



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 PM GMT

PDB ID : 4KOD  
Title : Structure of p97 N-D1 R155H mutant in complex with ADP  
Authors : Xia, D.; Tang, W.K.  
Deposited on : 2013-05-11  
Resolution : 2.96 Å(reported)

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

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

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

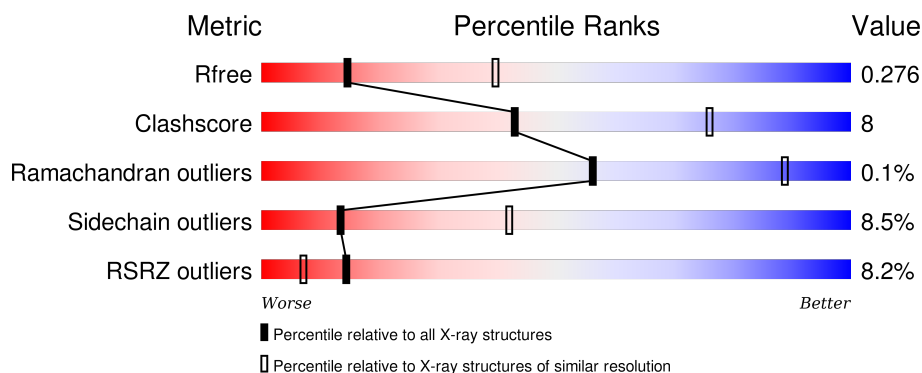
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	489	<div> <div>8%</div> <div>72% 16% • 10%</div> </div>
1	B	489	<div> <div>4%</div> <div>69% 20% • 10%</div> </div>
1	C	489	<div> <div>6%</div> <div>68% 20% • 10%</div> </div>
1	D	489	<div> <div>7%</div> <div>70% 19% • 10%</div> </div>
1	E	489	<div> <div>12%</div> <div>70% 18% • 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	489	
1	G	489	
1	H	489	
1	I	489	
1	J	489	
1	K	489	
1	L	489	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 41760 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3430	2154	607	651	18			
1	B	439	Total	C	N	O	S	0	0	0
			3438	2158	609	653	18			
1	C	438	Total	C	N	O	S	0	0	0
			3427	2152	605	652	18			
1	D	439	Total	C	N	O	S	0	0	0
			3438	2158	609	653	18			
1	E	439	Total	C	N	O	S	0	0	0
			3434	2157	606	653	18			
1	F	438	Total	C	N	O	S	0	0	0
			3427	2152	605	652	18			
1	G	437	Total	C	N	O	S	0	0	0
			3419	2148	603	650	18			
1	H	438	Total	C	N	O	S	0	0	0
			3430	2154	607	651	18			
1	I	440	Total	C	N	O	S	0	0	0
			3447	2164	611	654	18			
1	J	445	Total	C	N	O	S	0	0	0
			3486	2187	619	662	18			
1	K	438	Total	C	N	O	S	0	0	0
			3427	2152	605	652	18			
1	L	442	Total	C	N	O	S	0	0	0
			3465	2175	615	657	18			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
A	482	ARG	-	EXPRESSION TAG	UNP P55072
A	483	SER	-	EXPRESSION TAG	UNP P55072
A	484	HIS	-	EXPRESSION TAG	UNP P55072
A	485	HIS	-	EXPRESSION TAG	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	486	HIS	-	EXPRESSION TAG	UNP P55072
A	487	HIS	-	EXPRESSION TAG	UNP P55072
A	488	HIS	-	EXPRESSION TAG	UNP P55072
A	489	HIS	-	EXPRESSION TAG	UNP P55072
B	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
B	482	ARG	-	EXPRESSION TAG	UNP P55072
B	483	SER	-	EXPRESSION TAG	UNP P55072
B	484	HIS	-	EXPRESSION TAG	UNP P55072
B	485	HIS	-	EXPRESSION TAG	UNP P55072
B	486	HIS	-	EXPRESSION TAG	UNP P55072
B	487	HIS	-	EXPRESSION TAG	UNP P55072
B	488	HIS	-	EXPRESSION TAG	UNP P55072
B	489	HIS	-	EXPRESSION TAG	UNP P55072
C	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
C	482	ARG	-	EXPRESSION TAG	UNP P55072
C	483	SER	-	EXPRESSION TAG	UNP P55072
C	484	HIS	-	EXPRESSION TAG	UNP P55072
C	485	HIS	-	EXPRESSION TAG	UNP P55072
C	486	HIS	-	EXPRESSION TAG	UNP P55072
C	487	HIS	-	EXPRESSION TAG	UNP P55072
C	488	HIS	-	EXPRESSION TAG	UNP P55072
C	489	HIS	-	EXPRESSION TAG	UNP P55072
D	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
D	482	ARG	-	EXPRESSION TAG	UNP P55072
D	483	SER	-	EXPRESSION TAG	UNP P55072
D	484	HIS	-	EXPRESSION TAG	UNP P55072
D	485	HIS	-	EXPRESSION TAG	UNP P55072
D	486	HIS	-	EXPRESSION TAG	UNP P55072
D	487	HIS	-	EXPRESSION TAG	UNP P55072
D	488	HIS	-	EXPRESSION TAG	UNP P55072
D	489	HIS	-	EXPRESSION TAG	UNP P55072
E	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
E	482	ARG	-	EXPRESSION TAG	UNP P55072
E	483	SER	-	EXPRESSION TAG	UNP P55072
E	484	HIS	-	EXPRESSION TAG	UNP P55072
E	485	HIS	-	EXPRESSION TAG	UNP P55072
E	486	HIS	-	EXPRESSION TAG	UNP P55072
E	487	HIS	-	EXPRESSION TAG	UNP P55072
E	488	HIS	-	EXPRESSION TAG	UNP P55072
E	489	HIS	-	EXPRESSION TAG	UNP P55072
F	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
F	482	ARG	-	EXPRESSION TAG	UNP P55072

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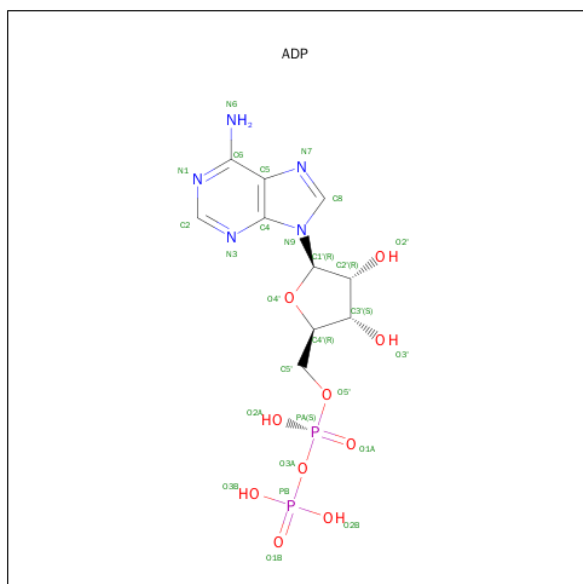
Chain	Residue	Modelled	Actual	Comment	Reference
F	483	SER	-	EXPRESSION TAG	UNP P55072
F	484	HIS	-	EXPRESSION TAG	UNP P55072
F	485	HIS	-	EXPRESSION TAG	UNP P55072
F	486	HIS	-	EXPRESSION TAG	UNP P55072
F	487	HIS	-	EXPRESSION TAG	UNP P55072
F	488	HIS	-	EXPRESSION TAG	UNP P55072
F	489	HIS	-	EXPRESSION TAG	UNP P55072
G	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
G	482	ARG	-	EXPRESSION TAG	UNP P55072
G	483	SER	-	EXPRESSION TAG	UNP P55072
G	484	HIS	-	EXPRESSION TAG	UNP P55072
G	485	HIS	-	EXPRESSION TAG	UNP P55072
G	486	HIS	-	EXPRESSION TAG	UNP P55072
G	487	HIS	-	EXPRESSION TAG	UNP P55072
G	488	HIS	-	EXPRESSION TAG	UNP P55072
G	489	HIS	-	EXPRESSION TAG	UNP P55072
H	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
H	482	ARG	-	EXPRESSION TAG	UNP P55072
H	483	SER	-	EXPRESSION TAG	UNP P55072
H	484	HIS	-	EXPRESSION TAG	UNP P55072
H	485	HIS	-	EXPRESSION TAG	UNP P55072
H	486	HIS	-	EXPRESSION TAG	UNP P55072
H	487	HIS	-	EXPRESSION TAG	UNP P55072
H	488	HIS	-	EXPRESSION TAG	UNP P55072
H	489	HIS	-	EXPRESSION TAG	UNP P55072
I	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
I	482	ARG	-	EXPRESSION TAG	UNP P55072
I	483	SER	-	EXPRESSION TAG	UNP P55072
I	484	HIS	-	EXPRESSION TAG	UNP P55072
I	485	HIS	-	EXPRESSION TAG	UNP P55072
I	486	HIS	-	EXPRESSION TAG	UNP P55072
I	487	HIS	-	EXPRESSION TAG	UNP P55072
I	488	HIS	-	EXPRESSION TAG	UNP P55072
I	489	HIS	-	EXPRESSION TAG	UNP P55072
J	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
J	482	ARG	-	EXPRESSION TAG	UNP P55072
J	483	SER	-	EXPRESSION TAG	UNP P55072
J	484	HIS	-	EXPRESSION TAG	UNP P55072
J	485	HIS	-	EXPRESSION TAG	UNP P55072
J	486	HIS	-	EXPRESSION TAG	UNP P55072
J	487	HIS	-	EXPRESSION TAG	UNP P55072
J	488	HIS	-	EXPRESSION TAG	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
J	489	HIS	-	EXPRESSION TAG	UNP P55072
K	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
K	482	ARG	-	EXPRESSION TAG	UNP P55072
K	483	SER	-	EXPRESSION TAG	UNP P55072
K	484	HIS	-	EXPRESSION TAG	UNP P55072
K	485	HIS	-	EXPRESSION TAG	UNP P55072
K	486	HIS	-	EXPRESSION TAG	UNP P55072
K	487	HIS	-	EXPRESSION TAG	UNP P55072
K	488	HIS	-	EXPRESSION TAG	UNP P55072
K	489	HIS	-	EXPRESSION TAG	UNP P55072
L	155	HIS	ARG	ENGINEERED MUTATION	UNP P55072
L	482	ARG	-	EXPRESSION TAG	UNP P55072
L	483	SER	-	EXPRESSION TAG	UNP P55072
L	484	HIS	-	EXPRESSION TAG	UNP P55072
L	485	HIS	-	EXPRESSION TAG	UNP P55072
L	486	HIS	-	EXPRESSION TAG	UNP P55072
L	487	HIS	-	EXPRESSION TAG	UNP P55072
L	488	HIS	-	EXPRESSION TAG	UNP P55072
L	489	HIS	-	EXPRESSION TAG	UNP P55072

