
1	E	426	ALA	5.4
2	C	86	LEU	5.4
2	D	241	ALA	5.4
1	A	155	PHE	5.4
1	E	257	SER	5.4
2	D	278	ASP	5.3
1	E	722	LEU	5.3
1	A	477	ILE	5.3
1	E	494	THR	5.3
1	E	241	LEU	5.3
1	A	258	ILE	5.3
1	B	546	ALA	5.3
2	C	82	SER	5.3

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Mol	Chain	Res	Type	RSRZ
2	C	66	ASP	5.3
1	A	722	LEU	5.3
1	J	425	ILE	5.3
2	H	181	ALA	5.3
2	K	71	ALA	5.3
1	J	276	ASN	5.3
2	H	241	ALA	5.3
2	G	293	GLU	5.3
1	B	607	ARG	5.3
1	E	486	PRO	5.3
2	D	80	ILE	5.3
1	B	627	THR	5.3
1	I	776	ALA	5.3
1	J	346	GLY	5.3
2	C	285	GLN	5.3
1	E	708	ALA	5.3
2	G	189	LEU	5.3
2	L	20	VAL	5.3
1	B	244	ALA	5.3
2	D	207	GLN	5.3
1	A	725	PHE	5.2
1	F	774	ALA	5.2
2	H	136	PRO	5.2
2	L	178	ILE	5.2
1	E	677	THR	5.2
1	B	781	VAL	5.2
1	J	498	ALA	5.2
2	H	137	ALA	5.2
1	A	773	LEU	5.2
2	G	179	ALA	5.2
2	H	208	LYS	5.2
1	I	239	ALA	5.2
1	B	755	THR	5.2
1	E	782	PRO	5.2
1	E	160	PRO	5.2
1	J	725	PHE	5.2
1	F	241	LEU	5.2
2	K	180	LEU	5.2
2	C	71	ALA	5.2
2	K	284	GLN	5.2
1	I	514	LEU	5.2
1	I	691	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	J	659	ALA	5.2
1	F	481	GLN	5.2
2	L	172	ASP	5.2
1	J	359	THR	5.2
2	G	55	ARG	5.2
1	J	240	LEU	5.2
1	I	458	THR	5.2
2	L	220	PHE	5.2
1	J	465	VAL	5.2
2	D	208	LYS	5.2
1	F	335	THR	5.2
1	E	261	GLU	5.2
1	B	709	TRP	5.2
2	H	298	GLN	5.1
1	J	159	GLU	5.1
1	I	221	ASP	5.1
1	I	782	PRO	5.1
1	J	479	ARG	5.1
2	D	286	PRO	5.1
1	E	145	TYR	5.1
2	G	90	ILE	5.1
1	I	469	ALA	5.1
1	A	760	HIS	5.1
1	B	570	PRO	5.1
2	G	20	VAL	5.1
2	L	148	LEU	5.1
1	F	155	PHE	5.1
1	E	771	TYR	5.1
2	D	291	TYR	5.1
1	B	778	LEU	5.1
2	G	199	TYR	5.1
1	A	579	ARG	5.1
1	I	422	GLY	5.1
1	J	483	HIS	5.1
1	A	158	SER	5.1
2	G	180	LEU	5.1
1	A	276	ASN	5.1
1	F	730	PHE	5.1
2	C	88	ALA	5.1
2	L	125	ALA	5.1
2	H	55	ARG	5.1
2	D	277	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	507	LYS	5.1
1	J	239	ALA	5.1
1	E	570	PRO	5.1
1	A	756	ILE	5.1
1	I	521	LEU	5.1
2	L	86	LEU	5.1
2	D	266	ARG	5.1
1	J	419	VAL	5.1
1	I	473	TYR	5.1
1	I	778	LEU	5.1
2	K	119	GLU	5.1
1	J	339	GLN	5.1
2	H	239	TRP	5.1
1	J	342	LEU	5.1
1	E	229	ASN	5.1
1	E	510	GLU	5.1
2	C	51	ALA	5.1
1	A	750	LEU	5.1
1	F	450	LEU	5.1
1	F	762	VAL	5.1
1	J	237	ALA	5.0
1	F	523	LEU	5.0
1	I	212	GLN	5.0
2	D	64	LYS	5.0
1	E	242	GLN	5.0
1	B	189	LEU	5.0
1	I	189	LEU	5.0
2	D	280	LEU	5.0
2	G	207	GLN	5.0
1	I	723	THR	5.0
1	B	633	MET	5.0
1	J	528	TYR	5.0
2	G	45	ASP	5.0
2	G	67	GLU	5.0
2	G	175	ILE	5.0
2	H	326	VAL	5.0
1	B	693	ASP	5.0
2	D	180	LEU	5.0
1	F	595	PRO	5.0
1	B	750	LEU	5.0
2	G	292	LEU	5.0
1	I	527	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	156	ARG	5.0
1	E	633	MET	5.0
1	F	332	GLN	5.0
1	I	759	MET	5.0
2	L	124	TYR	5.0
1	E	482	SER	5.0
2	C	21	GLU	5.0
2	D	181	ALA	4.9
2	H	327	LEU	5.0
1	E	500	ARG	4.9
2	H	109	THR	4.9
1	J	770	SER	4.9
2	K	195	ILE	4.9
1	I	659	ALA	4.9
2	G	40	THR	4.9
2	D	225	LEU	4.9
2	K	73	ALA	4.9
1	I	646	GLU	4.9
2	C	198	GLN	4.9
1	J	630	ILE	4.9
2	G	138	ALA	4.9
2	G	241	ALA	4.9
1	E	427	SER	4.9
1	A	728	HIS	4.9
1	I	484	LEU	4.9
1	B	577	GLY	4.9
2	D	290	LEU	4.9
1	E	504	PRO	4.9
1	I	386	ASP	4.9
1	I	382	LEU	4.9
1	I	147	THR	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	636	ILE	4.9
1	J	778	LEU	4.9
2	L	330	LEU	4.9
2	G	266	ARG	4.9
1	B	629	LEU	4.9
2	D	63	ILE	4.9
1	E	729	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	782	PRO	4.8
1	I	603	LEU	4.8
1	B	472	GLY	4.8
1	E	260	MET	4.8
2	K	23	PRO	4.8
1	J	648	GLY	4.8
1	E	491	ARG	4.8
1	F	478	SER	4.8
1	B	149	ASP	4.8
2	G	330	LEU	4.8
1	I	135	ALA	4.8
2	D	137	ALA	4.8
1	A	239	ALA	4.8
1	A	364	ASP	4.8
1	I	333	ASP	4.8
1	J	686	GLU	4.8
2	H	138	ALA	4.8
2	L	171	ILE	4.8
1	E	497	ASN	4.8
1	A	470	VAL	4.8
1	B	245	LYS	4.8
1	B	772	GLY	4.8
1	B	773	LEU	4.8
1	F	314	PRO	4.8
1	I	419	VAL	4.8
1	J	341	VAL	4.8
1	J	447	LEU	4.8
2	C	215	ILE	4.8
2	H	92	LEU	4.8
2	D	268	ILE	4.8
1	B	260	MET	4.8
1	I	362	PRO	4.8
2	G	54	ILE	4.8
1	F	259	THR	4.8
1	J	695	ILE	4.8
2	L	226	ALA	4.8
1	E	262	ARG	4.7
1	B	485	ALA	4.7
1	I	698	GLY	4.7
1	J	497	ASN	4.7
1	A	607	ARG	4.7
1	J	608	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
2	G	171	ILE	4.7
1	B	748	ASP	4.7
1	B	237	ALA	4.7
1	J	238	GLY	4.7
1	A	775	VAL	4.7
1	F	773	LEU	4.7
2	K	140	PRO	4.7
2	D	224	ALA	4.7
2	D	90	ILE	4.7
1	F	424	VAL	4.7
1	A	489	TYR	4.7
2	C	212	LEU	4.7
1	B	775	VAL	4.7
1	I	472	GLY	4.7
1	J	692	MET	4.7
1	F	160	PRO	4.7
1	F	600	PRO	4.7
1	I	497	ASN	4.7
1	F	708	ALA	4.7
1	F	656	ARG	4.7
1	E	458	THR	4.7
1	I	774	ALA	4.7
1	J	423	GLY	4.7
2	K	72	LEU	4.7
1	E	615	PRO	4.7
1	E	675	THR	4.7
1	J	132	LEU	4.7
1	A	690	VAL	4.7
1	E	422	GLY	4.7
2	D	23	PRO	4.7
1	E	700	SER	4.7
1	F	609	MET	4.7
1	F	476	GLN	4.7
1	F	166	MET	4.7
1	J	538	HIS	4.7
2	L	132	VAL	4.7
1	F	258	ILE	4.7
1	J	655	THR	4.7
2	D	65	LYS	4.6
1	A	190	ILE	4.6
1	B	741	GLY	4.6
1	B	761	SER	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	387	SER	4.6
1	J	212	GLN	4.6
1	F	781	VAL	4.6
1	J	762	VAL	4.6
2	G	226	ALA	4.6
1	B	634	ALA	4.6
1	I	701	THR	4.6
1	B	470	VAL	4.6
2	K	30	LEU	4.6
1	F	727	THR	4.6
1	I	564	THR	4.6
2	K	241	ALA	4.6
1	I	525	LYS	4.6
1	E	469	ALA	4.6
1	F	593	ASN	4.6
1	J	751	GLU	4.6
2	G	184	ASP	4.6
1	F	179	LEU	4.6
2	D	330	LEU	4.6
1	B	484	LEU	4.6
1	E	223	VAL	4.6
1	J	144	GLY	4.6
1	J	625	ARG	4.6
1	E	148	LEU	4.6
1	J	170	LEU	4.6
1	E	653	ILE	4.6
