



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:02 PM GMT

PDB ID : 5AKC
Title : MutS in complex with the N-terminal domain of MutL - crystal form 2
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 : 6.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

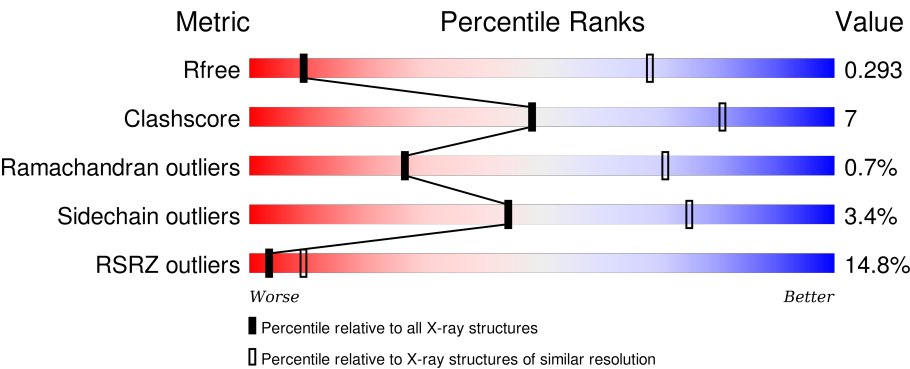
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	1014 (9.50-3.66)
Clashscore	102246	1062 (9.50-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	800	<div><div>10%</div><div><div></div><div>74%</div><div>8%</div><div>•</div><div>17%</div></div></div>
1	B	800	<div><div>8%</div><div><div></div><div>72%</div><div>10%</div><div>•</div><div>17%</div></div></div>
1	E	800	<div><div>11%</div><div><div></div><div>72%</div><div>10%</div><div>•</div><div>17%</div></div></div>
1	F	800	<div><div>8%</div><div><div></div><div>71%</div><div>11%</div><div>•</div><div>17%</div></div></div>
1	I	800	<div><div>14%</div><div><div></div><div>71%</div><div>12%</div><div>•</div><div>17%</div></div></div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	E	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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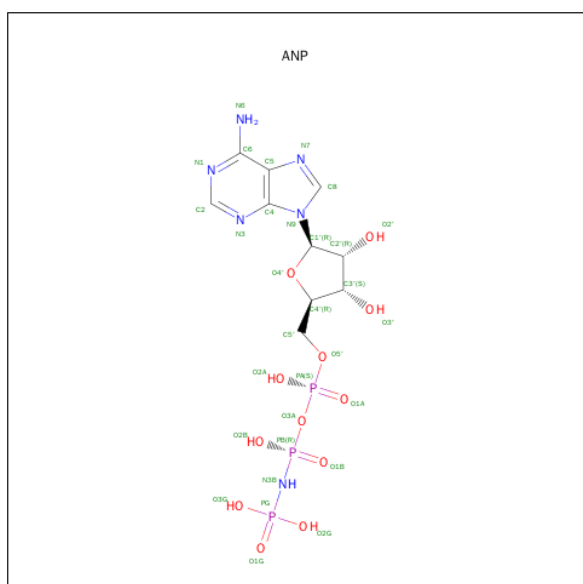
Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	SER	-	EXPRESSION TAG	UNP P23367
H	-8	SER	-	EXPRESSION TAG	UNP P23367
H	-7	GLY	-	EXPRESSION TAG	UNP P23367
H	-6	LEU	-	EXPRESSION TAG	UNP P23367
H	-5	VAL	-	EXPRESSION TAG	UNP P23367
H	-4	PRO	-	EXPRESSION TAG	UNP P23367
H	-3	ARG	-	EXPRESSION TAG	UNP P23367
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: $C_{10}H_{17}N_6O_{12}P_3$).

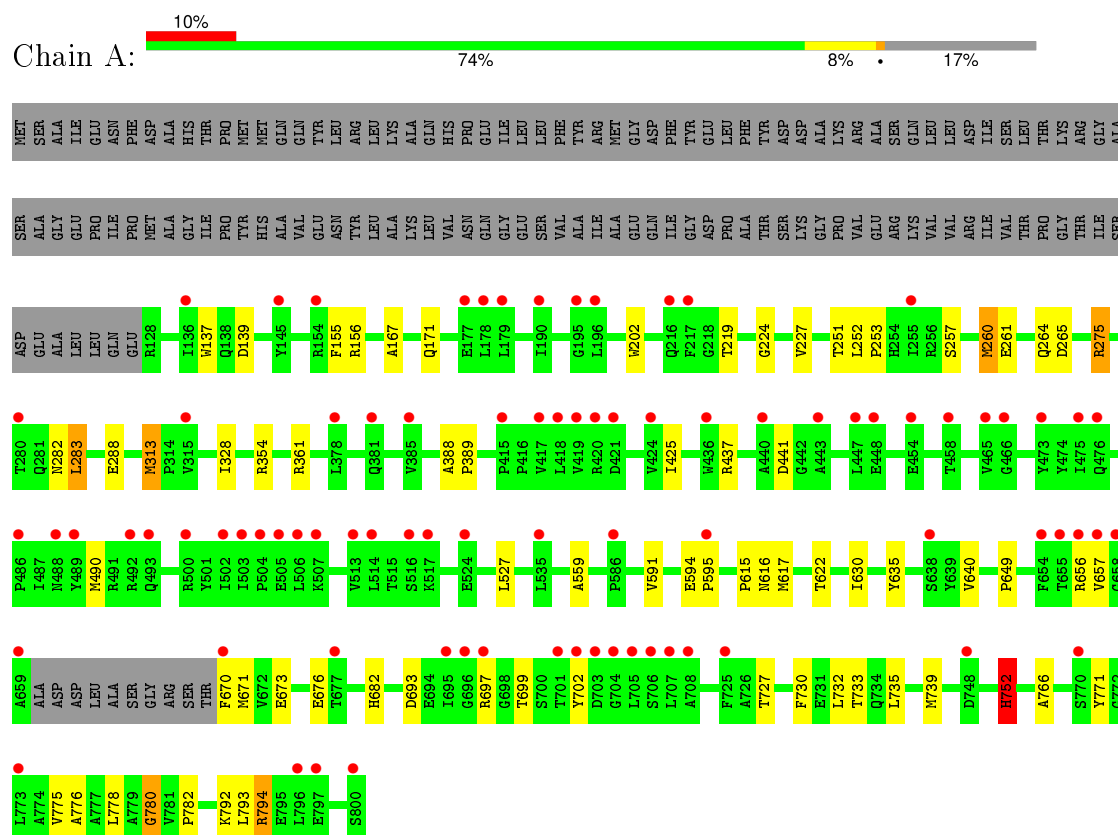


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

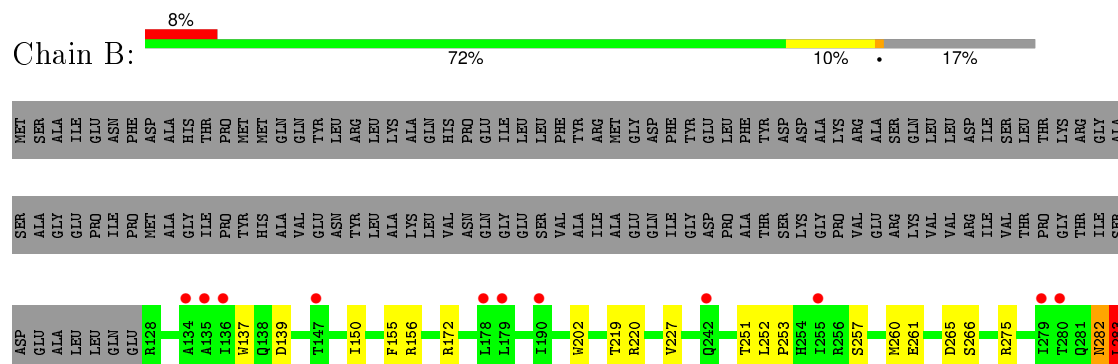
3 Residue-property plots [i](#)

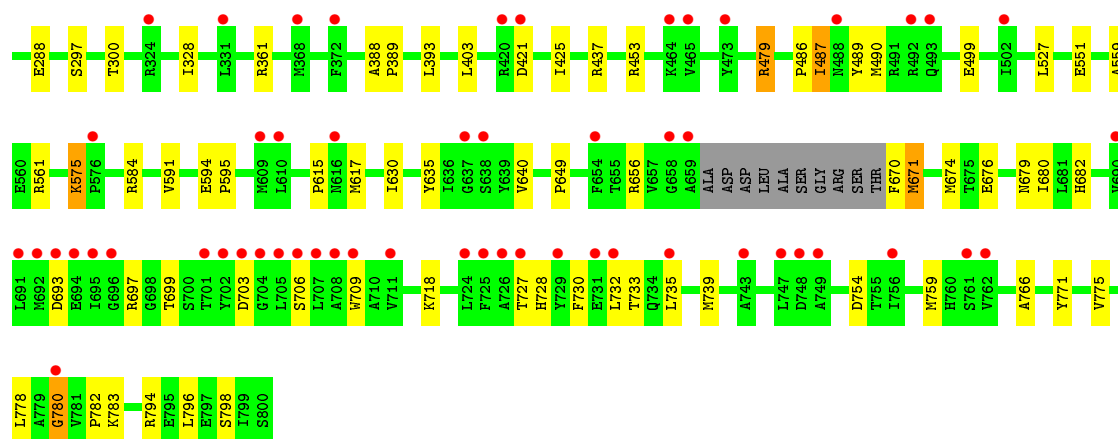
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

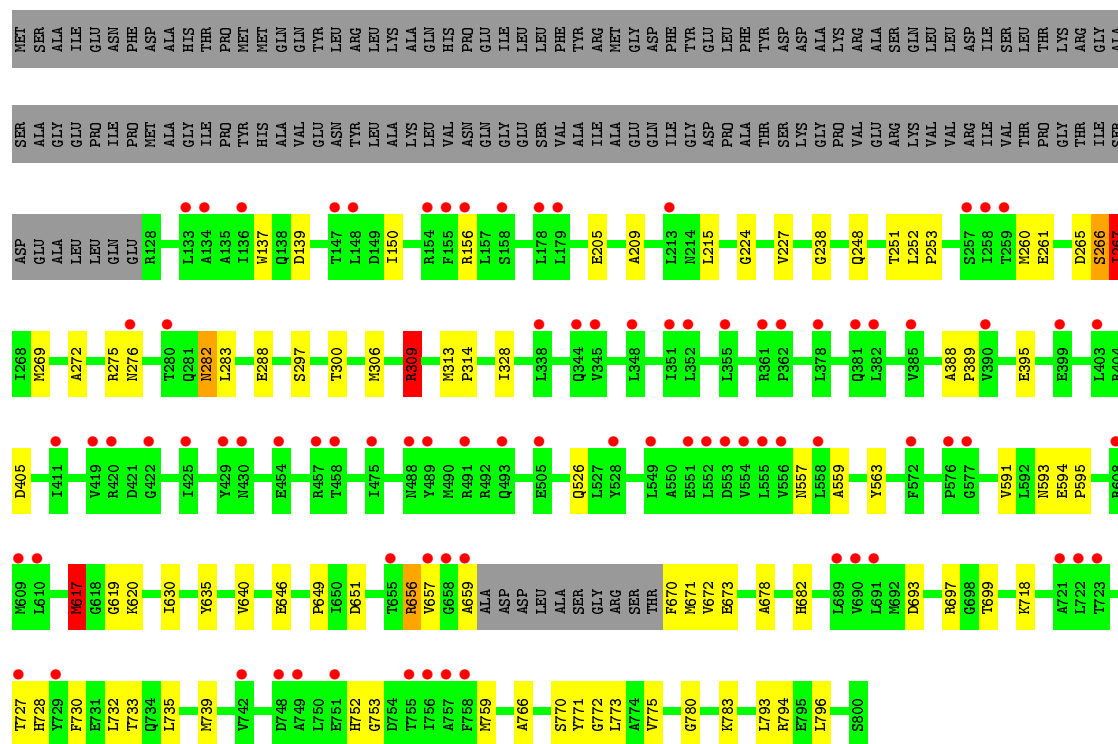
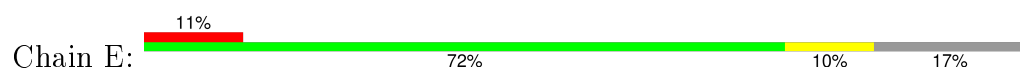