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	9	Total	O	0	0
			9	9		
3	C	14	Total	O	0	0
			14	14		
3	D	17	Total	O	0	0
			17	17		
3	E	17	Total	O	0	0
			17	17		
3	F	15	Total	O	0	0
			15	15		
3	G	11	Total	O	0	0
			11	11		
3	H	16	Total	O	0	0
			16	16		

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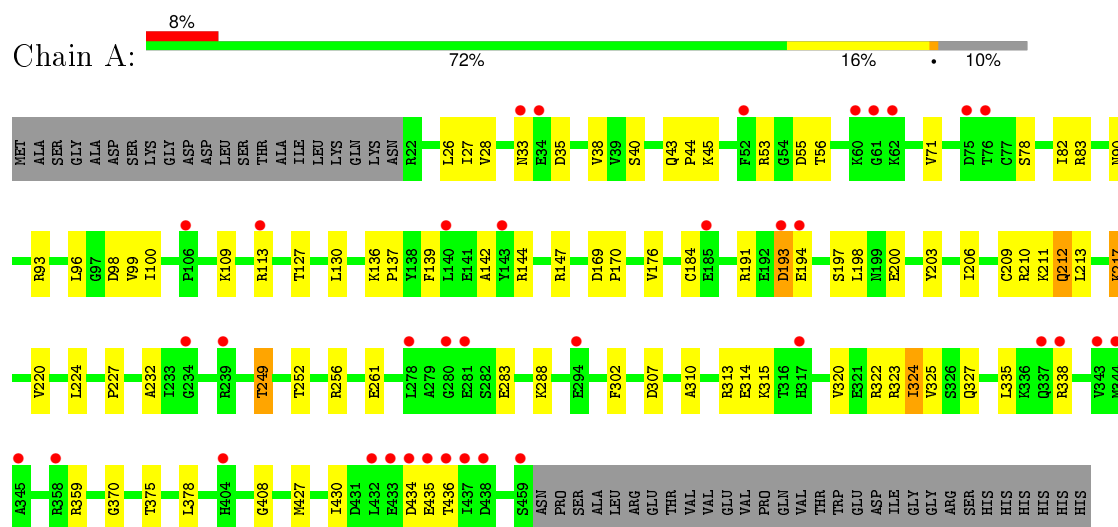
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	11	Total 11	O 11	0	0
3	J	17	Total 17	O 17	0	0
3	K	11	Total 11	O 11	0	0
3	L	16	Total 16	O 16	0	0

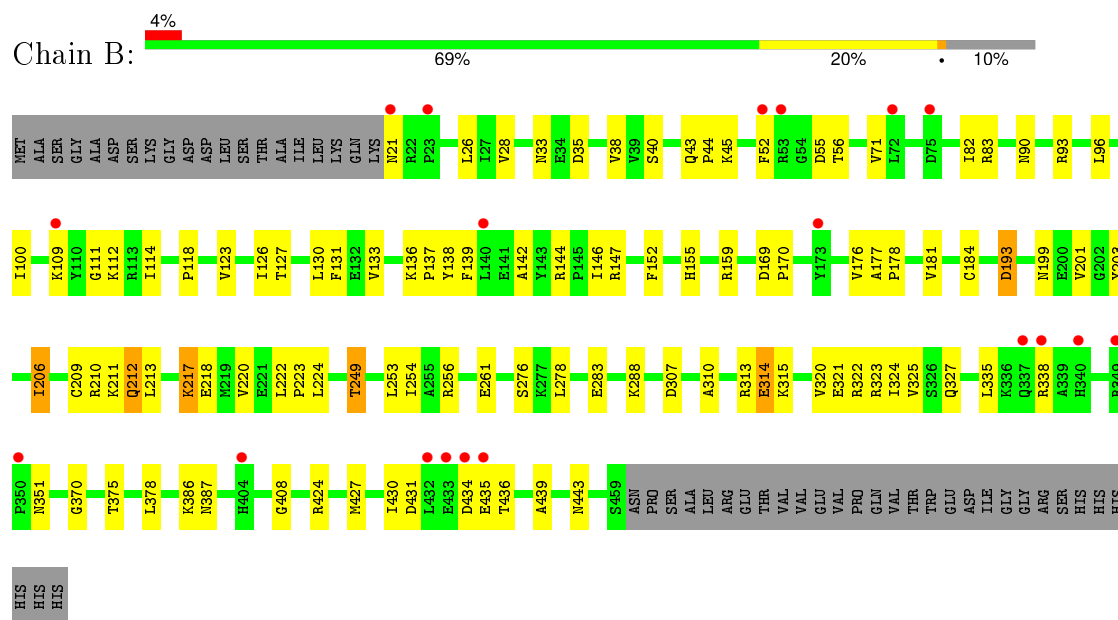
### 3 Residue-property plots [i](#)

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.

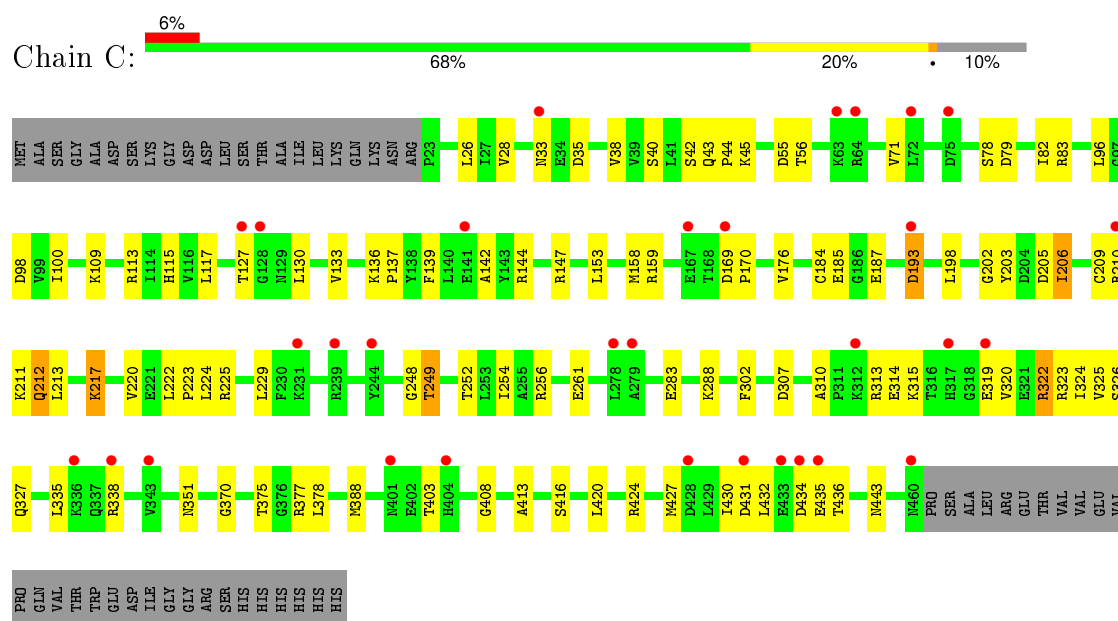
- Molecule 1: Transitional endoplasmic reticulum ATPase



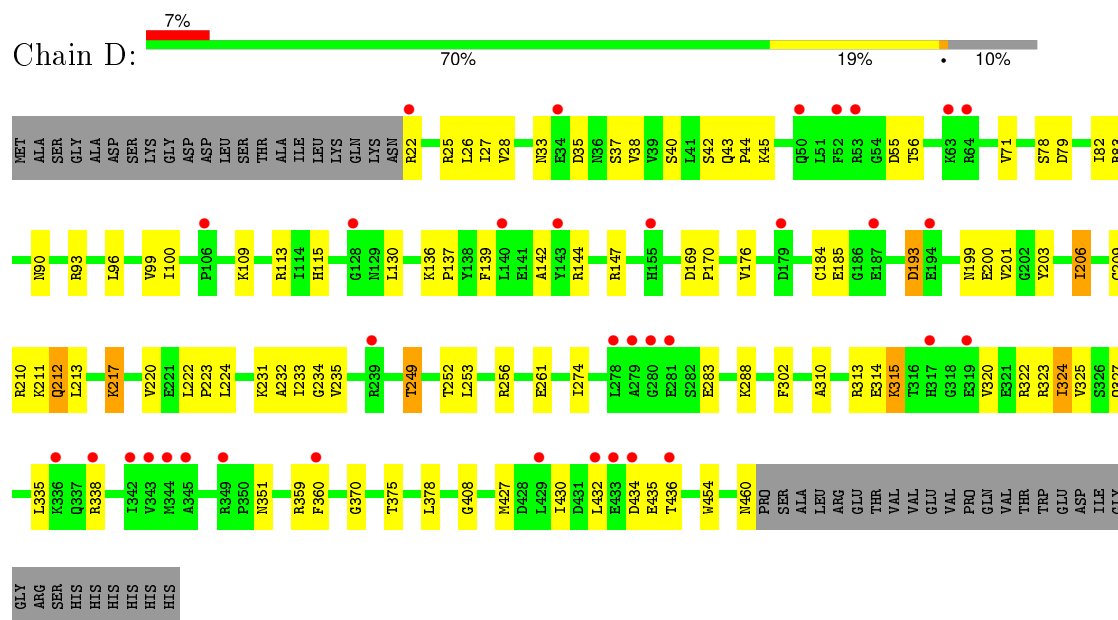
- Molecule 1: Transitional endoplasmic reticulum ATPase



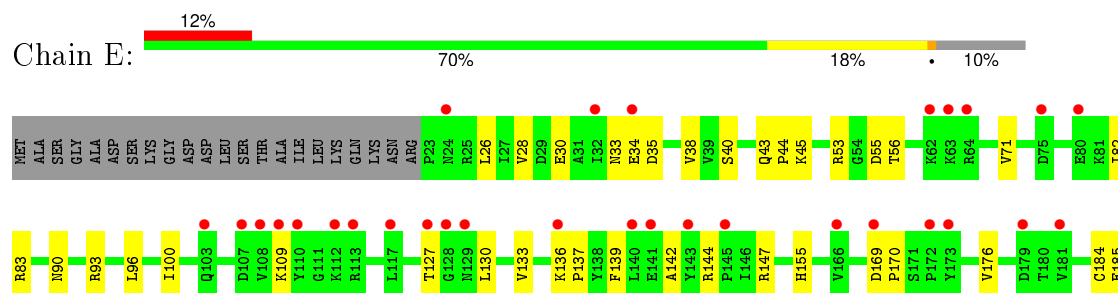
- Molecule 1: Transitional endoplasmic reticulum ATPase