2	L	224	ALA	4.6
2	G	203	PRO	4.6
1	E	430	ASN	4.6
1	J	696	GLY	4.6
1	B	481	GLN	4.6
1	E	463	LEU	4.6
1	I	605	PRO	4.6
1	B	689	LEU	4.6
2	H	21	GLU	4.6
1	I	467	PHE	4.6
1	I	647	ILE	4.6
2	C	87	GLU	4.6
1	A	600	PRO	4.6
1	E	636	ILE	4.5
1	A	524	GLU	4.5
2	L	265	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	657	VAL	4.5
2	C	183	PHE	4.5
2	L	176	ARG	4.5
1	I	748	ASP	4.5
1	A	655	THR	4.5
1	A	724	LEU	4.5
2	K	228	GLU	4.5
1	E	429	TYR	4.5
1	J	260	MET	4.5
1	A	601	LEU	4.5
1	E	238	GLY	4.5
1	E	244	ALA	4.5
1	A	460	LEU	4.5
1	E	381	GLN	4.5
2	K	95	ARG	4.5
1	I	511	ASP	4.5
2	D	122	GLN	4.5
1	F	772	GLY	4.5
1	A	603	LEU	4.5
1	A	578	ILE	4.5
2	H	240	VAL	4.5
2	K	66	ASP	4.5
1	I	241	LEU	4.5
2	G	267	LEU	4.5
2	H	323	TYR	4.5
1	E	693	ASP	4.5
1	A	178	LEU	4.5
1	A	481	GLN	4.5
2	C	85	ASP	4.5
1	B	595	PRO	4.5
2	H	220	PHE	4.5
1	E	778	LEU	4.5
1	F	158	SER	4.5
1	F	423	GLY	4.5
1	F	695	ILE	4.5
2	L	175	ILE	4.5
2	D	73	ALA	4.5
2	H	243	PRO	4.5
1	E	702	TYR	4.5
1	I	749	ALA	4.5
2	H	224	ALA	4.5
1	B	179	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	J	176	ALA	4.5
1	I	463	LEU	4.5
2	H	23	PRO	4.5
2	H	121	TRP	4.5
1	A	692	MET	4.5
1	F	522	ALA	4.5
1	F	654	PHE	4.5
1	J	515	THR	4.5
2	K	282	ALA	4.5
1	I	578	ILE	4.5
1	I	384	THR	4.5
2	H	179	ALA	4.5
2	D	123	ALA	4.5
1	E	498	ALA	4.4
2	D	69	ALA	4.4
1	J	647	ILE	4.4
1	B	148	LEU	4.4
2	L	183	PHE	4.4
2	D	136	PRO	4.4
1	F	484	LEU	4.4
1	I	690	VAL	4.4
2	K	82	SER	4.4
1	B	602	ASN	4.4
1	J	503	ILE	4.4
2	H	215	ILE	4.4
2	K	289	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
1	B	241	LEU	4.4
1	F	269	MET	4.4
2	G	167	GLU	4.4
2	G	198	GLN	4.4
2	L	87	GLU	4.4
1	A	241	LEU	4.4
1	B	247	THR	4.4
1	B	460	LEU	4.4
1	E	410	ALA	4.4
2	G	215	ILE	4.4
1	E	177	GLU	4.4
1	I	590	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
2	L	197	ARG	4.4
2	D	24	ALA	4.4
2	L	50	GLY	4.4
2	D	275	ALA	4.4
1	B	578	ILE	4.4
1	I	403	LEU	4.4
2	C	72	LEU	4.4
2	D	281	GLY	4.4
1	J	691	LEU	4.4
1	A	635	TYR	4.4
2	G	82	SER	4.4
1	J	241	LEU	4.4
1	A	522	ALA	4.4
1	E	178	LEU	4.4
1	I	331	LEU	4.4
1	I	347	ASP	4.4
1	F	780	GLY	4.4
1	I	134	ALA	4.4
1	A	451	GLU	4.4
2	H	223	GLN	4.4
1	E	472	GLY	4.3
1	I	423	GLY	4.3
1	F	612	ILE	4.3
1	A	360	ALA	4.3
2	D	70	LEU	4.3
1	B	458	THR	4.3
1	J	204	PHE	4.3
1	E	769	LYS	4.3
1	J	607	ARG	4.3
1	E	773	LEU	4.3
1	I	648	GLY	4.3
1	J	202	TRP	4.3
2	H	289	VAL	4.3
1	I	157	LEU	4.3
1	I	487	ILE	4.3
1	A	269	MET	4.3
1	B	551	GLU	4.3
2	L	212	LEU	4.3
1	A	312	HIS	4.3
1	A	708	ALA	4.3
2	L	24	ALA	4.3
1	E	495	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	717	ASN	4.3
1	B	549	LEU	4.3
1	E	704	GLY	4.3
2	H	146	GLU	4.3
1	E	652	ARG	4.3
1	A	495	LEU	4.3
1	B	381	GLN	4.3
2	D	81	ALA	4.3
2	K	276	TYR	4.3
2	G	209	GLU	4.3
2	K	118	GLN	4.3
2	G	233	ASP	4.3
1	A	580	ILE	4.3
1	A	652	ARG	4.3
1	B	134	ALA	4.3
1	B	712	ALA	4.3
1	F	525	LYS	4.3
1	J	726	ALA	4.3
1	J	424	VAL	4.3
1	J	511	ASP	4.3
2	C	50	GLY	4.3
1	E	324	ARG	4.3
1	E	459	GLY	4.3
1	F	157	LEU	4.3
1	B	135	ALA	4.3
1	E	499	GLU	4.3
2	L	108	LEU	4.3
1	J	234	LEU	4.2
1	F	148	LEU	4.2
1	A	776	ALA	4.2
2	G	202	VAL	4.2
2	C	124	TYR	4.2
1	B	151	SER	4.2
1	E	755	THR	4.2
1	B	762	VAL	4.2
1	J	227	VAL	4.2
1	B	192	GLY	4.2
1	B	716	ALA	4.2
1	A	763	GLN	4.2
1	I	755	THR	4.2
1	E	468	ASN	4.2
2	G	177	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	J	233	GLY	4.2
2	K	225	LEU	4.2
1	B	754	ASP	4.2
1	E	628	ALA	4.2
2	C	243	PRO	4.2
1	A	144	GLY	4.2
1	J	236	ALA	4.2
1	J	327	THR	4.2
2	D	256	PHE	4.2
2	K	29	GLU	4.2
1	I	483	HIS	4.2
1	F	243	TYR	4.2
1	F	410	ALA	4.2
1	J	597	ILE	4.2
1	I	334	PHE	4.2
2	G	63	ILE	4.2
2	G	162	ARG	4.2
2	H	95	ARG	4.2
1	B	203	GLU	4.2
1	I	263	GLU	4.2
1	F	463	LEU	4.2
1	J	506	LEU	4.2
1	I	243	TYR	4.2
2	H	276	TYR	4.2
1	I	397	MET	4.2
2	H	94	PHE	4.2
1	A	270	ASP	4.2
2	H	225	LEU	4.2
1	E	676	GLU	4.1
2	L	266	ARG	4.1
1	E	230	ALA	4.1
1	E	752	HIS	4.1
1	J	190	ILE	4.1
1	J	551	GLU	4.1
1	E	707	LEU	4.1
1	J	519	LYS	4.1
1	I	400	PHE	4.1
1	I	758	PHE	4.1
1	F	778	LEU	4.1
2	L	149	ASP	4.1
1	B	248	GLN	4.1
1	I	230	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	477	ILE	4.1
1	E	411	ILE	4.1
1	E	706	SER	4.1
1	A	475	ILE	4.1
1	A	478	SER	4.1
1	A	203	GLU	4.1
1	E	632	LEU	4.1
1	B	155	PHE	4.1
1	J	279	ILE	4.1
1	E	128	ARG	4.1
1	I	604	SER	4.1
1	J	484	LEU	4.1
1	B	751	GLU	4.1
1	E	524	GLU	4.1
2	G	182	ARG	4.1
1	B	501	TYR	4.1
1	E	221	ASP	4.1
1	I	327	THR	4.1
2	C	92	LEU	4.1
1	F	451	GLU	4.1
2	L	276	TYR	4.1
1	B	332	GLN	4.1
1	E	767	ALA	4.1
2	H	272	ILE	4.1
1	I	726	ALA	4.1
1	A	746	HIS	4.1
1	B	212	GLN	4.1
1	F	501	TYR	4.1
2	K	27	VAL	4.1
1	A	577	GLY	4.1
1	B	243	TYR	4.1
1	F	262	ARG	4.1
1	J	575	LYS	4.1
2	K	329	VAL	4.1
2	L	107	ARG	4.1
1	A	610	LEU	4.1
2	H	242	ASP	4.1
1	A	499	GLU	4.1
1	A	757	ALA	4.1
2	H	226	ALA	4.1
2	D	210	ARG	4.1
1	E	697	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	658	GLY	4.0
2	G	44	ILE	4.0
2	G	289	VAL	4.0
2	K	31	VAL	4.0
1	B	563	TYR	4.0
1	E	772	GLY	4.0
1	B	480	GLY	4.0
1	E	595	PRO	4.0
1	A	169	GLU	4.0
2	C	91	SER	4.0
1	J	769	LYS	4.0
1	F	559	ALA	4.0
1	E	674	MET	4.0
1	A	701	THR	4.0
1	B	738	LYS	4.0
1	J	694	GLU	4.0
2	K	21	GLU	4.0
1	J	422	GLY	4.0
1	J	615	PRO	4.0
1	I	531	LEU	4.0
1	E	159	GLU	4.0
1	B	345	VAL	4.0
2	D	83	LEU	4.0
1	B	158	SER	4.0
1	E	245	LYS	4.0