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

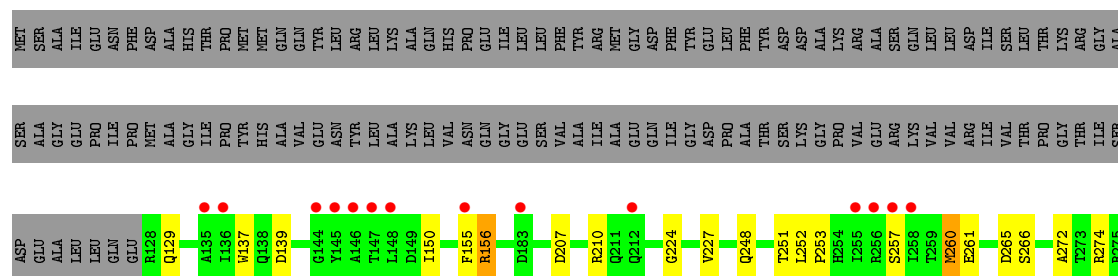


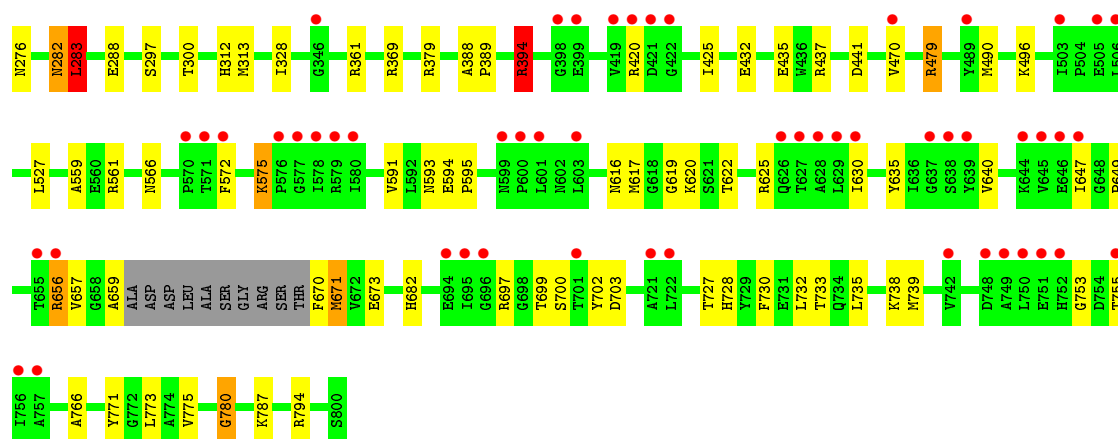


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

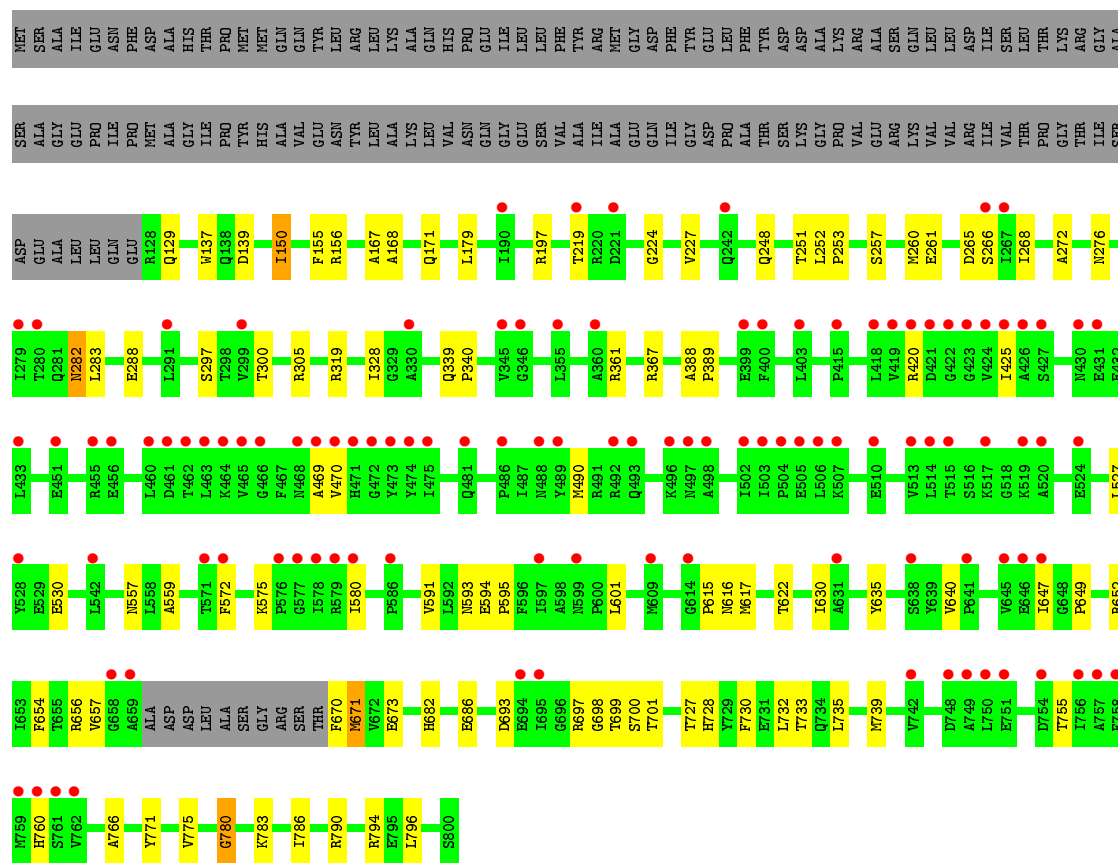


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

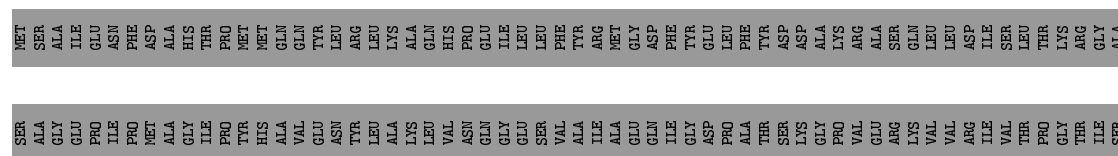


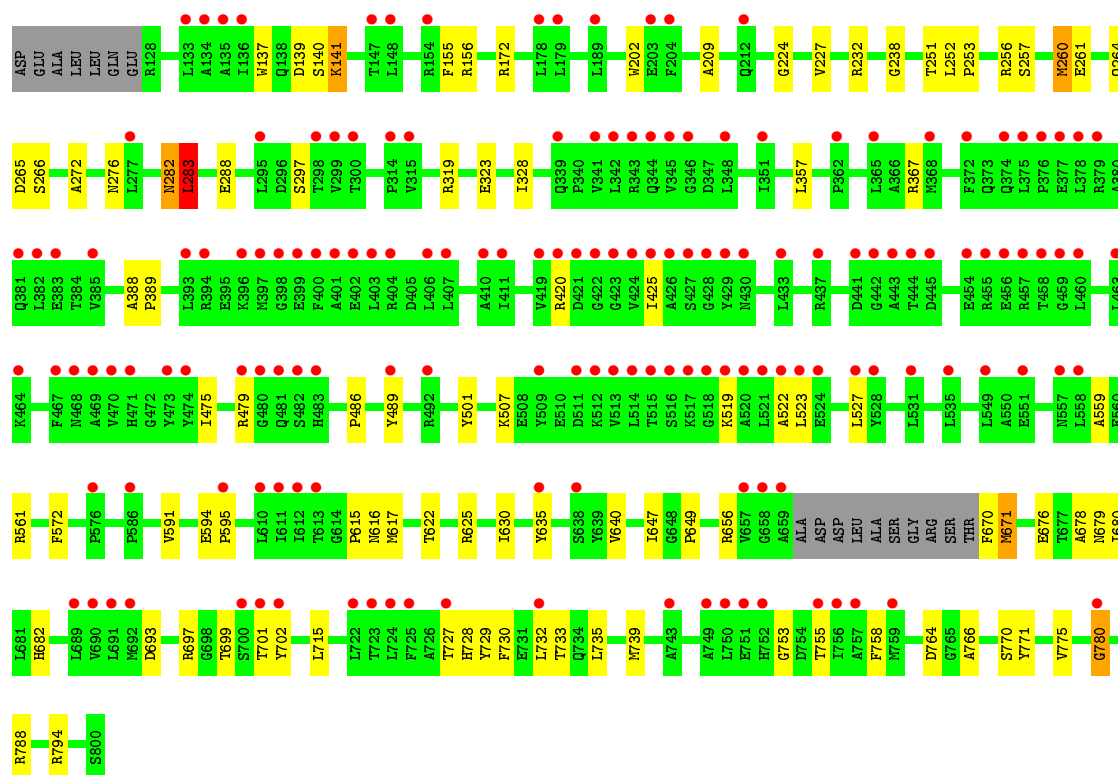


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

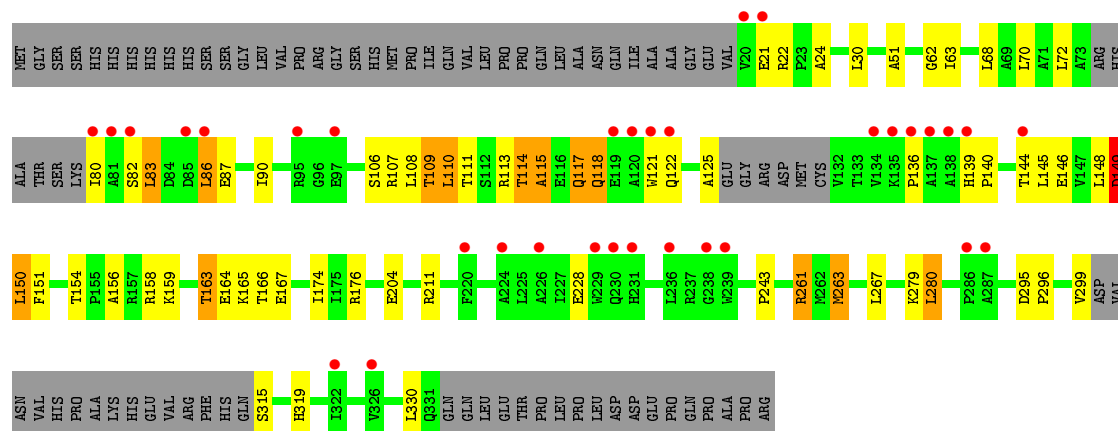


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

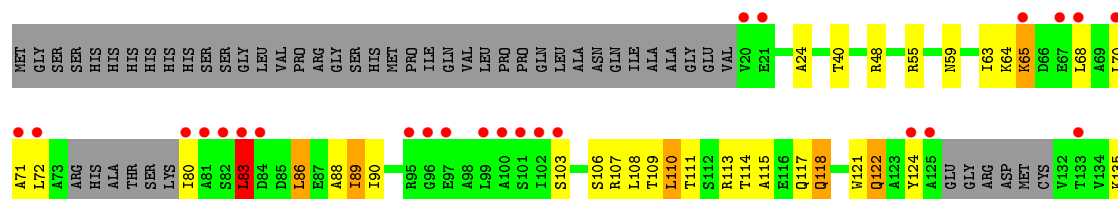


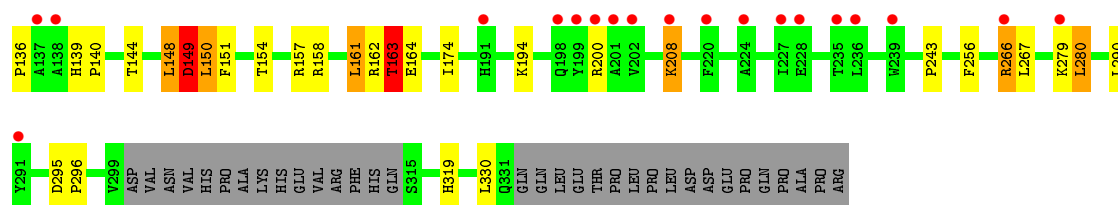


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

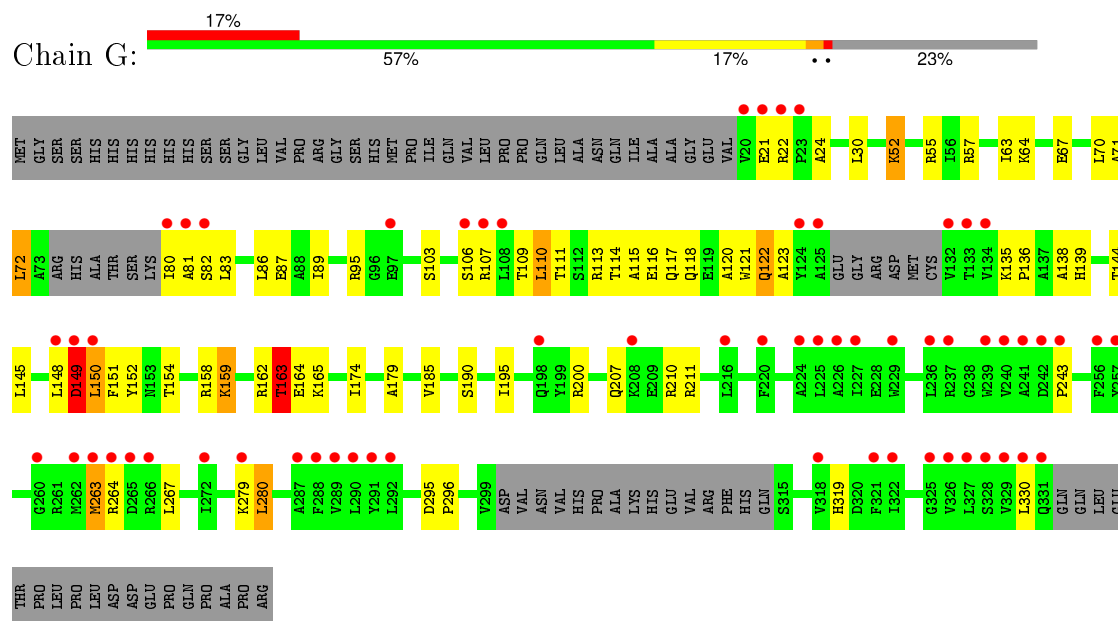


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

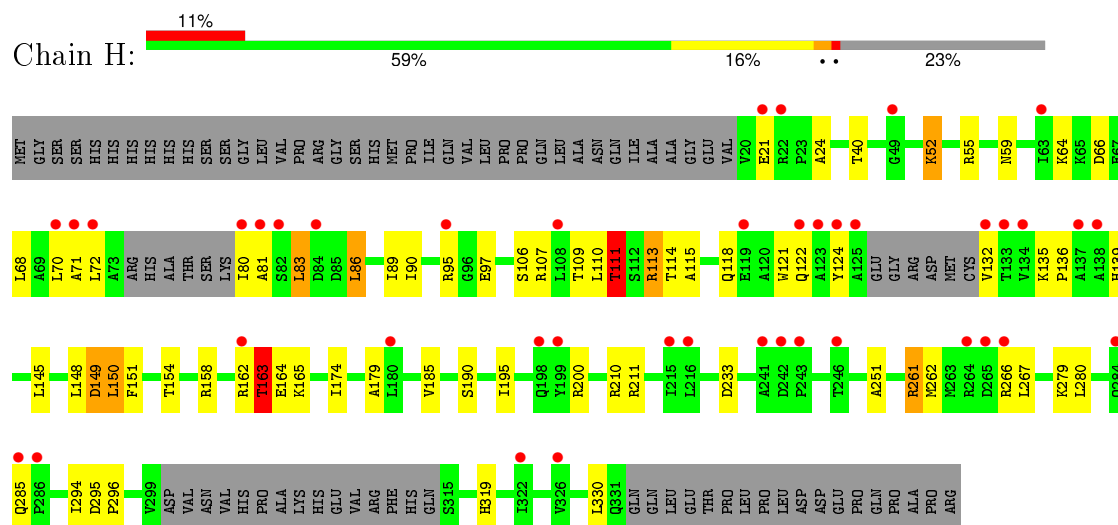


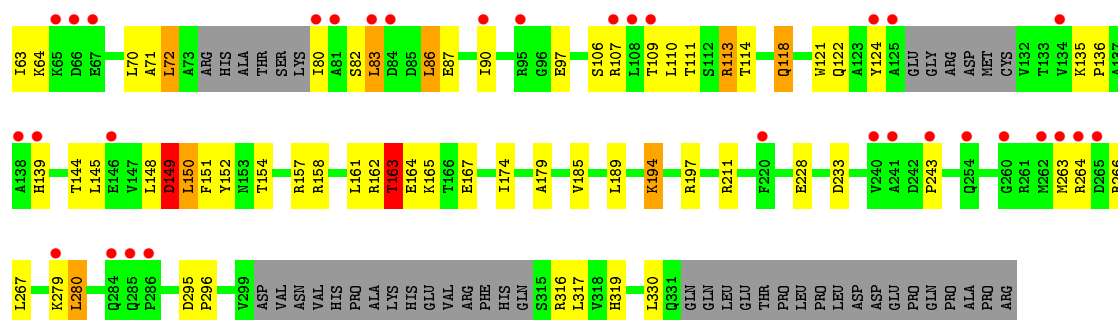


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

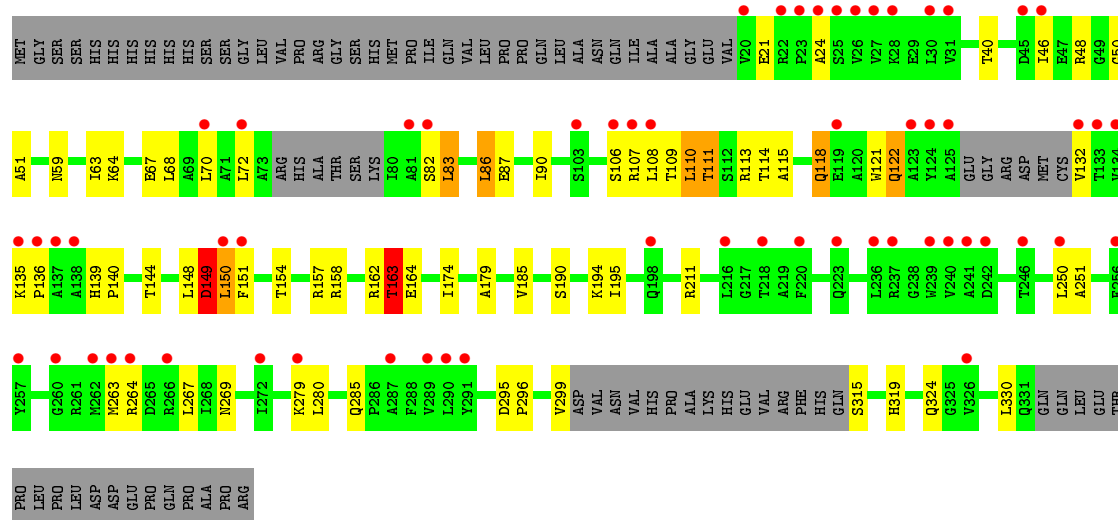


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL





• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	380.63Å 126.46Å 243.35Å 90.00° 91.41° 90.00°	Depositor
Resolution (Å)	243.28 – 6.60 49.94 – 6.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (243.28-6.60) 89.8 (49.94-6.60)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 6.68Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.259 , 0.291 0.266 , 0.293	Depositor DCC
R_{free} test set	1088 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	170.9	Xtriage
Anisotropy	0.989	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 383.0	EDS
Estimated twinning fraction	0.095 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 21274 reflections	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	45054	wwPDB-VP
Average B, all atoms (Å ²)	253.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.64	1/5311 (0.0%)	0.77	8/7186 (0.1%)
1	B	0.63	0/5311	0.81	18/7186 (0.3%)
1	E	0.67	1/5311 (0.0%)	0.78	6/7186 (0.1%)
1	F	0.67	2/5311 (0.0%)	0.84	17/7186 (0.2%)
1	I	0.58	0/5311	0.74	5/7186 (0.1%)
1	J	0.59	0/5311	0.78	15/7186 (0.2%)
2	C	0.68	1/2288 (0.0%)	0.87	8/3096 (0.3%)
2	D	0.77	1/2288 (0.0%)	0.90	10/3096 (0.3%)
2	G	0.65	0/2288	0.83	6/3096 (0.2%)
2	H	0.73	2/2288 (0.1%)	0.87	4/3096 (0.1%)
2	K	0.67	0/2288	0.84	5/3096 (0.2%)
2	L	0.62	1/2288 (0.0%)	0.81	2/3096 (0.1%)
All	All	0.65	9/45594 (0.0%)	0.81	104/61692 (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	A	0	1
1	B	0	1
1	I	0	2
2	C	0	1
2	H	0	1
2	K	0	2
2	L	0	1
All	All	0	9

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	208	LYS	CE-NZ	14.66	1.85	1.49
1	F	671	MET	CG-SD	13.22	2.15	1.81
1	E	718	LYS	CD-CE	8.36	1.72	1.51
2	C	228	GLU	CG-CD	7.86	1.63	1.51
1	F	129	GLN	CG-CD	5.82	1.64	1.51
2	L	194	LYS	CE-NZ	5.57	1.62	1.49
2	H	210	ARG	CD-NE	5.22	1.55	1.46
2	H	210	ARG	NE-CZ	5.09	1.39	1.33
1	A	676	GLU	CG-CD	5.08	1.59	1.51