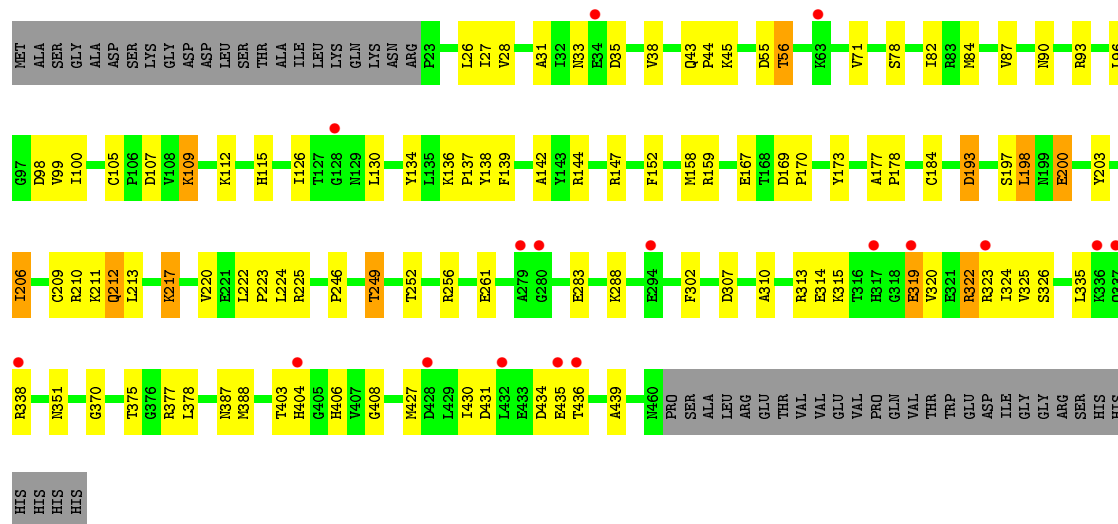
- Molecule 1: Transitional endoplasmic reticulum ATPase



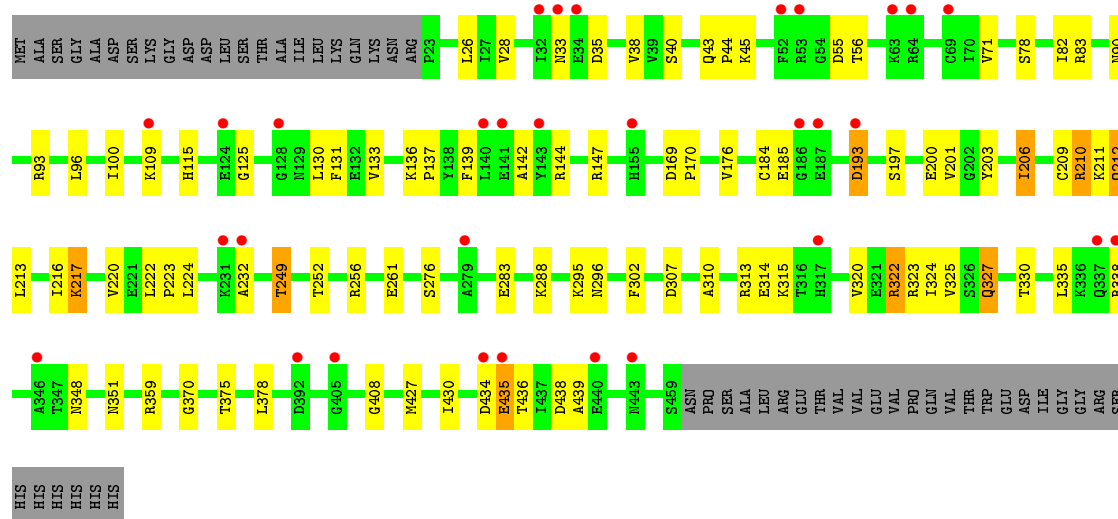
- Molecule 1: Transitional endoplasmic reticulum ATPase



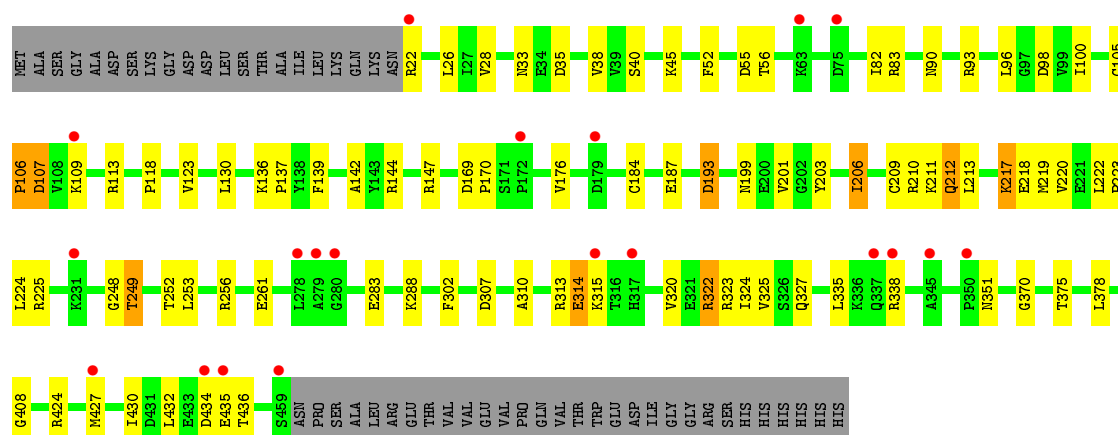
- Molecule 1: Transitional endoplasmic reticulum ATPase



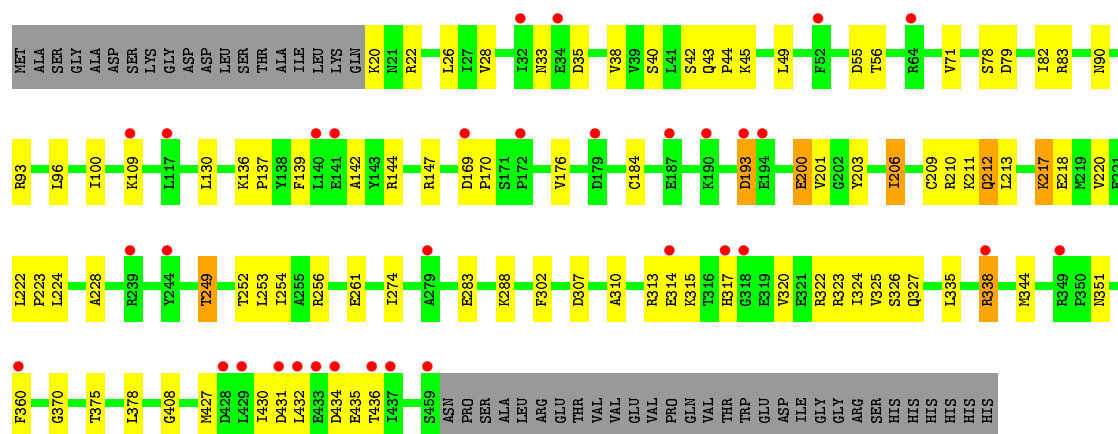
- Molecule 1: Transitional endoplasmic reticulum ATPase



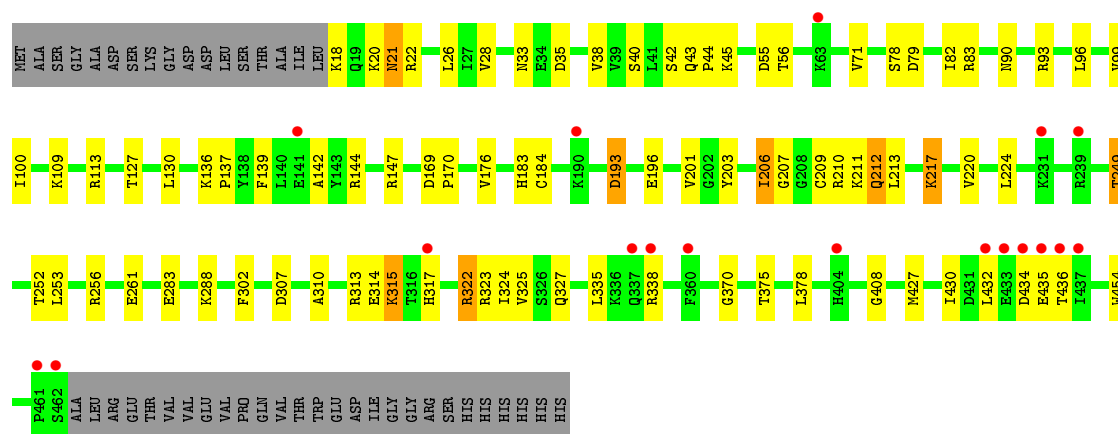
- Molecule 1: Transitional endoplasmic reticulum ATPase



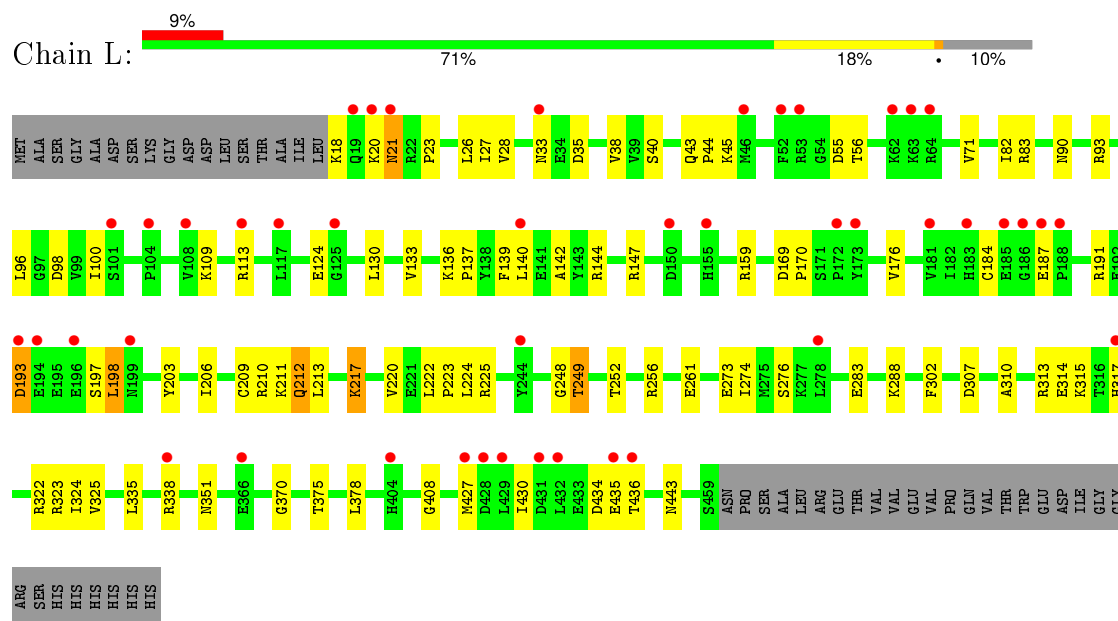
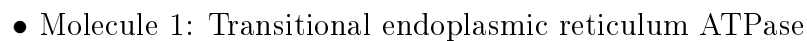
- Molecule 1: Transitional endoplasmic reticulum ATPase