1	I	724	LEU	4.0
1	B	190	ILE	4.0
2	H	279	LYS	4.0
2	H	213	GLY	4.0
2	K	70	LEU	4.0
2	L	55	ARG	4.0
2	H	207	GLN	4.0
2	D	220	PHE	4.0
1	A	496	LYS	4.0
1	B	150	ILE	4.0
1	B	492	ARG	4.0
2	H	96	GLY	4.0
2	L	216	LEU	4.0
1	A	519	LYS	4.0
1	F	696	GLY	4.0
1	I	202	TRP	4.0
1	A	471	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
2	C	109	THR	4.0
2	L	241	ALA	4.0
2	D	299	VAL	4.0
1	A	498	ALA	4.0
1	E	629	LEU	4.0
1	E	630	ILE	4.0
1	J	220	ARG	4.0
2	K	83	LEU	4.0
1	E	656	ARG	4.0
1	J	656	ARG	4.0
1	A	273	THR	4.0
1	J	510	GLU	4.0
1	J	731	GLU	4.0
1	B	739	MET	3.9
1	J	495	LEU	3.9
2	K	299	VAL	3.9
1	A	751	GLU	3.9
1	E	263	GLU	3.9
1	B	246	CYS	3.9
1	E	327	THR	3.9
1	I	489	TYR	3.9
1	A	758	PHE	3.9
1	F	217	PHE	3.9
1	J	325	GLN	3.9
2	G	315	SER	3.9
2	K	34	SER	3.9
2	L	54	ILE	3.9
1	E	328	ILE	3.9
1	I	360	ALA	3.9
2	H	214	ALA	3.9
1	J	445	ASP	3.9
1	J	451	GLU	3.9
2	K	182	ARG	3.9
1	F	564	THR	3.9
1	J	453	ARG	3.9
2	G	183	PHE	3.9
1	F	346	GLY	3.9
1	I	190	ILE	3.9
2	C	216	LEU	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
1	J	262	ARG	3.9
2	H	183	PHE	3.9
2	K	137	ALA	3.9
1	J	156	ARG	3.9
2	L	66	ASP	3.9
1	J	155	PHE	3.9
2	G	201	ALA	3.9
1	A	156	ARG	3.9
1	I	365	LEU	3.9
2	C	330	LEU	3.9
1	I	635	TYR	3.9
1	B	646	GLU	3.9
1	A	202	TRP	3.9
1	F	245	LYS	3.9
1	J	603	LEU	3.9
2	H	322	ILE	3.9
1	E	742	VAL	3.9
2	D	22	ARG	3.9
2	D	267	LEU	3.9
2	K	190	SER	3.9
1	E	479	ARG	3.9
1	A	653	ILE	3.9
2	D	274	GLN	3.9
1	J	462	THR	3.9
1	F	261	GLU	3.9
1	E	258	ILE	3.8
1	E	550	ALA	3.8
1	E	552	LEU	3.8
1	I	563	TYR	3.8
2	D	243	PRO	3.8
2	L	147	VAL	3.8
2	G	123	ALA	3.8
1	J	586	PRO	3.8
2	G	134	VAL	3.8
1	A	528	TYR	3.8
1	E	597	ILE	3.8
1	I	694	GLU	3.8
1	J	203	GLU	3.8
2	K	198	GLN	3.8
1	J	614	GLY	3.8
2	G	178	ILE	3.8
1	B	333	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	268	ILE	3.8
1	J	531	LEU	3.8
2	L	264	ARG	3.8
1	A	503	ILE	3.8
1	F	222	LEU	3.8
1	F	315	VAL	3.8
1	J	556	VAL	3.8
2	L	273	ARG	3.8
1	B	708	ALA	3.8
1	F	731	GLU	3.8
2	L	49	GLY	3.8
2	C	242	ASP	3.8
2	L	199	TYR	3.8
2	L	173	GLU	3.8
1	E	657	VAL	3.8
1	J	222	LEU	3.8
2	G	42	ILE	3.8
1	B	250	THR	3.8
1	E	627	THR	3.8
1	F	590	GLN	3.8
2	G	26	VAL	3.8
1	J	571	THR	3.8
1	J	138	GLN	3.8
2	C	178	ILE	3.8
2	G	50	GLY	3.8
1	F	216	GLN	3.8
1	E	485	ALA	3.8
1	A	658	GLY	3.8
1	B	639	TYR	3.8
1	I	460	LEU	3.8
1	A	180	TYR	3.8
1	B	510	GLU	3.8
1	B	673	GLU	3.8
1	F	599	ASN	3.8
1	I	276	ASN	3.8
2	C	125	ALA	3.8
2	K	90	ILE	3.8
2	G	173	GLU	3.8
2	C	107	ARG	3.8
2	H	145	LEU	3.8
1	B	360	ALA	3.8
2	D	284	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
2	G	174	ILE	3.8
1	A	450	LEU	3.8
1	B	156	ARG	3.8
1	A	212	GLN	3.8
2	C	175	ILE	3.8
1	A	732	LEU	3.8
1	A	731	GLU	3.8
2	G	124	TYR	3.8
2	D	329	VAL	3.8
1	A	479	ARG	3.8
1	I	158	SER	3.8
1	I	607	ARG	3.8
1	J	690	VAL	3.8
1	E	705	LEU	3.8
1	B	721	ALA	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	A	572	PHE	3.8
1	J	578	ILE	3.7
2	L	279	LYS	3.8
1	I	330	ALA	3.7
1	F	267	ILE	3.7
1	E	648	GLY	3.7
1	B	640	VAL	3.7
2	C	286	PRO	3.7
1	I	432	GLU	3.7
1	I	498	ALA	3.7
1	E	433	LEU	3.7
2	G	68	LEU	3.7
2	K	194	LYS	3.7
1	F	227	VAL	3.7
1	F	707	LEU	3.7
2	K	286	PRO	3.7
1	I	731	GLU	3.7
1	A	745	VAL	3.7
1	B	157	LEU	3.7
1	B	697	ARG	3.7
1	F	398	GLY	3.7
1	I	556	VAL	3.7
1	A	764	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	509	TYR	3.7
1	J	277	LEU	3.7
1	J	701	THR	3.7
2	C	151	PHE	3.7
1	B	193	ARG	3.7
2	G	146	GLU	3.7
2	H	182	ARG	3.7
1	I	708	ALA	3.7
1	E	519	LYS	3.7
1	F	133	LEU	3.7
2	G	212	LEU	3.7
2	G	149	ASP	3.7
1	A	538	HIS	3.7
2	D	315	SER	3.7
2	G	268	ILE	3.7
2	K	179	ALA	3.7
2	K	20	VAL	3.7
1	A	759	MET	3.7
2	C	20	VAL	3.7
1	F	712	ALA	3.7
1	I	238	GLY	3.7
2	D	255	TYR	3.7
1	B	711	VAL	3.7
1	F	419	VAL	3.7
1	B	334	PHE	3.7
1	I	555	LEU	3.7
2	G	43	ASP	3.7
1	B	475	ILE	3.7
1	J	218	GLY	3.7
1	E	341	VAL	3.7
1	I	526	GLN	3.7
1	A	597	ILE	3.7
2	K	84	ASP	3.7
2	K	178	ILE	3.7
1	B	729	TYR	3.7
1	F	563	TYR	3.7
1	B	262	ARG	3.7
2	D	259	ASN	3.7
1	I	725	PHE	3.7
1	I	730	PHE	3.7
1	J	458	THR	3.7
1	E	446	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	535	LEU	3.6
1	A	705	LEU	3.6
1	F	565	LEU	3.6
2	D	260	GLY	3.6
2	G	49	GLY	3.6
2	G	264	ARG	3.6
1	A	170	LEU	3.6
1	A	611	ILE	3.6
1	F	611	ILE	3.6
1	I	156	ARG	3.6
1	F	528	TYR	3.6
1	J	160	PRO	3.6
2	G	299	VAL	3.6
1	E	173	THR	3.6
1	E	549	LEU	3.6
1	I	228	GLU	3.6
2	G	170	HIS	3.6
1	A	608	ARG	3.6
2	G	51	ALA	3.6
1	A	316	ARG	3.6
2	K	45	ASP	3.6
1	F	348	LEU	3.6
2	C	153	ASN	3.6
2	D	264	ARG	3.6
1	E	413	ASP	3.6
1	A	261	GLU	3.6
1	I	510	GLU	3.6
1	J	612	ILE	3.6
2	L	239	TRP	3.6
2	D	162	ARG	3.6
1	F	268	ILE	3.6
1	F	520	ALA	3.6
2	D	71	ALA	3.6
2	G	66	ASP	3.6
1	B	552	LEU	3.6
1	A	183	ASP	3.6
2	D	253	ILE	3.6
1	A	523	LEU	3.6
1	F	236	ALA	3.6
1	F	479	ARG	3.6
2	G	64	LYS	3.6
1	A	772	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	553	ASP	3.6
1	I	722	LEU	3.6
1	E	572	PHE	3.6
2	K	116	GLU	3.6
1	A	743	ALA	3.6
2	C	246	THR	3.6
2	K	136	PRO	3.6
2	C	189	LEU	3.6
2	L	90	ILE	3.6
2	H	325	GLY	3.6
1	J	509	TYR	3.6
1	A	527	LEU	3.6
1	F	228	GLU	3.6
1	I	499	GLU	3.6
1	J	491	ARG	3.6
2	C	210	ARG	3.6
2	D	91	SER	3.6
1	J	143	PHE	3.6
2	K	193	GLY	3.6
1	E	338	LEU	3.6
1	I	535	LEU	3.6
2	D	263	MET	3.6
1	E	520	ALA	3.6
1	J	488	ASN	3.6
1	A	310	TRP	3.6
2	G	187	ILE	3.6
1	B	505	GLU	3.6
