



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:09 am 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

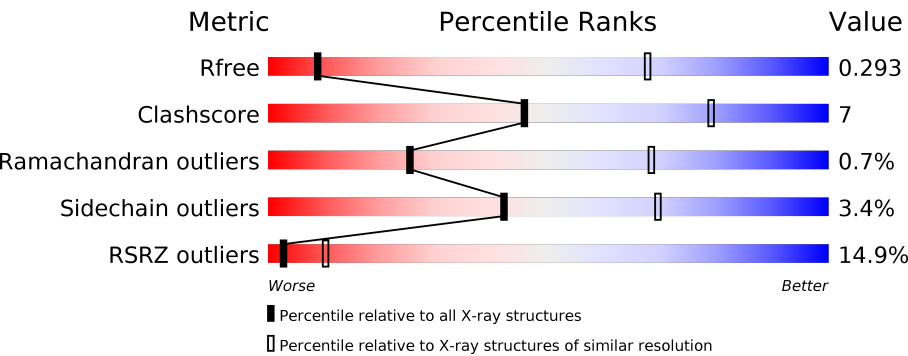
1 Overall quality at a glance i

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}	100719	1099 (9.50-3.70)
Clashscore	112137	1031 (9.00-3.80)
Ramachandran outliers	110173	1000 (9.00-3.76)
Sidechain outliers	110143	1097 (9.50-3.70)
RSRZ outliers	101464	1000 (9.00-3.72)

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>9%</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>
1	J	800	<div><div>20%</div><div><div></div><div>71%</div><div>11%</div><div>•</div><div>17%</div></div></div>

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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	-

2 Entry composition

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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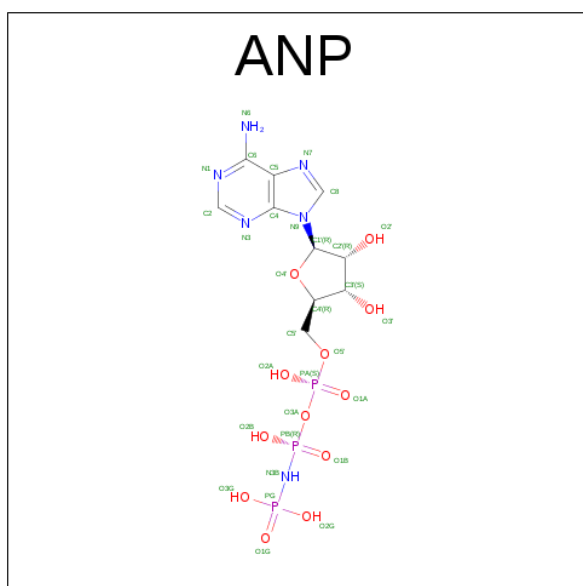
Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	SER	-	EXPRESSION TAG	UNP P23367
H	-8	SER	-	EXPRESSION TAG	UNP P23367
H	-7	GLY	-	EXPRESSION TAG	UNP P23367
H	-6	LEU	-	EXPRESSION TAG	UNP P23367
H	-5	VAL	-	EXPRESSION TAG	UNP P23367
H	-4	PRO	-	EXPRESSION TAG	UNP P23367
H	-3	ARG	-	EXPRESSION TAG	UNP P23367
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: $C_{10}H_{17}N_6O_{12}P_3$).

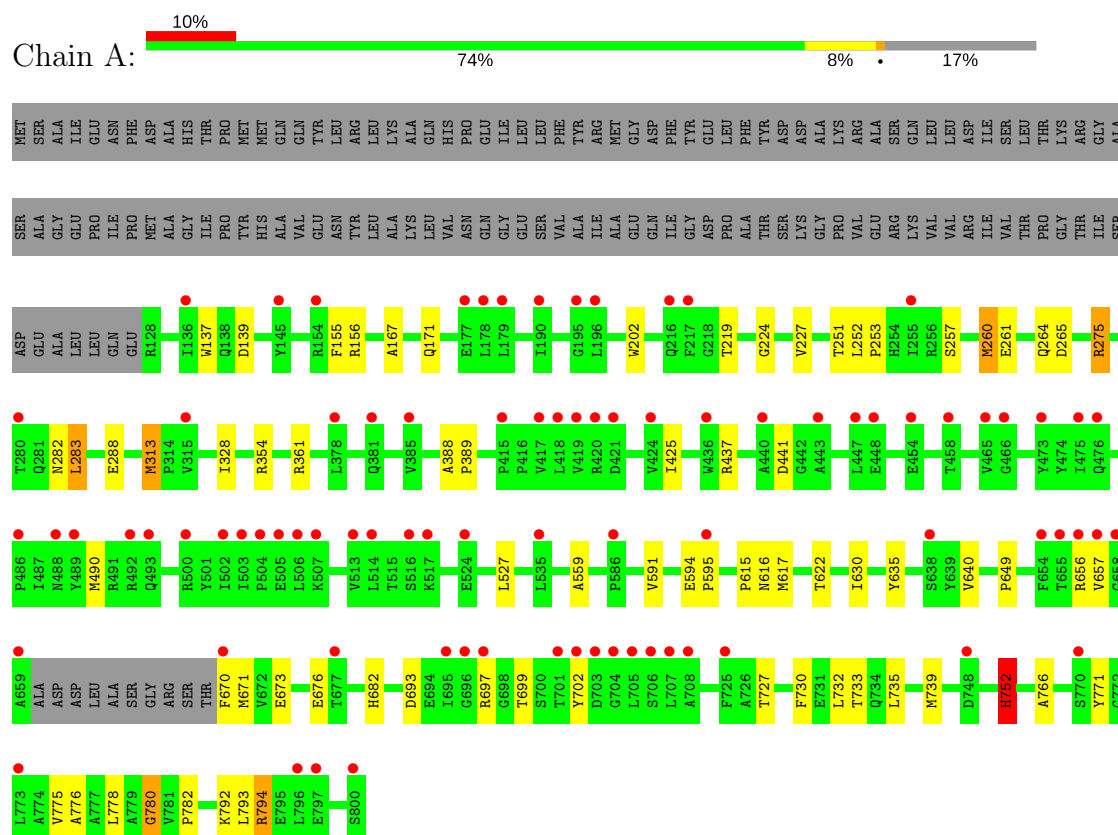


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

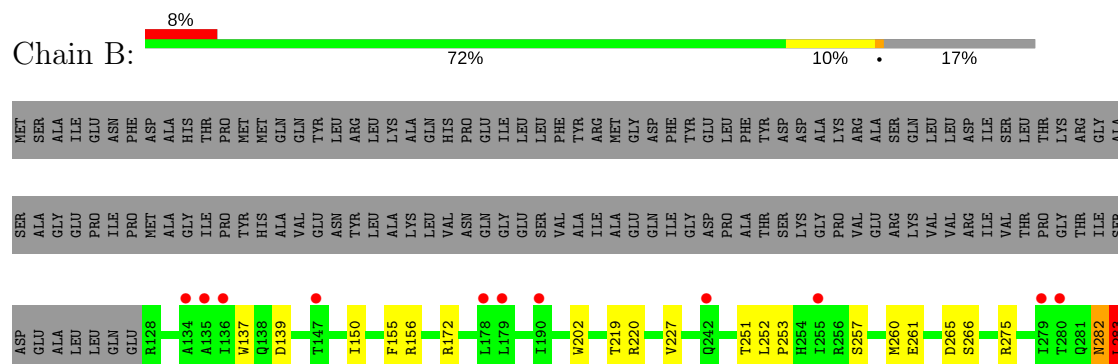
3 Residue-property plots [i](#)

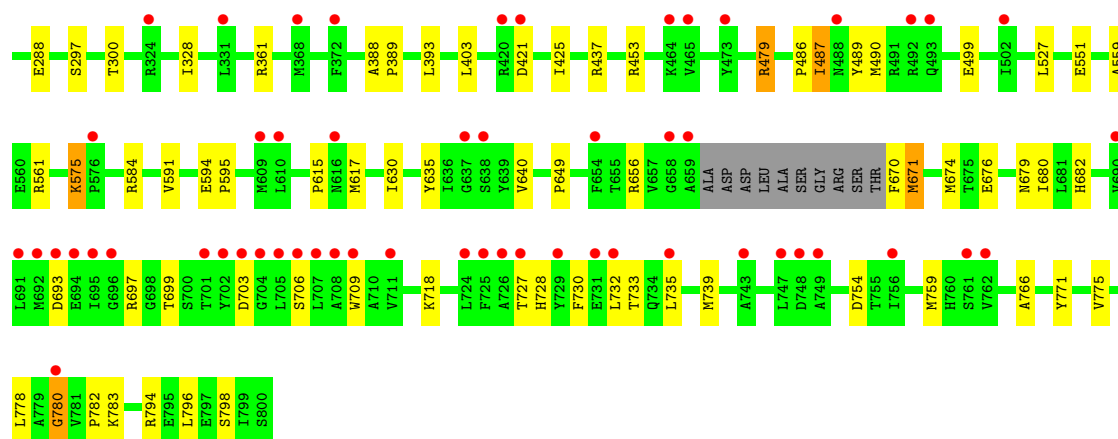
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

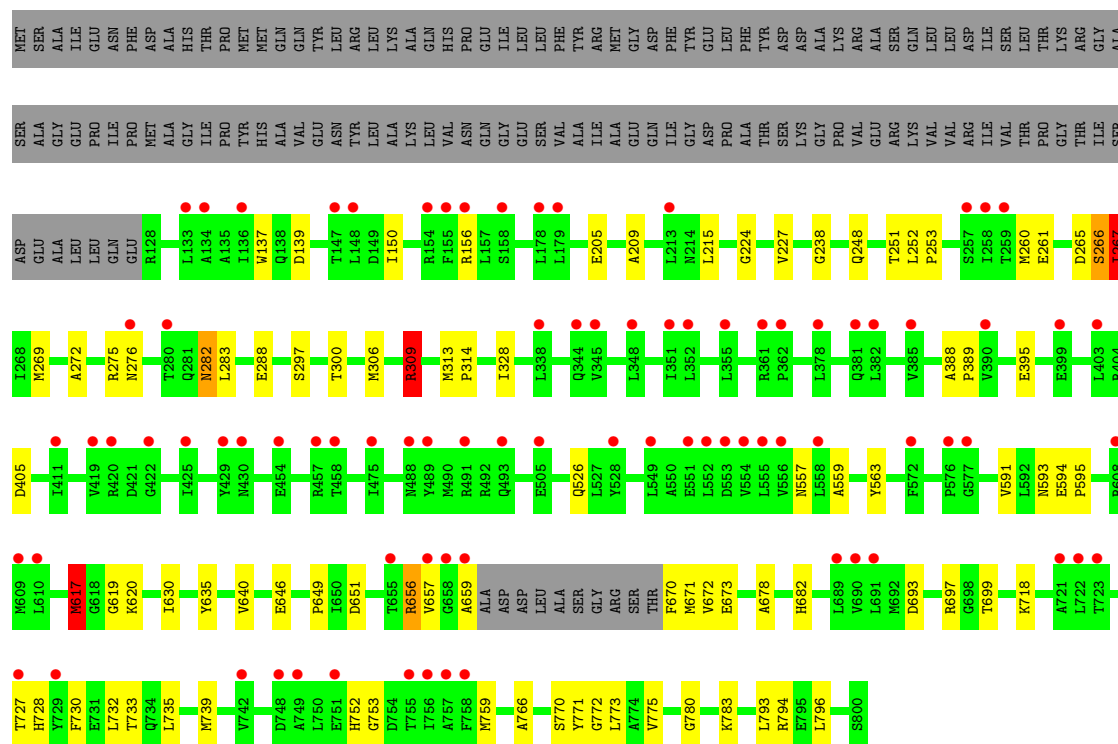
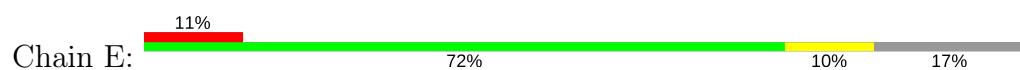