- Molecule 1: Transitional endoplasmic reticulum ATPase



- Molecule 1: Transitional endoplasmic reticulum ATPase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.52Å 170.74Å 256.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.99 – 2.96 21.99 – 2.96	Depositor EDS
% Data completeness (in resolution range)	88.0 (21.99-2.96) 88.3 (21.99-2.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.94Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.268 , 0.291 0.250 , 0.276	Depositor DCC
$R_{free}$ test set	5937 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.4	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 26.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 118226 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	41760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.37	0/3484	0.63	0/4708
1	B	0.47	0/3492	0.67	0/4719
1	C	0.38	0/3481	0.62	0/4704
1	D	0.39	0/3492	0.64	0/4719
1	E	0.40	1/3489 (0.0%)	0.68	3/4716 (0.1%)
1	F	0.48	0/3481	0.70	1/4704 (0.0%)
1	G	0.43	2/3473 (0.1%)	0.64	0/4693
1	H	0.42	0/3484	0.66	0/4708
1	I	0.40	0/3501	0.64	2/4730 (0.0%)
1	J	0.44	0/3541	0.66	0/4784
1	K	0.44	1/3481 (0.0%)	0.71	2/4704 (0.0%)
1	L	0.36	0/3519	0.62	0/4753
All	All	0.42	4/41918 (0.0%)	0.66	8/56642 (0.0%)

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	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	459	SER	C-N	8.47	1.53	1.34
1	E	193	ASP	CB-CG	-8.24	1.34	1.51
1	G	296	ASN	CG-ND2	-6.77	1.16	1.32
1	G	296	ASN	CG-OD1	-5.05	1.12	1.24