1	F	779	ALA	3.6
1	A	614	GLY	3.6
1	E	412	ILE	3.6
2	L	280	LEU	3.6
1	F	499	GLU	3.6
2	C	138	ALA	3.6
2	K	287	ALA	3.6
2	K	35	LEU	3.6
1	I	728	HIS	3.6
1	F	515	THR	3.6
1	F	518	GLY	3.6
1	I	579	ARG	3.6
1	F	498	ALA	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	707	LEU	3.5
1	E	747	LEU	3.5
1	A	777	ALA	3.5
1	A	193	ARG	3.5
1	F	560	GLU	3.5
1	E	450	LEU	3.5
1	B	550	ALA	3.5
1	F	653	ILE	3.5
1	A	324	ARG	3.5
1	I	703	ASP	3.5
1	J	192	GLY	3.5
1	A	216	GLN	3.5
1	E	709	TRP	3.5
1	I	390	VAL	3.5
1	J	606	GLN	3.5
2	H	31	VAL	3.5
1	A	267	ILE	3.5
1	E	246	CYS	3.5
1	A	709	TRP	3.5
2	C	155	PRO	3.5
1	F	657	VAL	3.5
1	I	752	HIS	3.5
2	C	123	ALA	3.5
2	D	257	TYR	3.5
1	A	236	ALA	3.5
1	B	227	VAL	3.5
1	A	627	THR	3.5
1	I	732	LEU	3.5
1	I	779	ALA	3.5
2	H	331	GLN	3.5
1	A	598	ALA	3.5
1	A	730	PHE	3.5
1	I	429	TYR	3.5
1	J	149	ASP	3.5
1	A	781	VAL	3.5
2	D	178	ILE	3.5
1	J	554	VAL	3.5
2	L	170	HIS	3.5
1	E	650	ILE	3.5
1	J	230	ALA	3.5
1	A	220	ARG	3.5
1	A	636	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
2	L	63	ILE	3.5
1	I	673	GLU	3.5
1	J	728	HIS	3.5
2	K	189	LEU	3.5
2	L	211	ARG	3.5
2	C	64	LYS	3.5
2	G	206	GLY	3.5
1	A	173	THR	3.5
1	A	576	PRO	3.5
1	F	514	LEU	3.5
1	B	497	ASN	3.5
1	I	559	ALA	3.5
1	F	255	ILE	3.5
1	F	260	MET	3.5
1	I	210	ARG	3.4
1	F	454	GLU	3.4
2	H	87	GLU	3.4
1	B	424	VAL	3.4
1	F	601	LEU	3.4
2	K	55	ARG	3.4
1	E	157	LEU	3.4
1	F	331	LEU	3.4
1	J	208	THR	3.4
1	A	488	ASN	3.4
1	F	263	GLU	3.4
1	I	342	LEU	3.4
2	D	72	LEU	3.4
2	H	56	ILE	3.4
2	H	86	LEU	3.4
2	D	134	VAL	3.4
1	I	148	LEU	3.4
2	H	49	GLY	3.4
1	I	416	PRO	3.4
1	I	677	THR	3.4
1	A	317	ASP	3.4
1	A	691	LEU	3.4
1	F	693	ASP	3.4
1	F	592	LEU	3.4
1	A	493	GLN	3.4
1	B	564	THR	3.4
1	B	606	GLN	3.4
1	I	410	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	G	291	TYR	3.4
2	K	243	PRO	3.4
1	I	383	GLU	3.4
1	J	473	TYR	3.4
2	H	54	ILE	3.4
1	A	628	ALA	3.4
1	E	175	PRO	3.4
1	F	562	ALA	3.4
1	I	146	ALA	3.4
1	J	235	SER	3.4
1	F	555	LEU	3.4
1	J	549	LEU	3.4
1	E	680	ILE	3.4
1	I	631	ALA	3.4
2	K	26	VAL	3.4
1	F	447	LEU	3.4
1	J	626	GLN	3.4
1	F	722	LEU	3.4
2	C	23	PRO	3.4
1	E	465	VAL	3.4
2	L	140	PRO	3.4
1	B	469	ALA	3.4
2	L	272	ILE	3.4
1	A	778	LEU	3.4
1	E	613	THR	3.4
2	G	186	THR	3.4
2	C	260	GLY	3.4
1	F	169	GLU	3.4
1	B	202	TRP	3.4
2	D	52	LYS	3.4
2	K	96	GLY	3.4
1	J	299	VAL	3.4
1	A	143	PHE	3.4
1	E	611	ILE	3.4
1	B	545	SER	3.4
2	G	122	GLN	3.4
2	D	27	VAL	3.4
2	D	124	TYR	3.4
1	A	741	GLY	3.3
1	J	344	GLN	3.4
1	J	783	LYS	3.3
2	G	205	GLY	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	208	THR	3.3
2	D	227	ILE	3.3
1	B	263	GLU	3.3
1	J	618	GLY	3.3
1	F	549	LEU	3.3
1	J	179	LEU	3.3
1	A	255	ILE	3.3
1	I	739	MET	3.3
2	D	54	ILE	3.3
1	A	157	LEU	3.3
1	A	348	LEU	3.3
1	A	604	SER	3.3
1	J	768	SER	3.3
2	K	280	LEU	3.3
1	A	454	GLU	3.3
1	J	527	LEU	3.3
2	G	242	ASP	3.3
1	B	625	ARG	3.3
1	B	632	LEU	3.3
2	G	136	PRO	3.3
2	H	324	GLN	3.3
2	H	283	ASP	3.3
2	L	233	ASP	3.3
1	I	512	LYS	3.3
2	L	242	ASP	3.3
2	D	82	SER	3.3
1	B	506	LEU	3.3
1	I	760	HIS	3.3
1	J	720	LYS	3.3
2	G	225	LEU	3.3
2	C	209	GLU	3.3
1	E	576	PRO	3.3
1	I	714	ASN	3.3
2	C	73	ALA	3.3
1	J	272	ALA	3.3
1	B	344	GLN	3.3
1	F	561	ARG	3.3
2	C	266	ARG	3.3
2	L	177	ARG	3.3
1	F	411	ILE	3.3
1	E	166	MET	3.3
2	H	64	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	372	PHE	3.3
2	D	51	ALA	3.3
1	J	557	ASN	3.3
2	C	211	ARG	3.3
2	H	267	LEU	3.3
1	B	468	ASN	3.3
1	A	221	ASP	3.3
1	E	614	GLY	3.3
1	F	154	ARG	3.3
1	F	709	TRP	3.3
1	J	214	ASN	3.3
2	D	182	ARG	3.3
2	G	200	ARG	3.3
2	D	331	GLN	3.3
1	A	638	SER	3.3
1	E	447	LEU	3.3
2	C	177	ARG	3.3
2	H	290	LEU	3.3
2	K	32	GLU	3.3
2	L	70	LEU	3.3
1	A	520	ALA	3.3
1	A	486	PRO	3.3
1	B	251	THR	3.3
2	L	225	LEU	3.3
2	H	274	GLN	3.3
2	D	326	VAL	3.3
2	L	168	PHE	3.3
1	A	651	ASP	3.3
1	E	496	LYS	3.3
1	I	381	GLN	3.3
1	I	738	LYS	3.3
1	J	541	ALA	3.3
2	C	241	ALA	3.3
1	A	637	GLY	3.3
1	B	636	ILE	3.3
2	H	268	ILE	3.3
2	L	268	ILE	3.3
2	G	89	ILE	3.2
1	A	704	GLY	3.2
1	I	208	THR	3.2
1	A	311	LEU	3.2
1	B	731	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	646	GLU	3.2
1	A	654	PHE	3.2
2	G	220	PHE	3.2
2	H	216	LEU	3.2
2	H	63	ILE	3.2
1	I	571	THR	3.2
1	J	786	ILE	3.2
1	B	659	ALA	3.2
1	I	399	GLU	3.2
1	I	773	LEU	3.2
1	J	177	GLU	3.2
1	J	323	GLU	3.2
2	D	161	LEU	3.2
1	A	480	GLY	3.2
1	F	470	VAL	3.2
1	J	397	MET	3.2
2	D	215	ILE	3.2
2	G	269	ASN	3.2
1	B	710	ALA	3.2
2	D	327	LEU	3.2
1	F	701	THR	3.2
2	G	147	VAL	3.2
2	H	65	LYS	3.2
2	H	30	LEU	3.2
1	A	351	ILE	3.2
1	I	277	LEU	3.2
1	E	464	LYS	3.2
1	E	555	LEU	3.2
1	J	785	VAL	3.2
2	C	202	VAL	3.2
2	G	135	LYS	3.2
1	A	650	ILE	3.2
1	I	229	ASN	3.2
2	C	264	ARG	3.2
1	A	515	THR	3.2
1	E	484	LEU	3.2
1	E	531	LEU	3.2
1	F	407	LEU	3.2
2	H	297	HIS	3.2
2	L	240	VAL	3.2
2	L	64	LYS	3.2
1	A	159	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	721	ALA	3.2
1	J	570	PRO	3.2
2	C	176	ARG	3.2
2	C	154	THR	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	185	VAL	3.2
1	J	500	ARG	3.2
2	L	198	GLN	3.2
1	B	348	LEU	3.2
1	J	514	LEU	3.2
2	G	132	VAL	3.2
1	B	478	SER	3.2
2	C	157	ARG	3.2
2	L	123	ALA	3.2
1	B	374	GLN	3.2
2	G	211	ARG	3.2
1	J	444	THR	3.2
2	H	119	GLU	3.2
2	D	271	ALA	3.2
1	I	601	LEU	3.2
2	C	184	ASP	3.2
1	B	133	LEU	3.2
1	E	474	TYR	3.2
2	C	95	ARG	3.2
2	D	132	VAL	3.2