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	283	LEU	CB-CG-CD2	-13.89	87.39	111.00
1	B	283	LEU	CB-CG-CD2	-11.85	90.85	111.00
1	J	283	LEU	CB-CG-CD2	-10.76	92.70	111.00
1	I	671	MET	CG-SD-CE	9.48	115.37	100.20
1	F	394	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	I	367	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	B	671	MET	CG-SD-CE	8.71	114.13	100.20
1	F	274	ARG	NE-CZ-NH2	-8.23	116.19	120.30
2	C	110	LEU	CA-CB-CG	-8.17	96.51	115.30
2	D	161	LEU	CB-CG-CD2	7.67	124.05	111.00
2	D	55	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	B	283	LEU	CA-CB-CG	7.58	132.74	115.30
1	B	671	MET	CA-CB-CG	7.55	126.14	113.30
1	F	575	LYS	CB-CG-CD	7.53	131.19	111.60
1	J	141	LYS	CD-CE-NZ	7.43	128.78	111.70
2	L	250	LEU	CB-CG-CD2	-7.20	98.77	111.00
1	A	283	LEU	CB-CG-CD2	-7.03	99.06	111.00
1	J	671	MET	CG-SD-CE	6.93	111.29	100.20
1	F	369	ARG	NE-CZ-NH2	-6.91	116.84	120.30
2	K	194	LYS	CD-CE-NZ	6.85	127.45	111.70
2	H	210	ARG	CD-NE-CZ	6.76	133.07	123.60
1	J	764	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	260	MET	CG-SD-CE	6.70	110.92	100.20
1	B	718	LYS	CD-CE-NZ	6.69	127.09	111.70
1	J	367	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	D	161	LEU	CB-CG-CD1	-6.62	99.75	111.00
1	F	283	LEU	CB-CG-CD1	6.61	122.23	111.00
1	F	210	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	575	LYS	CB-CG-CD	6.51	128.54	111.60
1	E	783	LYS	CA-CB-CG	6.47	127.64	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	283	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	313	MET	CA-CB-CG	6.36	124.11	113.30
2	L	110	LEU	CA-CB-CG	6.30	129.80	115.30
1	B	551	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	F	156	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	F	625	ARG	NE-CZ-NH2	6.17	123.39	120.30
2	H	294	ILE	C-N-CA	6.16	137.09	121.70
1	J	671	MET	CB-CG-SD	6.06	130.58	112.40
2	K	72	LEU	CA-CB-CG	6.03	129.16	115.30
1	B	718	LYS	CB-CG-CD	6.01	127.24	111.60
2	C	176	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	G	22	ARG	NE-CZ-NH1	5.95	123.27	120.30
2	C	261	ARG	NE-CZ-NH1	5.87	123.24	120.30
2	G	95	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	313	MET	CG-SD-CE	-5.86	90.83	100.20
1	E	656	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	E	395	GLU	OE1-CD-OE2	-5.83	116.30	123.30
1	J	260	MET	CG-SD-CE	5.82	109.52	100.20
1	I	361	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	J	479	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	E	646	GLU	OE1-CD-OE2	-5.80	116.34	123.30
2	C	228	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	B	759	MET	CG-SD-CE	5.76	109.42	100.20
1	F	420	ARG	NE-CZ-NH2	5.76	123.18	120.30
2	H	95	ARG	NE-CZ-NH2	-5.75	117.42	120.30
2	D	110	LEU	CA-CB-CG	5.74	128.49	115.30
1	J	172	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	F	260	MET	CG-SD-CE	5.70	109.32	100.20
1	A	676	GLU	OE1-CD-OE2	-5.69	116.47	123.30
1	F	394	ARG	NE-CZ-NH2	-5.69	117.45	120.30
2	G	110	LEU	CA-CB-CG	5.69	128.38	115.30
2	G	263	MET	CG-SD-CE	-5.67	91.13	100.20
1	E	617	MET	CB-CG-SD	5.60	129.21	112.40
1	A	354	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	K	157	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	C	167	GLU	OE1-CD-OE2	-5.54	116.66	123.30
1	F	283	LEU	CA-CB-CG	5.53	128.03	115.30
1	A	275	ARG	NE-CZ-NH1	5.53	123.07	120.30
2	K	161	LEU	CA-CB-CG	5.52	127.99	115.30
2	D	65	LYS	CD-CE-NZ	5.48	124.31	111.70
1	B	778	LEU	CB-CG-CD1	5.47	120.30	111.00
1	J	715	LEU	CB-CG-CD2	-5.46	101.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	D	83	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	B	421	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	E	309	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	J	507	LYS	CD-CE-NZ	5.31	123.91	111.70
2	G	110	LEU	CB-CA-C	-5.30	100.13	110.20
2	C	263	MET	CA-CB-CG	5.28	122.27	113.30
2	G	72	LEU	CA-CB-CG	5.27	127.42	115.30
1	F	787	LYS	CD-CE-NZ	5.26	123.81	111.70
1	B	403	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	F	773	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	B	486	PRO	N-CA-C	-5.24	98.48	112.10
1	J	625	ARG	NE-CZ-NH2	5.21	122.90	120.30
2	D	266	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	C	211	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	F	671	MET	CA-CB-CG	5.18	122.10	113.30
1	B	584	ARG	NE-CZ-NH2	-5.17	117.71	120.30
2	D	200	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	D	194	LYS	CD-CE-NZ	5.15	123.55	111.70
1	B	453	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	J	519	LYS	CD-CE-NZ	5.13	123.51	111.70
1	I	305	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	I	319	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	794	ARG	CB-CG-CD	5.08	124.81	111.60
2	K	124	TYR	CB-CA-C	-5.07	100.25	110.40
2	D	148	LEU	CB-CG-CD2	-5.07	102.38	111.00
2	H	113	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	437	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	393	LEU	CB-CG-CD2	5.04	119.57	111.00
1	F	656	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	C	22	ARG	CG-CD-NE	-5.03	101.25	111.80
1	J	357	LEU	CB-CG-CD2	5.00	119.50	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	752	HIS	Peptide
1	B	487	ILE	Peptide
2	C	86	LEU	Peptide
2	H	81	ALA	Peptide
1	I	129	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	I	755	THR	Peptide
2	K	113	ARG	Peptide
2	K	86	LEU	Peptide
2	L	86	LEU	Peptide