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

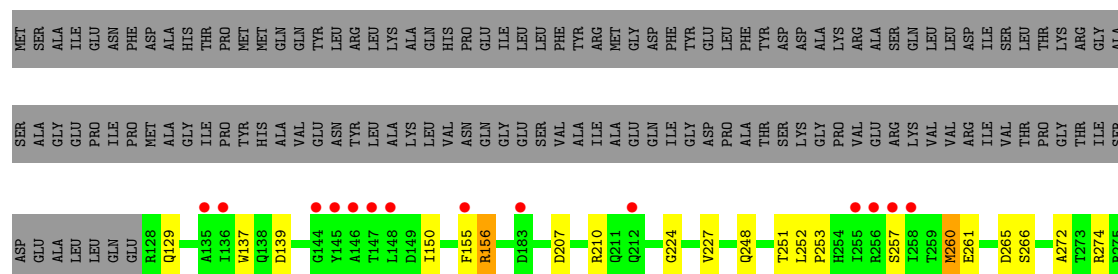


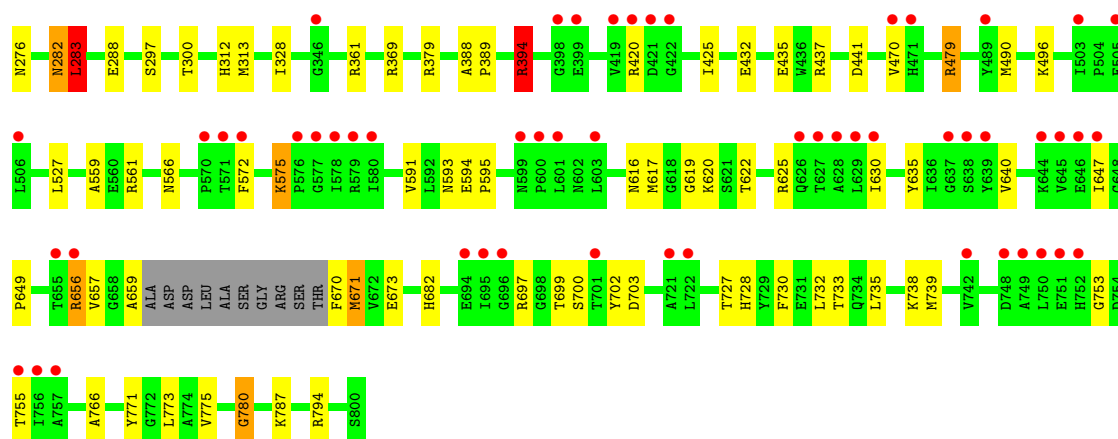


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

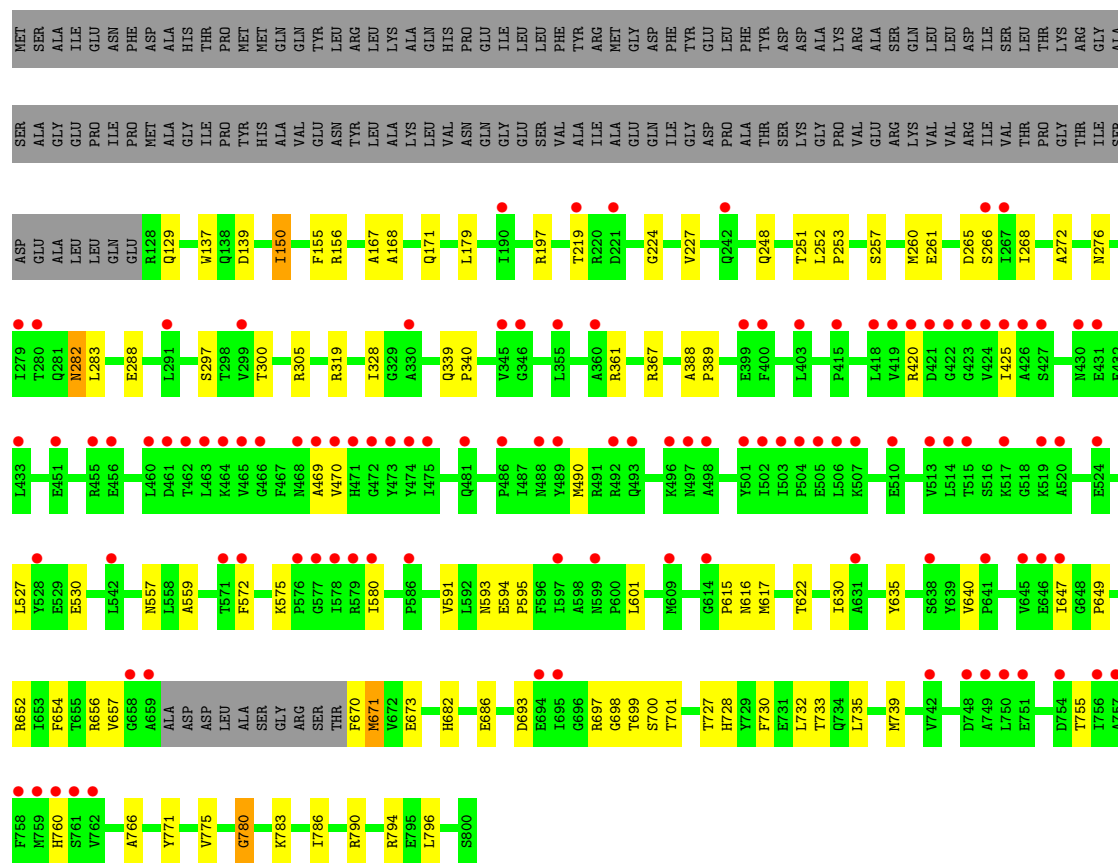


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

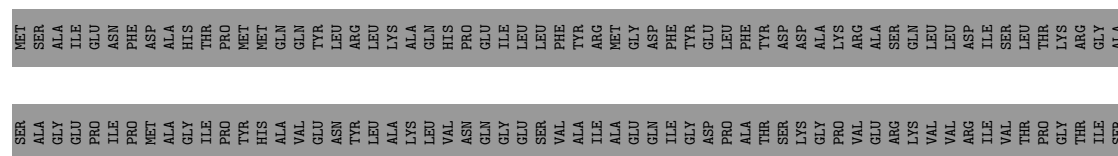


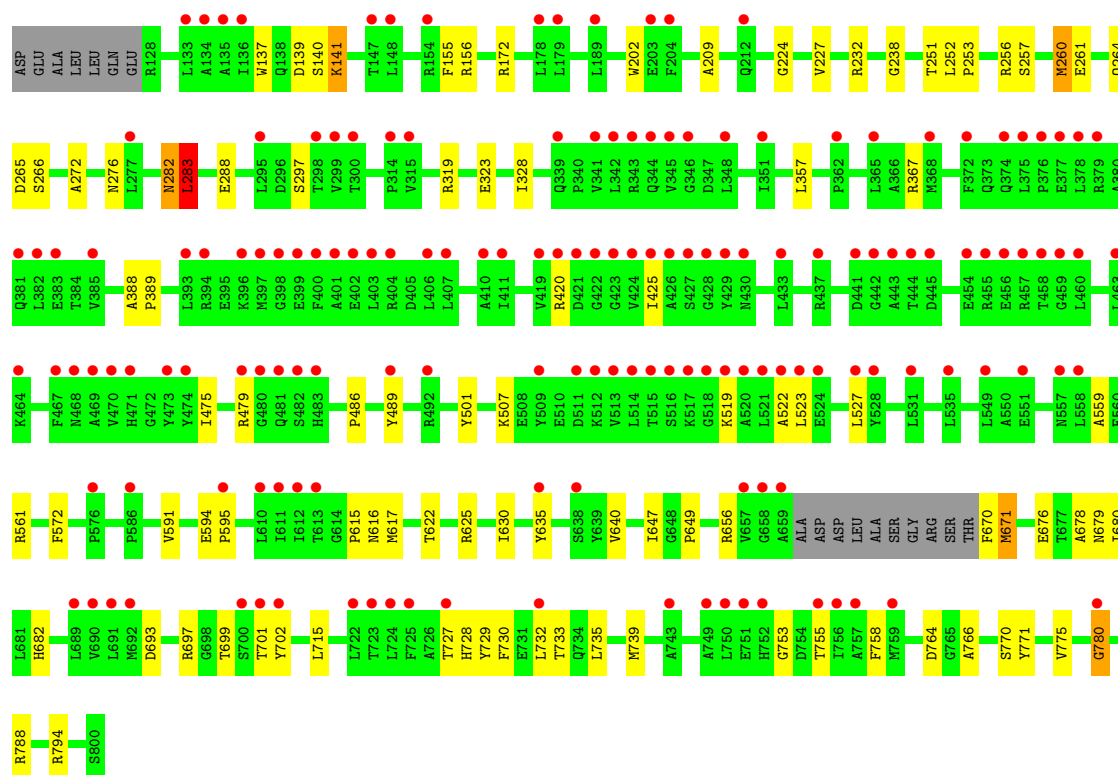


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

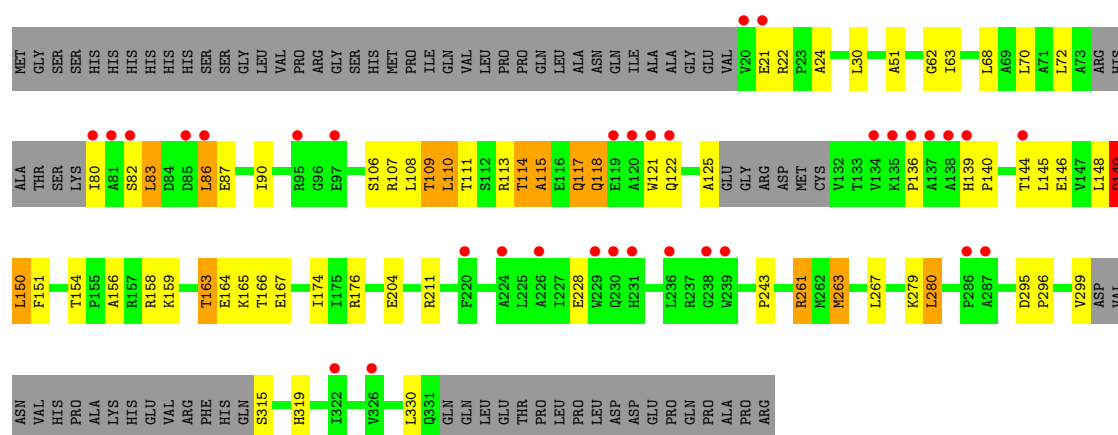


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

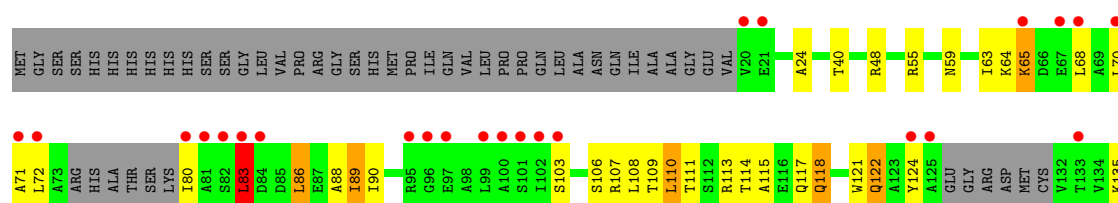


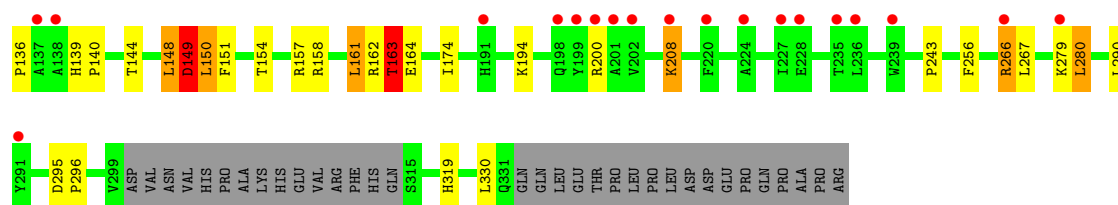


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

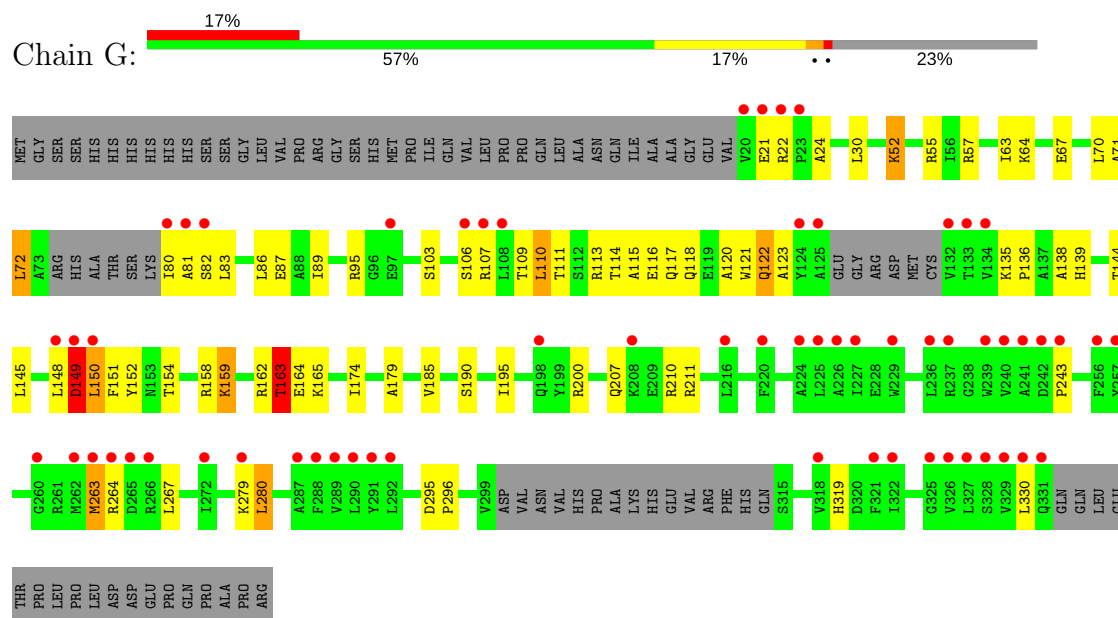


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

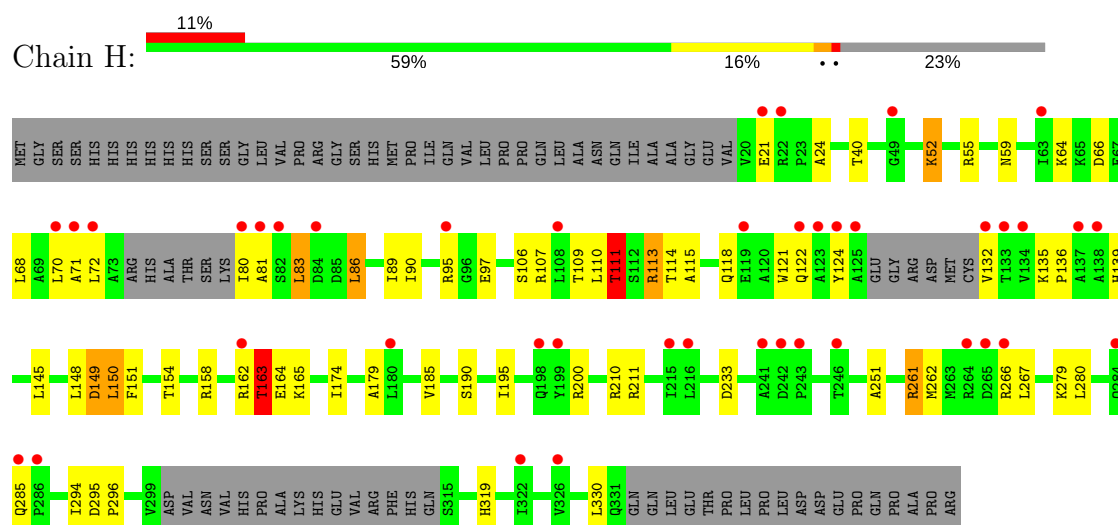




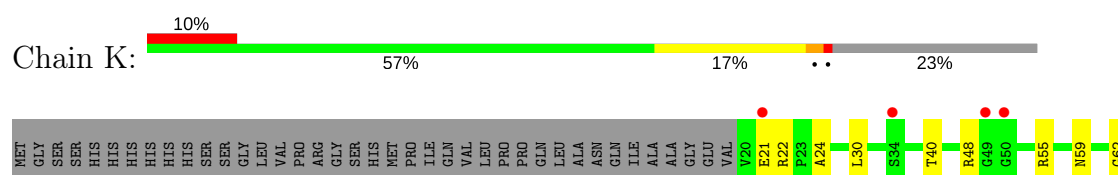
• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

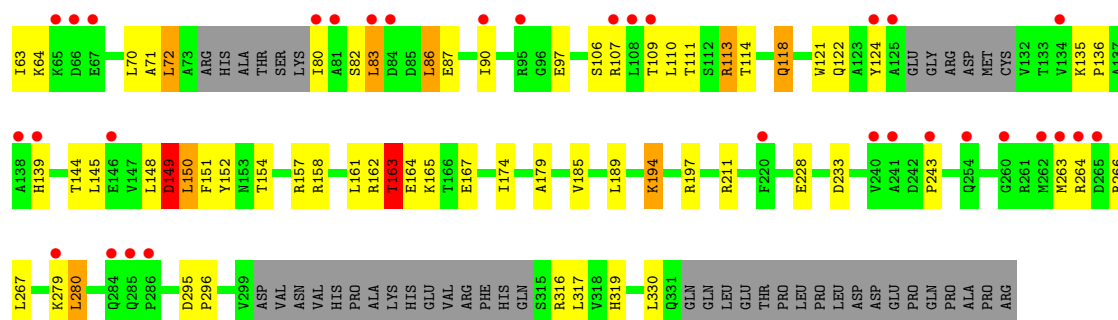


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

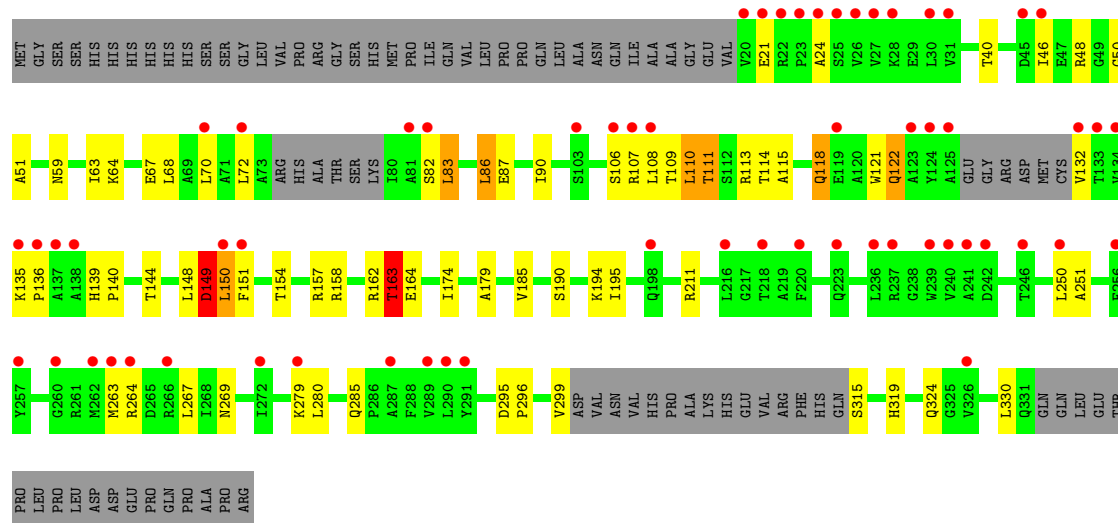


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL





• 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
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.095 for -h,-k,l	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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:NZ	2:D:208:LYS:CE	1.85	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:671:MET:SD	1:F:671:MET:CG	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
1:E:563:TYR:O	2:G:200:ARG:NH2	2.04	0.90
2:G:83:LEU:HA	2:G:87:GLU:CA	2.02	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:D:64:LYS:HD2	2:D:114:THR:HG21	1.68	0.76
2:L:299:VAL:CG1	2:L:315:SER:OG	2.34	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:F:432:GLU:O	1:F:435:GLU:HG2	1.92	0.70
1:I:697:ARG:HH22	1:J:697:ARG:CB	2.05	0.70
1:E:656:ARG:NH2	1:E:673:GLU:HA	2.06	0.70
1:F:394:ARG:CG	1:F:394:ARG:HH11	2.04	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:G:207:GLN:HG2	2:G:210:ARG:HG3	1.74	0.69
1:F:656:ARG:NH2	1:F:673:GLU:HA	2.07	0.69
2:L:111:THR:HG23	2:L:122:GLN:HB2	1.75	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)
1:A:697:ARG:NH1	1:B:697:ARG:CZ	2.57	0.66
2:K:106:SER:HB3	2:K:150:LEU:HD22	1.77	0.66
2:H:106:SER:HB3	2:H:150:LEU:HD22	1.77	0.66
2:H:90:ILE:CG2	2:K:266:ARG:NH2	2.58	0.66
1:I:150:ILE:HG21	1:I:248:GLN:NE2	2.11	0.66
1:I:656:ARG:NH1	1:I:657:VAL:O	2.28	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:G:162:ARG:O	2:G:163:THR:O	2.14	0.66
2:K:110:LEU:HD13	2:K:145:LEU:HG	1.78	0.66
2:C:163:THR:HB	2:C:166:THR:OG1	1.96	0.65
2:H:70:LEU:HD23	2:H:86:LEU:HD11	1.77	0.65
1:E:526:GLN:HE21	1:F:470:VAL:HG21	1.60	0.65
2:D:106:SER:HB3	2:D:150:LEU:HD22	1.79	0.65
2:H:162:ARG:O	2:H:163:THR:O	2.13	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:D:162:ARG:O	2:D:163:THR:O	2.15	0.64
2:L:299:VAL:CB	2:L:315:SER:OG	2.45	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:D:256:PHE:CE2	2:D:290:LEU:HB2	2.33	0.64
2:G:64:LYS:HA	2:G:118:GLN:HE22	1.63	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:110:LEU:HD12	2:G:123:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:86:LEU:HB3	2:G:89:ILE:HD12	1.79	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:A:137:TRP:CH2	1:A:139:ASP:HB3	2.35	0.61
2:G:159:LYS:HG2	2:G:159:LYS:O	1.98	0.61
1:I:219:THR:HG22	1:J:780:GLY:HA2	1.81	0.61
1:A:630:ILE:HG23	1:A:640:VAL:HG11	1.81	0.61
1:I:137:TRP:CH2	1:I:139:ASP:HB3	2.35	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:H:267:LEU:HD11	2:H:319:HIS:HB2	1.83	0.61
2:K:70:LEU:HB2	2:K:82:SER:HB2	1.82	0.61
1:B:137:TRP:CH2	1:B:139:ASP:HB3	2.35	0.61
1:E:617:MET:SD	1:F:671:MET:CG	2.89	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:C:106:SER:HB3	2:C:150:LEU:HD22	1.82	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
1:F:150:ILE:HG12	1:F:248:GLN:NE2	2.16	0.60
1:E:297:SER:OG	1:E:557:ASN:OD1	2.19	0.60
1:E:697:ARG:HH21	1:F:697:ARG:HB2	1.67	0.60
2:C:151:PHE:O	2:C:158:ARG:NH1	2.35	0.59
1:J:137:TRP:CH2	1:J:139:ASP:HB3	2.37	0.59
2:K:110:LEU:HD12	2:K:144:THR:O	2.02	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:F:617:MET:N	1:F:617:MET:SD	2.76	0.59