2	D	135	LYS	3.2
2	D	110	LEU	3.2
1	B	128	ARG	3.2
1	F	635	TYR	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	E	231	PRO	3.1
2	H	265	ASP	3.1
1	E	325	GLN	3.1
1	A	646	GLU	3.1
1	E	378	LEU	3.1
1	J	512	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	419	VAL	3.1
2	C	148	LEU	3.1
1	J	315	VAL	3.1
2	C	96	GLY	3.1
1	A	181	ALA	3.1
1	A	689	LEU	3.1
1	E	295	LEU	3.1
1	I	368	MET	3.1
1	J	464	LYS	3.1
1	E	224	GLY	3.1
2	C	49	GLY	3.1
2	C	84	ASP	3.1
1	F	473	TYR	3.1
1	F	705	LEU	3.1
1	J	755	THR	3.1
1	J	779	ALA	3.1
1	I	211	GLN	3.1
1	J	532	PHE	3.1
1	A	279	ILE	3.1
1	A	659	ALA	3.1
1	E	169	GLU	3.1
1	E	483	HIS	3.1
1	I	709	TRP	3.1
1	E	712	ALA	3.1
1	A	649	PRO	3.1
1	E	681	LEU	3.1
1	F	400	PHE	3.1
2	C	247	THR	3.1
2	G	329	VAL	3.1
1	B	191	GLU	3.1
1	E	763	GLN	3.1
1	E	155	PHE	3.1
1	F	270	ASP	3.1
1	F	128	ARG	3.1
1	J	389	PRO	3.1
2	D	133	THR	3.1
1	I	411	ILE	3.1
2	G	238	GLY	3.1
1	A	688	SER	3.1
1	B	368	MET	3.1
1	E	437	ARG	3.1
1	J	558	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	606	GLN	3.1
2	G	318	VAL	3.1
1	A	564	THR	3.1
1	F	558	LEU	3.1
1	I	237	ALA	3.1
2	G	109	THR	3.1
2	K	315	SER	3.1
1	F	316	ARG	3.1
1	I	560	GLU	3.1
1	F	521	LEU	3.1
2	D	270	HIS	3.1
1	A	531	LEU	3.1
1	J	539	LEU	3.1
2	D	45	ASP	3.1
2	H	22	ARG	3.1
2	G	227	ILE	3.1
1	F	437	ARG	3.1
1	A	262	ARG	3.1
1	A	703	ASP	3.1
2	G	163	THR	3.1
2	G	258	VAL	3.1
1	I	222	LEU	3.1
1	I	258	ILE	3.1
2	D	216	LEU	3.1
2	L	189	LEU	3.1
2	L	294	ILE	3.1
2	H	117	GLN	3.1
1	A	706	SER	3.1
1	E	557	ASN	3.1
1	J	213	LEU	3.1
2	C	220	PHE	3.1
2	C	250	LEU	3.1
2	D	292	LEU	3.1
1	E	649	PRO	3.1
2	L	299	VAL	3.1
2	C	272	ILE	3.1
2	D	179	ALA	3.1
2	G	263	MET	3.1
1	E	339	GLN	3.0
1	I	216	GLN	3.0
1	J	263	GLU	3.0
1	J	321	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	213	LEU	3.0
1	A	361	ARG	3.0
1	B	154	ARG	3.0
1	B	499	GLU	3.0
1	E	528	TYR	3.0
2	H	115	ALA	3.0
1	B	204	PHE	3.0
1	I	751	GLU	3.0
1	B	677	THR	3.0
2	L	51	ALA	3.0
2	H	112	SER	3.0
1	A	208	THR	3.0
1	F	161	ALA	3.0
2	C	83	LEU	3.0
2	D	92	LEU	3.0
2	H	291	TYR	3.0
2	H	116	GLU	3.0
1	J	189	LEU	3.0
1	J	535	LEU	3.0
1	I	591	VAL	3.0
1	F	244	ALA	3.0
2	G	224	ALA	3.0
2	L	25	SER	3.0
1	E	523	LEU	3.0
1	J	523	LEU	3.0
2	G	322	ILE	3.0
1	I	389	PRO	3.0
1	B	771	TYR	3.0
1	E	276	ASN	3.0
1	E	532	PHE	3.0
1	F	659	ALA	3.0
1	J	502	ILE	3.0
1	E	678	ALA	3.0
1	E	698	GLY	3.0
2	C	122	GLN	3.0
1	E	699	THR	3.0
1	J	298	THR	3.0
1	F	220	ARG	3.0
2	L	254	GLN	3.0
1	A	335	THR	3.0
2	G	326	VAL	3.0
2	G	65	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	273	ARG	3.0
2	K	22	ARG	3.0
1	B	637	GLY	3.0
2	H	45	ASP	3.0
2	H	278	ASP	3.0
2	L	89	ILE	3.0
1	B	528	TYR	3.0
1	J	194	ARG	3.0
1	J	529	GLU	3.0
2	H	238	GLY	3.0
1	I	628	ALA	3.0
1	J	210	ARG	3.0
1	A	175	PRO	3.0
1	B	327	THR	3.0
1	E	247	THR	3.0
1	A	346	GLY	3.0
1	B	328	ILE	3.0
2	C	239	TRP	3.0
1	J	178	LEU	3.0
1	J	338	LEU	3.0
2	L	269	ASN	3.0
1	I	300	THR	3.0
2	D	198	GLN	3.0
2	C	63	ILE	3.0
1	B	331	LEU	3.0
1	E	355	LEU	3.0
1	I	178	LEU	3.0
1	J	337	GLY	3.0
1	B	230	ALA	3.0
1	B	425	ILE	3.0
2	H	155	PRO	3.0
1	J	205	GLU	3.0
1	B	324	ARG	2.9
1	F	144	GLY	2.9
2	K	36	ASP	2.9
1	J	520	ALA	2.9
1	B	555	LEU	2.9
2	L	267	LEU	2.9
2	C	199	TYR	2.9
1	A	272	ALA	2.9
2	H	50	GLY	2.9
2	L	65	LYS	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	J	649	PRO	2.9
1	A	196	LEU	2.9
1	I	188	SER	2.9
1	I	761	SER	2.9
2	G	190	SER	2.9
2	L	56	ILE	2.9
2	L	68	LEU	2.9
1	A	526	GLN	2.9
1	J	624	MET	2.9
1	I	415	PRO	2.9
1	J	209	ALA	2.9
2	K	288	PHE	2.9
1	A	448	GLU	2.9
1	E	624	MET	2.9
2	L	318	VAL	2.9
1	B	152	SER	2.9
1	E	639	TYR	2.9
1	A	189	LEU	2.9
2	L	174	ILE	2.9
2	C	244	ASN	2.9
1	I	393	LEU	2.9
1	I	553	ASP	2.9
1	I	576	PRO	2.9
2	H	198	GLN	2.9
1	I	513	VAL	2.9
1	F	526	GLN	2.9
2	C	291	TYR	2.9
2	D	89	ILE	2.9
2	D	21	GLU	2.9
1	E	754	ASP	2.9
2	C	245	HIS	2.9
1	J	530	GLU	2.9
2	L	286	PRO	2.9
1	I	775	VAL	2.9
1	B	146	ALA	2.9
2	D	211	ARG	2.9
2	C	253	ILE	2.9
2	D	195	ILE	2.9
1	B	740	GLU	2.9
1	F	506	LEU	2.9
1	A	570	PRO	2.9
1	A	605	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	571	THR	2.9
2	H	222	GLU	2.9
2	K	265	ASP	2.9
2	C	208	LYS	2.9
1	A	274	ARG	2.9
2	G	56	ILE	2.9
2	L	281	GLY	2.9
1	A	260	MET	2.9
1	I	367	ARG	2.9
1	I	707	LEU	2.9
1	B	503	ILE	2.9
1	I	155	PHE	2.9
2	K	294	ILE	2.9
1	J	492	ARG	2.9
1	E	352	LEU	2.9
1	F	527	LEU	2.9
2	G	181	ALA	2.8
1	I	394	ARG	2.8
1	E	599	ASN	2.8
1	J	245	LYS	2.8
1	J	474	TYR	2.8
1	F	234	LEU	2.8
2	L	326	VAL	2.8
1	B	713	GLU	2.8
1	F	552	LEU	2.8
2	K	139	HIS	2.8
1	A	742	VAL	2.8
1	A	177	GLU	2.8
2	K	266	ARG	2.8
2	K	272	ILE	2.8
2	L	295	ASP	2.8
1	B	259	THR	2.8
1	B	235	SER	2.8
1	E	556	VAL	2.8
1	J	542	LEU	2.8
2	C	108	LEU	2.8
2	G	84	ASP	2.8
1	F	677	THR	2.8
1	I	705	LEU	2.8
1	E	428	GLY	2.8
1	F	711	VAL	2.8
1	J	181	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	587	VAL	2.8
2	C	265	ASP	2.8
2	H	178	ILE	2.8
1	J	463	LEU	2.8
1	B	249	ARG	2.8
1	I	785	VAL	2.8
2	G	234	LEU	2.8
2	H	200	ARG	2.8
1	A	271	ALA	2.8
1	B	624	MET	2.8
2	L	26	VAL	2.8
1	A	482	SER	2.8
1	E	647	ILE	2.8
2	G	235	THR	2.8
1	B	370	HIS	2.8
1	J	231	PRO	2.8
1	A	497	ASN	2.8
1	A	766	ALA	2.8
1	B	371	ALA	2.8
1	E	234	LEU	2.8
1	E	298	THR	2.8
1	I	159	GLU	2.8
1	I	462	THR	2.8
1	I	676	GLU	2.8
2	K	154	THR	2.8
1	F	368	MET	2.8
1	F	578	ILE	2.8