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	51	0
1	B	5226	0	5283	57	0
1	E	5226	0	5283	79	0
1	F	5226	0	5283	74	0
1	I	5226	0	5283	84	0
1	J	5226	0	5283	87	0
2	C	2252	0	2272	69	0
2	D	2252	0	2272	51	0
2	G	2252	0	2271	59	0
2	H	2252	0	2272	58	0
2	K	2252	0	2272	66	0
2	L	2252	0	2272	49	0
3	A	31	0	13	2	0
3	B	31	0	13	1	0
3	E	31	0	13	9	0
3	F	31	0	13	4	0
3	I	31	0	13	3	0
3	J	31	0	13	5	0
All	All	45054	0	45407	655	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (655) 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:D:208:LYS:CE	2:D:208:LYS:NZ	1.85	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:671:MET:CG	1:F:671:MET:SD	2.15	1.34
2:C:110:LEU:CD2	2:C:145:LEU:HA	1.64	1.26
2:C:110:LEU:HD21	2:C:145:LEU:CA	1.76	1.14
2:G:83:LEU:HA	2:G:87:GLU:HA	1.18	1.13
2:H:97:GLU:HA	2:K:266:ARG:NH1	1.68	1.07
2:C:110:LEU:HD22	2:C:144:THR:O	1.56	1.05
2:D:88:ALA:O	2:D:89:ILE:HG13	1.60	1.00
2:C:62:GLY:C	2:C:114:THR:HG23	1.80	1.00
2:C:299:VAL:HG12	2:C:315:SER:OG	1.60	1.00
1:E:697:ARG:NH2	1:F:697:ARG:HB2	1.78	0.96
2:C:156:ALA:HA	2:C:159:LYS:HE3	1.48	0.96
1:E:267:ILE:HD11	1:E:314:PRO:HG2	1.49	0.95
1:E:670:PHE:N	3:F:1801:ANP:O1G	2.00	0.95
2:H:97:GLU:HA	2:K:266:ARG:HH12	1.29	0.95
2:H:70:LEU:HD22	2:H:86:LEU:HD21	1.48	0.94
2:H:266:ARG:NH2	2:K:90:ILE:HG21	1.84	0.93
1:A:670:PHE:N	3:B:1801:ANP:O1G	2.03	0.90
2:G:83:LEU:HA	2:G:87:GLU:CA	2.02	0.90
1:E:563:TYR:O	2:G:200:ARG:NH2	2.04	0.90
1:I:697:ARG:HB2	1:J:697:ARG:NH2	1.86	0.89
2:G:83:LEU:CA	2:G:87:GLU:HA	2.03	0.89
2:H:266:ARG:NH2	2:K:90:ILE:CG2	2.36	0.88
1:A:167:ALA:O	1:A:171:GLN:OE1	1.92	0.88
1:F:394:ARG:HG3	1:F:394:ARG:HH11	1.39	0.88
1:I:697:ARG:HH22	1:J:697:ARG:HB2	1.40	0.87
1:J:656:ARG:HG2	1:J:680:ILE:HD11	1.55	0.87
2:L:299:VAL:HG12	2:L:315:SER:OG	1.74	0.86
2:C:110:LEU:O	2:C:122:GLN:HA	1.75	0.86
2:H:97:GLU:HG2	2:K:266:ARG:HG3	1.58	0.85
2:K:110:LEU:O	2:K:122:GLN:HA	1.76	0.85
1:B:656:ARG:HG2	1:B:680:ILE:HD11	1.59	0.85
2:C:110:LEU:HD21	2:C:145:LEU:HA	0.86	0.83
1:I:617:MET:SD	1:J:671:MET:HA	2.17	0.83
2:D:110:LEU:O	2:D:122:GLN:HA	1.79	0.83
2:L:110:LEU:O	2:L:122:GLN:HA	1.78	0.83
1:I:780:GLY:O	1:J:678:ALA:HB1	1.79	0.82
1:A:752:HIS:CG	2:C:136:PRO:HG2	2.17	0.80
2:C:110:LEU:CD2	2:C:144:THR:O	2.29	0.80
2:H:70:LEU:HD22	2:H:86:LEU:CD2	2.11	0.79
1:E:267:ILE:HD11	1:E:314:PRO:CG	2.13	0.79
1:J:656:ARG:HG2	1:J:680:ILE:CD1	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:90:ILE:CG2	2:K:266:ARG:HH21	1.96	0.78
2:C:110:LEU:HD11	2:C:145:LEU:HD23	1.67	0.77
1:I:656:ARG:HH21	1:I:673:GLU:HA	1.48	0.77
2:D:117:GLN:OE1	1:E:405:ASP:OD1	2.02	0.77
2:C:299:VAL:CG1	2:C:315:SER:OG	2.32	0.77
1:F:620:LYS:NZ	3:F:1801:ANP:O1B	2.17	0.77
2:H:90:ILE:HG21	2:K:266:ARG:HH21	1.50	0.76
2:L:299:VAL:CG1	2:L:315:SER:OG	2.34	0.76
2:D:64:LYS:HD2	2:D:114:THR:HG21	1.68	0.76
1:I:656:ARG:NH2	1:I:673:GLU:HA	2.00	0.75
1:B:656:ARG:HG2	1:B:680:ILE:CD1	2.16	0.75
2:D:157:ARG:O	2:D:161:LEU:CD1	2.35	0.75
1:B:656:ARG:NE	1:B:676:GLU:HB3	2.04	0.73
1:A:656:ARG:HH21	1:A:673:GLU:HA	1.54	0.72
1:E:619:GLY:HA2	3:E:1801:ANP:H8	1.70	0.72
1:J:617:MET:HA	3:J:1801:ANP:H5'1	1.71	0.72
1:E:617:MET:SD	1:F:671:MET:HB2	2.29	0.72
1:E:656:ARG:HH21	1:E:673:GLU:HA	1.53	0.72
2:H:64:LYS:HD2	2:H:114:THR:HG21	1.72	0.72
1:A:682:HIS:CE1	1:B:782:PRO:HD3	2.24	0.72
1:I:796:LEU:HD13	1:J:702:TYR:HB3	1.73	0.71
1:I:697:ARG:NH2	1:J:697:ARG:HB2	2.05	0.71
1:E:267:ILE:CD1	1:E:314:PRO:HG2	2.20	0.71
1:A:656:ARG:NH2	1:A:673:GLU:HA	2.05	0.71
1:F:656:ARG:HH21	1:F:673:GLU:HA	1.56	0.70
1:I:697:ARG:HH22	1:J:697:ARG:CB	2.05	0.70
1:F:432:GLU:O	1:F:435:GLU:HG2	1.92	0.70
1:F:394:ARG:CG	1:F:394:ARG:HH11	2.04	0.70
1:E:656:ARG:NH2	1:E:673:GLU:HA	2.06	0.70
1:J:656:ARG:NE	1:J:676:GLU:HB3	2.06	0.70
2:H:266:ARG:HG3	2:K:97:GLU:HG2	1.75	0.69
2:L:111:THR:HG23	2:L:122:GLN:HB2	1.75	0.69
1:F:656:ARG:NH2	1:F:673:GLU:HA	2.07	0.69
2:G:207:GLN:HG2	2:G:210:ARG:HG3	1.74	0.69
2:L:107:ARG:HB3	2:L:148:LEU:HB2	1.73	0.69
1:I:697:ARG:HB2	1:J:697:ARG:HH22	1.56	0.68
2:C:109:THR:O	2:C:110:LEU:HD23	1.92	0.68
2:C:62:GLY:CA	2:C:114:THR:HG23	2.23	0.67
1:B:479:ARG:NH1	1:B:499:GLU:OE1	2.27	0.67
2:K:162:ARG:O	2:K:163:THR:O	2.12	0.67
1:E:770:SER:HB3	1:F:700:SER:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:106:SER:HB3	2:K:150:LEU:HD22	1.77	0.66
1:A:697:ARG:NH1	1:B:697:ARG:CZ	2.57	0.66
2:H:90:ILE:CG2	2:K:266:ARG:NH2	2.58	0.66
2:H:106:SER:HB3	2:H:150:LEU:HD22	1.77	0.66
1:I:656:ARG:NH1	1:I:657:VAL:O	2.28	0.66
1:I:150:ILE:HG21	1:I:248:GLN:NE2	2.11	0.66
2:L:162:ARG:O	2:L:163:THR:O	2.14	0.66
1:A:699:THR:HA	1:B:728:HIS:ND1	2.11	0.66
1:B:630:ILE:HG23	1:B:640:VAL:HG11	1.78	0.66
2:K:110:LEU:HD13	2:K:145:LEU:HG	1.78	0.66
2:G:162:ARG:O	2:G:163:THR:O	2.14	0.66
2:H:70:LEU:HD23	2:H:86:LEU:HD11	1.77	0.65
2:C:163:THR:HB	2:C:166:THR:OG1	1.96	0.65
1:E:526:GLN:HE21	1:F:470:VAL:HG21	1.60	0.65
2:H:162:ARG:O	2:H:163:THR:O	2.13	0.65
2:D:106:SER:HB3	2:D:150:LEU:HD22	1.79	0.65
2:H:266:ARG:HH22	2:K:90:ILE:HG22	1.59	0.65
2:C:109:THR:O	2:C:110:LEU:CD2	2.44	0.65
1:I:780:GLY:O	1:J:678:ALA:CB	2.45	0.65
1:F:656:ARG:NH1	1:F:657:VAL:O	2.30	0.65
2:D:107:ARG:NH2	2:D:124:TYR:OH	2.30	0.65
1:I:699:THR:HA	1:J:728:HIS:ND1	2.12	0.65
1:A:656:ARG:NH1	1:A:657:VAL:O	2.30	0.65
1:E:630:ILE:HG23	1:E:640:VAL:HG11	1.78	0.65
2:C:299:VAL:C	2:C:315:SER:OG	2.35	0.64
1:F:630:ILE:HG23	1:F:640:VAL:HG11	1.80	0.64
2:L:299:VAL:CB	2:L:315:SER:OG	2.45	0.64
2:D:162:ARG:O	2:D:163:THR:O	2.15	0.64
1:J:630:ILE:HG23	1:J:640:VAL:HG11	1.78	0.64
1:A:615:PRO:HA	1:B:699:THR:HG21	1.80	0.64
2:D:88:ALA:O	2:D:89:ILE:CG1	2.41	0.64
2:G:64:LYS:HA	2:G:118:GLN:HE22	1.63	0.64
2:D:256:PHE:CE2	2:D:290:LEU:HB2	2.33	0.64
1:I:150:ILE:H	1:I:150:ILE:HD12	1.62	0.63
1:I:630:ILE:HG23	1:I:640:VAL:HG11	1.81	0.63
1:F:150:ILE:HD11	1:F:252:LEU:CD2	2.29	0.63
2:C:70:LEU:HB3	2:C:82:SER:HB2	1.78	0.63
1:E:620:LYS:NZ	3:E:1801:ANP:O1B	2.26	0.63
2:H:266:ARG:NH2	2:K:90:ILE:HG22	2.13	0.63
2:G:106:SER:HB3	2:G:150:LEU:HD22	1.81	0.63
2:G:86:LEU:HB3	2:G:89:ILE:HD12	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:110:LEU:HD12	2:G:123:ALA:HB3	1.81	0.62
1:I:760:HIS:HB3	3:I:1801:ANP:N6	2.13	0.62
1:J:755:THR:HG21	2:L:135:LYS:NZ	2.15	0.62
1:I:671:MET:HA	1:J:617:MET:SD	2.39	0.62
2:L:106:SER:HB3	2:L:150:LEU:HD22	1.81	0.62
1:E:137:TRP:CH2	1:E:139:ASP:HB3	2.35	0.62
2:K:267:LEU:HD11	2:K:319:HIS:HB2	1.82	0.62
1:I:219:THR:HG22	1:J:780:GLY:HA2	1.81	0.61
2:G:159:LYS:HG2	2:G:159:LYS:O	1.98	0.61
1:A:137:TRP:CH2	1:A:139:ASP:HB3	2.35	0.61
1:I:137:TRP:CH2	1:I:139:ASP:HB3	2.35	0.61
1:A:630:ILE:HG23	1:A:640:VAL:HG11	1.81	0.61
1:E:205:GLU:HG2	2:H:52:LYS:NZ	2.15	0.61
1:J:727:THR:HG21	1:J:732:LEU:HD12	1.82	0.61
2:K:70:LEU:HB2	2:K:82:SER:HB2	1.82	0.61
2:H:267:LEU:HD11	2:H:319:HIS:HB2	1.83	0.61
1:E:617:MET:SD	1:F:671:MET:CG	2.89	0.61
1:B:137:TRP:CH2	1:B:139:ASP:HB3	2.35	0.61
1:E:770:SER:HB3	1:F:700:SER:CB	2.31	0.60
1:E:150:ILE:HD11	1:E:252:LEU:CD2	2.30	0.60
1:E:678:ALA:HB1	1:F:780:GLY:O	2.02	0.60
1:E:267:ILE:HA	1:E:651:ASP:O	2.01	0.60
1:I:616:ASN:ND2	1:J:670:PHE:CD2	2.70	0.60
2:G:151:PHE:O	2:G:158:ARG:NH1	2.35	0.60
1:J:141:LYS:HD3	1:J:232:ARG:HH21	1.67	0.60
2:C:106:SER:HB3	2:C:150:LEU:HD22	1.82	0.60
1:F:150:ILE:HG12	1:F:248:GLN:NE2	2.16	0.60
1:E:697:ARG:HH21	1:F:697:ARG:HB2	1.67	0.60
1:E:297:SER:OG	1:E:557:ASN:OD1	2.19	0.60
2:K:110:LEU:HD12	2:K:144:THR:O	2.02	0.59
1:J:137:TRP:CH2	1:J:139:ASP:HB3	2.37	0.59
2:C:151:PHE:O	2:C:158:ARG:NH1	2.35	0.59
1:A:752:HIS:ND1	2:C:136:PRO:HG2	2.17	0.59
1:E:617:MET:SD	1:F:671:MET:CB	2.90	0.59
1:I:697:ARG:HH22	1:J:697:ARG:CA	2.16	0.59
1:F:617:MET:N	1:F:617:MET:SD	2.76	0.59
2:C:107:ARG:HB2	2:C:148:LEU:HB2	1.85	0.58
1:B:656:ARG:HE	1:B:676:GLU:HB3	1.67	0.58
2:G:24:ALA:HB1	2:G:174:ILE:HD12	1.84	0.58
2:L:299:VAL:HB	2:L:315:SER:OG	2.04	0.58
1:F:137:TRP:CH2	1:F:139:ASP:HB3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1801:ANP:O1G	1:B:670:PHE:HB3	2.02	0.58
2:D:157:ARG:O	2:D:161:LEU:HD13	2.02	0.58
1:F:727:THR:HG21	1:F:732:LEU:HD12	1.85	0.58
2:D:256:PHE:CD2	2:D:290:LEU:HB2	2.39	0.58
2:L:24:ALA:HB1	2:L:174:ILE:HD12	1.85	0.58
2:D:83:LEU:CD1	2:D:90:ILE:HD12	2.33	0.58
1:E:659:ALA:C	1:F:659:ALA:HB2	2.24	0.57
1:F:593:ASN:O	2:H:55:ARG:NH2	2.37	0.57
1:F:150:ILE:CD1	1:F:252:LEU:CD2	2.82	0.57
2:L:151:PHE:O	2:L:158:ARG:NH1	2.37	0.57
2:H:90:ILE:HG22	2:K:266:ARG:NH2	2.19	0.57
1:E:656:ARG:NH1	1:E:657:VAL:O	2.38	0.57
2:K:82:SER:O	2:K:87:GLU:HA	2.05	0.57
1:E:771:TYR:N	1:F:699:THR:OG1	2.35	0.57
2:D:151:PHE:O	2:D:158:ARG:NH1	2.37	0.57
2:K:24:ALA:HB1	2:K:174:ILE:HD12	1.87	0.57
2:D:24:ALA:HB1	2:D:174:ILE:HD12	1.87	0.57
1:I:297:SER:OG	1:I:557:ASN:OD1	2.19	0.57
1:A:782:PRO:HD3	1:B:682:HIS:CE1	2.40	0.57
2:C:63:ILE:N	2:C:114:THR:HG23	2.19	0.57
2:L:82:SER:O	2:L:87:GLU:HA	2.05	0.57
1:J:656:ARG:HE	1:J:676:GLU:HB3	1.69	0.56
2:D:139:HIS:HE2	2:D:144:THR:HG1	1.52	0.56
2:C:82:SER:O	2:C:87:GLU:HA	2.05	0.56
1:I:615:PRO:HA	1:J:699:THR:HG21	1.87	0.56
1:F:312:HIS:O	1:F:313:MET:HE3	2.04	0.56
2:H:111:THR:HA	2:H:121:TRP:O	2.05	0.56
2:L:111:THR:HA	2:L:121:TRP:O	2.05	0.56
2:C:110:LEU:CD1	2:C:145:LEU:HD23	2.34	0.56
1:F:312:HIS:O	1:F:313:MET:CE	2.53	0.56
1:B:754:ASP:OD2	2:D:135:LYS:HE2	2.05	0.56
1:E:796:LEU:HD13	1:F:702:TYR:HB3	1.88	0.56
1:B:656:ARG:HH21	1:B:679:ASN:HB3	1.71	0.56
1:F:635:TYR:OH	1:F:649:PRO:HA	2.06	0.56
1:E:266:SER:O	1:E:267:ILE:HG23	2.05	0.56
2:L:83:LEU:HD22	2:L:90:ILE:HG12	1.88	0.56
1:E:306:MET:HA	1:E:309:ARG:NE	2.19	0.55
1:J:656:ARG:HH21	1:J:679:ASN:HB3	1.71	0.55
2:H:279:LYS:HE2	2:H:330:LEU:HB3	1.87	0.55
1:E:595:PRO:HG3	2:G:57:ARG:HD2	1.88	0.55
1:J:264:GLN:HG2	1:J:264:GLN:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:PHE:O	2:H:158:ARG:NH1	2.39	0.55
1:E:617:MET:CE	3:E:1801:ANP:H4'	2.36	0.55
1:I:697:ARG:HH12	1:J:697:ARG:HB2	1.70	0.55
1:I:470:VAL:HG11	1:J:523:LEU:HD13	1.89	0.55
1:J:635:TYR:OH	1:J:649:PRO:HA	2.05	0.55
1:E:727:THR:HG21	1:E:732:LEU:HD12	1.88	0.55
1:A:635:TYR:OH	1:A:649:PRO:HA	2.06	0.55
2:K:316:ARG:CG	2:K:317:LEU:N	2.69	0.55
1:E:635:TYR:OH	1:E:649:PRO:HA	2.07	0.55
1:J:617:MET:HA	3:J:1801:ANP:C5'	2.36	0.55
2:D:113:ARG:NE	2:D:118:GLN:O	2.30	0.55
2:H:64:LYS:HB3	2:H:66:ASP:OD1	2.06	0.55
2:H:261:ARG:HD3	2:H:262:MET:H	1.72	0.55
2:K:107:ARG:HB2	2:K:148:LEU:HB2	1.88	0.55
1:I:469:ALA:HB1	1:J:522:ALA:HB1	1.89	0.55
2:C:24:ALA:HB1	2:C:174:ILE:HD12	1.88	0.54
1:E:150:ILE:HD11	1:E:252:LEU:HD21	1.90	0.54
2:K:316:ARG:HG3	2:K:317:LEU:N	2.21	0.54
1:I:635:TYR:OH	1:I:649:PRO:HA	2.07	0.54
1:E:697:ARG:HB2	1:F:697:ARG:NH2	2.21	0.54
1:E:671:MET:HG2	1:E:672:VAL:H	1.72	0.54
2:G:80:ILE:HG12	2:G:81:ALA:H	1.73	0.54
1:J:622:THR:OG1	3:J:1801:ANP:H8	2.07	0.54
2:G:83:LEU:HD23	2:G:87:GLU:O	2.07	0.54
2:C:111:THR:HA	2:C:121:TRP:O	2.08	0.54
1:I:227:VAL:HG12	1:I:260:MET:HB2	1.90	0.54
2:K:151:PHE:O	2:K:158:ARG:NH1	2.40	0.54
2:D:158:ARG:HA	2:D:161:LEU:HD13	1.89	0.54
2:C:299:VAL:CG1	2:C:315:SER:HG	2.20	0.53
2:K:139:HIS:HE2	2:K:144:THR:HG1	1.56	0.53
1:E:150:ILE:CD1	1:E:252:LEU:CD2	2.86	0.53
2:K:107:ARG:CZ	2:K:152:TYR:HD2	2.20	0.53
1:F:735:LEU:O	1:F:739:MET:N	2.38	0.53
1:B:635:TYR:OH	1:B:649:PRO:HA	2.07	0.53
2:K:279:LYS:HE2	2:K:330:LEU:HB3	1.90	0.53
2:D:107:ARG:HB2	2:D:148:LEU:HB2	1.90	0.53
2:L:279:LYS:HE2	2:L:330:LEU:HB3	1.90	0.53
1:I:701:THR:HG1	1:J:729:TYR:HD1	1.54	0.53
2:G:295:ASP:CG	2:G:296:PRO:HD2	2.29	0.53
2:L:299:VAL:HB	2:L:315:SER:HG	1.74	0.53
2:L:299:VAL:C	2:L:315:SER:OG	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:GLU:HG2	2:H:52:LYS:HZ3	1.71	0.53
2:C:279:LYS:HE2	2:C:330:LEU:HB3	1.90	0.53
1:I:617:MET:HG3	1:J:671:MET:HB2	1.91	0.53
1:I:727:THR:HG21	1:I:732:LEU:HD12	1.89	0.53
2:D:295:ASP:CG	2:D:296:PRO:HD2	2.28	0.53
1:E:594:GLU:HB2	1:E:595:PRO:CD	2.39	0.53
2:G:111:THR:OG1	2:G:144:THR:HB	2.09	0.52
2:D:279:LYS:HE2	2:D:330:LEU:HB3	1.89	0.52
1:E:617:MET:HE3	3:E:1801:ANP:H4'	1.91	0.52
2:H:295:ASP:CG	2:H:296:PRO:HD2	2.29	0.52
1:I:268:ILE:HG21	1:I:652:ARG:HH21	1.74	0.52
2:H:24:ALA:HB1	2:H:174:ILE:HD12	1.92	0.52
2:L:267:LEU:HD11	2:L:319:HIS:HB2	1.92	0.52
2:C:110:LEU:HD13	2:C:145:LEU:HG	1.92	0.52
2:C:62:GLY:C	2:C:114:THR:CG2	2.68	0.52
2:K:70:LEU:HD12	2:K:71:ALA:N	2.25	0.52
2:G:64:LYS:HB2	2:G:67:GLU:HG3	1.91	0.52
1:E:593:ASN:O	2:G:55:ARG:CZ	2.58	0.52
1:A:699:THR:HG21	1:B:615:PRO:HA	1.92	0.52
2:L:295:ASP:CG	2:L:296:PRO:HD2	2.30	0.52
2:D:72:LEU:HD23	2:D:103:SER:CB	2.39	0.52
2:D:72:LEU:HD23	2:D:103:SER:HB2	1.92	0.52
2:G:107:ARG:CZ	2:G:152:TYR:HD2	2.23	0.52
2:G:107:ARG:HB2	2:G:148:LEU:HB2	1.91	0.52
2:H:70:LEU:HD12	2:H:71:ALA:N	2.25	0.52
1:J:489:TYR:HD2	1:J:501:TYR:HB2	1.75	0.52
2:D:151:PHE:O	2:D:158:ARG:CZ	2.58	0.51
1:E:759:MET:SD	2:G:138:ALA:HB1	2.50	0.51
1:A:793:LEU:HD13	1:B:703:ASP:HA	1.92	0.51
2:C:299:VAL:CB	2:C:315:SER:OG	2.58	0.51
1:E:251:THR:O	1:E:252:LEU:HD23	2.10	0.51
1:B:754:ASP:HB2	2:D:135:LYS:NZ	2.25	0.51
2:H:107:ARG:HB2	2:H:148:LEU:HB2	1.91	0.51
1:F:150:ILE:HD11	1:F:252:LEU:HD21	1.91	0.51
2:C:267:LEU:HD11	2:C:319:HIS:HB2	1.93	0.51
2:K:164:GLU:HG3	2:K:165:LYS:N	2.25	0.51
1:I:670:PHE:HB3	3:J:1801:ANP:O1G	2.11	0.51
1:I:783:LYS:NZ	1:J:256:ARG:HB2	2.26	0.51
1:I:617:MET:SD	1:J:671:MET:CA	2.95	0.51
2:L:107:ARG:HG2	2:L:148:LEU:HD13	1.91	0.51
2:G:151:PHE:O	2:G:158:ARG:CZ	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:82:SER:O	2:G:87:GLU:N	2.33	0.51
1:F:394:ARG:HG3	1:F:394:ARG:NH1	2.12	0.51
1:E:252:LEU:N	1:E:253:PRO:CD	2.74	0.51
1:J:735:LEU:O	1:J:739:MET:N	2.38	0.51
2:H:164:GLU:HG2	2:H:165:LYS:N	2.26	0.51
3:E:1801:ANP:O2G	1:F:670:PHE:N	2.45	0.50
2:G:116:GLU:O	2:G:118:GLN:N	2.44	0.50
1:A:264:GLN:O	1:A:264:GLN:HG2	2.10	0.50
2:K:295:ASP:CG	2:K:296:PRO:HD2	2.32	0.50
2:K:179:ALA:HB1	2:K:211:ARG:HH12	1.76	0.50
1:A:735:LEU:O	1:A:739:MET:N	2.39	0.50
3:E:1801:ANP:O1G	1:F:670:PHE:HB3	2.12	0.50
1:B:733:THR:HG21	1:B:766:ALA:HB1	1.93	0.50
1:A:617:MET:SD	1:B:671:MET:HA	2.52	0.50
2:L:264:ARG:HB2	2:L:264:ARG:CZ	2.41	0.50
2:C:295:ASP:CG	2:C:296:PRO:HD2	2.32	0.50
1:J:252:LEU:N	1:J:253:PRO:CD	2.75	0.50
2:H:90:ILE:HG21	2:K:266:ARG:NH2	2.20	0.50
1:I:735:LEU:O	1:I:739:MET:N	2.38	0.50
2:G:70:LEU:HD12	2:G:71:ALA:N	2.26	0.50
1:F:394:ARG:CG	1:F:394:ARG:NH1	2.68	0.50
1:E:772:GLY:HA3	1:F:703:ASP:OD2	2.12	0.50
2:D:267:LEU:HD11	2:D:319:HIS:HB2	1.94	0.50
2:H:70:LEU:CD2	2:H:86:LEU:HD11	2.40	0.50
2:K:83:LEU:HD22	2:K:90:ILE:HG12	1.93	0.50
1:J:251:THR:O	1:J:252:LEU:HD23	2.12	0.50
1:A:733:THR:HG21	1:A:766:ALA:HB1	1.93	0.50
2:L:48:ARG:HG2	2:L:164:GLU:OE1	2.12	0.50
2:C:72:LEU:HD13	2:C:125:ALA:HB2	1.93	0.49
1:A:594:GLU:HB2	1:A:595:PRO:CD	2.42	0.49
1:I:388:ALA:HB3	1:I:389:PRO:HD3	1.94	0.49
1:I:616:ASN:OD1	1:J:670:PHE:HB3	2.13	0.49