1:I:697:ARG:HH22	1:J:697:ARG:CA	2.16	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
3:A:1801:ANP:O1G	1:B:670:PHE:HB3	2.02	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)
2:L:299:VAL:HB	2:L:315:SER:OG	2.04	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:F:593:ASN:O	2:H:55:ARG:NH2	2.37	0.57
1:E:659:ALA:C	1:F:659:ALA:HB2	2.24	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
1:E:771:TYR:N	1:F:699:THR:OG1	2.35	0.57
2:K:82:SER:O	2:K:87:GLU:HA	2.05	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
2:D:139:HIS:HE2	2:D:144:THR:HG1	1.52	0.56
1:J:656:ARG:HE	1:J:676:GLU:HB3	1.69	0.56
2:C:82:SER:O	2:C:87:GLU:HA	2.05	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
1:I:615:PRO:HA	1:J:699:THR:HG21	1.87	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:E:595:PRO:HG3	2:G:57:ARG:HD2	1.88	0.55
2:H:279:LYS:HE2	2:H:330:LEU:HB3	1.87	0.55
1:J:264:GLN:HG2	1:J:264:GLN:O	2.06	0.55
1:J:656:ARG:HH21	1:J:679:ASN:HB3	1.71	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:A:635:TYR:OH	1:A:649:PRO:HA	2.06	0.55
1:E:635:TYR:OH	1:E:649:PRO:HA	2.07	0.55
1:E:727:THR:HG21	1:E:732:LEU:HD12	1.88	0.55
2:K:316:ARG:CG	2:K:317:LEU:N	2.69	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:261:ARG:HD3	2:H:262:MET:H	1.72	0.55
2:H:64:LYS:HB3	2:H:66:ASP:OD1	2.06	0.55
1:I:469:ALA:HB1	1:J:522:ALA:HB1	1.89	0.55
2:K:107:ARG:HB2	2:K:148:LEU:HB2	1.88	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:C:111:THR:HA	2:C:121:TRP:O	2.08	0.54
2:G:83:LEU:HD23	2:G:87:GLU:O	2.07	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:B:635:TYR:OH	1:B:649:PRO:HA	2.07	0.53
1:F:735:LEU:O	1:F:739:MET:N	2.38	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:G:295:ASP:CG	2:G:296:PRO:HD2	2.29	0.53
1:I:701:THR:HG1	1:J:729:TYR:HD1	1.54	0.53
2:L:279:LYS:HE2	2:L:330:LEU:HB3	1.90	0.53
2:C:279:LYS:HE2	2:C:330:LEU:HB3	1.90	0.53
1:E:205:GLU:HG2	2:H:52:LYS:HZ3	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:299:VAL:C	2:L:315:SER:OG	2.47	0.53
2:L:299:VAL:HB	2:L:315:SER:HG	1.74	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:D:279:LYS:HE2	2:D:330:LEU:HB3	1.89	0.52
2:G:111:THR:OG1	2:G:144:THR:HB	2.09	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
1:E:593:ASN:O	2:G:55:ARG:CZ	2.58	0.52
2:G:64:LYS:HB2	2:G:67:GLU:HG3	1.91	0.52
2:K:70:LEU:HD12	2:K:71:ALA:N	2.25	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
1:A:793:LEU:HD13	1:B:703:ASP:HA	1.92	0.51
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:B:754:ASP:HB2	2:D:135:LYS:NZ	2.25	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
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
2:G:151:PHE:O	2:G:158:ARG:CZ	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:LEU:N	1:E:253:PRO:CD	2.74	0.51
1:F:394:ARG:HG3	1:F:394:ARG:NH1	2.12	0.51
2:G:82:SER:O	2:G:87:GLU:N	2.33	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
1:A:264:GLN:O	1:A:264:GLN:HG2	2.10	0.50
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:735:LEU:O	1:A:739:MET:N	2.39	0.50
2:K:179:ALA:HB1	2:K:211:ARG:HH12	1.76	0.50
2:K:295:ASP:CG	2:K:296:PRO:HD2	2.32	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:C:295:ASP:CG	2:C:296:PRO:HD2	2.32	0.50
2:L:264:ARG:CZ	2:L:264:ARG:HB2	2.41	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:D:267:LEU:HD11	2:D:319:HIS:HB2	1.94	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:G:70:LEU:HD12	2:G:71:ALA:N	2.26	0.50
1:A:733:THR:HG21	1:A:766:ALA:HB1	1.93	0.50
2:H:70:LEU:CD2	2:H:86:LEU:HD11	2.40	0.50
1:J:251:THR:O	1:J:252:LEU:HD23	2.12	0.50
2:K:83:LEU:HD22	2:K:90:ILE:HG12	1.93	0.50
2:L:48:ARG:HG2	2:L:164:GLU:OE1	2.12	0.50
1:A:594:GLU:HB2	1:A:595:PRO:CD	2.42	0.49
2:C:72:LEU:HD13	2:C:125:ALA:HB2	1.93	0.49
1:I:388:ALA:HB3	1:I:389:PRO:HD3	1.94	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
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:A:778:LEU:HD21	1:B:220:ARG:CZ	2.42	0.49
1:I:700:SER:HB2	1:J:770:SER:HB3	1.94	0.49
2:H:97:GLU:CA	2:K:266:ARG:HH12	2.14	0.49
2:C:164:GLU:HG2	2:C:165:LYS:N	2.27	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