1	B	359	THR	2.8
1	E	673	GLU	2.8
1	I	323	GLU	2.8
1	J	211	GLN	2.8
2	D	258	VAL	2.8
1	B	234	LEU	2.8
1	I	433	LEU	2.8
1	E	220	ARG	2.8
2	H	269	ASN	2.8
1	E	273	THR	2.8
1	E	535	LEU	2.8
1	I	133	LEU	2.8
2	G	262	MET	2.8
1	A	744	ASN	2.8
1	F	652	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	465	VAL	2.8
2	D	237	ARG	2.8
1	E	414	THR	2.8
2	K	68	LEU	2.8
1	A	137	TRP	2.8
2	H	260	GLY	2.8
1	J	460	LEU	2.8
1	A	768	SER	2.8
1	J	461	ASP	2.8
1	I	436	TRP	2.8
1	F	738	LYS	2.8
1	B	186	GLU	2.7
2	C	269	ASN	2.7
1	A	623	TYR	2.7
1	E	331	LEU	2.7
1	F	732	LEU	2.7
1	J	191	GLU	2.7
2	K	69	ALA	2.7
1	A	347	ASP	2.7
1	E	574	ASP	2.7
1	A	398	GLY	2.7
1	E	256	ARG	2.7
1	J	650	ILE	2.7
1	J	217	PHE	2.7
2	C	137	ALA	2.7
2	C	249	ALA	2.7
1	B	707	LEU	2.7
1	B	502	ILE	2.7
1	I	503	ILE	2.7
1	J	688	SER	2.7
2	H	227	ILE	2.7
1	B	378	LEU	2.7
1	F	551	GLU	2.7
1	F	381	GLN	2.7
1	A	275	ARG	2.7
2	G	160	PHE	2.7
1	F	333	ASP	2.7
1	F	453	ARG	2.7
2	D	84	ASP	2.7
2	L	196	VAL	2.7
1	F	586	PRO	2.7
1	B	783	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	711	VAL	2.7
1	A	259	THR	2.7
1	B	586	PRO	2.7
1	B	701	THR	2.7
1	E	514	LEU	2.7
1	I	741	GLY	2.7
2	G	110	LEU	2.7
2	G	216	LEU	2.7
2	C	251	ALA	2.7
2	K	63	ILE	2.7
1	A	624	MET	2.7
1	E	739	MET	2.7
1	I	552	LEU	2.7
1	J	784	GLU	2.7
2	G	25	SER	2.7
2	G	125	ALA	2.7
2	K	291	TYR	2.7
2	H	33	ASN	2.7
1	B	569	SER	2.7
2	L	253	ILE	2.7
1	B	479	ARG	2.7
1	J	295	LEU	2.7
2	C	150	LEU	2.7
1	E	679	ASN	2.7
1	F	602	ASN	2.7
1	I	244	ALA	2.7
1	A	172	ARG	2.7
1	B	670	PHE	2.7
1	J	596	PHE	2.7
2	C	254	GLN	2.7
2	G	279	LYS	2.7
2	L	52	LYS	2.7
1	I	704	GLY	2.7
1	F	497	ASN	2.7
1	I	587	VAL	2.7
2	D	53	LEU	2.7
2	K	212	LEU	2.7
1	A	313	MET	2.7
1	B	511	ASP	2.7
2	K	155	PRO	2.7
1	A	318	THR	2.7
1	A	792	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	94	PHE	2.7
1	I	391	GLN	2.7
2	H	266	ARG	2.7
1	J	355	LEU	2.7
2	D	50	GLY	2.7
2	K	150	LEU	2.7
1	F	360	ALA	2.7
2	H	206	GLY	2.7
1	B	752	HIS	2.7
1	J	296	ASP	2.7
2	C	200	ARG	2.7
2	C	259	ASN	2.7
1	A	712	ALA	2.7
1	A	518	GLY	2.7
2	K	99	LEU	2.7
1	A	571	THR	2.7
1	E	342	LEU	2.7
1	F	556	VAL	2.7
2	H	202	VAL	2.7
1	A	204	PHE	2.7
1	I	634	ALA	2.7
1	I	597	ILE	2.7
2	C	65	LYS	2.7
2	C	268	ILE	2.7
1	B	221	ASP	2.6
1	J	700	SER	2.7
2	C	207	GLN	2.6
1	B	732	LEU	2.6
1	E	269	MET	2.6
1	E	745	VAL	2.6
1	A	218	GLY	2.6
1	B	184	PHE	2.6
2	L	27	VAL	2.6
2	H	144	THR	2.6
1	B	258	ILE	2.6
1	F	213	LEU	2.6
1	I	339	GLN	2.6
1	J	131	ASN	2.6
1	J	291	LEU	2.6
1	A	711	VAL	2.6
1	E	345	VAL	2.6
1	I	713	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	329	VAL	2.6
2	L	329	VAL	2.6
1	A	192	GLY	2.6
2	K	157	ARG	2.6
1	B	461	ASP	2.6
1	F	397	MET	2.6
2	L	263	MET	2.6
1	F	401	ALA	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	B	579	ARG	2.6
1	J	361	ARG	2.6
1	F	680	ILE	2.6
2	G	243	PRO	2.6
1	E	521	LEU	2.6
1	B	714	ASN	2.6
1	F	589	GLU	2.6
2	G	137	ALA	2.6
1	E	558	LEU	2.6
1	F	230	ALA	2.6
1	F	433	LEU	2.6
1	I	338	LEU	2.6
1	I	426	ALA	2.6
2	L	45	ASP	2.6
1	E	545	SER	2.6
1	E	176	ALA	2.6
2	C	289	VAL	2.6
1	E	189	LEU	2.6
1	I	234	LEU	2.6
1	I	715	LEU	2.6
2	K	28	LYS	2.6
1	B	361	ARG	2.6
1	A	365	LEU	2.6
2	D	109	THR	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	E	259	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	280	THR	2.6
2	K	268	ILE	2.6
1	A	449	ARG	2.6
1	A	648	GLY	2.6
1	J	518	GLY	2.6
1	B	547	SER	2.6
1	J	613	THR	2.6
1	E	608	ARG	2.6
1	J	343	ARG	2.6
1	F	650	ILE	2.6
1	J	487	ILE	2.6
2	C	146	GLU	2.6
1	I	712	ALA	2.6
2	K	279	LYS	2.6
1	F	567	TYR	2.6
1	B	418	LEU	2.6
1	F	266	SER	2.6
1	F	190	ILE	2.6
1	F	579	ARG	2.6
1	I	501	TYR	2.6
2	C	213	GLY	2.6
1	I	699	THR	2.6
1	B	211	GLN	2.6
1	J	573	ILE	2.6
2	C	288	PHE	2.6
2	G	298	GLN	2.6
1	F	706	SER	2.6
1	J	548	ALA	2.6
2	C	224	ALA	2.6
1	J	340	PRO	2.6
2	C	255	TYR	2.6
1	A	263	GLU	2.6
1	B	178	LEU	2.6
2	D	200	ARG	2.6
2	H	284	GLN	2.6
1	F	505	GLU	2.6
1	J	585	HIS	2.6
2	G	204	GLU	2.6
1	A	537	PRO	2.6
2	L	44	ILE	2.6
1	I	348	LEU	2.6
2	H	162	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	721	ALA	2.6
1	J	522	ALA	2.6
1	E	297	SER	2.6
2	K	102	ILE	2.6
2	K	322	ILE	2.6
2	C	110	LEU	2.6
2	D	148	LEU	2.6
1	J	742	VAL	2.6
2	L	316	ARG	2.6
1	A	563	TYR	2.6
1	F	580	ILE	2.6
1	B	504	PRO	2.6
2	H	163	THR	2.6
1	A	191	GLU	2.5
1	F	557	ASN	2.5
1	B	420	ARG	2.5
1	B	498	ALA	2.5
1	E	217	PHE	2.5
1	F	229	ASN	2.5
2	D	146	GLU	2.5
2	G	53	LEU	2.5
2	K	64	LYS	2.5
2	L	146	GLU	2.5
1	A	458	THR	2.5
1	B	524	GLU	2.5
1	E	374	GLN	2.5
1	E	467	PHE	2.5
1	A	565	LEU	2.5
1	E	542	LEU	2.5
1	I	610	LEU	2.5
2	G	236	LEU	2.5
2	H	320	ASP	2.5
1	F	603	LEU	2.5
1	J	351	ILE	2.5
1	J	443	ALA	2.5
2	G	41	ARG	2.5
2	K	331	GLN	2.5
1	E	277	LEU	2.5
1	F	733	THR	2.5
2	L	133	THR	2.5
1	F	191	GLU	2.5
1	F	312	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	355	LEU	2.5
1	B	565	LEU	2.5
1	J	732	LEU	2.5
1	A	331	LEU	2.5
1	B	228	GLU	2.5
1	B	626	GLN	2.5
2	C	97	GLU	2.5
1	I	609	MET	2.5
2	G	290	LEU	2.5
1	A	555	LEU	2.5
1	B	352	LEU	2.5
1	B	423	GLY	2.5
1	B	715	LEU	2.5
1	A	368	MET	2.5
1	F	143	PHE	2.5
1	J	433	LEU	2.5
1	J	689	LEU	2.5
2	H	219	ALA	2.5
2	G	27	VAL	2.5
1	F	212	GLN	2.5
1	J	228	GLU	2.5
2	K	151	PHE	2.5
1	F	761	SER	2.5
1	F	782	PRO	2.5
1	B	558	LEU	2.5
1	J	300	THR	2.5
1	J	466	GLY	2.5
1	A	530	GLU	2.5
1	E	548	ALA	2.5