1:I:697:ARG:NH1	1:J:697:ARG:HB2	2.27	0.49
1:F:594:GLU:HB2	1:F:595:PRO:CD	2.42	0.49
2:H:179:ALA:HB1	2:H:211:ARG:HH12	1.76	0.49
2:H:97:GLU:CA	2:K:266:ARG:HH12	2.14	0.49
1:I:700:SER:HB2	1:J:770:SER:HB3	1.94	0.49
1:A:778:LEU:HD21	1:B:220:ARG:CZ	2.42	0.49
1:F:733:THR:HG21	1:F:766:ALA:HB1	1.95	0.49
2:K:64:LYS:HD2	2:K:114:THR:HG21	1.93	0.49
2:C:164:GLU:HG2	2:C:165:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:619:GLY:HA2	3:E:1801:ANP:C8	2.39	0.49
2:K:82:SER:O	2:K:86:LEU:O	2.29	0.49
2:K:113:ARG:NE	2:K:118:GLN:O	2.30	0.49
1:J:156:ARG:HD2	1:J:261:GLU:HG3	1.94	0.49
2:C:110:LEU:CD1	2:C:145:LEU:HG	2.42	0.49
2:H:97:GLU:CG	2:K:266:ARG:HG3	2.35	0.49
1:F:252:LEU:N	1:F:253:PRO:CD	2.76	0.49
2:C:151:PHE:O	2:C:158:ARG:CZ	2.61	0.49
1:A:251:THR:O	1:A:252:LEU:HD23	2.12	0.49
2:D:70:LEU:O	2:D:80:ILE:HD11	2.12	0.49
1:F:388:ALA:HB3	1:F:389:PRO:HD3	1.94	0.49
1:A:202:TRP:CZ2	2:D:158:ARG:NH2	2.81	0.49
1:A:252:LEU:N	1:A:253:PRO:CD	2.76	0.49
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.94	0.49
1:J:328:ILE:HG23	1:J:559:ALA:HA	1.93	0.49
2:G:279:LYS:HE2	2:G:330:LEU:HB3	1.94	0.49
1:I:622:THR:OG1	3:I:1801:ANP:C8	2.61	0.49
2:L:151:PHE:O	2:L:158:ARG:CZ	2.60	0.49
1:A:727:THR:HG21	1:A:732:LEU:HD12	1.94	0.49
1:I:252:LEU:N	1:I:253:PRO:CD	2.75	0.49
2:H:251:ALA:HB1	2:H:285:GLN:HB3	1.94	0.49
1:A:780:GLY:HA2	1:B:219:THR:HG22	1.94	0.49
2:C:30:LEU:HD22	2:C:145:LEU:HD22	1.94	0.49
1:F:150:ILE:HD13	1:F:248:GLN:HG3	1.94	0.49
1:E:150:ILE:HG12	1:E:248:GLN:NE2	2.27	0.49
1:E:594:GLU:HB2	1:E:595:PRO:HD3	1.95	0.49
1:E:735:LEU:O	1:E:739:MET:N	2.42	0.48
2:G:164:GLU:OE1	2:G:164:GLU:N	2.42	0.48
2:C:156:ALA:HA	2:C:159:LYS:HG2	1.95	0.48
2:K:110:LEU:CD1	2:K:144:THR:O	2.61	0.48
1:J:622:THR:HG21	3:J:1801:ANP:N7	2.28	0.48
1:F:251:THR:O	1:F:252:LEU:HD23	2.13	0.48
2:L:63:ILE:N	2:L:114:THR:HG22	2.28	0.48
1:J:733:THR:HG21	1:J:766:ALA:HB1	1.94	0.48
1:I:328:ILE:HG23	1:I:559:ALA:HA	1.94	0.48
1:F:156:ARG:HD2	1:F:261:GLU:HG3	1.96	0.48
1:I:251:THR:O	1:I:252:LEU:HD23	2.13	0.48
1:A:671:MET:HA	1:B:617:MET:SD	2.53	0.48
1:I:733:THR:HG21	1:I:766:ALA:HB1	1.96	0.48
1:A:616:ASN:CG	1:B:670:PHE:CD2	2.87	0.48
2:H:151:PHE:O	2:H:158:ARG:CZ	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:268:ILE:HG21	1:I:652:ARG:NH2	2.28	0.48
1:A:793:LEU:HD13	1:B:706:SER:OG	2.13	0.48
2:H:266:ARG:HB3	2:K:80:ILE:HD11	1.96	0.48
2:L:113:ARG:HD3	2:L:139:HIS:O	2.14	0.48
2:G:263:MET:HG3	2:G:264:ARG:N	2.29	0.48
2:G:113:ARG:NE	2:G:118:GLN:O	2.31	0.48
1:I:701:THR:CG2	1:J:701:THR:HG23	2.44	0.48
2:D:70:LEU:HD12	2:D:71:ALA:N	2.28	0.48
1:A:793:LEU:CD1	1:B:706:SER:OG	2.62	0.47
2:L:139:HIS:HE2	2:L:144:THR:HG1	1.59	0.47
2:G:80:ILE:HG12	2:G:81:ALA:N	2.29	0.47
1:B:487:ILE:HA	1:B:489:TYR:H	1.80	0.47
1:A:792:LYS:HE2	1:B:709:TRP:CE3	2.49	0.47
2:C:110:LEU:CD1	2:C:145:LEU:CD2	2.92	0.47
2:D:86:LEU:HD22	2:D:89:ILE:HD12	1.96	0.47
1:E:266:SER:C	1:E:267:ILE:HG23	2.35	0.47
1:I:698:GLY:O	1:J:728:HIS:CG	2.67	0.47
1:F:297:SER:OG	1:F:561:ARG:HD3	2.15	0.47
2:D:149:ASP:N	2:D:149:ASP:OD1	2.47	0.47
2:C:113:ARG:NE	2:C:118:GLN:O	2.31	0.47
2:D:83:LEU:HD11	2:D:90:ILE:CD1	2.44	0.47
2:L:82:SER:O	2:L:86:LEU:O	2.31	0.47
2:K:151:PHE:O	2:K:158:ARG:CZ	2.63	0.47
2:C:82:SER:O	2:C:86:LEU:O	2.32	0.47
2:D:83:LEU:HD11	2:D:90:ILE:HD12	1.96	0.47
1:I:728:HIS:ND1	1:J:699:THR:HA	2.28	0.47
2:K:62:GLY:HA3	2:K:114:THR:HA	1.97	0.47
1:B:252:LEU:N	1:B:253:PRO:CD	2.77	0.47
2:G:72:LEU:HD23	2:G:103:SER:CB	2.45	0.47
1:B:388:ALA:HB3	1:B:389:PRO:HD3	1.97	0.47
1:E:227:VAL:HG12	1:E:260:MET:HB2	1.96	0.47
1:I:594:GLU:HB2	1:I:595:PRO:CD	2.45	0.47
1:A:776:ALA:HB2	1:B:674:MET:SD	2.55	0.47
2:G:30:LEU:HD22	2:G:145:LEU:HD22	1.97	0.47
2:L:251:ALA:HB1	2:L:285:GLN:HB3	1.97	0.47
2:C:299:VAL:HB	2:C:315:SER:HG	1.78	0.47
2:G:110:LEU:O	2:G:122:GLN:HG2	2.15	0.47
1:I:786:ILE:HG22	1:I:790:ARG:HE	1.80	0.47
2:C:110:LEU:HD11	2:C:145:LEU:CD2	2.40	0.46
2:D:157:ARG:O	2:D:161:LEU:HD11	2.15	0.46
1:I:699:THR:HG21	1:J:615:PRO:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:113:ARG:HD3	2:C:139:HIS:O	2.16	0.46
1:B:251:THR:O	1:B:252:LEU:HD23	2.13	0.46
1:F:328:ILE:HG23	1:F:559:ALA:HA	1.98	0.46
1:J:771:TYR:O	1:J:775:VAL:HG23	2.15	0.46
2:G:113:ARG:HD3	2:G:139:HIS:O	2.16	0.46
1:B:798:SER:HA	1:F:496:LYS:HZ1	1.80	0.46
2:G:267:LEU:HD11	2:G:319:HIS:HB2	1.98	0.46
2:K:83:LEU:C	2:K:87:GLU:HB2	2.36	0.46
1:E:678:ALA:CB	1:F:780:GLY:O	2.63	0.46
2:D:68:LEU:CD1	2:D:121:TRP:HB2	2.46	0.46
1:J:272:ALA:O	1:J:276:ASN:HB2	2.16	0.46
2:H:113:ARG:NE	2:H:118:GLN:O	2.31	0.46
1:J:425:ILE:CD1	1:J:527:LEU:HB2	2.45	0.46
2:L:83:LEU:C	2:L:87:GLU:HB2	2.35	0.46
1:A:156:ARG:HD2	1:A:261:GLU:HG3	1.98	0.46
2:D:48:ARG:HG2	2:D:164:GLU:OE1	2.16	0.46
1:E:620:LYS:N	3:E:1801:ANP:O1A	2.49	0.46
2:D:83:LEU:HD21	2:D:90:ILE:CD1	2.45	0.46
1:E:617:MET:HA	3:E:1801:ANP:H5'1	1.98	0.46
1:I:219:THR:CG2	1:J:780:GLY:HA2	2.46	0.46
2:C:72:LEU:C	2:C:72:LEU:HD12	2.36	0.46
2:H:113:ARG:HD3	2:H:139:HIS:O	2.16	0.46
1:E:388:ALA:HB3	1:E:389:PRO:HD3	1.97	0.46
1:J:594:GLU:HB3	1:J:595:PRO:CD	2.46	0.46
1:B:297:SER:OG	1:B:561:ARG:HD3	2.16	0.46
1:A:697:ARG:HH12	1:B:697:ARG:CZ	2.27	0.46
2:C:109:THR:OG1	2:C:146:GLU:HB2	2.16	0.45
2:H:97:GLU:HA	2:K:266:ARG:HH11	1.68	0.45
2:L:114:THR:OG1	2:L:118:GLN:OE1	2.35	0.45
1:E:733:THR:HG21	1:E:766:ALA:HB1	1.97	0.45
2:H:72:LEU:C	2:H:72:LEU:HD12	2.36	0.45
1:J:388:ALA:HB3	1:J:389:PRO:HD3	1.98	0.45
1:A:702:TYR:HB3	1:B:796:LEU:HD13	1.97	0.45
2:K:30:LEU:HD22	2:K:145:LEU:HD22	1.99	0.45
2:K:149:ASP:OD1	2:K:149:ASP:N	2.49	0.45
1:B:156:ARG:HD2	1:B:261:GLU:HG3	1.97	0.45
1:I:425:ILE:CD1	1:I:527:LEU:HB2	2.47	0.45
1:A:388:ALA:HB3	1:A:389:PRO:HD3	1.99	0.45
2:G:149:ASP:OD1	2:G:149:ASP:N	2.49	0.45
1:E:617:MET:SD	1:F:671:MET:HG3	2.57	0.45
1:E:671:MET:HG2	1:E:672:VAL:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:72:LEU:HD23	2:G:103:SER:HB2	1.99	0.45
2:C:70:LEU:HD22	2:C:82:SER:HA	1.98	0.45
2:K:48:ARG:HG2	2:K:164:GLU:OE1	2.17	0.45
1:F:227:VAL:HG12	1:F:260:MET:HB2	1.99	0.45
2:L:149:ASP:OD1	2:L:149:ASP:N	2.49	0.45
2:C:110:LEU:CD2	2:C:145:LEU:CA	2.58	0.45
1:I:698:GLY:O	1:J:728:HIS:CD2	2.70	0.45
1:J:755:THR:HG21	2:L:135:LYS:HZ2	1.82	0.45
1:I:771:TYR:O	1:I:775:VAL:HG23	2.17	0.45
2:C:299:VAL:CB	2:C:315:SER:HG	2.30	0.45
2:K:113:ARG:HD3	2:K:139:HIS:O	2.17	0.45
1:A:778:LEU:HD21	1:B:220:ARG:NH1	2.32	0.45
1:I:224:GLY:O	1:I:682:HIS:ND1	2.50	0.45
2:D:113:ARG:HD3	2:D:139:HIS:O	2.16	0.45
2:G:64:LYS:HD2	2:G:114:THR:HG21	1.99	0.45
1:B:771:TYR:O	1:B:775:VAL:HG23	2.16	0.45
1:J:656:ARG:HE	1:J:676:GLU:CB	2.30	0.44
1:B:727:THR:HG21	1:B:732:LEU:HD12	1.97	0.44
1:E:670:PHE:CD2	1:F:616:ASN:ND2	2.85	0.44
1:I:697:ARG:CZ	1:J:697:ARG:HB2	2.47	0.44
1:E:526:GLN:NE2	1:F:470:VAL:HG21	2.28	0.44
1:E:772:GLY:N	1:F:699:THR:OG1	2.50	0.44
1:I:594:GLU:HB2	1:I:595:PRO:HD3	1.99	0.44
1:B:594:GLU:HB3	1:B:595:PRO:CD	2.48	0.44
2:L:135:LYS:HB2	2:L:136:PRO:CD	2.48	0.44
2:L:113:ARG:NE	2:L:118:GLN:O	2.32	0.44
2:G:190:SER:HA	2:G:195:ILE:HA	2.00	0.44
2:L:72:LEU:HD12	2:L:72:LEU:C	2.38	0.44
2:C:83:LEU:C	2:C:87:GLU:HB2	2.38	0.44
1:A:780:GLY:HA2	1:B:219:THR:CG2	2.48	0.44
2:L:190:SER:HA	2:L:195:ILE:HA	2.00	0.44
1:I:272:ALA:O	1:I:276:ASN:HB2	2.17	0.44
1:F:619:GLY:HA2	3:F:1801:ANP:C8	2.47	0.44
2:G:107:ARG:NH2	2:G:152:TYR:HD2	2.15	0.44
1:A:771:TYR:O	1:A:775:VAL:HG23	2.18	0.44
2:K:111:THR:HA	2:K:121:TRP:O	2.18	0.44
2:H:68:LEU:CD1	2:H:121:TRP:HB2	2.48	0.44
2:K:107:ARG:NH2	2:K:152:TYR:HD2	2.14	0.44
1:E:215:LEU:HD22	2:H:124:TYR:CE2	2.52	0.44
1:J:297:SER:OG	1:J:561:ARG:HD3	2.17	0.44
1:F:755:THR:HG21	2:H:135:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:656:ARG:HA	1:E:656:ARG:HD2	1.75	0.44
2:L:107:ARG:CG	2:L:148:LEU:HD13	2.47	0.44
1:I:616:ASN:CG	1:J:670:PHE:HB3	2.38	0.43
2:G:70:LEU:HB2	2:G:82:SER:HB2	2.00	0.43
2:H:83:LEU:HD23	2:H:86:LEU:HD23	2.00	0.43
1:F:379:ARG:HG2	1:F:394:ARG:HH12	1.83	0.43
2:C:121:TRP:CZ3	2:C:136:PRO:HG3	2.54	0.43
1:E:771:TYR:O	1:E:775:VAL:HG23	2.17	0.43
2:G:164:GLU:CD	2:G:165:LYS:H	2.21	0.43
2:C:149:ASP:OD1	2:C:149:ASP:N	2.52	0.43
1:J:788:ARG:HD3	1:J:788:ARG:HA	1.82	0.43
1:E:156:ARG:HD2	1:E:261:GLU:HG3	2.00	0.43
1:I:700:SER:HA	1:J:728:HIS:O	2.18	0.43
1:B:328:ILE:HG23	1:B:559:ALA:HA	2.00	0.43
2:L:64:LYS:HB2	2:L:67:GLU:HG3	1.99	0.43
1:F:224:GLY:O	1:F:682:HIS:ND1	2.51	0.43
1:E:752:HIS:ND1	2:G:136:PRO:HG2	2.33	0.43
1:E:267:ILE:CG1	1:E:314:PRO:HG2	2.47	0.43
2:K:80:ILE:HG23	2:K:80:ILE:O	2.19	0.43
2:C:163:THR:CB	2:C:166:THR:OG1	2.63	0.43
1:B:487:ILE:C	1:B:489:TYR:N	2.71	0.43
1:B:798:SER:HA	1:F:496:LYS:CE	2.49	0.43
1:F:566:ASN:OD1	2:H:200:ARG:NH2	2.51	0.43
2:G:179:ALA:HB1	2:G:211:ARG:HH12	1.83	0.43
2:D:108:LEU:HD11	2:D:110:LEU:HD23	2.01	0.43
2:G:110:LEU:CD1	2:G:123:ALA:HB3	2.49	0.43
1:E:328:ILE:HG23	1:E:559:ALA:HA	2.00	0.43
1:J:209:ALA:CB	1:J:238:GLY:HA3	2.49	0.43
1:I:420:ARG:NH2	1:J:420:ARG:NH2	2.67	0.43
1:A:425:ILE:CD1	1:A:527:LEU:HB2	2.49	0.43
2:H:110:LEU:CD1	2:H:145:LEU:HG	2.48	0.43
2:D:63:ILE:N	2:D:114:THR:HG22	2.33	0.43
1:A:656:ARG:HA	1:A:656:ARG:HD2	1.76	0.43
2:G:111:THR:O	2:G:111:THR:OG1	2.37	0.43
1:A:227:VAL:HG12	1:A:260:MET:HB2	2.00	0.43
1:F:425:ILE:CD1	1:F:527:LEU:HB2	2.49	0.43
2:G:87:GLU:O	2:G:89:ILE:N	2.48	0.43
1:I:656:ARG:HA	1:I:656:ARG:HD2	1.72	0.43
1:E:593:ASN:O	2:G:55:ARG:NE	2.52	0.43
1:I:593:ASN:O	2:K:55:ARG:CZ	2.67	0.43
1:B:425:ILE:CD1	1:B:527:LEU:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:PHE:HB3	1:F:257:SER:O	2.19	0.43
2:D:114:THR:OG1	2:D:118:GLN:OE1	2.37	0.43
1:J:755:THR:HG21	2:L:135:LYS:HZ3	1.83	0.43
2:K:40:THR:HG22	2:K:59:ASN:HD21	1.84	0.43
1:I:156:ARG:HD2	1:I:261:GLU:HG3	2.00	0.43
1:J:282:ASN:O	1:J:283:LEU:C	2.57	0.43
2:G:164:GLU:CG	2:G:165:LYS:N	2.81	0.42
1:F:771:TYR:O	1:F:775:VAL:HG23	2.19	0.42
2:D:139:HIS:ND1	2:D:140:PRO:O	2.53	0.42
2:K:63:ILE:C	2:K:114:THR:OG1	2.58	0.42
2:K:263:MET:HG3	2:K:264:ARG:N	2.34	0.42
1:I:580:ILE:HD12	1:I:601:LEU:HD23	2.01	0.42
1:F:432:GLU:HA	1:F:435:GLU:HG2	2.02	0.42
2:L:179:ALA:HB1	2:L:211:ARG:HH12	1.83	0.42
2:K:189:LEU:HB3	2:K:197:ARG:HB2	2.02	0.42
2:C:156:ALA:O	2:C:159:LYS:HG2	2.20	0.42
2:C:108:LEU:HD13	2:C:109:THR:N	2.34	0.42
1:J:615:PRO:HB2	1:J:758:PHE:HE1	1.83	0.42
1:E:224:GLY:O	1:E:682:HIS:ND1	2.51	0.42
1:E:209:ALA:CB	1:E:238:GLY:HA3	2.49	0.42
2:C:109:THR:OG1	2:C:146:GLU:O	2.36	0.42
1:I:670:PHE:HB3	1:J:616:ASN:ND2	2.34	0.42
1:I:155:PHE:HB3	1:I:257:SER:O	2.19	0.42
2:C:80:ILE:HG23	2:C:80:ILE:O	2.19	0.42
1:I:282:ASN:O	1:I:283:LEU:C	2.58	0.42
2:C:83:LEU:HD22	2:C:90:ILE:HG12	2.00	0.42
2:D:80:ILE:O	2:D:80:ILE:HG23	2.19	0.42
1:E:282:ASN:O	1:E:283:LEU:C	2.58	0.42
2:L:68:LEU:CD1	2:L:121:TRP:HB2	2.49	0.42
1:I:656:ARG:NH2	1:I:673:GLU:CA	2.78	0.42
1:F:272:ALA:O	1:F:276:ASN:HB2	2.20	0.42
1:F:572:PHE:HA	1:F:647:ILE:O	2.20	0.42
1:B:227:VAL:HG12	1:B:260:MET:HB2	2.02	0.42
2:K:135:LYS:HB2	2:K:136:PRO:CD	2.50	0.42
2:C:68:LEU:CD1	2:C:121:TRP:HB2	2.50	0.42
1:I:671:MET:CA	1:J:617:MET:SD	3.08	0.42
2:G:63:ILE:N	2:G:114:THR:HG22	2.34	0.42
2:G:243:PRO:HB2	2:G:280:LEU:HD21	2.02	0.42
2:L:108:LEU:HD11	2:L:110:LEU:HD23	2.02	0.41
2:D:111:THR:HA	2:D:121:TRP:O	2.20	0.41
2:G:121:TRP:CZ3	2:G:136:PRO:HG3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:ASN:O	1:F:283:LEU:C	2.58	0.41
2:C:243:PRO:HB2	2:C:280:LEU:HD21	2.01	0.41
1:I:167:ALA:O	1:I:171:GLN:OE1	2.37	0.41
1:I:622:THR:OG1	3:I:1801:ANP:H8	2.20	0.41
1:E:728:HIS:ND1	1:F:699:THR:HA	2.35	0.41
2:C:139:HIS:ND1	2:C:140:PRO:O	2.53	0.41
2:C:110:LEU:CD2	2:C:145:LEU:HG	2.49	0.41
1:B:656:ARG:HE	1:B:676:GLU:CB	2.31	0.41
1:B:656:ARG:NE	1:B:676:GLU:CB	2.81	0.41
2:L:83:LEU:HA	2:L:87:GLU:HA	2.02	0.41
2:G:135:LYS:HB2	2:G:136:PRO:CD	2.50	0.41
1:J:572:PHE:HA	1:J:647:ILE:O	2.19	0.41
1:J:224:GLY:O	1:J:682:HIS:ND1	2.51	0.41
1:A:219:THR:CG2	1:B:780:GLY:HA2	2.51	0.41
2:C:110:LEU:HD21	2:C:145:LEU:CB	2.48	0.41
1:I:616:ASN:CG	1:J:670:PHE:CD2	2.94	0.41
2:H:135:LYS:HB2	2:H:136:PRO:CD	2.51	0.41
1:I:168:ALA:HA	1:I:171:GLN:OE1	2.20	0.41
2:H:90:ILE:HG22	2:K:266:ARG:HH21	1.73	0.41
2:G:139:HIS:NE2	2:G:144:THR:OG1	2.54	0.41
1:A:224:GLY:O	1:A:682:HIS:ND1	2.53	0.41
2:G:185:VAL:O	2:G:211:ARG:NH2	2.53	0.41
1:I:572:PHE:HA	1:I:647:ILE:O	2.21	0.41
1:J:155:PHE:HB3	1:J:257:SER:O	2.20	0.41
2:D:83:LEU:CD2	2:D:90:ILE:HD12	2.51	0.41
2:H:40:THR:HG22	2:H:59:ASN:HD21	1.86	0.41
2:D:243:PRO:HB2	2:D:280:LEU:HD21	2.03	0.41
1:J:656:ARG:CG	1:J:680:ILE:CD1	2.95	0.41
1:A:622:THR:HG21	3:A:1801:ANP:N7	2.35	0.41
1:E:671:MET:HG2	1:E:672:VAL:HG23	2.02	0.41
2:H:185:VAL:O	2:H:211:ARG:NH2	2.53	0.41
1:E:699:THR:HA	1:F:728:HIS:ND1	2.35	0.41
2:C:109:THR:C	2:C:110:LEU:HG	2.41	0.41
1:I:699:THR:OG1	1:J:771:TYR:N	2.47	0.41
2:L:139:HIS:ND1	2:L:140:PRO:O	2.54	0.41
1:F:207:ASP:HB2	2:G:52:LYS:HE3	2.02	0.41
1:E:773:LEU:HD12	1:E:793:LEU:HD22	2.03	0.41
2:D:40:THR:HG22	2:D:59:ASN:HD21	1.86	0.41
1:B:202:TRP:CZ2	2:C:158:ARG:NH2	2.89	0.41
1:I:783:LYS:HZ3	1:J:256:ARG:HB2	1.85	0.41
1:A:437:ARG:O	1:A:441:ASP:N	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:40:THR:HG22	2:L:59:ASN:HD21	1.86	0.41
1:I:339:GLN:N	1:I:340:PRO:CD	2.84	0.41
1:B:282:ASN:O	1:B:283:LEU:C	2.60	0.41
2:H:80:ILE:HG23	2:H:80:ILE:O	2.21	0.41
1:E:272:ALA:O	1:E:276:ASN:HB2	2.21	0.41
1:J:486:PRO:HD2	1:J:489:TYR:CD1	2.56	0.40
1:B:155:PHE:HB3	1:B:257:SER:O	2.22	0.40
1:J:319:ARG:HD3	1:J:319:ARG:HA	1.74	0.40
2:C:114:THR:O	2:C:115:ALA:C	2.60	0.40
1:F:622:THR:OG1	3:F:1801:ANP:C8	2.70	0.40
2:D:121:TRP:CZ3	2:D:136:PRO:HG3	2.56	0.40
2:K:185:VAL:O	2:K:211:ARG:NH2	2.54	0.40
2:L:185:VAL:O	2:L:211:ARG:NH2	2.54	0.40
1:B:735:LEU:O	1:B:739:MET:N	2.42	0.40
1:B:150:ILE:HD12	1:B:150:ILE:C	2.42	0.40
1:F:437:ARG:O	1:F:441:ASP:N	2.48	0.40
2:K:121:TRP:CZ3	2:K:136:PRO:HG3	2.56	0.40
2:K:111:THR:HG22	2:K:122:GLN:HB2	2.03	0.40
1:I:671:MET:HB2	1:J:617:MET:HG3	2.03	0.40
2:H:66:ASP:N	2:H:66:ASP:OD1	2.55	0.40
1:I:652:ARG:CZ	1:I:654:PHE:HZ	2.34	0.40
1:A:219:THR:HG21	1:B:780:GLY:HA2	2.03	0.40
2:K:243:PRO:HB2	2:K:280:LEU:HD21	2.03	0.40
1:A:155:PHE:HB3	1:A:257:SER:O	2.22	0.40
2:L:46:ILE:HG13	2:L:50:GLY:HA2	2.03	0.40
1:J:227:VAL:HG12	1:J:260:MET:HB2	2.02	0.40
2:K:22:ARG:NE	2:K:167:GLU:OE2	2.55	0.40
1:F:479:ARG:HA	1:F:479:ARG:HD2	1.69	0.40
1:J:656:ARG:HE	1:J:676:GLU:C	2.24	0.40
2:G:120:ALA:HB2	2:G:139:HIS:HB3	2.04	0.40
2:H:190:SER:HA	2:H:195:ILE:HA	2.02	0.40
1:I:179:LEU:HD23	1:I:197:ARG:HB2	2.03	0.40
2:H:86:LEU:HG	2:H:89:ILE:HD12	2.03	0.40
2:K:110:LEU:HD12	2:K:111:THR:N	2.37	0.40
2:D:135:LYS:HB3	2:D:136:PRO:CD	2.51	0.40
1:J:202:TRP:CZ2	2:K:158:ARG:NH2	2.90	0.40
1:J:475:ILE:HG21	1:J:489:TYR:HE2	1.87	0.40
2:L:51:ALA:O	2:L:149:ASP:CA	2.69	0.40
2:C:51:ALA:O	2:C:149:ASP:CA	2.69	0.40