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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
1:J:156:ARG:HD2	1:J:261:GLU:HG3	1.94	0.49
2:K:113:ARG:NE	2:K:118:GLN:O	2.30	0.49
2:K:82:SER:O	2:K:86:LEU:O	2.29	0.49
1:A:251:THR:O	1:A:252:LEU:HD23	2.12	0.49
2:C:110:LEU:CD1	2:C:145:LEU:HG	2.42	0.49
2:C:151:PHE:O	2:C:158:ARG:CZ	2.61	0.49
2:D:70:LEU:O	2:D:80:ILE:HD11	2.12	0.49
1:F:252:LEU:N	1:F:253:PRO:CD	2.76	0.49
1:F:388:ALA:HB3	1:F:389:PRO:HD3	1.94	0.49
2:H:97:GLU:CG	2:K:266:ARG:HG3	2.35	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
2:G:279:LYS:HE2	2:G:330:LEU:HB3	1.94	0.49
1:J:328:ILE:HG23	1:J:559:ALA:HA	1.93	0.49
1:A:727:THR:HG21	1:A:732:LEU:HD12	1.94	0.49
2:H:251:ALA:HB1	2:H:285:GLN:HB3	1.94	0.49
1:I:252:LEU:N	1:I:253:PRO:CD	2.75	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: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: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:F:150:ILE:HD13	1:F:248:GLN:HG3	1.94	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
1:F:251:THR:O	1:F:252:LEU:HD23	2.13	0.48
1:J:622:THR:HG21	3:J:1801:ANP:N7	2.28	0.48
2:K:110:LEU:CD1	2:K:144:THR:O	2.61	0.48
1:I:328:ILE:HG23	1:I:559:ALA:HA	1.94	0.48
1:J:733:THR:HG21	1:J:766:ALA:HB1	1.94	0.48
2:L:63:ILE:N	2:L:114:THR:HG22	2.28	0.48
1:F:156:ARG:HD2	1:F:261:GLU:HG3	1.96	0.48
1:A:671:MET:HA	1:B:617:MET:SD	2.53	0.48
1:I:251:THR:O	1:I:252:LEU:HD23	2.13	0.48
1:I:733:THR:HG21	1:I:766:ALA:HB1	1.96	0.48
1:A:793:LEU:HD13	1:B:706:SER:OG	2.13	0.48
1:A:616:ASN:CG	1:B:670:PHE:CD2	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:151:PHE:O	2:H:158:ARG:CZ	2.61	0.48
1:I:268:ILE:HG21	1:I:652:ARG:NH2	2.28	0.48
2:H:266:ARG:HB3	2:K:80:ILE:HD11	1.96	0.48
2:G:263:MET:HG3	2:G:264:ARG:N	2.29	0.48
2:L:113:ARG:HD3	2:L:139:HIS:O	2.14	0.48
2:D:70:LEU:HD12	2:D:71:ALA:N	2.28	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
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:A:792:LYS:HE2	1:B:709:TRP:CE3	2.49	0.47
1:B:487:ILE:HA	1:B:489:TYR:H	1.80	0.47
2:C:113:ARG:NE	2:C:118:GLN:O	2.31	0.47
2:C:110:LEU:CD1	2:C:145:LEU:CD2	2.92	0.47
2:D:149:ASP:OD1	2:D:149:ASP:N	2.47	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:F:297:SER:OG	1:F:561:ARG:HD3	2.15	0.47
1:I:698:GLY:O	1:J:728:HIS:CG	2.67	0.47
2:D:83:LEU:HD11	2:D:90:ILE:CD1	2.44	0.47
2:K:151:PHE:O	2:K:158:ARG:CZ	2.63	0.47
2:L:82:SER:O	2:L:86:LEU:O	2.31	0.47
1:B:252:LEU:N	1:B:253:PRO:CD	2.77	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
2:G:72:LEU:HD23	2:G:103:SER:CB	2.45	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:A:776:ALA:HB2	1:B:674:MET:SD	2.55	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
2:G:30:LEU:HD22	2:G:145:LEU:HD22	1.97	0.47
1:I:594:GLU:HB2	1:I:595:PRO:CD	2.45	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:B:251:THR:O	1:B:252:LEU:HD23	2.13	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:F:328:ILE:HG23	1:F:559:ALA:HA	1.98	0.46
1:I:699:THR:HG21	1:J:615:PRO:HA	1.96	0.46
1:B:798:SER:HA	1:F:496:LYS:HZ1	1.80	0.46
2:G:113:ARG:HD3	2:G:139:HIS:O	2.16	0.46
2:G:267:LEU:HD11	2:G:319:HIS:HB2	1.98	0.46
1:J:771:TYR:O	1:J:775:VAL:HG23	2.15	0.46
2:D:68:LEU:CD1	2:D:121:TRP:HB2	2.46	0.46
1:E:678:ALA:CB	1:F:780:GLY:O	2.63	0.46
2:H:113:ARG:NE	2:H:118:GLN:O	2.31	0.46
1:J:272:ALA:O	1:J:276:ASN:HB2	2.16	0.46
2:K:83:LEU:C	2:K:87:GLU:HB2	2.36	0.46
1:J:425:ILE:CD1	1:J:527:LEU:HB2	2.45	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
2:L:83:LEU:C	2:L:87:GLU:HB2	2.35	0.46
2:D:83:LEU:HD21	2:D:90:ILE:CD1	2.45	0.46
1:E:620:LYS:N	3:E:1801:ANP:O1A	2.49	0.46
1:B:297:SER:OG	1:B:561:ARG:HD3	2.16	0.46
2:C:72:LEU:C	2:C:72:LEU:HD12	2.36	0.46
1:E:617:MET:HA	3:E:1801:ANP:H5'1	1.98	0.46
1:E:388:ALA:HB3	1:E:389:PRO:HD3	1.97	0.46
2:H:113:ARG:HD3	2:H:139:HIS:O	2.16	0.46
1:I:219:THR:CG2	1:J:780:GLY:HA2	2.46	0.46
1:J:594:GLU:HB3	1:J:595:PRO:CD	2.46	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
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
2:H:97:GLU:HA	2:K:266:ARG:HH11	1.68	0.45
1:J:388:ALA:HB3	1:J:389:PRO:HD3	1.98	0.45
2:L:114:THR:OG1	2:L:118:GLN:OE1	2.35	0.45
1:A:702:TYR:HB3	1:B:796:LEU:HD13	1.97	0.45
2:K:149:ASP:OD1	2:K:149:ASP:N	2.49	0.45
2:K:30:LEU:HD22	2:K:145:LEU:HD22	1.99	0.45
1:A:388:ALA:HB3	1:A:389:PRO:HD3	1.99	0.45
1:B:156:ARG:HD2	1:B:261:GLU:HG3	1.97	0.45
2:G:149:ASP:OD1	2:G:149:ASP:N	2.49	0.45
1:I:425:ILE:CD1	1:I:527:LEU:HB2	2.47	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
1:F:227:VAL:HG12	1:F:260:MET:HB2	1.99	0.45
2:K:48:ARG:HG2	2:K:164:GLU:OE1	2.17	0.45
2:L:149:ASP:N	2:L:149:ASP:OD1	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:I:771:TYR:O	1:I:775:VAL:HG23	2.17	0.45
1:J:755:THR:HG21	2:L:135:LYS:HZ2	1.82	0.45
1:A:778:LEU:HD21	1:B:220:ARG:NH1	2.32	0.45
2:C:299:VAL:CB	2:C:315:SER:HG	2.30	0.45
1:I:224:GLY:O	1:I:682:HIS:ND1	2.50	0.45
2:K:113:ARG:HD3	2:K:139:HIS:O	2.17	0.45
1:B:771:TYR:O	1:B:775:VAL:HG23	2.16	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:727:THR:HG21	1:B:732:LEU:HD12	1.97	0.44
1:J:656:ARG:HE	1:J:676:GLU:CB	2.30	0.44
1:B:594:GLU:HB3	1:B:595:PRO:CD	2.48	0.44
1:E:772:GLY:N	1:F:699:THR:OG1	2.50	0.44
1:E:526:GLN:NE2	1:F:470:VAL:HG21	2.28	0.44
1:E:670:PHE:CD2	1:F:616:ASN:ND2	2.85	0.44
1:I:594:GLU:HB2	1:I:595:PRO:HD3	1.99	0.44
1:I:697:ARG:CZ	1:J:697:ARG:HB2	2.47	0.44
2:G:190:SER:HA	2:G:195:ILE:HA	2.00	0.44
2:L:113:ARG:NE	2:L:118:GLN:O	2.32	0.44
2:L:135:LYS:HB2	2:L:136:PRO:CD	2.48	0.44
2:L:72:LEU:HD12	2:L:72:LEU:C	2.38	0.44
1:A:780:GLY:HA2	1:B:219:THR:CG2	2.48	0.44
2:C:83:LEU:C	2:C:87:GLU:HB2	2.38	0.44
1:I:272:ALA:O	1:I:276:ASN:HB2	2.17	0.44
2:L:190:SER:HA	2:L:195:ILE:HA	2.00	0.44
1:F:619:GLY:HA2	3:F:1801:ANP:C8	2.47	0.44
1:A:771:TYR:O	1:A:775:VAL:HG23	2.18	0.44
2:G:107:ARG:NH2	2:G:152:TYR:HD2	2.15	0.44
1:F:755:THR:HG21	2:H:135:LYS:HD2	2.00	0.44
1:E:215:LEU:HD22	2:H:124:TYR:CE2	2.52	0.44
2:H:68:LEU:CD1	2:H:121:TRP:HB2	2.48	0.44
1:J:297:SER:OG	1:J:561:ARG:HD3	2.17	0.44
2:K:111:THR:HA	2:K:121:TRP:O	2.18	0.44
2:K:107:ARG:NH2	2:K:152:TYR:HD2	2.14	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
2:G:70:LEU:HB2	2:G:82:SER:HB2	2.00	0.43
1:I:616:ASN:CG	1:J:670:PHE:HB3	2.38	0.43
2:C:121:TRP:CZ3	2:C:136:PRO:HG3	2.54	0.43
2:C:149:ASP:OD1	2:C:149:ASP:N	2.52	0.43
1:E:771:TYR:O	1:E:775:VAL:HG23	2.17	0.43