1	E	694	GLU	2.5
1	F	728	HIS	2.5
1	A	581	THR	2.5
1	I	454	GLU	2.5
1	B	346	GLY	2.5
1	B	519	LYS	2.5
1	J	739	MET	2.5
1	E	527	LEU	2.5
1	E	731	GLU	2.5
2	D	31	VAL	2.5
2	H	270	HIS	2.5
2	H	318	VAL	2.5
2	K	318	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	220	ARG	2.5
1	I	754	ASP	2.5
1	F	531	LEU	2.5
2	C	188	ASN	2.5
2	C	284	GLN	2.5
1	E	577	GLY	2.5
1	I	632	LEU	2.5
1	E	683	ASN	2.5
1	E	161	ALA	2.5
1	I	716	ALA	2.5
1	J	320	VAL	2.5
1	J	470	VAL	2.5
2	D	246	THR	2.5
2	G	73	ALA	2.5
2	L	73	ALA	2.5
2	G	52	LYS	2.5
2	K	281	GLY	2.5
1	J	250	THR	2.5
2	L	227	ILE	2.5
1	B	717	ASN	2.5
2	K	65	LYS	2.5
2	L	57	ARG	2.5
1	E	623	TYR	2.5
1	J	201	LEU	2.5
2	H	319	HIS	2.5
1	F	535	LEU	2.5
2	D	147	VAL	2.4
1	B	372	PHE	2.4
1	B	674	MET	2.4
1	E	511	ASP	2.4
1	E	513	VAL	2.4
1	F	334	PHE	2.4
1	F	591	VAL	2.4
1	J	169	GLU	2.4
2	D	26	VAL	2.4
1	E	344	GLN	2.4
1	A	230	ALA	2.4
1	F	681	LEU	2.4
1	I	783	LYS	2.4
2	H	288	PHE	2.4
2	K	259	ASN	2.4
1	A	634	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	149	ASP	2.4
1	A	501	TYR	2.4
1	J	717	ASN	2.4
2	L	134	VAL	2.4
1	A	521	LEU	2.4
1	B	421	ASP	2.4
1	E	646	GLU	2.4
1	F	436	TRP	2.4
2	D	262	MET	2.4
2	H	27	VAL	2.4
1	I	213	LEU	2.4
2	C	52	LYS	2.4
2	G	296	PRO	2.4
1	J	259	THR	2.4
1	J	767	ALA	2.4
2	G	255	TYR	2.4
2	L	322	ILE	2.4
2	L	223	GLN	2.4
1	F	426	ALA	2.4
1	J	232	ARG	2.4
2	D	56	ILE	2.4
1	A	767	ALA	2.4
1	E	372	PHE	2.4
1	J	459	GLY	2.4
1	E	578	ILE	2.4
1	E	594	GLU	2.4
1	J	457	ARG	2.4
2	H	287	ALA	2.4
1	F	408	GLU	2.4
1	J	513	VAL	2.4
2	C	225	LEU	2.4
2	H	35	LEU	2.4
1	A	161	ALA	2.4
1	E	522	ALA	2.4
1	F	430	ASN	2.4
2	G	46	ILE	2.4
1	B	341	VAL	2.4
1	J	574	ASP	2.4
1	B	671	MET	2.4
2	C	326	VAL	2.4
1	I	538	HIS	2.4
1	J	533	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	263	MET	2.4
2	K	200	ARG	2.4
1	A	425	ILE	2.4
2	L	53	LEU	2.4
1	E	337	GLY	2.4
1	A	534	LEU	2.4
1	A	656	ARG	2.4
2	G	70	LEU	2.4
2	K	54	ILE	2.4
1	J	166	MET	2.4
1	E	236	ALA	2.4
1	E	746	HIS	2.4
2	H	277	GLU	2.4
1	F	225	PHE	2.4
1	I	427	SER	2.4
1	E	651	ASP	2.4
1	F	246	CYS	2.4
1	J	420	ARG	2.4
2	L	115	ALA	2.4
1	A	516	SER	2.4
2	K	103	SER	2.4
1	J	593	ASN	2.4
1	A	536	LEU	2.3
1	F	345	VAL	2.3
1	I	492	ARG	2.3
1	I	586	PRO	2.3
2	L	287	ALA	2.3
1	A	233	GLY	2.3
1	B	252	LEU	2.3
1	F	674	MET	2.3
1	J	364	ASP	2.3
2	D	150	LEU	2.3
2	C	294	ILE	2.3
1	E	310	TRP	2.3
1	E	598	ALA	2.3
1	A	277	LEU	2.3
1	A	582	GLU	2.3
1	E	174	ASN	2.3
1	I	508	GLU	2.3
2	D	228	GLU	2.3
2	H	161	LEU	2.3
1	F	800	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	214	ALA	2.3
1	B	476	GLN	2.3
1	B	601	LEU	2.3
1	E	203	GLU	2.3
1	I	530	GLU	2.3
2	D	46	ILE	2.3
1	E	554	VAL	2.3
1	I	457	ARG	2.3
2	H	29	GLU	2.3
1	F	375	LEU	2.3
2	C	147	VAL	2.3
2	G	287	ALA	2.3
2	C	322	ILE	2.3
2	K	93	GLY	2.3
1	A	505	GLU	2.3
1	A	645	VAL	2.3
1	F	448	GLU	2.3
2	L	46	ILE	2.3
2	C	132	VAL	2.3
1	I	706	SER	2.3
1	I	245	LYS	2.3
2	L	109	THR	2.3
1	F	364	ASP	2.3
2	D	111	THR	2.3
1	E	671	MET	2.3
2	L	195	ILE	2.3
2	L	277	GLU	2.3
2	H	199	TYR	2.3
2	K	290	LEU	2.3
1	J	172	ARG	2.3
2	H	34	SER	2.3
2	H	261	ARG	2.3
1	E	711	VAL	2.3
1	E	744	ASN	2.3
1	J	698	GLY	2.3
2	H	85	ASP	2.3
2	D	88	ALA	2.3
1	A	558	LEU	2.3
1	J	273	THR	2.3
1	A	184	PHE	2.3
1	I	199	ARG	2.3
1	A	138	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	612	ILE	2.3
1	I	191	GLU	2.3
1	A	162	ASP	2.3
2	C	115	ALA	2.3
2	D	261	ARG	2.3
2	K	210	ARG	2.3
1	B	335	THR	2.3
1	E	132	LEU	2.3
1	E	645	VAL	2.3
2	H	258	VAL	2.3
1	B	137	TRP	2.3
1	I	343	ARG	2.3
2	H	295	ASP	2.3
1	J	184	PHE	2.3
1	E	144	GLY	2.3
1	I	255	ILE	2.3
1	B	507	LYS	2.3
1	I	674	MET	2.3
1	J	139	ASP	2.3
2	K	247	THR	2.3
1	F	546	ALA	2.3
2	H	120	ALA	2.3
1	B	496	LYS	2.3
1	E	770	SER	2.3
1	A	733	THR	2.3
1	E	180	TYR	2.3
1	E	219	THR	2.3
1	I	431	GLU	2.3
1	I	627	THR	2.3
2	K	285	GLN	2.3
1	J	617	MET	2.3
1	F	429	TYR	2.3
1	B	153	GLY	2.3
1	I	689	LEU	2.3
1	J	540	GLU	2.3
1	B	138	GLN	2.3
1	B	422	GLY	2.3
1	F	382	LEU	2.3
2	H	292	LEU	2.3
1	I	451	GLU	2.3
1	A	586	PRO	2.3
1	B	199	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	22	ARG	2.3
1	E	658	GLY	2.2
1	I	772	GLY	2.2
2	G	260	GLY	2.2
1	J	545	SER	2.2
2	C	257	TYR	2.2
1	B	349	GLU	2.2
1	E	377	GLU	2.2
1	F	165	THR	2.2
1	I	532	PHE	2.2
1	J	354	ARG	2.2
2	K	50	GLY	2.2
2	L	69	ALA	2.2
1	B	580	ILE	2.2
1	F	162	ASP	2.2
1	F	413	ASP	2.2
1	I	295	LEU	2.2
2	D	107	ARG	2.2
2	H	32	GLU	2.2
1	J	368	MET	2.2
2	D	298	GLN	2.2
2	H	26	VAL	2.2
2	G	288	PHE	2.2
1	B	548	ALA	2.2
2	D	219	ALA	2.2
1	A	525	LYS	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	H	28	LYS	2.2
1	A	779	ALA	2.2
1	A	500	ARG	2.2
1	F	273	THR	2.2
1	B	209	ALA	2.2
1	F	710	ALA	2.2
1	B	384	THR	2.2
1	J	318	THR	2.2
2	L	208	LYS	2.2
1	A	644	LYS	2.2
1	B	562	ALA	2.2
2	H	271	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	638	SER	2.2
1	I	184	PHE	2.2
1	E	369	ARG	2.2
1	F	704	GLY	2.2
1	I	328	ILE	2.2
2	C	226	ALA	2.2
1	J	730	PHE	2.2
2	D	30	LEU	2.2
2	D	250	LEU	2.2
1	A	631	ALA	2.2
1	B	325	GLN	2.2
1	B	493	GLN	2.2
1	E	371	ALA	2.2
1	F	767	ALA	2.2
2	D	87	GLU	2.2
2	L	88	ALA	2.2
1	A	629	LEU	2.2
1	A	551	GLU	2.2
1	E	360	ALA	2.2
1	E	515	THR	2.2
1	F	138	GLN	2.2
1	J	713	GLU	2.2
1	E	732	LEU	2.2
2	G	151	PHE	2.2
1	A	225	PHE	2.2
1	A	459	GLY	2.2
1	B	623	TYR	2.2
1	B	213	LEU	2.2
1	I	192	GLY	2.2