There are no symmetry-related clashes.

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%)	626 (95%)	31 (5%)	2 (0%)	46	83
1	B	659/800 (82%)	627 (95%)	30 (5%)	2 (0%)	46	83
1	E	659/800 (82%)	629 (95%)	27 (4%)	3 (0%)	34	77
1	F	659/800 (82%)	630 (96%)	26 (4%)	3 (0%)	34	77
1	I	659/800 (82%)	627 (95%)	31 (5%)	1 (0%)	52	86
1	J	659/800 (82%)	631 (96%)	25 (4%)	3 (0%)	34	77
2	C	277/369 (75%)	255 (92%)	18 (6%)	4 (1%)	14	58
2	D	277/369 (75%)	252 (91%)	20 (7%)	5 (2%)	11	53
2	G	277/369 (75%)	250 (90%)	22 (8%)	5 (2%)	11	53
2	H	277/369 (75%)	247 (89%)	25 (9%)	5 (2%)	11	53
2	K	277/369 (75%)	253 (91%)	21 (8%)	3 (1%)	17	63
2	L	277/369 (75%)	255 (92%)	18 (6%)	4 (1%)	14	58
All	All	5616/7014 (80%)	5282 (94%)	294 (5%)	40 (1%)	26	71

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	115	ALA
2	D	89	ILE
2	D	115	ALA
2	D	163	THR
2	G	115	ALA
2	G	163	THR
2	H	115	ALA
2	H	163	THR
2	K	163	THR
2	L	115	ALA
2	L	163	THR
2	C	149	ASP

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Mol	Chain	Res	Type
2	D	149	ASP
2	D	150	LEU
1	E	267	ILE
2	G	117	GLN
2	G	149	ASP
2	H	149	ASP
2	H	150	LEU
2	K	149	ASP
2	K	150	LEU
2	L	149	ASP
2	L	150	LEU
2	C	150	LEU
1	F	283	LEU
2	G	150	LEU
1	J	283	LEU
1	A	283	LEU
2	H	111	THR
1	A	780	GLY
1	B	283	LEU
1	F	780	GLY
1	J	780	GLY
1	B	780	GLY
2	C	117	GLN
1	E	780	GLY
1	F	753	GLY
1	I	780	GLY
1	E	753	GLY
1	J	753	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%)	538 (98%)	12 (2%)	60	83
1	B	550/662 (83%)	534 (97%)	16 (3%)	50	78
1	E	550/662 (83%)	535 (97%)	15 (3%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	550/662 (83%)	535 (97%)	15 (3%)	52	79
1	I	550/662 (83%)	536 (98%)	14 (2%)	55	81
1	J	550/662 (83%)	539 (98%)	11 (2%)	63	85
2	C	235/308 (76%)	222 (94%)	13 (6%)	27	63
2	D	235/308 (76%)	224 (95%)	11 (5%)	32	68
2	G	235/308 (76%)	226 (96%)	9 (4%)	40	73
2	H	235/308 (76%)	221 (94%)	14 (6%)	24	60
2	K	235/308 (76%)	223 (95%)	12 (5%)	29	66
2	L	235/308 (76%)	219 (93%)	16 (7%)	20	57
All	All	4710/5820 (81%)	4552 (97%)	158 (3%)	44	75

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	ASP
1	A	275	ARG
1	A	282	ASN
1	A	288	GLU
1	A	313	MET
1	A	361	ARG
1	A	490	MET
1	A	591	VAL
1	A	693	ASP
1	A	730	PHE
1	A	752	HIS
1	A	794	ARG
1	B	265	ASP
1	B	266	SER
1	B	275	ARG
1	B	282	ASN
1	B	283	LEU
1	B	288	GLU
1	B	300	THR
1	B	361	ARG
1	B	479	ARG
1	B	490	MET
1	B	575	LYS
1	B	591	VAL
1	B	693	ASP

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Mol	Chain	Res	Type
1	B	730	PHE
1	B	783	LYS
1	B	794	ARG
2	C	21	GLU
2	C	83	LEU
2	C	109	THR
2	C	114	THR
2	C	117	GLN
2	C	118	GLN
2	C	149	ASP
2	C	154	THR
2	C	163	THR
2	C	204	GLU
2	C	261	ARG
2	C	263	MET
2	C	280	LEU
2	D	65	LYS
2	D	83	LEU
2	D	86	LEU
2	D	109	THR
2	D	118	GLN
2	D	122	GLN
2	D	149	ASP
2	D	154	THR
2	D	163	THR
2	D	266	ARG
2	D	280	LEU
1	E	265	ASP
1	E	266	SER
1	E	267	ILE
1	E	269	MET
1	E	275	ARG
1	E	282	ASN
1	E	288	GLU
1	E	300	THR
1	E	309	ARG
1	E	313	MET
1	E	591	VAL
1	E	617	MET
1	E	693	ASP
1	E	730	PHE
1	E	794	ARG

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Mol	Chain	Res	Type
1	F	265	ASP
1	F	266	SER
1	F	282	ASN
1	F	283	LEU
1	F	288	GLU
1	F	300	THR
1	F	361	ARG
1	F	394	ARG
1	F	479	ARG
1	F	490	MET
1	F	575	LYS
1	F	591	VAL
1	F	730	PHE
1	F	738	LYS
1	F	794	ARG
2	G	21	GLU
2	G	52	LYS
2	G	109	THR
2	G	122	GLN
2	G	149	ASP
2	G	154	THR
2	G	159	LYS
2	G	163	THR
2	G	280	LEU
2	H	21	GLU
2	H	52	LYS
2	H	83	LEU
2	H	86	LEU
2	H	109	THR
2	H	111	THR
2	H	122	GLN
2	H	132	VAL
2	H	149	ASP
2	H	154	THR
2	H	163	THR
2	H	233	ASP
2	H	261	ARG
2	H	280	LEU
1	I	150	ILE
1	I	265	ASP
1	I	266	SER
1	I	282	ASN

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Mol	Chain	Res	Type
1	I	288	GLU
1	I	300	THR
1	I	490	MET
1	I	530	GLU
1	I	575	LYS
1	I	591	VAL
1	I	686	GLU
1	I	693	ASP
1	I	730	PHE
1	I	794	ARG
1	J	140	SER
1	J	265	ASP
1	J	266	SER
1	J	282	ASN
1	J	283	LEU
1	J	288	GLU
1	J	323	GLU
1	J	591	VAL
1	J	693	ASP
1	J	730	PHE
1	J	794	ARG
2	K	21	GLU
2	K	72	LEU
2	K	83	LEU
2	K	109	THR
2	K	118	GLN
2	K	149	ASP
2	K	154	THR
2	K	163	THR
2	K	194	LYS
2	K	228	GLU
2	K	233	ASP
2	K	280	LEU
2	L	21	GLU
2	L	70	LEU
2	L	83	LEU
2	L	109	THR
2	L	111	THR
2	L	118	GLN
2	L	122	GLN
2	L	132	VAL
2	L	149	ASP