1:F:379:ARG:HG2	1:F:394:ARG:HH12	1.83	0.43
2:G:164:GLU:CD	2:G:165:LYS:H	2.21	0.43
2:H:83:LEU:HD23	2:H:86:LEU:HD23	2.00	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:B:328:ILE:HG23	1:B:559:ALA:HA	2.00	0.43
1:E:752:HIS:ND1	2:G:136:PRO:HG2	2.33	0.43
1:F:224:GLY:O	1:F:682:HIS:ND1	2.51	0.43
1:I:700:SER:HA	1:J:728:HIS:O	2.18	0.43
2:L:64:LYS:HB2	2:L:67:GLU:HG3	1.99	0.43
1:B:487:ILE:C	1:B:489:TYR:N	2.71	0.43
2:C:163:THR:CB	2:C:166:THR:OG1	2.63	0.43
1:E:267:ILE:CG1	1:E:314:PRO:HG2	2.47	0.43
1:B:798:SER:HA	1:F:496:LYS:CE	2.49	0.43
2:G:179:ALA:HB1	2:G:211:ARG:HH12	1.83	0.43
1:F:566:ASN:OD1	2:H:200:ARG:NH2	2.51	0.43
2:K:80:ILE:HG23	2:K:80:ILE:O	2.19	0.43
2:D:108:LEU:HD11	2:D:110:LEU:HD23	2.01	0.43
1:E:328:ILE:HG23	1:E:559:ALA:HA	2.00	0.43
2:G:110:LEU:CD1	2:G:123:ALA:HB3	2.49	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
1:A:227:VAL:HG12	1:A:260:MET:HB2	2.00	0.43
1:A:656:ARG:HA	1:A:656:ARG:HD2	1.76	0.43
2:D:63:ILE:N	2:D:114:THR:HG22	2.33	0.43
1:F:425:ILE:CD1	1:F:527:LEU:HB2	2.49	0.43
2:G:111:THR:O	2:G:111:THR:OG1	2.37	0.43
1:B:425:ILE:CD1	1:B:527:LEU:HB2	2.49	0.43
1:F:155:PHE:HB3	1:F:257:SER:O	2.19	0.43
1:E:593:ASN:O	2:G:55:ARG:NE	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:593:ASN:O	2:K:55:ARG:CZ	2.67	0.43
2:D:114:THR:OG1	2:D:118:GLN:OE1	2.37	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
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:F:771:TYR:O	1:F:775:VAL:HG23	2.19	0.42
2:G:164:GLU:CG	2:G:165:LYS:N	2.81	0.42
2:D:139:HIS:ND1	2:D:140:PRO:O	2.53	0.42
1:I:580:ILE:HD12	1:I:601:LEU:HD23	2.01	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:F:432:GLU:HA	1:F:435:GLU:HG2	2.02	0.42
2:K:189:LEU:HB3	2:K:197:ARG:HB2	2.02	0.42
2:L:179:ALA:HB1	2:L:211:ARG:HH12	1.83	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: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
1:J:615:PRO:HB2	1:J:758:PHE:HE1	1.83	0.42
2:C:109:THR:OG1	2:C:146:GLU:O	2.36	0.42
2:C:80:ILE:HG23	2:C:80:ILE:O	2.19	0.42
1:I:155:PHE:HB3	1:I:257:SER:O	2.19	0.42
1:I:282:ASN:O	1:I:283:LEU:C	2.58	0.42
1:I:670:PHE:HB3	1:J:616:ASN:ND2	2.34	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
1:B:227:VAL:HG12	1:B:260:MET:HB2	2.02	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:I:656:ARG:NH2	1:I:673:GLU:CA	2.78	0.42
2:L:68:LEU:CD1	2:L:121:TRP:HB2	2.49	0.42
2:C:68:LEU:CD1	2:C:121:TRP:HB2	2.50	0.42
2:K:135:LYS:HB2	2:K:136:PRO:CD	2.50	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
1:I:671:MET:CA	1:J:617:MET:SD	3.08	0.42
2:C:243:PRO:HB2	2:C:280:LEU:HD21	2.01	0.41
2:D:111:THR:HA	2:D:121:TRP:O	2.20	0.41
1:F:282:ASN:O	1:F:283:LEU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:121:TRP:CZ3	2:G:136:PRO:HG3	2.54	0.41
1:I:167:ALA:O	1:I:171:GLN:OE1	2.37	0.41
2:L:108:LEU:HD11	2:L:110:LEU:HD23	2.02	0.41
2:C:139:HIS:ND1	2:C:140:PRO:O	2.53	0.41
1:E:728:HIS:ND1	1:F:699:THR:HA	2.35	0.41
1:I:622:THR:OG1	3:I:1801:ANP:H8	2.20	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
1:A:219:THR:CG2	1:B:780:GLY:HA2	2.51	0.41
2:C:110:LEU:CD2	2:C:145:LEU:HG	2.49	0.41
2:G:135:LYS:HB2	2:G:136:PRO:CD	2.50	0.41
1:J:224:GLY:O	1:J:682:HIS:ND1	2.51	0.41
1:J:572:PHE:HA	1:J:647:ILE:O	2.19	0.41
2:L:83:LEU:HA	2:L:87:GLU:HA	2.02	0.41
2:C:110:LEU:HD21	2:C:145:LEU:CB	2.48	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
1:I:616:ASN:CG	1:J:670:PHE:CD2	2.94	0.41
2:G:139:HIS:NE2	2:G:144:THR:OG1	2.54	0.41
2:H:90:ILE:HG22	2:K:266:ARG:HH21	1.73	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:243:PRO:HB2	2:D:280:LEU:HD21	2.03	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
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
1:E:699:THR:HA	1:F:728:HIS:ND1	2.35	0.41
2:H:185:VAL:O	2:H:211:ARG:NH2	2.53	0.41
1:J:656:ARG:CG	1:J:680:ILE:CD1	2.95	0.41
1:F:207:ASP:HB2	2:G:52:LYS:HE3	2.02	0.41
2:C:109:THR:C	2:C:110:LEU:HG	2.41	0.41
2:D:40:THR:HG22	2:D:59:ASN:HD21	1.86	0.41
1:E:773:LEU:HD12	1:E:793:LEU:HD22	2.03	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:A:437:ARG:O	1:A:441:ASP:N	2.47	0.41
1:B:282:ASN:O	1:B:283:LEU:C	2.60	0.41
1:B:202:TRP:CZ2	2:C:158:ARG:NH2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:ALA:O	1:E:276:ASN:HB2	2.21	0.41
2:H:80:ILE:O	2:H:80:ILE:HG23	2.21	0.41
1:I:339:GLN:N	1:I:340:PRO:CD	2.84	0.41
1:I:783:LYS:HZ3	1:J:256:ARG:HB2	1.85	0.41
2:L:40:THR:HG22	2:L:59:ASN:HD21	1.86	0.41
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
1:J:486:PRO:HD2	1:J:489:TYR:CD1	2.56	0.40
1:B:150:ILE:HD12	1:B:150:ILE:C	2.42	0.40
1:B:735:LEU:O	1:B:739:MET:N	2.42	0.40
2:C:114:THR:O	2:C:115:ALA:C	2.60	0.40
2:D:121:TRP:CZ3	2:D:136:PRO:HG3	2.56	0.40
1:F:437:ARG:O	1:F:441:ASP:N	2.48	0.40
1:F:622:THR:OG1	3:F:1801:ANP:C8	2.70	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:A:155:PHE:HB3	1:A:257:SER:O	2.22	0.40
1:A:219:THR:HG21	1:B:780:GLY:HA2	2.03	0.40
1:F:479:ARG:HA	1:F:479:ARG:HD2	1.69	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:I:671:MET:HB2	1:J:617:MET:HG3	2.03	0.40
1:J:227:VAL:HG12	1:J:260:MET:HB2	2.02	0.40
2:K:111:THR:HG22	2:K:122:GLN:HB2	2.03	0.40
2:K:121:TRP:CZ3	2:K:136:PRO:HG3	2.56	0.40
2:K:22:ARG:NE	2:K:167:GLU:OE2	2.55	0.40
2:K:243:PRO:HB2	2:K:280:LEU:HD21	2.03	0.40
2:L:46:ILE:HG13	2:L:50:GLY:HA2	2.03	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
1:J:656:ARG:HE	1:J:676:GLU:C	2.24	0.40
2:C:51:ALA:O	2:C:149:ASP:CA	2.69	0.40
2:D:135:LYS:HB3	2:D:136:PRO:CD	2.51	0.40
2:H:86:LEU:HG	2:H:89:ILE:HD12	2.03	0.40
1:J:475:ILE:HG21	1:J:489:TYR:HE2	1.87	0.40
2:K:110:LEU:HD12	2:K:111:THR:N	2.37	0.40
1:J:202:TRP:CZ2	2:K:158:ARG:NH2	2.90	0.40
2:L:51:ALA:O	2:L: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%)	44	81
1	B	659/800 (82%)	627 (95%)	30 (5%)	2 (0%)	44	81
1	E	659/800 (82%)	629 (95%)	27 (4%)	3 (0%)	32	74
1	F	659/800 (82%)	630 (96%)	26 (4%)	3 (0%)	32	74
1	I	659/800 (82%)	627 (95%)	31 (5%)	1 (0%)	51	84
1	J	659/800 (82%)	631 (96%)	25 (4%)	3 (0%)	32	74
2	C	277/369 (75%)	255 (92%)	18 (6%)	4 (1%)	13	54
2	D	277/369 (75%)	252 (91%)	20 (7%)	5 (2%)	10	49
2	G	277/369 (75%)	250 (90%)	22 (8%)	5 (2%)	10	49
2	H	277/369 (75%)	247 (89%)	25 (9%)	5 (2%)	10	49
2	K	277/369 (75%)	253 (91%)	21 (8%)	3 (1%)	17	60
2	L	277/369 (75%)	255 (92%)	18 (6%)	4 (1%)	13	54
All	All	5616/7014 (80%)	5282 (94%)	294 (5%)	40 (1%)	25	68