All (8) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	193	ASP	CB-CG-OD1	-16.01	103.89	118.30
1	E	193	ASP	CB-CG-OD2	7.36	124.93	118.30
1	I	360	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	K	242	LEU	CA-CB-CG	5.54	128.04	115.30
1	F	319	GLU	CB-CA-C	-5.48	99.43	110.40
1	E	193	ASP	CB-CA-C	-5.25	99.90	110.40
1	K	335	LEU	CA-CB-CG	5.23	127.34	115.30
1	I	360	PHE	CB-CG-CD2	5.11	124.38	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	239	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3430	0	3480	44	0
1	B	3438	0	3486	66	1
1	C	3427	0	3474	74	0
1	D	3438	0	3486	61	0
1	E	3434	0	3481	60	0
1	F	3427	0	3474	71	1
1	G	3419	0	3468	55	1
1	H	3430	0	3480	54	0
1	I	3447	0	3499	49	1
1	J	3486	0	3538	46	0
1	K	3427	0	3474	132	0
1	L	3465	0	3520	56	0
2	A	27	0	12	2	0
2	B	27	0	12	2	0
2	C	27	0	12	4	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	F	27	0	12	3	0
2	G	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	27	0	12	3	0
2	I	27	0	12	2	0
2	J	27	0	12	2	0
2	K	27	0	12	3	0
2	L	27	0	12	4	0
3	A	14	0	0	2	0
3	B	9	0	0	0	0
3	C	14	0	0	0	0
3	D	17	0	0	1	0
3	E	17	0	0	2	0
3	F	15	0	0	0	0
3	G	11	0	0	4	0
3	H	16	0	0	0	0
3	I	11	0	0	1	0
3	J	17	0	0	2	0
3	K	11	0	0	1	0
3	L	16	0	0	0	0
All	All	41760	0	42004	681	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (681) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:433:GLU:HG3	1:K:436:THR:HG21	1.29	1.12
1:C:159:ARG:HD2	1:D:232:ALA:O	1.53	1.09
1:B:276:SER:HB3	1:F:326:SER:HB3	1.33	1.08
1:C:158:MET:HB2	1:D:233:ILE:HG22	1.36	1.07
1:I:209:CYS:HB2	1:I:212:GLN:HG2	1.36	1.03
1:K:240:GLY:HA3	1:K:363:PHE:CD1	1.95	1.02
1:J:209:CYS:HB2	1:J:212:GLN:HG2	1.41	1.00
1:D:209:CYS:HB2	1:D:212:GLN:HG2	1.52	0.91
1:B:209:CYS:HB2	1:B:212:GLN:HG2	1.53	0.90
1:C:413:ALA:HB2	1:D:360:PHE:HE1	1.36	0.90
1:K:256:ARG:HA	1:K:266:PHE:CE2	2.06	0.89
1:K:430:ILE:HG22	1:K:433:GLU:CB	2.03	0.88
1:L:209:CYS:HB2	1:L:212:GLN:HG2	1.56	0.88
1:I:209:CYS:HB2	1:I:212:GLN:CG	2.03	0.88
1:E:406:HIS:CD2	1:E:461:PRO:HB3	2.10	0.87
1:K:433:GLU:HG3	1:K:436:THR:CG2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:322:ARG:HH22	1:J:317:HIS:HB2	1.41	0.85
1:C:209:CYS:HB2	1:C:212:GLN:HG2	1.59	0.85
1:G:438:ASP:HA	3:G:910:HOH:O	1.77	0.84
1:B:276:SER:CB	1:F:326:SER:HB3	2.06	0.84
1:B:320:VAL:HG21	1:F:319:GLU:OE2	1.78	0.84
1:K:433:GLU:CG	1:K:436:THR:HG21	2.07	0.84
1:K:209:CYS:HB2	1:K:212:GLN:HG2	1.61	0.83
1:A:209:CYS:HB2	1:A:212:GLN:HG2	1.59	0.83
1:B:276:SER:HA	1:F:326:SER:HB2	1.59	0.83
1:K:430:ILE:HG22	1:K:433:GLU:HB2	1.59	0.82
1:K:298:PRO:HA	1:K:340:HIS:O	1.80	0.82
1:E:209:CYS:HB2	1:E:212:GLN:HG2	1.60	0.82
1:K:313:ARG:NH1	1:K:325:VAL:O	2.13	0.81
1:K:322:ARG:HA	1:K:325:VAL:HB	1.63	0.80
1:K:433:GLU:CG	1:K:436:THR:CG2	2.59	0.80
1:G:133:VAL:HG21	1:G:439:ALA:HB3	1.64	0.79
1:K:365:ARG:O	1:K:365:ARG:HG2	1.82	0.78
1:K:241:ILE:HD11	1:K:342:ILE:HG23	1.65	0.78
1:F:403:THR:HB	1:F:406:HIS:ND1	1.97	0.78
1:B:431:ASP:HB2	1:F:99:VAL:HG11	1.65	0.77
1:K:240:GLY:HA3	1:K:363:PHE:CE1	2.20	0.77
1:K:241:ILE:HG12	1:K:343:VAL:O	1.85	0.76
1:H:209:CYS:HB2	1:H:212:GLN:HG2	1.67	0.76
1:G:232:ALA:O	1:L:159:ARG:HD2	1.86	0.76
1:L:139:PHE:HA	1:L:142:ALA:HB2	1.68	0.75
1:K:256:ARG:HA	1:K:266:PHE:HE2	1.52	0.75
1:I:431:ASP:HB2	1:J:99:VAL:HG11	1.67	0.75
1:K:242:LEU:HD22	1:K:243:LEU:N	2.02	0.74
1:H:203:TYR:CE2	1:H:261:GLU:HG2	2.22	0.74
1:J:203:TYR:CE2	1:J:261:GLU:HG2	2.23	0.73
1:C:326:SER:HB3	1:E:276:SER:HB3	1.71	0.73
1:F:209:CYS:HB2	1:F:212:GLN:HG2	1.70	0.73
1:C:431:ASP:HB2	1:D:99:VAL:CG1	2.19	0.73
1:A:139:PHE:HA	1:A:142:ALA:HB2	1.70	0.73
1:K:347:THR:HG22	1:K:348:ASN:H	1.54	0.72
1:K:139:PHE:HA	1:K:142:ALA:HB2	1.71	0.72
1:G:276:SER:HB3	1:K:326:SER:HB2	1.69	0.72
1:F:139:PHE:HA	1:F:142:ALA:HB2	1.71	0.72
1:I:200:GLU:OE1	1:I:201:VAL:N	2.19	0.72
1:C:139:PHE:HA	1:C:142:ALA:HB2	1.71	0.72
1:B:320:VAL:CG2	1:F:319:GLU:OE2	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:ASP:OD1	1:E:193:ASP:N	2.18	0.72
1:I:139:PHE:HA	1:I:142:ALA:HB2	1.71	0.72
1:B:201:VAL:HG11	1:B:253:LEU:HD12	1.72	0.72
1:B:276:SER:HB3	1:F:326:SER:CB	2.18	0.72
1:D:139:PHE:HA	1:D:142:ALA:HB2	1.72	0.72
1:G:435:GLU:HG2	1:K:228:ALA:HB3	1.72	0.72
1:C:432:LEU:HA	1:D:25:ARG:HH21	1.55	0.71
1:G:139:PHE:HA	1:G:142:ALA:HB2	1.70	0.71
1:H:139:PHE:HA	1:H:142:ALA:HB2	1.72	0.71
1:E:139:PHE:HA	1:E:142:ALA:HB2	1.72	0.71
1:C:319:GLU:OE2	1:E:320:VAL:CG2	2.38	0.71
1:C:416:SER:HA	1:D:235:VAL:HG13	1.73	0.70
1:K:433:GLU:CB	1:K:436:THR:HG22	2.20	0.70
1:K:242:LEU:HD22	1:K:243:LEU:H	1.56	0.70
1:K:363:PHE:HE1	1:K:365:ARG:HB3	1.56	0.70
1:J:139:PHE:HA	1:J:142:ALA:HB2	1.71	0.70
1:J:201:VAL:HG11	1:J:253:LEU:HD12	1.72	0.70
1:E:203:TYR:CE2	1:E:261:GLU:HG2	2.26	0.70
1:F:98:ASP:OD1	1:F:225:ARG:NH2	2.24	0.70
1:B:276:SER:CB	1:F:326:SER:CB	2.70	0.69
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.27	0.69
1:D:209:CYS:HB2	1:D:212:GLN:CG	2.22	0.68
1:C:431:ASP:HB2	1:D:99:VAL:HG11	1.74	0.68
1:B:139:PHE:HA	1:B:142:ALA:HB2	1.73	0.68
1:F:158:MET:HA	1:F:387:ASN:O	1.93	0.68
1:F:203:TYR:CE2	1:F:261:GLU:HG2	2.28	0.68
1:B:276:SER:CA	1:F:326:SER:HB2	2.23	0.68
1:I:326:SER:HB2	1:K:276:SER:HB3	1.76	0.68
1:K:241:ILE:HA	1:K:365:ARG:NH1	2.09	0.68
1:F:115:HIS:CD2	1:F:167:GLU:OE2	2.47	0.68
1:C:158:MET:HB2	1:D:233:ILE:CG2	2.21	0.67
1:E:193:ASP:HB3	1:G:295:LYS:HE3	1.75	0.67
1:G:133:VAL:HG21	1:G:439:ALA:CB	2.24	0.67
1:K:127:THR:HB	1:K:438:ASP:OD1	1.94	0.67
1:G:209:CYS:HB2	1:G:212:GLN:HG2	1.76	0.67
1:H:106:PRO:HD2	1:H:107:ASP:OD1	1.93	0.67
1:A:53:ARG:NH2	3:A:909:HOH:O	2.26	0.67
1:I:249:THR:HG21	1:I:370:GLY:O	1.94	0.67
1:G:203:TYR:CE2	1:G:261:GLU:HG2	2.30	0.67
1:B:278:LEU:HA	1:F:323:ARG:NH1	2.10	0.66
1:F:126:ILE:HB	1:F:439:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:317:HIS:HB2	1:J:322:ARG:HH22	1.61	0.66
1:K:287:ARG:HA	1:K:290:PHE:HB2	1.76	0.66
1:J:249:THR:HG21	1:J:370:GLY:O	1.95	0.66
1:K:240:GLY:O	1:K:241:ILE:HD12	1.94	0.66
1:F:249:THR:HG21	1:F:370:GLY:O	1.97	0.65
1:I:203:TYR:CE2	1:I:261:GLU:HG2	2.32	0.65
1:B:276:SER:CA	1:F:326:SER:CB	2.74	0.65
1:L:203:TYR:CE2	1:L:261:GLU:HG2	2.30	0.65
1:C:249:THR:HG21	1:C:370:GLY:O	1.96	0.65
1:C:432:LEU:HA	1:D:25:ARG:NH2	2.12	0.64
1:H:432:LEU:HD21	1:L:21:ASN:HD22	1.61	0.64
1:K:203:TYR:CE2	1:K:261:GLU:HG2	2.32	0.64
1:L:98:ASP:OD1	1:L:225:ARG:NH2	2.31	0.64
1:K:136:LYS:HB3	1:K:137:PRO:HD3	1.80	0.64
1:H:249:THR:HG21	1:H:370:GLY:O	1.97	0.64
1:E:249:THR:HG21	1:E:370:GLY:O	1.98	0.64
1:B:209:CYS:HB2	1:B:212:GLN:CG	2.24	0.63
1:A:249:THR:HG21	1:A:370:GLY:O	1.98	0.63
1:C:413:ALA:HB2	1:D:360:PHE:CE1	2.26	0.63
1:E:187:GLU:HG3	1:L:124:GLU:HG2	1.80	0.63
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.81	0.63
1:J:209:CYS:HB2	1:J:212:GLN:CG	2.21	0.62
1:B:136:LYS:HB3	1:B:137:PRO:HD3	1.81	0.62
1:D:136:LYS:HB3	1:D:137:PRO:HD3	1.81	0.62
1:F:136:LYS:HB3	1:F:137:PRO:HD3	1.81	0.62
1:B:249:THR:HG21	1:B:370:GLY:O	1.99	0.62
1:C:158:MET:O	1:D:234:GLY:N	2.32	0.62
1:E:136:LYS:HB3	1:E:137:PRO:HD3	1.82	0.62
1:C:136:LYS:HB3	1:C:137:PRO:HD3	1.81	0.62
1:A:203:TYR:CE2	1:A:261:GLU:HG2	2.35	0.62
1:D:201:VAL:HG11	1:D:253:LEU:HD11	1.82	0.62
1:L:249:THR:HG21	1:L:370:GLY:O	1.99	0.62