1	I	205	GLU	2.2
1	J	244	ALA	2.2
2	H	273	ARG	2.2
2	H	286	PRO	2.2
2	K	37	ALA	2.2
2	C	35	LEU	2.2
1	A	647	ILE	2.2
2	G	31	VAL	2.2
2	L	255	TYR	2.2
1	F	770	SER	2.2
1	A	788	ARG	2.2
2	K	233	ASP	2.2
2	C	248	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	430	ASN	2.2
1	J	714	ASN	2.2
1	F	253	PRO	2.2
1	F	449	ARG	2.2
1	I	252	LEU	2.2
1	I	418	LEU	2.2
2	C	295	ASP	2.2
2	K	158	ARG	2.2
2	K	295	ASP	2.2
2	D	322	ILE	2.2
1	J	432	GLU	2.2
2	G	48	ARG	2.2
2	C	31	VAL	2.2
1	A	222	LEU	2.2
1	F	516	SER	2.2
2	H	315	SER	2.2
2	K	25	SER	2.2
1	F	420	ARG	2.2
1	E	682	HIS	2.2
2	D	25	SER	2.2
1	B	500	ARG	2.2
1	B	654	PHE	2.2
1	F	159	GLU	2.2
1	F	414	THR	2.2
1	J	317	ASP	2.2
2	C	172	ASP	2.2
1	J	534	LEU	2.1
1	I	344	GLN	2.1
1	J	517	LYS	2.1
2	G	331	GLN	2.1
1	A	436	TRP	2.1
1	A	566	ASN	2.1
1	F	658	GLY	2.1
2	L	187	ILE	2.1
1	A	517	LYS	2.1
1	E	326	GLN	2.1
2	L	114	THR	2.1
1	E	735	LEU	2.1
1	J	229	ASN	2.1
1	I	299	VAL	2.1
2	C	292	LEU	2.1
2	G	196	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	561	ARG	2.1
2	K	101	SER	2.1
1	E	368	MET	2.1
1	E	296	ASP	2.1
1	E	375	LEU	2.1
1	F	517	LYS	2.1
1	F	757	ALA	2.1
1	J	292	ALA	2.1
1	I	629	LEU	2.1
2	C	171	ILE	2.1
1	F	233	GLY	2.1
2	G	157	ARG	2.1
2	L	91	SER	2.1
2	K	257	TYR	2.1
1	E	517	LYS	2.1
2	K	260	GLY	2.1
1	A	584	ARG	2.1
1	A	615	PRO	2.1
1	A	782	PRO	2.1
1	I	790	ARG	2.1
1	F	462	THR	2.1
1	A	243	TYR	2.1
1	B	489	TYR	2.1
1	B	567	TYR	2.1
1	I	149	ASP	2.1
2	K	242	ASP	2.1
1	B	593	ASN	2.1
1	A	491	ARG	2.1
1	F	352	LEU	2.1
1	I	256	ARG	2.1
1	I	549	LEU	2.1
1	F	310	TRP	2.1
2	L	137	ALA	2.1
2	D	28	LYS	2.1
1	I	650	ILE	2.1
1	A	397	MET	2.1
1	B	542	LEU	2.1
1	I	565	LEU	2.1
1	J	398	GLY	2.1
2	C	262	MET	2.1
2	G	111	THR	2.1
1	E	415	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	203	PRO	2.1
1	B	454	GLU	2.1
1	A	583	GLY	2.1
1	J	687	TYR	2.1
2	H	259	ASN	2.1
2	K	100	ALA	2.1
1	B	735	LEU	2.1
1	J	385	VAL	2.1
2	L	200	ARG	2.1
1	F	313	MET	2.1
1	F	464	LYS	2.1
1	J	536	LEU	2.1
1	J	442	GLY	2.1
1	A	424	VAL	2.1
1	F	167	ALA	2.1
1	J	316	ARG	2.1
2	H	201	ALA	2.1
2	L	244	ASN	2.1
1	B	364	ASP	2.1
1	E	385	VAL	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
2	K	192	ASN	2.1
1	F	748	ASP	2.1
2	C	299	VAL	2.1
2	L	184	ASP	2.1
1	B	407	LEU	2.1
1	E	457	ARG	2.1
1	A	245	LYS	2.1
1	I	268	ILE	2.1
1	A	559	ALA	2.1
1	E	764	ASP	2.1
2	C	252	GLU	2.1
1	J	365	LEU	2.1
1	B	641	PRO	2.1
1	B	365	LEU	2.1
1	B	369	ARG	2.1
1	I	702	TYR	2.1
2	C	270	HIS	2.1
1	I	428	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	625	ARG	2.1
1	I	363	ARG	2.1
1	J	311	LEU	2.1
2	G	88	ALA	2.1
1	B	145	TYR	2.1
2	D	160	PHE	2.1
1	A	174	ASN	2.1
1	F	756	ILE	2.1
1	I	534	LEU	2.0
2	L	145	LEU	2.0
1	A	205	GLU	2.0
1	B	180	TYR	2.0
1	I	654	PHE	2.0
1	B	277	LEU	2.0
1	E	393	LEU	2.0
1	F	403	LEU	2.0
2	D	184	ASP	2.0
2	H	218	THR	2.0
1	E	235	SER	2.0
1	J	258	ILE	2.0
1	A	785	VAL	2.0
1	J	521	LEU	2.0
2	D	221	LEU	2.0
1	F	422	GLY	2.0
2	K	231	HIS	2.0
1	B	231	PRO	2.0
1	E	538	HIS	2.0
1	B	523	LEU	2.0
2	H	97	GLU	2.0
1	I	220	ARG	2.0
1	B	356	ALA	2.0
1	E	766	ALA	2.0
1	F	184	PHE	2.0
2	L	162	ARG	2.0
1	F	628	ALA	2.0
1	I	259	THR	2.0
2	H	24	ALA	2.0
2	G	91	SER	2.0
1	A	154	ARG	2.0
1	A	532	PHE	2.0
1	E	600	PRO	2.0
1	I	407	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	606	GLN	2.0
1	E	138	GLN	2.0
1	E	533	ASP	2.0
2	K	44	ILE	2.0
1	B	410	ALA	2.0
1	F	311	LEU	2.0
1	F	365	LEU	2.0
1	F	496	LYS	2.0
1	J	331	LEU	2.0
1	J	738	LYS	2.0
2	G	69	ALA	2.0
1	B	229	ASN	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	791	GLN	2.0
1	E	356	ALA	2.0
1	I	291	LEU	2.0
1	J	130	ASP	2.0
2	C	315	SER	2.0
1	A	321	LEU	2.0
1	A	552	LEU	2.0
1	A	687	TYR	2.0
1	I	561	ARG	2.0
2	K	62	GLY	2.0
2	K	132	VAL	2.0
1	I	680	ILE	2.0
1	A	511	ASP	2.0
1	J	735	LEU	2.0
2	K	236	LEU	2.0
1	J	278	GLU	2.0
2	G	158	ARG	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 ⓘ

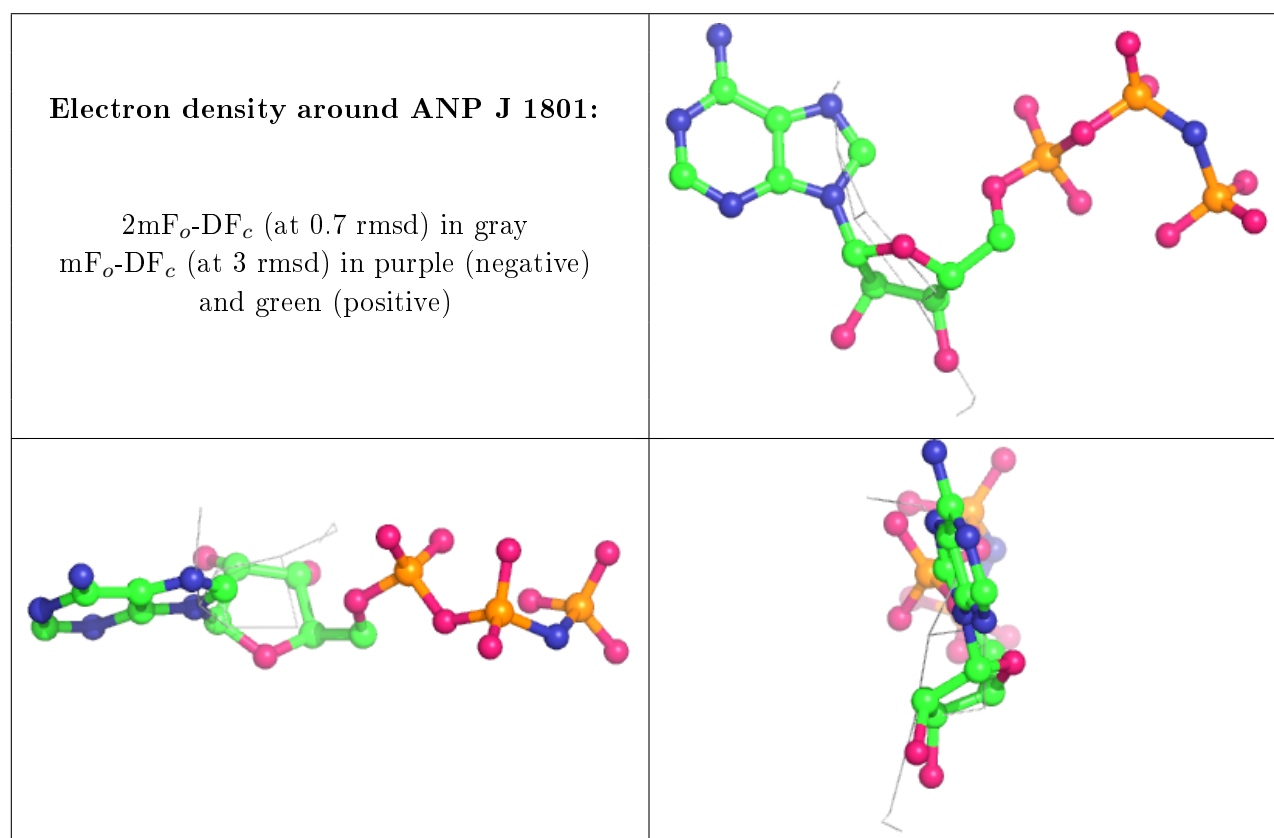
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ANP	J	1801	31/31	0.64	0.49	193,199,212,213	0
3	ANP	E	1801	31/31	0.70	0.51	204,216,227,232	0
3	ANP	I	1801	31/31	0.70	0.41	177,180,186,187	0
3	ANP	B	1801	31/31	0.72	0.31	165,174,179,181	0
3	ANP	A	1801	31/31	0.81	0.51	156,164,170,171	0
3	ANP	F	1801	31/31	0.85	0.30	154,162,169,174	0

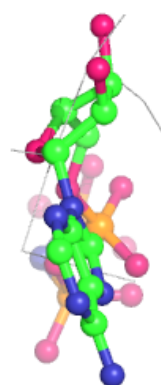
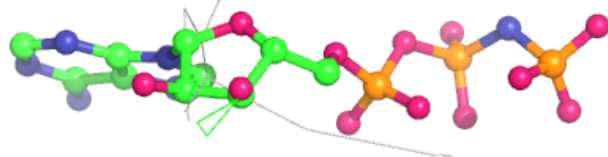
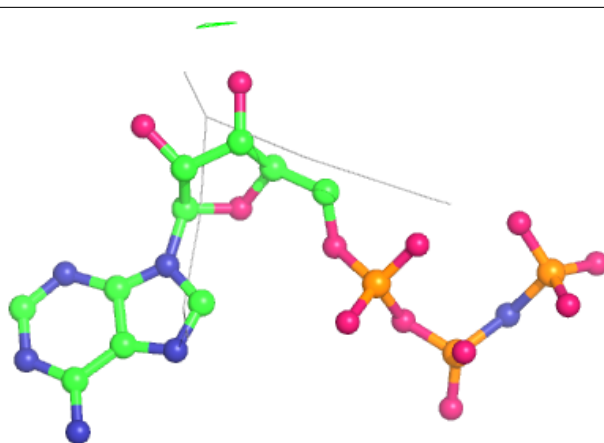
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



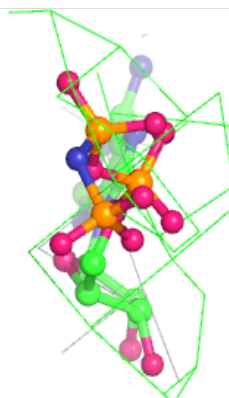
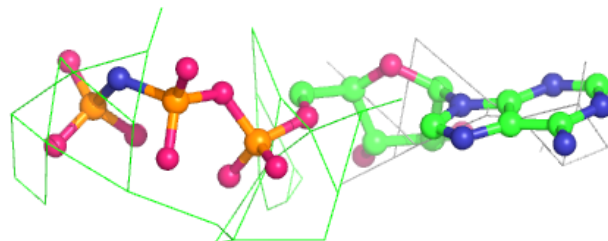
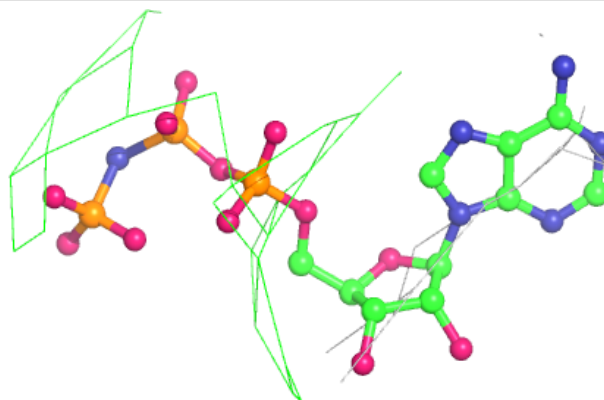


**Electron density around ANP E 1801:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

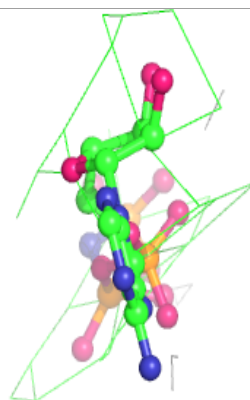
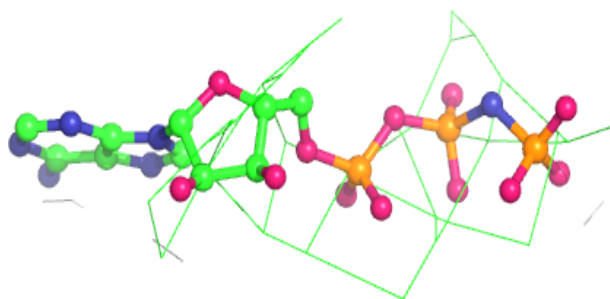
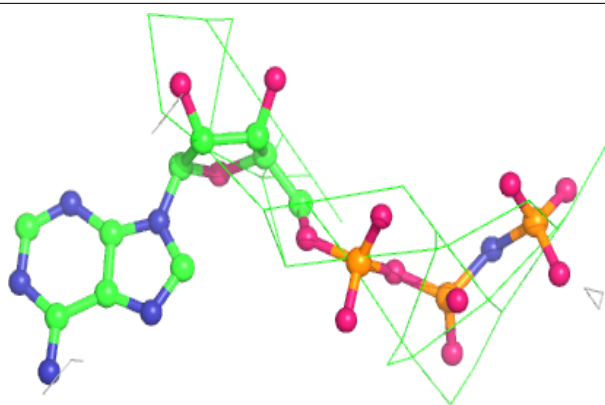
**Electron density around ANP I 1801:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

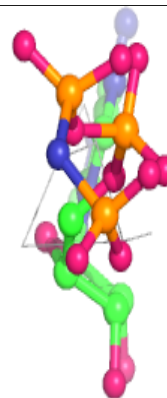
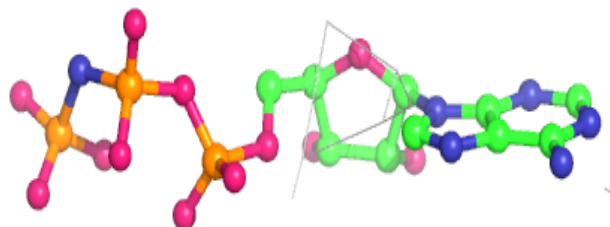
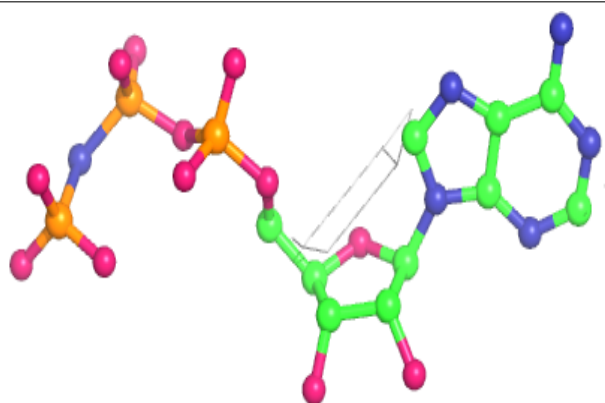


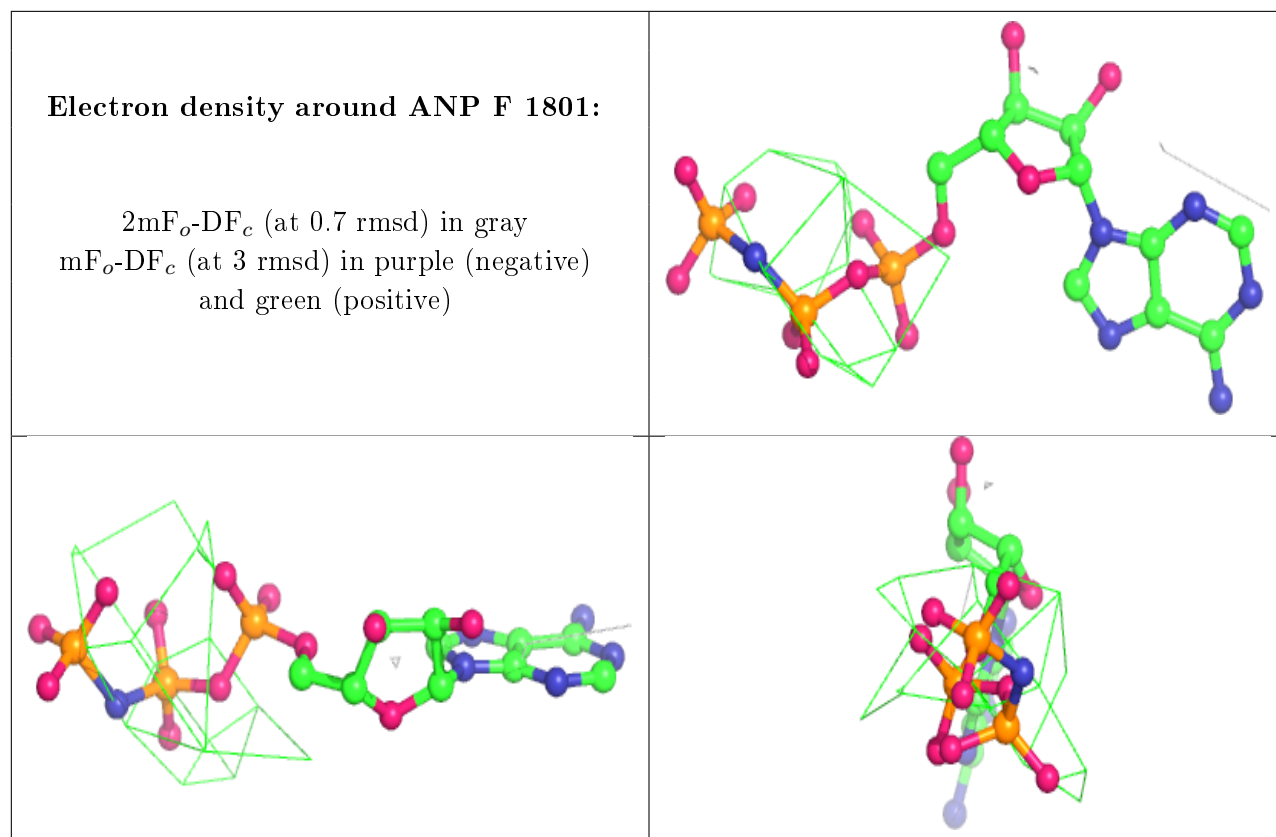
**Electron density around ANP B 1801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ANP A 1801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.