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%)	57	79
1	B	550/662 (83%)	534 (97%)	16 (3%)	48	73
1	E	550/662 (83%)	535 (97%)	15 (3%)	50	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	550/662 (83%)	535 (97%)	15 (3%)	50	74
1	I	550/662 (83%)	536 (98%)	14 (2%)	53	77
1	J	550/662 (83%)	539 (98%)	11 (2%)	60	82
2	C	235/308 (76%)	222 (94%)	13 (6%)	25	58
2	D	235/308 (76%)	224 (95%)	11 (5%)	30	62
2	G	235/308 (76%)	226 (96%)	9 (4%)	38	67
2	H	235/308 (76%)	221 (94%)	14 (6%)	22	55
2	K	235/308 (76%)	223 (95%)	12 (5%)	28	60
2	L	235/308 (76%)	219 (93%)	16 (7%)	18	51
All	All	4710/5820 (81%)	4552 (97%)	158 (3%)	42	69

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	2.11	10 (34%)	28,52,52	2.93	13 (46%)
3	ANP	B	1801	-	29,33,33	2.34	11 (37%)	28,52,52	2.11	7 (25%)
3	ANP	E	1801	-	29,33,33	1.81	7 (24%)	28,52,52	2.18	7 (25%)
3	ANP	F	1801	-	29,33,33	2.08	8 (27%)	28,52,52	2.11	9 (32%)
3	ANP	I	1801	1	29,33,33	2.08	8 (27%)	28,52,52	2.33	8 (28%)
3	ANP	J	1801	-	29,33,33	1.78	7 (24%)	28,52,52	2.33	9 (32%)

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	-3.47	1.47	1.56
3	J	1801	ANP	PG-O2G	-3.41	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1801	ANP	PB-O2B	-3.24	1.47	1.56
3	F	1801	ANP	PG-O3G	-3.18	1.48	1.56
3	E	1801	ANP	PG-O3G	-3.09	1.48	1.56
3	I	1801	ANP	PG-O3G	-3.08	1.48	1.56
3	J	1801	ANP	PB-O2B	-3.06	1.48	1.56
3	J	1801	ANP	PG-O3G	-2.91	1.48	1.56
3	B	1801	ANP	PB-O2B	-2.88	1.48	1.56
3	A	1801	ANP	PB-O2B	-2.84	1.48	1.56
3	E	1801	ANP	PB-O2B	-2.67	1.49	1.56
3	B	1801	ANP	PG-O2G	-2.63	1.49	1.56
3	B	1801	ANP	PG-O3G	-2.55	1.49	1.56
3	I	1801	ANP	PG-O2G	-2.53	1.49	1.56
3	A	1801	ANP	PG-O3G	-2.52	1.49	1.56
3	F	1801	ANP	PG-O2G	-2.46	1.50	1.56
3	A	1801	ANP	PG-O2G	-2.15	1.50	1.56
3	F	1801	ANP	PB-O2B	-2.07	1.51	1.56
3	B	1801	ANP	PG-O1G	2.27	1.48	1.46
3	J	1801	ANP	PB-O1B	2.50	1.48	1.46
3	J	1801	ANP	PG-N3B	2.65	1.70	1.63
3	I	1801	ANP	C2-N3	2.78	1.36	1.32
3	A	1801	ANP	C2-N3	2.79	1.36	1.32
3	B	1801	ANP	O4'-C1'	2.79	1.45	1.41
3	E	1801	ANP	C5-C4	2.93	1.47	1.40
3	E	1801	ANP	C2-N3	2.96	1.37	1.32
3	A	1801	ANP	O4'-C1'	3.02	1.45	1.41
3	I	1801	ANP	PB-O1B	3.06	1.49	1.46
3	A	1801	ANP	PG-O1G	3.09	1.49	1.46
3	A	1801	ANP	PB-O1B	3.09	1.49	1.46
3	A	1801	ANP	PB-N3B	3.20	1.71	1.63
3	J	1801	ANP	C5-C4	3.27	1.47	1.40
3	F	1801	ANP	C5-C4	3.48	1.48	1.40
3	F	1801	ANP	C2-N3	3.52	1.38	1.32
3	B	1801	ANP	C2-N3	3.55	1.38	1.32
3	B	1801	ANP	PB-O3A	3.63	1.63	1.59
3	E	1801	ANP	PG-N3B	3.68	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	A	1801	ANP	C5-C4	4.17	1.49	1.40
3	F	1801	ANP	PB-O1B	4.18	1.50	1.46
3	J	1801	ANP	PB-N3B	4.24	1.74	1.63
3	E	1801	ANP	PB-N3B	4.42	1.75	1.63
3	B	1801	ANP	PB-N3B	4.49	1.75	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1801	ANP	PG-N3B	4.69	1.75	1.63
3	I	1801	ANP	PB-N3B	4.71	1.75	1.63
3	A	1801	ANP	PG-N3B	4.74	1.75	1.63
3	F	1801	ANP	PB-N3B	4.85	1.76	1.63
3	I	1801	ANP	PG-N3B	4.87	1.76	1.63
3	F	1801	ANP	PG-N3B	5.04	1.76	1.63
3	B	1801	ANP	PB-O1B	5.28	1.52	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	ANP	O1G-PG-N3B	-8.53	99.03	111.79
3	E	1801	ANP	N3-C2-N1	-6.88	122.87	128.86
3	J	1801	ANP	N3-C2-N1	-6.26	123.40	128.86
3	I	1801	ANP	N3-C2-N1	-6.11	123.54	128.86
3	F	1801	ANP	N3-C2-N1	-5.88	123.74	128.86
3	A	1801	ANP	N3-C2-N1	-5.78	123.82	128.86
3	J	1801	ANP	O1G-PG-N3B	-5.40	103.71	111.79
3	B	1801	ANP	N3-C2-N1	-5.32	124.22	128.86
3	B	1801	ANP	O1G-PG-N3B	-5.23	103.97	111.79
3	B	1801	ANP	C4-C5-N7	-4.73	104.84	109.41
3	I	1801	ANP	O1G-PG-N3B	-4.70	104.76	111.79
3	F	1801	ANP	O1G-PG-N3B	-4.44	105.15	111.79
3	A	1801	ANP	C4-C5-N7	-4.04	105.51	109.41
3	A	1801	ANP	O1B-PB-N3B	-3.74	106.20	111.79
3	E	1801	ANP	PA-O3A-PB	-3.71	119.27	132.38
3	J	1801	ANP	C4-C5-N7	-3.44	106.08	109.41
3	F	1801	ANP	C4-C5-N7	-3.40	106.13	109.41
3	J	1801	ANP	PA-O3A-PB	-3.30	120.74	132.38
3	I	1801	ANP	C4-C5-N7	-3.02	106.49	109.41
3	E	1801	ANP	O1G-PG-N3B	-2.83	107.55	111.79
3	I	1801	ANP	PA-O3A-PB	-2.81	122.45	132.38
3	B	1801	ANP	O2'-C2'-C3'	-2.24	104.64	111.83
3	J	1801	ANP	O1B-PB-N3B	-2.24	108.44	111.79
3	A	1801	ANP	PA-O3A-PB	-2.20	124.62	132.38
3	F	1801	ANP	PA-O3A-PB	-2.17	124.73	132.38
3	E	1801	ANP	O1B-PB-N3B	-2.12	108.62	111.79
3	F	1801	ANP	O2'-C2'-C3'	-2.06	105.23	111.83
3	J	1801	ANP	O2'-C2'-C1'	2.01	117.90	111.61
3	F	1801	ANP	C2-N1-C6	2.02	122.30	118.77
3	A	1801	ANP	C2-N1-C6	2.03	122.31	118.77
3	F	1801	ANP	C1'-N9-C4	2.07	130.21	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1801	ANP	C2'-C3'-C4'	2.08	106.67	102.62
3	A	1801	ANP	O3G-PG-O2G	2.11	113.59	107.69
3	I	1801	ANP	O3G-PG-O2G	2.11	113.59	107.69
3	J	1801	ANP	O3G-PG-O2G	2.13	113.64	107.69
3	A	1801	ANP	O4'-C4'-C5'	2.16	116.71	109.40
3	B	1801	ANP	O3G-PG-O2G	2.32	114.19	107.69
3	E	1801	ANP	N6-C6-N1	2.41	123.55	118.77
3	J	1801	ANP	O3A-PB-N3B	2.49	113.50	106.59
3	B	1801	ANP	C1'-N9-C4	2.66	131.24	126.64
3	F	1801	ANP	O2B-PB-O1B	2.70	115.49	109.87
3	E	1801	ANP	O3G-PG-O2G	2.74	115.36	107.69
3	I	1801	ANP	O2B-PB-O1B	2.81	115.71	109.87
3	B	1801	ANP	C4'-O4'-C1'	3.13	113.11	109.77
3	A	1801	ANP	O5'-C5'-C4'	3.28	120.63	109.00
3	F	1801	ANP	C4'-O4'-C1'	3.42	113.41	109.77
3	I	1801	ANP	C1'-N9-C4	3.46	132.61	126.64
3	A	1801	ANP	C1'-N9-C4	3.52	132.72	126.64
3	E	1801	ANP	O2B-PB-O1B	4.46	119.14	109.87
3	A	1801	ANP	C4'-O4'-C1'	4.85	114.93	109.77
3	A	1801	ANP	O2B-PB-O1B	4.99	120.24	109.87
3	J	1801	ANP	O2B-PB-O1B	5.13	120.53	109.87
3	I	1801	ANP	C4'-O4'-C1'	5.29	115.40	109.77

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	663/800 (82%)	0.79	83 (12%) 4 12	177, 220, 306, 373	0
1	B	663/800 (82%)	0.75	66 (9%) 8 15	196, 245, 311, 362	0
1	E	663/800 (82%)	0.80	84 (12%) 4 12	191, 224, 348, 398	0
1	F	663/800 (82%)	0.73	68 (10%) 7 14	181, 220, 296, 350	0
1	I	663/800 (82%)	1.12	111 (16%) 2 9	198, 244, 528, 643	0
1	J	663/800 (82%)	1.25	158 (23%) 1 7	213, 266, 510, 602	0
2	C	285/369 (77%)	0.81	33 (11%) 5 13	200, 237, 282, 323	0
2	D	285/369 (77%)	0.89	43 (15%) 3 10	193, 234, 273, 296	0
2	G	285/369 (77%)	1.08	61 (21%) 1 7	217, 239, 319, 347	0
2	H	285/369 (77%)	0.93	41 (14%) 3 10	210, 227, 268, 294	0
2	K	285/369 (77%)	0.90	36 (12%) 4 12	197, 233, 295, 329	0
2	L	285/369 (77%)	1.05	61 (21%) 1 7	233, 264, 336, 375	0
All	All	5688/7014 (81%)	0.92	845 (14%) 3 10	177, 237, 355, 643	0

All (845) 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	7.3
1	I	471	HIS	7.2
1	I	461	ASP	7.1
1	J	459	GLY	6.9