1:G:283:GLU:OE2	1:G:323:ARG:HG2	2.00	0.61
1:E:133:VAL:HG13	1:E:443:ASN:HB2	1.82	0.61
1:G:249:THR:HG21	1:G:370:GLY:O	1.99	0.61
1:K:306:LEU:HA	1:K:346:ALA:O	2.01	0.61
1:H:136:LYS:HB3	1:H:137:PRO:HD3	1.82	0.61
1:C:222:LEU:HD11	1:E:424:ARG:HG3	1.83	0.61
1:E:406:HIS:CD2	1:E:461:PRO:CB	2.84	0.61
1:A:434:ASP:HA	1:A:436:THR:H	1.66	0.61
1:J:136:LYS:HB3	1:J:137:PRO:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ARG:CZ	1:E:321:GLU:OE1	2.49	0.61
1:G:136:LYS:HB3	1:G:137:PRO:HD3	1.82	0.61
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.37	0.60
1:K:249:THR:HG21	1:K:370:GLY:O	2.01	0.60
1:H:206:ILE:CD1	1:H:209:CYS:SG	2.89	0.60
1:E:213:LEU:O	1:E:217:LYS:HG3	2.02	0.60
1:J:283:GLU:OE2	1:J:323:ARG:HG2	2.02	0.60
1:F:158:MET:N	1:F:387:ASN:O	2.34	0.60
1:G:232:ALA:O	1:L:159:ARG:CD	2.50	0.60
1:L:209:CYS:HB2	1:L:212:GLN:CG	2.30	0.60
1:J:201:VAL:HG11	1:J:253:LEU:CD1	2.31	0.60
1:K:433:GLU:HB3	1:K:436:THR:HG22	1.83	0.59
1:I:136:LYS:HB3	1:I:137:PRO:HD3	1.84	0.59
1:G:327:GLN:HE21	1:L:276:SER:HB2	1.67	0.59
1:H:434:ASP:HA	1:H:436:THR:H	1.67	0.59
1:D:249:THR:HG21	1:D:370:GLY:O	2.01	0.59
1:K:302:PHE:HA	1:K:344:MET:O	2.02	0.59
1:I:222:LEU:HD11	1:K:424:ARG:HG3	1.84	0.59
1:G:359:ARG:NH2	2:L:800:ADP:O3B	2.36	0.59
1:E:434:ASP:HA	1:E:436:THR:H	1.68	0.58
1:I:434:ASP:HA	1:I:436:THR:H	1.68	0.58
1:B:434:ASP:HA	1:B:436:THR:H	1.69	0.58
1:L:136:LYS:HB3	1:L:137:PRO:HD3	1.85	0.58
1:B:276:SER:O	1:F:323:ARG:HG3	2.03	0.58
1:D:283:GLU:OE2	1:D:323:ARG:HG2	2.03	0.58
1:A:209:CYS:HB2	1:A:212:GLN:CG	2.32	0.58
1:C:283:GLU:OE2	1:C:323:ARG:HG2	2.04	0.58
1:F:434:ASP:HA	1:F:436:THR:H	1.69	0.58
1:E:283:GLU:OE2	1:E:323:ARG:HG2	2.04	0.57
1:J:206:ILE:HG13	1:J:207:GLY:N	2.18	0.57
1:D:434:ASP:HA	1:D:436:THR:H	1.69	0.57
1:J:434:ASP:HA	1:J:436:THR:H	1.68	0.57
1:K:301:ILE:HD12	1:K:343:VAL:HG22	1.87	0.57
1:C:213:LEU:O	1:C:217:LYS:HG3	2.05	0.57
1:A:283:GLU:OE2	1:A:323:ARG:HG2	2.04	0.57
1:A:213:LEU:O	1:A:217:LYS:HG3	2.04	0.57
1:D:35:ASP:HB3	1:D:38:VAL:HG12	1.87	0.57
1:K:285:ASN:HD21	1:K:288:LYS:HD2	1.69	0.57
1:F:213:LEU:O	1:F:217:LYS:HG3	2.05	0.57
1:L:35:ASP:HB3	1:L:38:VAL:HG12	1.88	0.56
1:K:241:ILE:CD1	1:K:342:ILE:HG23	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:434:ASP:HA	1:G:436:THR:H	1.70	0.56
1:K:213:LEU:O	1:K:217:LYS:HG3	2.05	0.56
1:E:201:VAL:HG11	1:E:253:LEU:HD12	1.88	0.56
1:F:82:ILE:HG21	1:F:100:ILE:HD11	1.87	0.56
1:F:158:MET:CA	1:F:387:ASN:O	2.54	0.56
1:C:434:ASP:HA	1:C:436:THR:H	1.70	0.56
1:L:434:ASP:HA	1:L:436:THR:H	1.69	0.56
1:J:35:ASP:HB3	1:J:38:VAL:HG12	1.86	0.56
1:L:20:LYS:C	1:L:21:ASN:OD1	2.44	0.56
1:I:220:VAL:HB	1:I:224:LEU:HD12	1.88	0.56
1:E:35:ASP:HB3	1:E:38:VAL:HG12	1.88	0.56
1:I:35:ASP:HB3	1:I:38:VAL:HG12	1.88	0.56
1:G:193:ASP:N	1:G:193:ASP:OD1	2.39	0.56
1:K:347:THR:CG2	1:K:348:ASN:H	2.19	0.56
1:C:209:CYS:HB2	1:C:212:GLN:CG	2.34	0.56
1:E:220:VAL:HB	1:E:224:LEU:HD12	1.88	0.56
1:D:201:VAL:HG11	1:D:253:LEU:CD1	2.36	0.55
1:E:53:ARG:N	3:E:905:HOH:O	2.38	0.55
1:L:213:LEU:O	1:L:217:LYS:HG3	2.05	0.55
1:L:220:VAL:HB	1:L:224:LEU:HD12	1.88	0.55
1:K:35:ASP:HB3	1:K:38:VAL:HG12	1.88	0.55
1:B:142:ALA:HB1	1:B:144:ARG:HG3	1.88	0.55
1:K:285:ASN:ND2	1:K:288:LYS:HB3	2.21	0.55
1:C:133:VAL:HG13	1:C:443:ASN:HB2	1.87	0.55
1:J:220:VAL:HB	1:J:224:LEU:HD12	1.88	0.55
1:D:220:VAL:HB	1:D:224:LEU:HD12	1.88	0.55
1:A:220:VAL:HB	1:A:224:LEU:HD12	1.88	0.55
1:K:297:ALA:HB1	1:K:340:HIS:O	2.07	0.55
1:B:201:VAL:HG11	1:B:253:LEU:CD1	2.35	0.55
1:K:304:ASP:HA	1:K:346:ALA:HB3	1.89	0.55
1:K:306:LEU:HA	1:K:347:THR:HA	1.88	0.55
1:F:158:MET:HG2	1:F:388:MET:HB3	1.88	0.55
1:H:220:VAL:HB	1:H:224:LEU:HD12	1.89	0.55
1:J:21:ASN:HA	1:J:22:ARG:HG2	1.88	0.55
1:G:206:ILE:HD11	1:G:209:CYS:SG	2.47	0.55
1:B:220:VAL:HB	1:B:224:LEU:HD12	1.88	0.55
1:K:301:ILE:HB	1:K:343:VAL:HG13	1.88	0.55
1:I:218:GLU:OE1	1:K:454:TRP:HZ2	1.88	0.55
1:B:213:LEU:O	1:B:217:LYS:HG3	2.07	0.55
1:F:283:GLU:OE2	1:F:323:ARG:HG2	2.06	0.55
1:C:319:GLU:OE2	1:E:320:VAL:HG21	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:ASP:OD1	1:C:225:ARG:NH2	2.39	0.54
1:D:193:ASP:N	1:D:193:ASP:OD1	2.40	0.54
1:B:133:VAL:HG13	1:B:443:ASN:HB2	1.89	0.54
1:G:125:GLY:HA2	1:K:231:LYS:HB3	1.89	0.54
1:F:142:ALA:HB1	1:F:144:ARG:HG3	1.90	0.54
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.88	0.54
1:K:193:ASP:OD1	1:K:193:ASP:N	2.39	0.54
1:A:35:ASP:HB3	1:A:38:VAL:HG12	1.88	0.54
1:B:35:ASP:HB3	1:B:38:VAL:HG12	1.90	0.54
1:C:35:ASP:HB3	1:C:38:VAL:HG12	1.89	0.54
1:G:35:ASP:HB3	1:G:38:VAL:HG12	1.87	0.54
1:H:35:ASP:HB3	1:H:38:VAL:HG12	1.89	0.54
1:F:206:ILE:O	1:F:206:ILE:CG1	2.54	0.54
1:K:209:CYS:HB2	1:K:212:GLN:CG	2.35	0.54
1:H:218:GLU:OE1	1:J:454:TRP:HZ2	1.91	0.54
1:C:222:LEU:HD11	1:E:424:ARG:CG	2.37	0.54
1:I:432:LEU:HD23	1:J:21:ASN:HB2	1.90	0.54
1:G:220:VAL:HB	1:G:224:LEU:HD12	1.88	0.54
1:K:300:ILE:HD11	1:K:344:MET:HG3	1.90	0.54
1:L:283:GLU:OE2	1:L:323:ARG:HG2	2.08	0.54
1:E:187:GLU:CG	1:L:124:GLU:HG2	2.38	0.54
1:G:322:ARG:HH22	1:L:317:HIS:HB2	1.73	0.54
1:F:220:VAL:HB	1:F:224:LEU:HD12	1.90	0.53
1:H:213:LEU:O	1:H:217:LYS:HG3	2.08	0.53
1:K:322:ARG:CA	1:K:325:VAL:HB	2.36	0.53
1:H:434:ASP:HA	1:H:436:THR:N	2.24	0.53
1:H:26:LEU:HD21	1:H:45:LYS:HE2	1.90	0.53
1:K:220:VAL:HB	1:K:224:LEU:HD12	1.91	0.53
1:G:213:LEU:O	1:G:217:LYS:HG3	2.09	0.53
1:J:249:THR:N	2:J:800:ADP:O2B	2.42	0.53
1:E:209:CYS:HB2	1:E:212:GLN:CG	2.33	0.53
1:D:203:TYR:CE2	1:D:261:GLU:HG2	2.43	0.53
1:F:197:SER:HB3	1:F:200:GLU:HG3	1.90	0.53
1:C:193:ASP:N	1:C:193:ASP:OD1	2.42	0.53
1:I:283:GLU:OE2	1:I:323:ARG:HG2	2.09	0.53
1:A:434:ASP:HA	1:A:436:THR:N	2.24	0.53
1:F:169:ASP:HB3	1:F:170:PRO:HD3	1.91	0.53
1:C:220:VAL:HB	1:C:224:LEU:HD12	1.89	0.53
1:K:300:ILE:HG13	1:K:342:ILE:O	2.08	0.53
1:F:35:ASP:HB3	1:F:38:VAL:HG12	1.90	0.53
1:G:125:GLY:HA3	1:K:231:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:HG21	1:C:100:ILE:HD11	1.91	0.53
1:F:26:LEU:HD21	1:F:45:LYS:HE2	1.91	0.52
1:H:424:ARG:HG3	1:L:222:LEU:HD11	1.91	0.52
1:B:55:ASP:O	1:B:71:VAL:HG12	2.09	0.52
1:H:82:ILE:HG21	1:H:100:ILE:HD11	1.91	0.52
1:K:282:SER:O	1:K:324:ILE:HG21	2.09	0.52
1:J:193:ASP:OD1	1:J:193:ASP:N	2.42	0.52
1:I:326:SER:CB	1:K:276:SER:HB3	2.38	0.52
1:K:436:THR:O	1:K:436:THR:HG23	2.07	0.52
1:E:434:ASP:HA	1:E:436:THR:N	2.24	0.52
1:D:434:ASP:HA	1:D:436:THR:N	2.24	0.52
1:J:434:ASP:HA	1:J:436:THR:N	2.24	0.52
1:B:434:ASP:HA	1:B:436:THR:N	2.25	0.52
1:K:82:ILE:HG21	1:K:100:ILE:HD11	1.92	0.52
1:I:193:ASP:OD1	1:I:193:ASP:N	2.41	0.52
1:I:434:ASP:HA	1:I:436:THR:N	2.24	0.52
1:F:90:ASN:O	1:F:93:ARG:NH1	2.43	0.52
1:A:227:PRO:HD2	3:A:906:HOH:O	2.10	0.52
1:I:432:LEU:CD2	1:J:21:ASN:HB2	2.39	0.52
1:J:82:ILE:HG21	1:J:100:ILE:HD11	1.91	0.52
1:L:434:ASP:HA	1:L:436:THR:N	2.26	0.51
1:H:219:MET:HE2	3:J:917:HOH:O	2.09	0.51
1:H:106:PRO:HD2	1:H:107:ASP:H	1.75	0.51
1:F:434:ASP:HA	1:F:436:THR:N	2.26	0.51
1:A:82:ILE:HG21	1:A:100:ILE:HD11	1.92	0.51
1:I:130:LEU:HD23	1:I:130:LEU:H	1.75	0.51
1:B:249:THR:N	2:B:800:ADP:O2B	2.44	0.51
1:I:213:LEU:O	1:I:217:LYS:HG3	2.10	0.51
1:K:139:PHE:CE1	1:K:176:VAL:HG11	2.46	0.51
1:C:139:PHE:CE1	1:C:176:VAL:HG11	2.46	0.51
1:D:139:PHE:CE1	1:D:176:VAL:HG11	2.46	0.51