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Mol	Chain	Res	Type
2	L	154	THR
2	L	157	ARG
2	L	163	THR
2	L	263	MET
2	L	269	ASN
2	L	280	LEU
2	L	324	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	GLN
1	A	344	GLN
1	A	493	GLN
2	C	324	GLN
2	D	118	GLN
2	D	324	GLN
1	E	248	GLN
1	E	526	GLN
1	F	248	GLN
2	G	118	GLN
2	G	324	GLN
2	H	118	GLN
2	H	324	GLN
1	I	248	GLN
1	I	526	GLN
2	K	118	GLN
2	K	198	GLN
2	K	324	GLN
2	L	118	GLN
2	L	198	GLN
2	L	324	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ANP	A	1801	-	29,33,33	2.10	10 (34%)	26,52,52	2.51	8 (30%)
3	ANP	B	1801	-	29,33,33	2.33	11 (37%)	26,52,52	1.92	6 (23%)
3	ANP	E	1801	-	29,33,33	1.81	7 (24%)	26,52,52	2.26	5 (19%)
3	ANP	F	1801	-	29,33,33	2.06	8 (27%)	26,52,52	2.05	7 (26%)
3	ANP	I	1801	1	29,33,33	2.07	8 (27%)	26,52,52	2.36	6 (23%)
3	ANP	J	1801	-	29,33,33	1.78	7 (24%)	26,52,52	2.18	8 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	B	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	E	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	F	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	I	1801	1	-	0/13/38/38	0/3/3/3
3	ANP	J	1801	-	-	0/13/38/38	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1801	ANP	PG-O2G	-3.55	1.47	1.56
3	J	1801	ANP	PG-O2G	-3.49	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1801	ANP	PB-O2B	-3.32	1.47	1.56
3	F	1801	ANP	PG-O3G	-3.25	1.48	1.56
3	E	1801	ANP	PG-O3G	-3.16	1.48	1.56
3	I	1801	ANP	PG-O3G	-3.16	1.48	1.56
3	J	1801	ANP	PB-O2B	-3.13	1.48	1.56
3	J	1801	ANP	PG-O3G	-2.98	1.48	1.56
3	B	1801	ANP	PB-O2B	-2.95	1.48	1.56
3	A	1801	ANP	PB-O2B	-2.91	1.48	1.56
3	E	1801	ANP	PB-O2B	-2.73	1.49	1.56
3	B	1801	ANP	PG-O2G	-2.69	1.49	1.56
3	B	1801	ANP	PG-O3G	-2.61	1.49	1.56
3	I	1801	ANP	PG-O2G	-2.60	1.49	1.56
3	A	1801	ANP	PG-O3G	-2.58	1.49	1.56
3	F	1801	ANP	PG-O2G	-2.52	1.50	1.56
3	A	1801	ANP	PG-O2G	-2.21	1.50	1.56
3	F	1801	ANP	PB-O2B	-2.12	1.51	1.56
3	B	1801	ANP	PG-O1G	2.38	1.48	1.46
3	J	1801	ANP	PG-N3B	2.61	1.70	1.63
3	J	1801	ANP	PB-O1B	2.62	1.48	1.46
3	I	1801	ANP	C2-N3	2.63	1.36	1.32
3	A	1801	ANP	C2-N3	2.64	1.36	1.32
3	B	1801	ANP	O4'-C1'	2.72	1.45	1.41
3	E	1801	ANP	C2-N3	2.81	1.37	1.32
3	E	1801	ANP	C5-C4	2.93	1.47	1.40
3	A	1801	ANP	O4'-C1'	2.94	1.45	1.41
3	A	1801	ANP	PB-N3B	3.13	1.71	1.63
3	I	1801	ANP	PB-O1B	3.22	1.49	1.46
3	A	1801	ANP	PG-O1G	3.24	1.49	1.46
3	A	1801	ANP	PB-O1B	3.24	1.49	1.46
3	J	1801	ANP	C5-C4	3.27	1.47	1.40
3	F	1801	ANP	C2-N3	3.33	1.38	1.32
3	B	1801	ANP	C2-N3	3.36	1.38	1.32
3	F	1801	ANP	C5-C4	3.48	1.48	1.40
3	B	1801	ANP	PB-O3A	3.57	1.63	1.59
3	E	1801	ANP	PG-N3B	3.58	1.73	1.63
3	I	1801	ANP	C5-C4	3.71	1.48	1.40
3	B	1801	ANP	C5-C4	4.07	1.49	1.40
3	J	1801	ANP	PB-N3B	4.12	1.74	1.63
3	A	1801	ANP	C5-C4	4.17	1.49	1.40
3	E	1801	ANP	PB-N3B	4.29	1.75	1.63
3	B	1801	ANP	PB-N3B	4.35	1.75	1.63
3	F	1801	ANP	PB-O1B	4.39	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1801	ANP	PG-N3B	4.54	1.75	1.63
3	I	1801	ANP	PB-N3B	4.56	1.75	1.63
3	A	1801	ANP	PG-N3B	4.59	1.75	1.63
3	F	1801	ANP	PB-N3B	4.69	1.76	1.63
3	I	1801	ANP	PG-N3B	4.71	1.76	1.63
3	F	1801	ANP	PG-N3B	4.87	1.76	1.63
3	B	1801	ANP	PB-O1B	5.56	1.52	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1801	ANP	N3-C2-N1	-7.64	122.87	128.87
3	J	1801	ANP	N3-C2-N1	-6.96	123.40	128.87
3	I	1801	ANP	N3-C2-N1	-6.79	123.54	128.87
3	F	1801	ANP	N3-C2-N1	-6.53	123.74	128.87
3	A	1801	ANP	N3-C2-N1	-6.43	123.82	128.87
3	B	1801	ANP	N3-C2-N1	-5.92	124.22	128.87
3	E	1801	ANP	PA-O3A-PB	-3.70	119.27	132.71
3	J	1801	ANP	PA-O3A-PB	-3.30	120.74	132.71
3	I	1801	ANP	PA-O3A-PB	-2.83	122.45	132.71
3	B	1801	ANP	O2'-C2'-C3'	-2.23	104.64	111.86
3	A	1801	ANP	PA-O3A-PB	-2.23	124.62	132.71
3	F	1801	ANP	PA-O3A-PB	-2.20	124.73	132.71
3	F	1801	ANP	O2'-C2'-C3'	-2.05	105.23	111.86
3	J	1801	ANP	O2'-C2'-C1'	2.01	117.90	111.61
3	J	1801	ANP	C4'-O4'-C1'	2.03	111.80	109.64
3	A	1801	ANP	O3G-PG-O2G	2.04	113.59	107.67
3	I	1801	ANP	O3G-PG-O2G	2.04	113.59	107.67
3	J	1801	ANP	O3G-PG-O2G	2.06	113.64	107.67
3	J	1801	ANP	O4'-C1'-N9	2.07	112.02	108.11
3	A	1801	ANP	O4'-C4'-C5'	2.07	116.71	109.29
3	F	1801	ANP	N6-C6-N1	2.13	122.08	118.52
3	B	1801	ANP	O3G-PG-O2G	2.24	114.19	107.67
3	B	1801	ANP	O4'-C1'-N9	2.33	112.51	108.11
3	E	1801	ANP	O3G-PG-O2G	2.65	115.36	107.67
3	J	1801	ANP	O3A-PB-N3B	2.70	113.50	106.07
3	F	1801	ANP	O2B-PB-O1B	2.78	115.49	110.02
3	I	1801	ANP	O2B-PB-O1B	2.89	115.71	110.02
3	E	1801	ANP	N6-C6-N1	3.00	123.55	118.52
3	F	1801	ANP	C1'-N9-C4	3.05	130.21	126.81
3	A	1801	ANP	O5'-C5'-C4'	3.20	120.63	109.09
3	B	1801	ANP	C4'-O4'-C1'	3.27	113.11	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1801	ANP	C4'-O4'-C1'	3.56	113.41	109.64
3	B	1801	ANP	C1'-N9-C4	3.97	131.24	126.81
3	E	1801	ANP	O2B-PB-O1B	4.63	119.14	110.02
3	A	1801	ANP	C4'-O4'-C1'	4.99	114.93	109.64
3	A	1801	ANP	O2B-PB-O1B	5.19	120.24	110.02
3	I	1801	ANP	C1'-N9-C4	5.20	132.61	126.81
3	A	1801	ANP	C1'-N9-C4	5.30	132.72	126.81
3	J	1801	ANP	O2B-PB-O1B	5.33	120.53	110.02
3	I	1801	ANP	C4'-O4'-C1'	5.43	115.40	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1801	ANP	2	0
3	B	1801	ANP	1	0
3	E	1801	ANP	9	0
3	F	1801	ANP	4	0
3	I	1801	ANP	3	0
3	J	1801	ANP	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	663/800 (82%)	0.79	83 (12%)	5 11	177, 220, 306, 373	0
1	B	663/800 (82%)	0.74	66 (9%)	9 14	196, 245, 311, 362	0
1	E	663/800 (82%)	0.80	84 (12%)	5 11	191, 224, 348, 398	0
1	F	663/800 (82%)	0.73	67 (10%)	9 14	181, 220, 296, 350	0
1	I	663/800 (82%)	1.12	110 (16%)	2 8	198, 244, 528, 643	0
1	J	663/800 (82%)	1.24	158 (23%)	1 6	213, 266, 510, 602	0
2	C	285/369 (77%)	0.81	33 (11%)	6 12	200, 237, 282, 323	0
2	D	285/369 (77%)	0.89	43 (15%)	3 9	193, 234, 273, 296	0
2	G	285/369 (77%)	1.07	61 (21%)	1 6	217, 239, 319, 347	0
2	H	285/369 (77%)	0.92	41 (14%)	3 9	210, 227, 268, 294	0
2	K	285/369 (77%)	0.90	36 (12%)	5 11	197, 233, 295, 329	0
2	L	285/369 (77%)	1.04	60 (21%)	1 6	233, 264, 336, 375	0
All	All	5688/7014 (81%)	0.91	842 (14%)	3 9	177, 237, 355, 643	0

All (842) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	421	ASP	13.9
1	I	422	GLY	13.1
1	I	749	ALA	8.3
1	J	515	THR	8.3
1	I	420	ARG	7.8
2	C	138	ALA	7.7
1	I	419	VAL	7.3
1	J	429	TYR	7.2
1	I	471	HIS	7.2
1	I	461	ASP	7.1
1	J	459	GLY	6.8