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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	6.7
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	5.8
1	E	609	MET	5.7
1	F	646	GLU	5.6
1	J	519	LYS	5.5
1	I	423	GLY	5.5
2	K	264	ARG	5.5
2	G	81	ALA	5.5
1	J	722	LEU	5.4
1	F	638	SER	5.4
1	J	514	LEU	5.4
1	I	473	TYR	5.4
1	F	577	GLY	5.2
2	G	240	VAL	5.2
1	I	577	GLY	5.2
1	I	757	ALA	5.2
1	A	659	ALA	5.1
1	J	381	GLN	5.1
1	J	410	ALA	5.1
1	J	512	LYS	5.1
1	A	702	TYR	5.1
1	I	498	ALA	5.1
1	J	443	ALA	5.0
2	G	331	GLN	5.0
1	J	659	ALA	5.0
1	J	422	GLY	5.0
1	E	723	THR	5.0
1	J	427	SER	5.0
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	4.9
1	J	136	ILE	4.8
1	I	515	THR	4.8
1	A	503	ILE	4.8
1	J	397	MET	4.7
2	G	289	VAL	4.7
1	I	489	TYR	4.7
1	F	578	ILE	4.7
1	I	748	ASP	4.6
1	E	756	ILE	4.6
1	E	489	TYR	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	J	480	GLY	4.5
1	I	472	GLY	4.4
1	A	177	GLU	4.4
1	E	659	ALA	4.4
1	I	759	MET	4.4
2	G	287	ALA	4.4
2	D	82	SER	4.4
1	B	705	LEU	4.4
2	G	239	TRP	4.4
2	K	125	ALA	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
1	I	646	GLU	4.3
2	H	82	SER	4.3
2	L	107	ARG	4.3
2	G	22	ARG	4.3
1	J	425	ILE	4.3
1	F	749	ALA	4.2
2	D	83	LEU	4.2
1	J	375	LEU	4.2
2	K	285	GLN	4.2
2	L	124	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	264	ARG	4.2
1	J	148	LEU	4.2
1	J	470	VAL	4.2
1	A	701	THR	4.1
2	H	49	GLY	4.1
1	B	178	LEU	4.1
1	J	420	ARG	4.1
1	J	658	GLY	4.1
2	G	20	VAL	4.1
1	E	362	PRO	4.1
1	I	758	PHE	4.1
1	B	727	THR	4.1
1	J	411	ILE	4.1
1	J	423	GLY	4.1
2	C	82	SER	4.1
1	I	751	GLU	4.1
1	J	751	GLU	4.0
1	F	750	LEU	4.0
2	G	322	ILE	4.0
1	E	148	LEU	4.0
1	J	442	GLY	4.0
1	J	378	LEU	4.0
1	J	407	LEU	4.0
1	J	518	GLY	4.0
1	A	697	ARG	4.0
2	C	139	HIS	4.0
2	G	325	GLY	4.0
1	E	382	LEU	3.9
1	J	362	PRO	3.9
1	F	742	VAL	3.9
1	J	511	ASP	3.9
2	L	198	GLN	3.9
2	H	71	ALA	3.9
2	H	123	ALA	3.9
2	L	291	TYR	3.9
2	K	286	PRO	3.9
2	L	279	LYS	3.9
2	G	107	ARG	3.9
2	G	290	LEU	3.9
1	J	524	GLU	3.9
1	J	372	PHE	3.9
1	B	707	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	749	ALA	3.8
2	C	80	ILE	3.8
1	J	750	LEU	3.8
2	G	21	GLU	3.8
1	J	178	LEU	3.8
1	J	690	VAL	3.8
1	B	749	ALA	3.8
1	J	457	ARG	3.8
1	E	610	LEU	3.8
1	I	465	VAL	3.8
1	I	761	SER	3.8
1	B	280	THR	3.8
1	E	552	LEU	3.7
1	J	345	VAL	3.7
1	I	647	ILE	3.7
1	E	655	THR	3.7
1	I	475	ILE	3.7
1	F	637	GLY	3.7
1	J	433	LEU	3.7
1	I	481	GLN	3.7
1	B	748	ASP	3.7
1	J	523	LEU	3.7
2	G	288	PHE	3.7
1	F	721	ALA	3.7
1	J	755	THR	3.7
2	D	20	VAL	3.7
2	K	243	PRO	3.7
1	E	381	GLN	3.7
2	H	198	GLN	3.7
1	I	460	LEU	3.6
1	J	612	ILE	3.6
2	L	150	LEU	3.6
1	J	368	MET	3.6
1	J	428	GLY	3.6
1	J	520	ALA	3.6
1	J	204	PHE	3.6
2	G	256	PHE	3.6
2	K	21	GLU	3.6
1	B	493	GLN	3.6
1	J	595	PRO	3.6
1	B	693	ASP	3.6
1	J	374	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
2	G	329	VAL	3.6
2	K	134	VAL	3.6
1	F	136	ILE	3.6
2	L	262	MET	3.5
1	J	382	LEU	3.5
1	E	576	PRO	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	I	345	VAL	3.5
1	B	638	SER	3.5
1	J	342	LEU	3.5
1	E	551	GLU	3.5
1	J	419	VAL	3.5
1	J	430	ASN	3.5
2	K	138	ALA	3.5
2	G	266	ARG	3.5
1	B	732	LEU	3.5
1	I	399	GLU	3.5
1	B	659	ALA	3.5
1	J	521	LEU	3.5
1	E	689	LEU	3.4
1	I	609	MET	3.4
1	A	595	PRO	3.4
1	B	465	VAL	3.4
1	I	463	LEU	3.4
2	L	242	ASP	3.4
1	B	136	ILE	3.4
1	F	695	ILE	3.4
2	L	137	ALA	3.4
1	B	709	TRP	3.4
1	J	531	LEU	3.4
2	C	119	GLU	3.4
1	A	656	ARG	3.4
1	A	797	GLU	3.4
1	J	749	ALA	3.4
1	F	256	ARG	3.4
1	J	481	GLN	3.4
1	J	460	LEU	3.4
1	A	696	GLY	3.4
2	G	326	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	464	LYS	3.3
1	E	658	GLY	3.3
2	C	137	ALA	3.3
2	K	265	ASP	3.3
1	J	134	ALA	3.3
1	J	471	HIS	3.3
1	J	343	ARG	3.3
2	C	136	PRO	3.3
2	H	241	ALA	3.3
2	L	27	VAL	3.3
1	E	425	ILE	3.3
1	E	155	PHE	3.3
2	H	132	VAL	3.3
2	L	81	ALA	3.3
1	J	341	VAL	3.3
1	E	555	LEU	3.3
1	E	721	ALA	3.3
1	I	400	PHE	3.3
2	C	239	TRP	3.3
1	J	509	TYR	3.3
2	G	272	ILE	3.3
1	F	571	THR	3.3
2	G	82	SER	3.2
2	L	24	ALA	3.2
1	F	420	ARG	3.2
2	L	20	VAL	3.2
1	E	454	GLU	3.2
2	H	133	THR	3.2
1	B	706	SER	3.2
1	I	514	LEU	3.2
1	I	599	ASN	3.2
2	D	99	LEU	3.2
2	K	284	GLN	3.2
1	I	346	GLY	3.2
1	B	708	ALA	3.2
1	A	502	ILE	3.2
2	G	243	PRO	3.2
2	H	243	PRO	3.2
2	L	22	ARG	3.2
1	B	695	ILE	3.2
1	E	385	VAL	3.2
1	B	372	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	216	GLN	3.2
2	L	125	ALA	3.2
1	A	420	ARG	3.2
2	H	266	ARG	3.2
2	K	263	MET	3.2
1	J	469	ALA	3.2
1	I	750	LEU	3.2
1	J	689	LEU	3.2
1	J	424	VAL	3.2
1	E	276	ASN	3.1
1	J	752	HIS	3.1
1	E	690	VAL	3.1
1	F	398	GLY	3.1
1	F	756	ILE	3.1
2	L	290	LEU	3.1
2	H	72	LEU	3.1
1	E	136	ILE	3.1
2	G	227	ILE	3.1
1	B	702	TYR	3.1
1	E	352	LEU	3.1
2	K	49	GLY	3.1
1	J	344	GLN	3.1
1	B	701	THR	3.1
1	J	610	LEU	3.1
1	A	465	VAL	3.1
2	K	124	TYR	3.1
2	L	263	MET	3.1
1	E	488	ASN	3.1
2	L	241	ALA	3.1
1	I	469	ALA	3.1
2	K	109	THR	3.1
1	J	724	LEU	3.1
1	A	419	VAL	3.1
1	I	462	THR	3.1
1	J	339	GLN	3.0
2	G	124	TYR	3.0
2	C	231	HIS	3.0
2	D	84	ASP	3.0
2	H	122	GLN	3.0
1	B	696	GLY	3.0
1	B	726	ALA	3.0
1	J	522	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	80	ILE	3.0
2	L	237	ARG	3.0
1	B	762	VAL	3.0
1	F	212	GLN	3.0
1	A	196	LEU	3.0
2	C	81	ALA	3.0
1	E	458	THR	3.0
2	K	66	ASP	3.0
1	J	657	VAL	3.0
2	C	220	PHE	3.0
1	J	516	SER	3.0
2	G	328	SER	3.0
1	F	576	PRO	3.0
1	A	504	PRO	3.0
1	A	703	ASP	3.0
1	J	401	ALA	3.0
1	A	516	SER	3.0
1	J	517	LYS	3.0
1	B	420	ARG	3.0
1	A	492	ARG	3.0
1	A	586	PRO	3.0
2	K	260	GLY	3.0
1	A	255	ILE	2.9
1	I	360	ALA	3.0
1	B	179	LEU	2.9
2	H	286	PRO	2.9
1	J	377	GLU	2.9
1	J	385	VAL	2.9
1	F	183	ASP	2.9
1	B	637	GLY	2.9
1	I	576	PRO	2.9
1	A	707	LEU	2.9
2	L	25	SER	2.9
2	K	241	ALA	2.9
1	I	572	PHE	2.9
1	I	756	ILE	2.9
1	F	155	PHE	2.9
1	F	600	PRO	2.9
2	K	108	LEU	2.9
1	J	406	LEU	2.9
2	K	84	ASP	2.9
1	B	747	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	755	THR	2.9
1	A	473	TYR	2.9
2	D	21	GLU	2.9
1	J	586	PRO	2.9
1	B	703	ASP	2.9
1	E	554	VAL	2.9
1	A	796	LEU	2.8
1	I	645	VAL	2.8
1	F	601	LEU	2.8
1	I	280	THR	2.8
1	J	133	LEU	2.8
1	I	597	ILE	2.8
1	I	586	PRO	2.8
2	D	137	ALA	2.8
2	D	138	ALA	2.8
2	G	125	ALA	2.8
1	F	572	PHE	2.8
2	L	240	VAL	2.8
2	G	80	ILE	2.8
2	H	138	ALA	2.8
1	F	630	ILE	2.8
1	I	510	GLU	2.8
2	K	220	PHE	2.8
2	G	279	LYS	2.8
1	I	219	THR	2.8
1	J	492	ARG	2.8
2	K	139	HIS	2.8
1	B	658	GLY	2.8
2	D	102	ILE	2.8
2	G	236	LEU	2.8
2	K	107	ARG	2.8
1	I	519	LYS	2.8
2	D	199	TYR	2.8
1	E	457	ARG	2.8
2	K	50	GLY	2.8
2	D	239	TRP	2.8
1	I	641	PRO	2.8
2	D	208	LYS	2.8
2	K	146	GLU	2.8
2	L	31	VAL	2.8
1	J	638	SER	2.8
2	D	220	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	644	LYS	2.8
1	F	751	GLU	2.8
2	K	90	ILE	2.8
1	E	134	ALA	2.8
2	L	257	TYR	2.8
1	A	421	ASP	2.7
1	F	701	THR	2.7
1	F	748	ASP	2.7
2	L	106	SER	2.7
2	G	108	LEU	2.7
1	A	488	ASN	2.7
1	B	694	GLU	2.7
1	I	493	GLN	2.7
1	J	394	ARG	2.7
1	A	475	ILE	2.7
2	C	226	ALA	2.7
2	D	97	GLU	2.7
1	A	748	ASP	2.7
1	A	505	GLU	2.7
1	A	658	GLY	2.7
1	J	147	THR	2.7
1	J	535	LEU	2.7
1	E	577	GLY	2.7
1	F	580	ILE	2.7
1	J	454	GLU	2.7
2	G	257	TYR	2.7
2	G	318	VAL	2.7
1	I	695	ILE	2.7
1	E	751	GLU	2.7
1	J	445	ASP	2.7
2	G	242	ASP	2.7
1	J	403	LEU	2.7
1	J	468	ASN	2.7
1	B	725	PHE	2.7
2	H	63	ILE	2.7
1	E	420	ARG	2.7
1	J	725	PHE	2.7
2	H	81	ALA	2.7
1	A	506	LEU	2.7
1	E	345	VAL	2.7
1	I	694	GLU	2.7
2	L	151	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	700	SER	2.7
2	L	82	SER	2.7
1	A	381	GLN	2.7
1	F	627	THR	2.7
1	E	179	LEU	2.6
1	I	579	ARG	2.6