1:H:139:PHE:CE1	1:H:176:VAL:HG11	2.46	0.51
1:L:193:ASP:OD1	1:L:193:ASP:N	2.43	0.51
1:G:310:ALA:HA	1:G:325:VAL:HG22	1.93	0.51
1:D:82:ILE:HG21	1:D:100:ILE:HD11	1.92	0.51
1:B:283:GLU:OE2	1:B:323:ARG:HG2	2.10	0.51
1:B:310:ALA:HA	1:B:325:VAL:HG22	1.93	0.51
1:D:310:ALA:HA	1:D:325:VAL:HG22	1.92	0.51
1:C:249:THR:N	2:C:800:ADP:O2B	2.44	0.51
1:E:155:HIS:HB3	1:E:386:LYS:O	2.10	0.51
1:I:338:ARG:HD2	3:I:901:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:305:GLU:HG2	1:K:308:ALA:CB	2.40	0.51
1:L:133:VAL:HG13	1:L:443:ASN:HB2	1.93	0.51
1:K:241:ILE:HG12	1:K:343:VAL:C	2.31	0.50
1:H:206:ILE:HD11	1:H:209:CYS:SG	2.51	0.50
1:G:434:ASP:HA	1:G:436:THR:N	2.26	0.50
1:E:82:ILE:HG21	1:E:100:ILE:HD11	1.92	0.50
1:A:307:ASP:OD1	1:A:307:ASP:N	2.43	0.50
1:A:193:ASP:N	1:A:193:ASP:OD1	2.42	0.50
1:B:139:PHE:CE1	1:B:176:VAL:HG11	2.46	0.50
1:C:222:LEU:HD11	1:E:424:ARG:HH11	1.76	0.50
1:C:322:ARG:NE	1:E:321:GLU:OE1	2.44	0.50
1:B:193:ASP:N	1:B:193:ASP:OD1	2.44	0.50
1:F:310:ALA:HA	1:F:325:VAL:HG22	1.93	0.50
1:G:82:ILE:HG21	1:G:100:ILE:HD11	1.92	0.50
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.93	0.50
1:L:55:ASP:O	1:L:71:VAL:HG12	2.12	0.50
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.94	0.50
1:C:434:ASP:HA	1:C:436:THR:N	2.27	0.50
1:A:194:GLU:HB2	1:K:193:ASP:OD2	2.11	0.50
1:J:310:ALA:HA	1:J:325:VAL:HG22	1.94	0.50
1:H:106:PRO:CD	1:H:107:ASP:H	2.24	0.50
1:I:26:LEU:HD21	1:I:45:LYS:HE2	1.92	0.50
1:H:52:PHE:O	1:H:55:ASP:HB2	2.12	0.50
1:K:408:GLY:HA3	2:K:800:ADP:N7	2.27	0.50
1:J:213:LEU:O	1:J:217:LYS:HG3	2.12	0.50
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.94	0.50
1:L:169:ASP:HB3	1:L:170:PRO:HD3	1.94	0.50
1:F:377:ARG:NE	1:F:403:THR:O	2.45	0.50
1:H:206:ILE:HG13	1:H:206:ILE:O	2.12	0.50
1:A:142:ALA:HB1	1:A:144:ARG:HG3	1.94	0.50
1:K:430:ILE:HG22	1:K:433:GLU:HB3	1.92	0.49
1:K:305:GLU:CG	1:K:308:ALA:HA	2.42	0.49
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.94	0.49
1:H:314:GLU:HB2	1:J:315:LYS:NZ	2.27	0.49
1:B:424:ARG:HG3	1:F:222:LEU:HD11	1.95	0.49
1:F:130:LEU:H	1:F:130:LEU:HD23	1.78	0.49
1:K:26:LEU:HD21	1:K:45:LYS:HE2	1.93	0.49
1:C:326:SER:HB2	1:E:276:SER:HA	1.94	0.49
1:J:142:ALA:HB1	1:J:144:ARG:HG3	1.93	0.49
1:K:305:GLU:HG3	1:K:308:ALA:HA	1.93	0.49
1:I:307:ASP:N	1:I:307:ASP:OD1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:365:ARG:O	1:K:365:ARG:CG	2.56	0.49
1:I:201:VAL:HG11	1:I:253:LEU:HD12	1.95	0.49
1:D:213:LEU:O	1:D:217:LYS:HG3	2.11	0.49
1:G:169:ASP:HB3	1:G:170:PRO:HD3	1.94	0.49
1:L:40:SER:HB2	1:L:83:ARG:HB2	1.95	0.49
1:J:26:LEU:HD21	1:J:45:LYS:HE2	1.94	0.49
1:E:139:PHE:CE1	1:E:176:VAL:HG11	2.47	0.49
1:A:26:LEU:HD21	1:A:45:LYS:HE2	1.93	0.49
1:H:310:ALA:HA	1:H:325:VAL:HG22	1.94	0.49
1:B:278:LEU:HA	1:F:323:ARG:HH11	1.75	0.49
1:I:249:THR:N	2:I:800:ADP:O2B	2.46	0.49
1:G:133:VAL:HG11	1:G:439:ALA:HB1	1.94	0.49
1:E:142:ALA:HB1	1:E:144:ARG:HG3	1.95	0.49
1:F:408:GLY:HA3	2:F:800:ADP:N7	2.28	0.49
2:C:800:ADP:O3B	1:D:359:ARG:NH2	2.46	0.49
1:K:169:ASP:HB3	1:K:170:PRO:HD3	1.95	0.49
1:D:142:ALA:HB1	1:D:144:ARG:HG3	1.95	0.49
1:K:40:SER:HB2	1:K:83:ARG:HB2	1.95	0.49
1:H:169:ASP:HB3	1:H:170:PRO:HD3	1.95	0.49
1:F:56:THR:OG1	1:F:105:CYS:O	2.30	0.49
1:A:310:ALA:HA	1:A:325:VAL:HG22	1.94	0.49
1:K:126:ILE:HB	1:K:439:ALA:HB2	1.94	0.48
1:B:26:LEU:HD21	1:B:45:LYS:HE2	1.94	0.48
1:H:283:GLU:OE2	1:H:323:ARG:HG2	2.13	0.48
1:H:408:GLY:HA3	2:H:800:ADP:N7	2.28	0.48
1:L:249:THR:N	2:L:800:ADP:O2B	2.47	0.48
1:K:306:LEU:HD23	1:K:346:ALA:HB1	1.95	0.48
1:C:252:THR:HA	1:C:302:PHE:CE2	2.48	0.48
1:I:82:ILE:HG21	1:I:100:ILE:HD11	1.94	0.48
1:I:90:ASN:O	1:I:93:ARG:NH1	2.46	0.48
1:B:427:MET:HA	1:B:430:ILE:HD12	1.95	0.48
1:B:130:LEU:HD23	1:B:130:LEU:H	1.78	0.48
1:A:249:THR:N	2:A:800:ADP:O2B	2.46	0.48
1:I:169:ASP:HB3	1:I:170:PRO:HD3	1.95	0.48
1:E:310:ALA:HA	1:E:325:VAL:HG22	1.95	0.48
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.94	0.48
1:L:90:ASN:O	1:L:93:ARG:NH1	2.45	0.48
1:K:313:ARG:HD3	1:K:325:VAL:HG13	1.95	0.48
1:A:191:ARG:NH1	1:A:197:SER:HA	2.29	0.48
1:J:169:ASP:HB3	1:J:170:PRO:HD3	1.94	0.48
1:I:142:ALA:HB1	1:I:144:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:THR:N	2:F:800:ADP:O2B	2.46	0.48
1:H:98:ASP:OD1	1:H:225:ARG:NH2	2.45	0.48
1:B:206:ILE:CD1	1:B:254:ILE:HG12	2.43	0.48
1:L:82:ILE:HG21	1:L:100:ILE:HD11	1.96	0.48
1:G:55:ASP:O	1:G:71:VAL:HG12	2.14	0.48
1:G:130:LEU:H	1:G:130:LEU:HD23	1.78	0.48
1:J:130:LEU:H	1:J:130:LEU:HD23	1.78	0.48
1:K:130:LEU:HD23	1:K:130:LEU:H	1.79	0.48
1:K:347:THR:HG22	1:K:348:ASN:N	2.23	0.48
1:I:408:GLY:HA3	2:I:800:ADP:N7	2.29	0.48
1:K:286:LEU:O	1:K:290:PHE:CD1	2.67	0.48
1:C:153:LEU:HD13	1:C:198:LEU:HB2	1.94	0.48
1:G:26:LEU:HD21	1:G:45:LYS:HE2	1.96	0.48
1:K:266:PHE:CD1	1:K:300:ILE:HG22	2.49	0.48
1:I:139:PHE:CE1	1:I:176:VAL:HG11	2.49	0.48
1:G:249:THR:N	2:G:800:ADP:O2B	2.46	0.48
1:J:183:HIS:HB3	3:J:909:HOH:O	2.14	0.48
1:I:310:ALA:HA	1:I:325:VAL:HG22	1.95	0.48
1:K:142:ALA:HB1	1:K:144:ARG:HG3	1.96	0.48
1:L:26:LEU:HD21	1:L:45:LYS:HE2	1.95	0.48
1:K:230:PHE:CE1	1:K:237:PRO:HG3	2.49	0.48
1:C:26:LEU:HD21	1:C:45:LYS:HE2	1.95	0.48
1:D:169:ASP:HB3	1:D:170:PRO:HD3	1.95	0.48
1:F:138:TYR:CE2	1:F:152:PHE:CD2	3.02	0.47
1:D:130:LEU:HD23	1:D:130:LEU:H	1.78	0.47
1:A:408:GLY:HA3	2:A:800:ADP:N7	2.29	0.47
1:A:427:MET:HA	1:A:430:ILE:HD12	1.96	0.47
1:K:241:ILE:HD11	1:K:342:ILE:HD12	1.95	0.47
1:E:55:ASP:O	1:E:71:VAL:HG12	2.14	0.47
1:F:87:VAL:HA	1:F:198:LEU:HD11	1.95	0.47
1:D:427:MET:HA	1:D:430:ILE:HD12	1.97	0.47
1:G:408:GLY:HA3	2:G:800:ADP:N7	2.28	0.47
1:F:203:TYR:CD2	1:F:261:GLU:HG2	2.50	0.47
1:B:408:GLY:HA3	2:B:800:ADP:N7	2.30	0.47
1:E:34:GLU:N	3:E:909:HOH:O	2.27	0.47
1:F:109:LYS:NZ	1:F:173:TYR:O	2.47	0.47
1:H:130:LEU:H	1:H:130:LEU:HD23	1.79	0.47
1:E:26:LEU:HD21	1:E:45:LYS:HE2	1.95	0.47
1:E:249:THR:N	2:E:800:ADP:O2B	2.47	0.47
1:C:427:MET:HA	1:C:430:ILE:HD12	1.97	0.47
1:K:98:ASP:OD1	1:K:225:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:306:LEU:HB3	1:K:347:THR:HA	1.97	0.47
1:A:139:PHE:CE1	1:A:176:VAL:HG11	2.50	0.47
1:J:139:PHE:CE1	1:J:176:VAL:HG11	2.49	0.47
1:C:408:GLY:HA3	2:C:800:ADP:N7	2.30	0.47
1:A:130:LEU:H	1:A:130:LEU:HD23	1.80	0.47
1:A:232:ALA:O	1:F:159:ARG:NE	2.48	0.47
1:B:126:ILE:HB	1:B:439:ALA:HB2	1.95	0.47
1:L:408:GLY:HA3	2:L:800:ADP:N7	2.29	0.47
1:D:408:GLY:HA3	2:D:800:ADP:N7	2.30	0.47
1:D:252:THR:HA	1:D:302:PHE:CE2	2.50	0.47
1:K:269:ILE:HG23	1:K:269:ILE:O	2.15	0.47
1:E:185:GLU:OE2	1:L:187:GLU:OE1	2.33	0.47
1:I:222:LEU:HD11	1:K:424:ARG:CG	2.45	0.47
1:L:310:ALA:HA	1:L:325:VAL:HG22	1.96	0.47
1:L:139:PHE:CE1	1:L:176:VAL:HG11	2.50	0.46
1:G:142:ALA:HB1	1:G:144:ARG:HG3	1.96	0.46
1:J:427:MET:HA	1:J:430:ILE:HD12	1.97	0.46
1:L:427:MET:HA	1:L:430:ILE:HD12	1.97	0.46
1:C:55:ASP:O	1:C:71:VAL:HG12	2.15	0.46
1:K:348:ASN:ND2	1:K:348:ASN:N	2.63	0.46
1:D:55:ASP:O	1:D:71:VAL:HG12	2.15	0.46
1:F:307:ASP:N	1:F:307:ASP:OD1	2.47	0.46
1:K:430:ILE:CG2	1:K:433:GLU:CB	2.87	0.46
1:H:106:PRO:CD	1:H:107:ASP:N	2.76	0.46
1:I:427:MET:HA	1:I:430:ILE:HD12	1.97	0.46
1:C:130:LEU:H	1:C:130:LEU:HD23	1.81	0.46
1:E:130:LEU:H	1:E:130:LEU:HD23	1.80	0.46
1:F:427:MET:HA	1:F:430:ILE:HD12	1.97	0.46