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Mol	Chain	Res	Type	RSRZ
1	J	398	GLY	6.8
2	G	330	LEU	6.8
1	I	488	ASN	6.7
2	L	138	ALA	6.6
1	J	458	THR	6.6
1	I	492	ARG	6.4
2	G	241	ALA	6.1
1	J	399	GLU	6.1
1	F	645	VAL	6.1
1	J	513	VAL	6.0
1	J	426	ALA	5.9
2	L	23	PRO	5.8
1	I	497	ASN	5.7
1	E	609	MET	5.6
1	F	646	GLU	5.5
1	I	423	GLY	5.5
1	J	519	LYS	5.5
2	K	264	ARG	5.5
2	G	81	ALA	5.5
1	F	638	SER	5.4
1	J	514	LEU	5.4
1	J	722	LEU	5.4
1	I	473	TYR	5.4
1	F	577	GLY	5.2
1	I	577	GLY	5.2
2	G	240	VAL	5.2
1	A	659	ALA	5.1
1	J	381	GLN	5.1
1	I	757	ALA	5.1
1	J	410	ALA	5.1
1	J	512	LYS	5.1
1	A	702	TYR	5.1
1	I	498	ALA	5.0
2	G	331	GLN	5.0
1	J	659	ALA	5.0
1	J	443	ALA	5.0
1	J	422	GLY	5.0
1	E	723	THR	4.9
1	J	427	SER	4.9
1	E	722	LEU	4.9
1	I	470	VAL	4.9
1	J	756	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	J	757	ALA	4.8
1	I	515	THR	4.8
1	J	136	ILE	4.8
1	J	397	MET	4.7
1	A	503	ILE	4.7
2	G	289	VAL	4.7
1	E	489	TYR	4.6
1	F	578	ILE	4.6
1	E	756	ILE	4.6
1	I	489	TYR	4.6
1	I	748	ASP	4.6
1	J	444	THR	4.6
1	J	701	THR	4.6
1	B	692	MET	4.6
1	J	421	ASP	4.6
1	J	400	PHE	4.5
1	I	578	ILE	4.5
2	G	23	PRO	4.5
1	I	472	GLY	4.5
1	J	480	GLY	4.5
1	A	177	GLU	4.4
1	E	659	ALA	4.4
2	D	82	SER	4.4
2	G	287	ALA	4.4
1	I	759	MET	4.3
1	B	705	LEU	4.3
2	K	125	ALA	4.3
2	G	239	TRP	4.3
1	E	419	VAL	4.3
1	J	376	PRO	4.3
2	K	80	ILE	4.3
1	E	429	TYR	4.3
2	H	82	SER	4.3
1	I	646	GLU	4.3
2	G	22	ARG	4.3
2	L	107	ARG	4.3
1	J	375	LEU	4.2
2	D	83	LEU	4.2
1	J	425	ILE	4.2
1	F	749	ALA	4.2
2	K	285	GLN	4.2
2	H	264	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
2	L	124	TYR	4.2
1	J	470	VAL	4.2
1	J	148	LEU	4.2
2	H	49	GLY	4.1
2	G	20	VAL	4.1
1	B	178	LEU	4.1
1	A	701	THR	4.1
1	J	658	GLY	4.1
1	J	420	ARG	4.1
1	E	362	PRO	4.1
2	C	82	SER	4.1
1	J	411	ILE	4.1
1	I	758	PHE	4.1
1	J	751	GLU	4.0
1	J	423	GLY	4.0
1	I	751	GLU	4.0
1	B	727	THR	4.0
1	E	148	LEU	4.0
2	G	322	ILE	4.0
1	F	750	LEU	4.0
1	E	382	LEU	4.0
1	J	378	LEU	4.0
1	J	442	GLY	4.0
1	J	518	GLY	4.0
1	J	407	LEU	3.9
1	J	511	ASP	3.9
2	C	139	HIS	3.9
2	G	325	GLY	3.9
2	L	198	GLN	3.9
2	L	291	TYR	3.9
1	A	697	ARG	3.9
1	F	742	VAL	3.9
2	G	107	ARG	3.9
1	J	362	PRO	3.9
2	K	286	PRO	3.9
2	H	123	ALA	3.9
2	H	71	ALA	3.9
2	L	279	LYS	3.9
1	J	372	PHE	3.8
2	G	290	LEU	3.8
1	J	524	GLU	3.8
2	C	80	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	G	21	GLU	3.8
1	B	707	LEU	3.8
1	J	750	LEU	3.8
1	E	749	ALA	3.8
1	J	690	VAL	3.8
1	B	280	THR	3.8
1	J	178	LEU	3.8
1	J	457	ARG	3.8
1	B	749	ALA	3.8
1	I	465	VAL	3.8
1	E	610	LEU	3.7
1	I	761	SER	3.7
1	E	552	LEU	3.7
1	F	637	GLY	3.7
1	J	345	VAL	3.7
1	I	647	ILE	3.7
1	E	381	GLN	3.7
1	E	655	THR	3.7
1	I	475	ILE	3.7
1	J	433	LEU	3.7
2	D	20	VAL	3.7
1	I	481	GLN	3.7
1	B	748	ASP	3.7
2	K	243	PRO	3.7
1	J	755	THR	3.7
1	J	523	LEU	3.7
2	G	288	PHE	3.7
2	H	198	GLN	3.7
1	F	721	ALA	3.7
2	L	150	LEU	3.6
1	J	612	ILE	3.6
1	J	368	MET	3.6
1	I	460	LEU	3.6
1	J	204	PHE	3.6
1	J	428	GLY	3.6
1	J	520	ALA	3.6
2	G	256	PHE	3.6
2	K	21	GLU	3.6
1	B	493	GLN	3.6
1	J	374	GLN	3.6
2	L	262	MET	3.5
1	J	595	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	G	329	VAL	3.5
1	B	693	ASP	3.5
1	J	382	LEU	3.5
2	K	134	VAL	3.5
1	E	576	PRO	3.5
1	F	136	ILE	3.5
1	I	424	VAL	3.5
2	D	70	LEU	3.5
2	L	26	VAL	3.5
2	H	265	ASP	3.5
1	B	638	SER	3.5
1	J	342	LEU	3.5
1	I	345	VAL	3.5
1	E	551	GLU	3.5
1	J	430	ASN	3.5
2	G	266	ARG	3.5
1	B	732	LEU	3.5
1	J	419	VAL	3.5
1	J	521	LEU	3.5
1	B	659	ALA	3.4
1	I	609	MET	3.4
1	F	695	ILE	3.4
1	B	465	VAL	3.4
1	I	399	GLU	3.4
1	I	463	LEU	3.4
2	K	138	ALA	3.4
1	E	689	LEU	3.4
1	A	595	PRO	3.4
1	B	136	ILE	3.4
2	L	242	ASP	3.4
1	B	709	TRP	3.4
2	C	119	GLU	3.4
1	F	256	ARG	3.4
1	J	531	LEU	3.4
2	L	137	ALA	3.4
1	A	656	ARG	3.4
1	A	797	GLU	3.4
1	J	749	ALA	3.4
1	J	481	GLN	3.4
1	J	460	LEU	3.4
2	C	137	ALA	3.3
2	G	326	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	464	LYS	3.3
1	E	658	GLY	3.3
1	J	343	ARG	3.3
2	K	265	ASP	3.3
1	J	471	HIS	3.3
1	A	696	GLY	3.3
2	H	241	ALA	3.3
2	C	136	PRO	3.3
2	L	27	VAL	3.3
1	E	155	PHE	3.3
1	J	134	ALA	3.3
1	E	425	ILE	3.3
1	J	341	VAL	3.3
2	L	81	ALA	3.3
2	H	132	VAL	3.3
1	E	555	LEU	3.3
1	I	400	PHE	3.3
1	E	721	ALA	3.3
2	C	239	TRP	3.3
1	J	509	TYR	3.3
2	G	272	ILE	3.2
1	E	454	GLU	3.2
1	F	571	THR	3.2
1	I	514	LEU	3.2
2	G	82	SER	3.2
1	F	420	ARG	3.2
2	L	24	ALA	3.2
2	H	133	THR	3.2
2	L	20	VAL	3.2
1	E	385	VAL	3.2
2	D	99	LEU	3.2
1	I	599	ASN	3.2
2	K	284	GLN	3.2
1	B	706	SER	3.2
1	I	346	GLY	3.2
1	A	502	ILE	3.2
2	G	243	PRO	3.2
1	A	420	ARG	3.2
2	H	243	PRO	3.2
1	B	708	ALA	3.2
1	A	216	GLN	3.2
1	J	469	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	125	ALA	3.2
1	B	372	PHE	3.2
2	K	263	MET	3.2
2	L	22	ARG	3.2
2	H	266	ARG	3.2
1	J	689	LEU	3.1
1	B	695	ILE	3.1
2	L	290	LEU	3.1
1	E	276	ASN	3.1
1	J	752	HIS	3.1
1	I	750	LEU	3.1
1	J	424	VAL	3.1
1	F	756	ILE	3.1
1	F	398	GLY	3.1
1	E	136	ILE	3.1
1	E	690	VAL	3.1
1	E	352	LEU	3.1
2	H	72	LEU	3.1
1	E	488	ASN	3.1
1	J	344	GLN	3.1
2	K	49	GLY	3.1
2	G	227	ILE	3.1
1	B	702	TYR	3.1
2	L	263	MET	3.1
1	J	610	LEU	3.1
1	A	465	VAL	3.1
1	I	469	ALA	3.1
2	K	124	TYR	3.1
1	B	701	THR	3.1
2	L	241	ALA	3.1
1	A	419	VAL	3.1
2	G	124	TYR	3.1
1	J	339	GLN	3.1
1	J	724	LEU	3.0
1	J	522	ALA	3.0
2	H	80	ILE	3.0
1	I	462	THR	3.0
2	K	109	THR	3.0
2	L	237	ARG	3.0
2	C	231	HIS	3.0
2	D	84	ASP	3.0
1	F	212	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	458	THR	3.0
2	H	122	GLN	3.0
1	B	762	VAL	3.0
2	C	81	ALA	3.0
1	B	726	ALA	3.0
1	A	196	LEU	3.0
1	B	696	GLY	3.0
2	C	220	PHE	3.0
1	J	657	VAL	3.0
1	J	401	ALA	3.0
1	J	516	SER	3.0
1	A	516	SER	3.0
2	G	328	SER	3.0
1	B	420	ARG	3.0
2	K	66	ASP	3.0
1	F	576	PRO	3.0
1	J	517	LYS	3.0
2	K	260	GLY	3.0
1	A	255	ILE	3.0
1	A	504	PRO	3.0
1	A	586	PRO	2.9
1	I	360	ALA	2.9
1	A	703	ASP	2.9
1	A	492	ARG	2.9
2	H	286	PRO	2.9
1	J	377	GLU	2.9
1	B	637	GLY	2.9
1	B	179	LEU	2.9
2	K	241	ALA	2.9
1	F	183	ASP	2.9
1	J	385	VAL	2.9
1	A	707	LEU	2.9
1	F	155	PHE	2.9
1	I	576	PRO	2.9
2	L	25	SER	2.9
1	I	572	PHE	2.9
1	I	756	ILE	2.9
1	J	406	LEU	2.9
2	K	108	LEU	2.9
1	E	755	THR	2.9
2	D	21	GLU	2.9
2	K	84	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	600	PRO	2.9
1	A	473	TYR	2.9
1	B	747	LEU	2.9
1	E	554	VAL	2.9
1	J	586	PRO	2.9
1	B	703	ASP	2.8
1	A	796	LEU	2.8
1	I	645	VAL	2.8
1	I	280	THR	2.8
2	G	125	ALA	2.8
1	I	586	PRO	2.8
2	D	137	ALA	2.8
2	L	240	VAL	2.8
1	F	601	LEU	2.8
1	F	572	PHE	2.8
1	I	510	GLU	2.8
2	D	138	ALA	2.8
1	F	630	ILE	2.8
1	J	133	LEU	2.8
2	K	220	PHE	2.8
1	I	519	LYS	2.8
1	I	597	ILE	2.8
2	G	279	LYS	2.8
1	E	457	ARG	2.8
2	D	102	ILE	2.8
2	G	80	ILE	2.8
2	K	107	ARG	2.8
2	D	199	TYR	2.8
2	D	239	TRP	2.8
1	I	219	THR	2.8
1	J	492	ARG	2.8
2	K	50	GLY	2.8
2	D	208	LYS	2.8
2	D	220	PHE	2.8
2	H	138	ALA	2.8
1	I	641	PRO	2.8
2	G	236	LEU	2.8
1	B	658	GLY	2.8
2	L	31	VAL	2.8
1	A	421	ASP	2.8
1	J	638	SER	2.8
2	L	257	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	701	THR	2.8
1	F	751	GLU	2.8
2	K	146	GLU	2.7
2	L	106	SER	2.7
2	G	108	LEU	2.7
1	E	134	ALA	2.7
1	F	644	LYS	2.7
2	K	139	HIS	2.7
2	K	90	ILE	2.7
1	A	488	ASN	2.7
1	F	748	ASP	2.7
1	J	394	ARG	2.7
1	A	475	ILE	2.7
2	C	226	ALA	2.7
1	B	694	GLU	2.7
2	D	97	GLU	2.7
1	I	493	GLN	2.7
1	A	748	ASP	2.7
1	A	505	GLU	2.7
1	I	695	ILE	2.7
1	J	468	ASN	2.7
1	J	535	LEU	2.7
1	A	658	GLY	2.7
1	E	577	GLY	2.7
1	E	751	GLU	2.7
1	E	345	VAL	2.7
1	J	403	LEU	2.7
2	G	242	ASP	2.7
2	G	257	TYR	2.7
2	G	318	VAL	2.7
1	J	454	GLU	2.7
2	H	81	ALA	2.7
1	J	147	THR	2.7
1	J	445	ASP	2.7
1	B	725	PHE	2.7
1	E	420	ARG	2.7
1	I	694	GLU	2.7
2	L	151	PHE	2.7
1	F	580	ILE	2.7
2	H	63	ILE	2.7
1	A	506	LEU	2.7
1	F	627	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	725	PHE	2.7
1	J	700	SER	2.7
2	L	82	SER	2.7
1	A	381	GLN	2.6
1	I	579	ARG	2.6
1	F	626	GLN	2.6
1	E	179	LEU	2.6
1	B	654	PHE	2.6
1	E	430	ASN	2.6
1	F	752	HIS	2.6
2	D	198	GLN	2.6
1	A	695	ILE	2.6
1	B	135	ALA	2.6
1	E	258	ILE	2.6
1	J	346	GLY	2.6
1	E	549	LEU	2.6
1	F	145	TYR	2.6
1	F	603	LEU	2.6
2	G	150	LEU	2.6
1	F	399	GLU	2.6
1	F	639	TYR	2.6
1	A	440	ALA	2.6
1	A	454	GLU	2.6
1	B	492	ARG	2.6
2	G	327	LEU	2.6
2	L	264	ARG	2.6
1	I	455	ARG	2.6
1	I	760	HIS	2.6
2	G	132	VAL	2.6
1	J	441	ASP	2.6
1	A	178	LEU	2.6
1	A	486	PRO	2.6
1	I	742	VAL	2.6
2	H	125	ALA	2.6
2	K	279	LYS	2.6
1	B	147	THR	2.6
2	G	133	THR	2.6
1	E	351	ILE	2.6
1	F	258	ILE	2.6
1	I	466	GLY	2.6
2	L	289	VAL	2.6
1	I	418	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	212	GLN	2.6
2	H	21	GLU	2.6
1	E	147	THR	2.6
1	I	279	ILE	2.6
1	I	580	ILE	2.6
1	E	158	SER	2.6
1	J	348	LEU	2.6
2	D	202	VAL	2.5
1	B	134	ALA	2.5
1	J	558	LEU	2.5
2	G	229	TRP	2.5
1	J	691	LEU	2.5
1	J	723	THR	2.5
2	C	238	GLY	2.5
1	F	647	ILE	2.5
1	B	421	ASP	2.5
1	E	556	VAL	2.5
1	I	267	ILE	2.5
2	G	321	PHE	2.5
2	D	200	ARG	2.5
1	A	417	VAL	2.5
1	F	505	GLU	2.5
1	I	474	TYR	2.5
1	J	635	TYR	2.5
1	J	692	MET	2.5
1	I	496	LYS	2.5
1	A	489	TYR	2.5
1	B	691	LEU	2.5
1	B	704	GLY	2.5
2	H	180	LEU	2.5
2	D	71	ALA	2.5
2	L	250	LEU	2.5
2	G	198	GLN	2.5
2	C	135	LYS	2.5
2	G	237	ARG	2.5
2	G	262	MET	2.5
1	B	331	LEU	2.5
1	I	415	PRO	2.5
1	J	780	GLY	2.5
2	L	134	VAL	2.5
2	L	136	PRO	2.5
1	A	704	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	147	THR	2.5
1	A	385	VAL	2.5
1	I	638	SER	2.5
2	D	291	TYR	2.5
1	I	762	VAL	2.5
2	D	100	ALA	2.5
1	J	300	THR	2.5
1	E	178	LEU	2.4
1	E	259	THR	2.4
1	E	355	LEU	2.4
1	I	433	LEU	2.4
1	J	277	LEU	2.4
1	J	473	TYR	2.4
1	F	255	ILE	2.4
1	A	458	THR	2.4
2	D	68	LEU	2.4
2	C	286	PRO	2.4
1	B	279	ILE	2.4
1	E	608	ARG	2.4
1	I	456	GLU	2.4
1	J	611	ILE	2.4
1	I	221	ASP	2.4
1	A	705	LEU	2.4
2	D	96	GLY	2.4
2	G	224	ALA	2.4
2	H	216	LEU	2.4
1	A	524	GLU	2.4
1	A	476	GLN	2.4
2	H	124	TYR	2.4
1	I	614	GLY	2.4
1	J	379	ARG	2.4
1	J	299	VAL	2.4
1	J	298	THR	2.4
1	F	489	TYR	2.4
1	A	770	SER	2.4
2	H	285	GLN	2.4
1	F	696	GLY	2.4
1	E	154	ARG	2.4
1	E	572	PHE	2.4
1	E	729	TYR	2.4
2	G	148	LEU	2.4
2	L	326	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	344	GLN	2.4
1	A	415	PRO	2.4
1	J	743	ALA	2.4
1	B	324	ARG	2.4
1	E	338	LEU	2.4
1	J	549	LEU	2.4
1	J	557	ASN	2.4
2	H	95	ARG	2.4
2	K	262	MET	2.4
2	L	260	GLY	2.4
1	I	299	VAL	2.4
1	I	425	ILE	2.4
1	B	368	MET	2.4
1	F	579	ARG	2.4
1	J	351	ILE	2.4
1	I	464	LYS	2.4
2	D	201	ALA	2.4
2	D	228	GLU	2.4
1	E	657	VAL	2.4
1	I	266	SER	2.4
1	J	295	LEU	2.4
1	J	613	THR	2.4
1	B	731	GLU	2.4
2	C	224	ALA	2.4
1	I	430	ASN	2.4
2	G	149	ASP	2.4
1	J	479	ARG	2.4
1	F	144	GLY	2.4
2	K	65	LYS	2.3
1	A	424	VAL	2.3
1	F	419	VAL	2.3
2	D	124	TYR	2.3
1	F	503	ILE	2.3
1	E	558	LEU	2.3
2	C	86	LEU	2.3
2	G	220	PHE	2.3
1	E	475	ILE	2.3
2	L	246	THR	2.3
2	L	239	TRP	2.3
1	F	722	LEU	2.3
1	J	396	LYS	2.3
1	A	418	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	81	ALA	2.3
1	F	148	LEU	2.3
2	C	120	ALA	2.3
2	G	226	ALA	2.3
1	J	527	LEU	2.3
1	B	756	ILE	2.3
1	I	427	SER	2.3
1	J	482	SER	2.3
1	F	757	ALA	2.3
1	I	571	THR	2.3
1	A	706	SER	2.3
1	I	504	PRO	2.3
2	G	292	LEU	2.3
1	I	631	ALA	2.3
1	J	402	GLU	2.3
2	C	322	ILE	2.3
1	J	474	TYR	2.3
2	H	284	GLN	2.3
2	L	132	VAL	2.3
2	L	236	LEU	2.3
1	A	708	ALA	2.3
1	F	570	PRO	2.3
1	I	754	ASP	2.3
1	F	694	GLU	2.3
2	G	97	GLU	2.3
1	E	553	ASP	2.3
1	F	257	SER	2.3
2	K	34	SER	2.3
2	K	95	ARG	2.3
1	I	242	GLN	2.3
1	A	443	ALA	2.3
2	C	144	THR	2.3
1	E	493	GLN	2.3
1	I	502	ILE	2.3
2	L	287	ALA	2.3
1	F	421	ASP	2.3
1	J	189	LEU	2.3
1	B	690	VAL	2.3
1	J	467	PHE	2.3
2	C	20	VAL	2.3
1	I	517	LYS	2.3
1	F	506	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	322	ILE	2.3
1	F	755	THR	2.3
1	E	748	ASP	2.2
2	D	133	THR	2.2
1	I	486	PRO	2.2
1	E	505	GLU	2.2
1	F	655	THR	2.2
2	C	122	GLN	2.2
1	E	156	ARG	2.2
1	J	314	PRO	2.2
1	A	638	SER	2.2
2	H	162	ARG	2.2
2	D	125	ALA	2.2
2	L	133	THR	2.2
1	I	507	LYS	2.2
1	J	456	GLU	2.2
1	E	742	VAL	2.2
1	F	628	ALA	2.2
2	H	242	ASP	2.2
2	K	240	VAL	2.2
2	L	30	LEU	2.2
1	A	654	PHE	2.2
1	J	464	LYS	2.2
2	L	220	PHE	2.2
1	B	610	LEU	2.2
2	L	266	ARG	2.2
1	B	255	ILE	2.2
2	C	326	VAL	2.2
1	I	468	ASN	2.2
2	C	97	GLU	2.2
1	F	346	GLY	2.2
1	A	493	GLN	2.2
1	E	411	ILE	2.2
1	I	520	ALA	2.2
1	I	524	GLU	2.2
2	L	256	PHE	2.2
2	D	236	LEU	2.2
1	E	280	THR	2.2
1	A	447	LEU	2.2
1	J	179	LEU	2.2
1	F	656	ARG	2.2
2	G	264	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	506	LEU	2.2
1	A	315	VAL	2.2
2	D	101	SER	2.2
1	B	735	LEU	2.2
1	E	133	LEU	2.2
1	E	757	ALA	2.2
1	I	513	VAL	2.2
1	A	448	GLU	2.2
1	I	658	GLY	2.2
2	G	225	LEU	2.2
1	E	403	LEU	2.2
1	J	483	HIS	2.2
1	A	136	ILE	2.2
2	C	230	GLN	2.2
2	L	46	ILE	2.2
2	H	199	TYR	2.2
2	H	22	ARG	2.2
1	A	677	THR	2.2
1	E	758	PHE	2.2
1	F	599	ASN	2.2
2	D	81	ALA	2.2
2	G	208	LYS	2.2
1	J	154	ARG	2.2
1	A	670	PHE	2.2
1	B	724	LEU	2.2
1	A	800	SER	2.2
1	A	154	ARG	2.1
1	A	217	PHE	2.1
2	D	67	GLU	2.1
1	A	655	THR	2.1
1	I	426	ALA	2.1
1	B	743	ALA	2.1
2	L	223	GLN	2.1
1	B	780	GLY	2.1
1	E	399	GLU	2.1
1	I	330	ALA	2.1
2	D	227	ILE	2.1
2	D	95	ARG	2.1
1	E	727	THR	2.1
1	J	393	LEU	2.1
2	C	121	TRP	2.1
1	A	466	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	291	TYR	2.1
2	H	137	ALA	2.1
2	L	70	LEU	2.1
1	A	517	LYS	2.1
1	I	355	LEU	2.1
2	L	72	LEU	2.1
1	E	361	ARG	2.1
1	I	403	LEU	2.1
1	I	503	ILE	2.1
2	C	236	LEU	2.1
2	H	70	LEU	2.1
1	A	514	LEU	2.1
1	E	257	SER	2.1
1	F	629	LEU	2.1
2	G	265	ASP	2.1
1	A	436	TRP	2.1
1	A	195	GLY	2.1
1	B	488	ASN	2.1
2	L	218	THR	2.1
1	B	761	SER	2.1
1	I	190	ILE	2.1
1	J	528	TYR	2.1
1	J	727	THR	2.1
2	D	235	THR	2.1
2	D	224	ALA	2.1
2	L	123	ALA	2.1
1	J	383	GLU	2.1
2	D	279	LYS	2.1
2	L	119	GLU	2.1
1	E	213	LEU	2.1
2	G	260	GLY	2.1
2	H	215	ILE	2.1
2	K	83	LEU	2.1
1	J	315	VAL	2.1
2	H	134	VAL	2.1
1	I	431	GLU	2.1
1	I	451	GLU	2.1
2	K	67	GLU	2.1
1	J	455	ARG	2.1
2	K	254	GLN	2.1
1	A	535	LEU	2.1
1	E	378	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	291	LEU	2.1
2	G	263	MET	2.1
2	L	272	ILE	2.1
2	H	84	ASP	2.1
1	A	500	ARG	2.1
1	J	732	LEU	2.1
1	J	759	MET	2.1
1	J	551	GLU	2.1
1	J	437	ARG	2.1
2	D	191	HIS	2.1
2	L	216	LEU	2.1
1	B	609	MET	2.1
1	B	729	TYR	2.1
1	F	470	VAL	2.1
1	J	135	ALA	2.1
1	A	513	VAL	2.1
1	B	502	ILE	2.1
1	A	773	LEU	2.1
1	B	616	ASN	2.1
2	L	28	LYS	2.1
2	L	103	SER	2.1
1	A	190	ILE	2.1
1	J	489	TYR	2.1
2	H	326	VAL	2.1
1	J	404	ARG	2.1
1	J	702	TYR	2.1
2	C	85	ASP	2.1
1	I	659	ALA	2.1
2	H	119	GLU	2.1
1	E	390	VAL	2.0
2	C	95	ARG	2.0
2	H	246	THR	2.0
2	D	103	SER	2.0
2	G	106	SER	2.0
1	E	528	TYR	2.0
1	A	280	THR	2.0
1	J	365	LEU	2.0
1	F	146	ALA	2.0
1	F	422	GLY	2.0
2	G	216	LEU	2.0
1	B	576	PRO	2.0
1	E	422	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	65	LYS	2.0
2	C	21	GLU	2.0
1	J	576	PRO	2.0
2	C	229	TRP	2.0
2	C	287	ALA	2.0
2	D	80	ILE	2.0
2	L	45	ASP	2.0
1	J	203	GLU	2.0
2	C	134	VAL	2.0
1	I	528	TYR	2.0
2	L	108	LEU	2.0
1	B	190	ILE	2.0
1	E	491	ARG	2.0
1	B	473	TYR	2.0
1	E	348	LEU	2.0
1	B	242	GLN	2.0
1	B	711	VAL	2.0
1	A	179	LEU	2.0
1	E	691	LEU	2.0
1	A	507	LYS	2.0
1	F	135	ALA	2.0
1	I	505	GLU	2.0
1	I	542	LEU	2.0
2	D	266	ARG	2.0
2	H	108	LEU	2.0
1	A	657	VAL	2.0
1	A	378	LEU	2.0
1	A	725	PHE	2.0
1	J	463	LEU	2.0
2	D	72	LEU	2.0
1	A	145	TYR	2.0
2	G	134	VAL	2.0
2	L	135	LYS	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ANP	A	1801	31/31	0.86	0.32	-0.87	198,206,212,215	0
3	ANP	I	1801	31/31	0.84	0.38	-0.91	198,200,203,204	0
3	ANP	F	1801	31/31	0.88	0.33	-0.99	195,202,206,209	0
3	ANP	B	1801	31/31	0.78	0.33	-1.04	216,223,227,230	0
3	ANP	J	1801	31/31	0.91	0.23	-1.12	218,226,233,235	0
3	ANP	E	1801	31/31	0.93	0.28	-1.13	198,201,206,207	0

6.5 Other polymers [i](#)

There are no such residues in this entry.