1	A	695	ILE	2.6
1	F	626	GLN	2.6
1	E	430	ASN	2.6
1	B	135	ALA	2.6
1	B	492	ARG	2.6
1	F	145	TYR	2.6
1	F	752	HIS	2.6
1	F	603	LEU	2.6
1	B	654	PHE	2.6
2	D	198	GLN	2.6
1	F	399	GLU	2.6
1	E	258	ILE	2.6
1	I	760	HIS	2.6
1	J	346	GLY	2.6
1	E	549	LEU	2.6
2	G	327	LEU	2.6
1	A	454	GLU	2.6
1	J	441	ASP	2.6
2	H	125	ALA	2.6
1	F	639	TYR	2.6
2	G	150	LEU	2.6
2	L	264	ARG	2.6
1	I	455	ARG	2.6
1	A	440	ALA	2.6
1	B	147	THR	2.6
1	A	486	PRO	2.6
1	A	178	LEU	2.6
2	G	132	VAL	2.6
2	K	279	LYS	2.6
1	I	742	VAL	2.6
2	G	133	THR	2.6
1	E	351	ILE	2.6
1	F	258	ILE	2.6
1	I	418	LEU	2.6
1	I	466	GLY	2.6
2	H	21	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	147	THR	2.6
1	I	580	ILE	2.6
1	I	279	ILE	2.6
1	B	134	ALA	2.6
1	J	212	GLN	2.6
2	L	289	VAL	2.6
1	E	158	SER	2.6
1	J	348	LEU	2.6
2	D	202	VAL	2.5
2	G	229	TRP	2.5
1	J	723	THR	2.5
1	J	558	LEU	2.5
1	J	691	LEU	2.5
2	C	238	GLY	2.5
1	F	505	GLU	2.5
1	F	647	ILE	2.5
1	I	474	TYR	2.5
1	J	635	TYR	2.5
1	J	692	MET	2.5
2	G	321	PHE	2.5
1	B	704	GLY	2.5
1	I	267	ILE	2.5
1	B	421	ASP	2.5
1	E	556	VAL	2.5
1	I	496	LYS	2.5
2	D	200	ARG	2.5
1	A	417	VAL	2.5
1	A	489	TYR	2.5
2	G	198	GLN	2.5
2	G	237	ARG	2.5
1	A	704	GLY	2.5
1	B	691	LEU	2.5
2	L	136	PRO	2.5
1	I	415	PRO	2.5
2	D	71	ALA	2.5
1	F	147	THR	2.5
2	C	135	LYS	2.5
2	G	262	MET	2.5
2	H	180	LEU	2.5
2	L	134	VAL	2.5
2	L	250	LEU	2.5
1	J	780	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	331	LEU	2.5
1	I	638	SER	2.5
1	A	385	VAL	2.5
1	I	762	VAL	2.5
2	D	291	TYR	2.5
1	E	178	LEU	2.5
1	J	277	LEU	2.5
2	D	100	ALA	2.5
1	A	458	THR	2.5
1	E	259	THR	2.5
1	I	221	ASP	2.5
1	E	355	LEU	2.5
1	J	473	TYR	2.4
1	F	255	ILE	2.4
1	J	300	THR	2.4
1	E	608	ARG	2.4
1	J	611	ILE	2.4
1	A	705	LEU	2.4
2	D	68	LEU	2.4
1	I	433	LEU	2.4
2	D	96	GLY	2.4
2	G	224	ALA	2.4
1	A	476	GLN	2.4
1	F	489	TYR	2.4
1	A	770	SER	2.4
1	B	279	ILE	2.4
2	H	124	TYR	2.4
1	I	456	GLU	2.4
1	J	379	ARG	2.4
2	C	286	PRO	2.4
2	H	285	GLN	2.4
1	I	614	GLY	2.4
2	H	216	LEU	2.4
1	A	524	GLU	2.4
1	E	729	TYR	2.4
1	J	299	VAL	2.4
2	L	326	VAL	2.4
1	J	298	THR	2.4
1	E	572	PHE	2.4
2	H	95	ARG	2.4
1	J	743	ALA	2.4
1	A	415	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	154	ARG	2.4
1	F	579	ARG	2.4
1	F	696	GLY	2.4
1	J	557	ASN	2.4
1	J	549	LEU	2.4
2	K	262	MET	2.4
1	B	324	ARG	2.4
1	E	657	VAL	2.4
1	I	299	VAL	2.4
2	G	148	LEU	2.4
1	B	731	GLU	2.4
1	E	344	GLN	2.4
1	B	368	MET	2.4
1	I	464	LYS	2.4
1	E	338	LEU	2.4
1	J	351	ILE	2.4
2	K	65	LYS	2.4
2	L	260	GLY	2.4
1	J	613	THR	2.4
1	F	144	GLY	2.4
1	I	425	ILE	2.4
2	D	201	ALA	2.4
1	I	266	SER	2.4
1	J	295	LEU	2.4
1	J	479	ARG	2.4
2	C	224	ALA	2.4
2	D	228	GLU	2.4
1	F	503	ILE	2.4
1	I	430	ASN	2.4
2	G	149	ASP	2.4
1	F	419	VAL	2.3
1	A	424	VAL	2.3
1	E	558	LEU	2.3
2	G	220	PHE	2.3
2	L	246	THR	2.3
1	F	757	ALA	2.3
2	K	81	ALA	2.3
1	F	148	LEU	2.3
1	F	722	LEU	2.3
1	J	527	LEU	2.3
1	J	396	LYS	2.3
1	A	706	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	482	SER	2.3
2	D	124	TYR	2.3
2	G	226	ALA	2.3
1	I	504	PRO	2.3
1	E	475	ILE	2.3
2	C	86	LEU	2.3
2	C	120	ALA	2.3
2	L	239	TRP	2.3
1	A	418	LEU	2.3
1	B	756	ILE	2.3
1	I	571	THR	2.3
2	G	292	LEU	2.3
1	J	402	GLU	2.3
1	J	474	TYR	2.3
1	I	427	SER	2.3
2	C	322	ILE	2.3
2	H	284	GLN	2.3
1	A	708	ALA	2.3
1	I	631	ALA	2.3
2	K	34	SER	2.3
2	K	95	ARG	2.3
2	L	132	VAL	2.3
2	L	236	LEU	2.3
1	I	754	ASP	2.3
1	I	502	ILE	2.3
2	G	97	GLU	2.3
1	F	570	PRO	2.3
1	E	493	GLN	2.3
1	I	242	GLN	2.3
1	E	553	ASP	2.3
1	F	257	SER	2.3
1	F	694	GLU	2.3
2	C	144	THR	2.3
1	A	443	ALA	2.3
1	E	748	ASP	2.3
1	F	506	LEU	2.3
2	C	20	VAL	2.3
1	I	486	PRO	2.3
1	J	189	LEU	2.3
1	F	421	ASP	2.3
1	B	690	VAL	2.3
2	L	287	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	755	THR	2.3
2	H	322	ILE	2.3
1	J	314	PRO	2.3
1	J	467	PHE	2.3
2	C	122	GLN	2.2
1	E	505	GLU	2.2
2	D	133	THR	2.2
1	E	156	ARG	2.2
2	H	162	ARG	2.2
1	A	638	SER	2.2
1	F	655	THR	2.2
1	I	517	LYS	2.2
2	H	242	ASP	2.2
1	E	742	VAL	2.2
1	I	507	LYS	2.2
2	L	133	THR	2.2
2	L	30	LEU	2.2
1	J	456	GLU	2.2
1	J	464	LYS	2.2
1	B	610	LEU	2.2
1	F	346	GLY	2.2
2	C	326	VAL	2.2
1	E	280	THR	2.2
2	C	97	GLU	2.2
1	J	179	LEU	2.2
2	D	125	ALA	2.2
1	A	654	PHE	2.2
2	L	266	ARG	2.2
1	F	628	ALA	2.2
2	K	240	VAL	2.2
1	I	468	ASN	2.2
2	L	220	PHE	2.2
1	A	493	GLN	2.2
2	D	236	LEU	2.2
1	B	255	ILE	2.2
1	E	411	ILE	2.2
1	E	757	ALA	2.2
1	A	447	LEU	2.2
2	L	256	PHE	2.2
1	F	599	ASN	2.2
1	I	524	GLU	2.2
2	G	264	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	506	LEU	2.2
1	I	658	GLY	2.2
2	G	225	LEU	2.2
1	A	315	VAL	2.2
1	J	483	HIS	2.2
1	A	670	PHE	2.2
1	B	735	LEU	2.2
1	E	133	LEU	2.2
1	E	758	PHE	2.2
1	A	448	GLU	2.2
1	E	403	LEU	2.2
1	F	656	ARG	2.2
1	I	520	ALA	2.2
2	C	230	GLN	2.2
2	D	101	SER	2.2
1	J	154	ARG	2.2
2	L	46	ILE	2.2
2	G	208	LYS	2.2
1	A	136	ILE	2.2
1	A	677	THR	2.2
1	B	724	LEU	2.2
2	D	81	ALA	2.2
2	H	22	ARG	2.2
1	I	513	VAL	2.2
1	A	800	SER	2.2
2	H	199	TYR	2.2
1	B	780	GLY	2.2
1	A	655	THR	2.2
2	D	67	GLU	2.2
1	B	743	ALA	2.2
2	H	137	ALA	2.2
1	A	154	ARG	2.1
1	A	217	PHE	2.1
1	E	727	THR	2.1
2	L	223	GLN	2.1
1	B	488	ASN	2.1
1	J	393	LEU	2.1
2	D	95	ARG	2.1
1	I	426	ALA	2.1
2	G	291	TYR	2.1
1	E	399	GLU	2.1
1	I	503	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	236	LEU	2.1
2	D	227	ILE	2.1
1	A	466	GLY	2.1
2	H	70	LEU	2.1
2	L	70	LEU	2.1
1	E	361	ARG	2.1
1	I	330	ALA	2.1
2	L	119	GLU	2.1
2	C	121	TRP	2.1
1	J	528	TYR	2.1
2	L	72	LEU	2.1
1	B	761	SER	2.1
2	G	265	ASP	2.1
1	I	355	LEU	2.1
1	I	403	LEU	2.1
2	K	67	GLU	2.1
1	J	727	THR	2.1
1	A	517	LYS	2.1
2	D	235	THR	2.1
2	D	279	LYS	2.1
1	A	514	LEU	2.1
1	E	257	SER	2.1
1	I	190	ILE	2.1
1	J	315	VAL	2.1
1	J	383	GLU	2.1
1	A	195	GLY	2.1
2	L	218	THR	2.1
1	F	629	LEU	2.1
2	K	83	LEU	2.1
1	A	436	TRP	2.1
2	H	134	VAL	2.1
2	L	123	ALA	2.1
1	J	455	ARG	2.1
1	B	502	ILE	2.1
1	B	729	TYR	2.1
1	E	213	LEU	2.1
2	G	260	GLY	2.1
2	D	191	HIS	2.1
2	K	254	GLN	2.1
1	A	535	LEU	2.1
1	I	291	LEU	2.1
1	I	451	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	759	MET	2.1
2	G	263	MET	2.1
1	B	616	ASN	2.1
1	F	470	VAL	2.1
1	J	437	ARG	2.1
1	I	431	GLU	2.1
1	J	732	LEU	2.1
2	H	215	ILE	2.1
2	L	272	ILE	2.1
1	A	500	ARG	2.1
1	J	135	ALA	2.1
2	D	224	ALA	2.1
1	B	609	MET	2.1
1	J	551	GLU	2.1
2	H	84	ASP	2.1
1	E	378	LEU	2.1
1	A	773	LEU	2.1
1	J	489	TYR	2.1
2	L	28	LYS	2.1
2	H	119	GLU	2.1
1	J	702	TYR	2.1
1	A	513	VAL	2.1
1	I	659	ALA	2.1
2	L	216	LEU	2.1
1	A	190	ILE	2.1
2	C	95	ARG	2.1
2	H	326	VAL	2.1
2	L	103	SER	2.1
1	F	146	ALA	2.1
2	C	21	GLU	2.1
1	J	404	ARG	2.1
2	H	246	THR	2.1
1	J	365	LEU	2.1
2	C	85	ASP	2.1
1	E	528	TYR	2.0
2	G	216	LEU	2.0
2	L	45	ASP	2.0
1	E	422	GLY	2.0
2	C	229	TRP	2.0
1	E	390	VAL	2.0
1	B	576	PRO	2.0
2	D	103	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	280	THR	2.0
1	B	190	ILE	2.0
1	F	422	GLY	2.0
1	J	576	PRO	2.0
2	D	65	LYS	2.0
2	D	80	ILE	2.0
1	B	473	TYR	2.0
2	G	106	SER	2.0
1	E	691	LEU	2.0
2	C	287	ALA	2.0
1	B	242	GLN	2.0
1	B	711	VAL	2.0
2	C	134	VAL	2.0
1	E	491	ARG	2.0
1	A	179	LEU	2.0
1	F	471	HIS	2.0
2	L	108	LEU	2.0
1	J	203	GLU	2.0
1	A	507	LYS	2.0
1	E	348	LEU	2.0
1	F	135	ALA	2.0
2	D	266	ARG	2.0
1	I	501	TYR	2.0
1	I	528	TYR	2.0
1	I	542	LEU	2.0
1	A	657	VAL	2.0
1	I	505	GLU	2.0
1	J	463	LEU	2.0
2	L	135	LYS	2.0
1	A	725	PHE	2.0
1	A	378	LEU	2.0
2	H	108	LEU	2.0
2	L	21	GLU	2.0
2	D	72	LEU	2.0
1	A	145	TYR	2.0
2	G	134	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ANP	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	-1.11	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.