1:G:139:PHE:CE1	1:G:176:VAL:HG11	2.50	0.46
1:K:269:ILE:O	1:K:303:ILE:HA	2.16	0.46
1:D:26:LEU:HD21	1:D:45:LYS:HE2	1.97	0.46
1:K:427:MET:HA	1:K:430:ILE:HD12	1.97	0.46
1:K:433:GLU:CB	1:K:436:THR:CG2	2.88	0.46
1:K:239:ARG:HD3	1:K:342:ILE:CD1	2.45	0.46
1:C:142:ALA:HB1	1:C:144:ARG:HG3	1.97	0.46
1:E:408:GLY:HA3	2:E:800:ADP:N7	2.31	0.46
1:F:206:ILE:O	1:F:206:ILE:HG12	2.15	0.46
1:E:427:MET:HA	1:E:430:ILE:HD12	1.98	0.46
1:B:206:ILE:HD13	1:B:254:ILE:HG12	1.98	0.46
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.99	0.46
1:B:82:ILE:HG21	1:B:100:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:GLU:OE2	1:E:320:VAL:HG23	2.14	0.45
1:D:249:THR:N	2:D:800:ADP:O2B	2.48	0.45
1:L:137:PRO:HA	1:L:140:LEU:CD2	2.46	0.45
1:K:266:PHE:CD1	1:K:300:ILE:CG2	2.99	0.45
1:K:313:ARG:CZ	1:K:329:LEU:HD11	2.47	0.45
1:L:27:ILE:HA	1:L:98:ASP:O	2.16	0.45
1:L:140:LEU:O	1:L:140:LEU:HD12	2.15	0.45
1:H:201:VAL:HG11	1:H:253:LEU:HD12	1.97	0.45
1:K:354:ASP:OD2	1:K:356:ALA:HB3	2.17	0.45
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.98	0.45
1:E:252:THR:HA	1:E:302:PHE:CE2	2.52	0.45
1:C:202:GLY:O	1:C:205:ASP:HB2	2.16	0.45
1:F:320:VAL:HG22	1:F:323:ARG:NH2	2.32	0.45
1:J:408:GLY:HA3	2:J:800:ADP:N7	2.31	0.45
1:G:320:VAL:N	1:K:319:GLU:OE2	2.50	0.45
1:C:322:ARG:NH2	1:E:321:GLU:OE1	2.50	0.45
1:H:427:MET:HA	1:H:430:ILE:HD12	1.99	0.45
1:A:55:ASP:O	1:A:71:VAL:HG12	2.16	0.45
1:H:307:ASP:OD1	1:H:307:ASP:N	2.48	0.45
1:C:307:ASP:N	1:C:307:ASP:OD1	2.50	0.45
1:L:248:GLY:N	2:L:800:ADP:O3B	2.43	0.45
1:J:307:ASP:OD1	1:J:307:ASP:N	2.49	0.45
3:G:908:HOH:O	1:K:359:ARG:CG	2.65	0.45
1:A:90:ASN:O	1:A:93:ARG:NH1	2.49	0.45
1:F:43:GLN:N	1:F:44:PRO:HD2	2.32	0.45
1:D:90:ASN:O	1:D:93:ARG:NH1	2.50	0.45
1:F:193:ASP:N	1:F:193:ASP:OD1	2.48	0.45
1:K:322:ARG:HA	1:K:325:VAL:CB	2.41	0.45
1:H:22:ARG:HG2	1:J:432:LEU:HG	1.98	0.45
1:B:218:GLU:OE1	1:D:454:TRP:HZ2	2.00	0.45
1:K:242:LEU:O	1:K:366:GLU:HA	2.17	0.44
1:C:431:ASP:HB3	1:D:27:ILE:HD11	1.99	0.44
1:F:55:ASP:O	1:F:71:VAL:HG12	2.17	0.44
1:C:159:ARG:NH2	1:D:231:LYS:O	2.49	0.44
1:L:142:ALA:HB1	1:L:144:ARG:HG3	1.99	0.44
1:L:43:GLN:N	1:L:44:PRO:HD2	2.32	0.44
1:C:158:MET:HG2	1:C:388:MET:HB3	2.00	0.44
1:C:222:LEU:CD1	1:E:424:ARG:HH11	2.30	0.44
1:K:376:GLY:O	1:K:380:ILE:HG12	2.18	0.44
1:B:139:PHE:CD1	1:B:176:VAL:HG11	2.52	0.44
1:G:427:MET:HA	1:G:430:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:SER:O	1:E:200:GLU:HB2	2.17	0.44
1:D:43:GLN:N	1:D:44:PRO:HD2	2.32	0.44
3:G:908:HOH:O	1:K:359:ARG:HG3	2.16	0.44
1:J:40:SER:HB2	1:J:83:ARG:HB2	1.99	0.44
1:G:40:SER:HB2	1:G:83:ARG:HB2	1.99	0.44
1:K:90:ASN:O	1:K:93:ARG:NH1	2.50	0.44
1:E:307:ASP:OD1	1:E:307:ASP:N	2.48	0.44
1:L:307:ASP:N	1:L:307:ASP:OD1	2.50	0.44
1:B:276:SER:HA	1:F:326:SER:CB	2.35	0.44
1:A:359:ARG:NH2	2:F:800:ADP:O3B	2.51	0.44
1:F:112:LYS:HD2	1:F:169:ASP:OD2	2.18	0.44
1:G:197:SER:O	1:G:200:GLU:HB2	2.18	0.44
1:B:307:ASP:OD1	1:B:307:ASP:N	2.50	0.44
1:L:130:LEU:H	1:L:130:LEU:HD23	1.82	0.44
1:H:118:PRO:HB2	1:H:123:VAL:HG11	1.99	0.44
1:H:222:LEU:N	1:H:223:PRO:HD2	2.32	0.44
1:K:347:THR:CG2	1:K:348:ASN:N	2.81	0.44
1:C:420:LEU:HG	1:D:235:VAL:HG11	2.00	0.44
1:F:31:ALA:HB2	1:F:84:MET:C	2.38	0.44
1:F:252:THR:HA	1:F:302:PHE:CE2	2.53	0.44
1:K:133:VAL:HG13	1:K:443:ASN:HB2	2.00	0.44
1:H:139:PHE:CD1	1:H:176:VAL:HG11	2.53	0.43
1:K:249:THR:N	2:K:800:ADP:O2B	2.51	0.43
1:E:43:GLN:N	1:E:44:PRO:HD2	2.33	0.43
1:B:21:ASN:CA	1:D:432:LEU:HG	2.47	0.43
1:H:142:ALA:HB1	1:H:144:ARG:HG3	2.00	0.43
1:K:286:LEU:HD21	1:K:287:ARG:HH21	1.81	0.43
1:G:43:GLN:N	1:G:44:PRO:HD2	2.33	0.43
1:K:251:LYS:NZ	1:K:348:ASN:HB3	2.32	0.43
1:F:27:ILE:HA	1:F:98:ASP:O	2.19	0.43
1:K:285:ASN:ND2	1:K:288:LYS:CB	2.81	0.43
1:B:155:HIS:HB3	1:B:386:LYS:O	2.18	0.43
1:B:114:ILE:HD11	1:B:146:ILE:HD11	2.00	0.43
1:C:222:LEU:N	1:C:223:PRO:HD2	2.33	0.43
1:K:140:LEU:HD12	3:K:905:HOH:O	2.18	0.43
1:D:206:ILE:O	1:D:206:ILE:CG1	2.61	0.43
1:G:276:SER:O	1:K:323:ARG:O	2.36	0.43
1:H:249:THR:N	2:H:800:ADP:O2B	2.52	0.43
1:E:90:ASN:O	1:E:93:ARG:NH1	2.51	0.43
1:H:248:GLY:N	2:H:800:ADP:O3B	2.43	0.43
1:H:320:VAL:HG22	1:H:323:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:SER:HB2	1:E:83:ARG:HB2	2.01	0.43
1:E:320:VAL:HG22	1:E:323:ARG:NH2	2.34	0.43
1:H:113:ARG:HB3	1:H:169:ASP:HB2	2.00	0.43
1:B:222:LEU:N	1:B:223:PRO:HD2	2.32	0.43
1:L:191:ARG:NH1	1:L:197:SER:HA	2.34	0.43
1:B:314:GLU:HB2	1:D:315:LYS:NZ	2.34	0.43
1:K:239:ARG:HB3	1:K:335:LEU:HD12	2.01	0.43
1:K:55:ASP:O	1:K:71:VAL:HG12	2.18	0.43
1:H:40:SER:HB2	1:H:83:ARG:HB2	2.01	0.43
1:C:117:LEU:HD13	1:H:187:GLU:HG3	2.00	0.43
1:K:302:PHE:CZ	1:K:346:ALA:HB2	2.53	0.43
1:I:222:LEU:N	1:I:223:PRO:HD2	2.34	0.43
1:C:229:LEU:CD1	1:E:427:MET:HE3	2.49	0.43
1:J:55:ASP:O	1:J:71:VAL:HG12	2.19	0.42
1:K:43:GLN:N	1:K:44:PRO:HD2	2.34	0.42
1:D:42:SER:OG	1:D:79:ASP:HA	2.19	0.42
1:J:43:GLN:N	1:J:44:PRO:HD2	2.34	0.42
1:A:43:GLN:N	1:A:44:PRO:HD2	2.34	0.42
1:K:433:GLU:CA	1:K:436:THR:HG22	2.48	0.42
1:K:242:LEU:CD1	1:K:363:PHE:HE2	2.32	0.42
1:I:176:VAL:O	1:I:176:VAL:HG13	2.20	0.42
1:C:424:ARG:HG3	1:D:222:LEU:HD11	2.02	0.42
1:C:206:ILE:HD13	1:C:254:ILE:HG12	2.01	0.42
1:E:30:GLU:OE2	1:E:217:LYS:HE2	2.19	0.42
1:D:222:LEU:N	1:D:223:PRO:HD2	2.34	0.42
1:I:252:THR:HA	1:I:302:PHE:CE2	2.54	0.42
1:K:115:HIS:HE1	1:K:185:GLU:HB2	1.85	0.42
1:B:177:ALA:HB1	1:B:178:PRO:HD2	2.01	0.42
1:B:159:ARG:C	1:B:387:ASN:OD1	2.58	0.42
1:G:222:LEU:N	1:G:223:PRO:HD2	2.34	0.42
1:I:55:ASP:O	1:I:71:VAL:HG12	2.20	0.42
1:D:199:ASN:O	1:D:200:GLU:C	2.57	0.42
1:B:111:GLY:HA2	1:B:170:PRO:CD	2.50	0.42
1:I:43:GLN:N	1:I:44:PRO:HD2	2.34	0.42
1:F:177:ALA:HB1	1:F:178:PRO:HD2	2.01	0.42
1:J:252:THR:HA	1:J:302:PHE:CE2	2.55	0.42
1:G:115:HIS:HE1	1:G:185:GLU:HB2	1.85	0.42
1:G:307:ASP:N	1:G:307:ASP:OD1	2.52	0.42
1:I:40:SER:HB2	1:I:83:ARG:HB2	2.01	0.42
1:K:246:PRO:O	1:K:249:THR:OG1	2.38	0.42
1:C:187:GLU:HB2	1:H:187:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:330:THR:OG1	1:L:273:GLU:HA	2.19	0.42
1:H:252:THR:HA	1:H:302:PHE:CE2	2.55	0.42
1:A:27:ILE:HD11	1:F:431:ASP:HB3	2.01	0.42
1:C:229:LEU:HD12	1:E:427:MET:HE1	2.01	0.42
1:I:42:SER:OG	1:I:79:ASP:HA	2.20	0.42
1:C:40:SER:HB2	1:C:83:ARG:HB2	2.01	0.42
1:A:252:THR:HA	1:A:302:PHE:CE2	2.54	0.42
1:F:126:ILE:CB	1:F:439:ALA:HB2	2.47	0.42
1:B:320:VAL:HG22	1:B:323:ARG:NH2	2.34	0.42
1:J:203:TYR:CD2	1:J:261:GLU:HG2	2.54	0.42
1:L:20:LYS:CB	1:L:21:ASN:OD1	2.68	0.42
1:K:253:LEU:HD22	2:K:800:ADP:H2'	2.01	0.42
1:D:203:TYR:CE2	1:D:217:LYS:HD2	2.55	0.42
1:I:302:PHE:HA	1:I:344:MET:O	2.20	0.42
1:A:99:VAL:HG11	1:F:431:ASP:HB2	2.02	0.42
1:C:377:ARG:NE	1:C:403:THR:O	2.53	0.42
1:A:324:ILE:HG22	1:A:325:VAL:N	2.35	0.41
1:H:90:ASN:O	1:H:93:ARG:NH1	2.53	0.41
1:C:42:SER:OG	1:C:79:ASP:HA	2.20	0.41
1:J:90:ASN:O	1:J:93:ARG:NH1	2.53	0.41
1:K:310:ALA:N	1:K:311:PRO:HD3	2.35	0.41
1:G:252:THR:HA	1:G:302:PHE:CE2	2.55	0.41
1:L:198:LEU:HD22	1:L:198:LEU:HA	1.81	0.41
1:K:212:GLN:CD	1:K:212:GLN:H	2.24	0.41
1:G:320:VAL:HG22	1:G:323:ARG:NH2	2.35	0.41
1:F:222:LEU:N	1:F:223:PRO:HD2	2.35	0.41
1:J:42:SER:OG	1:J:79:ASP:HA	2.19	0.41
1:D:113:ARG:HB3	1:D:169:ASP:HB2	2.03	0.41
1:B:112:LYS:O	1:B:181:VAL:N	2.52	0.41
1:G:232:ALA:O	1:L:159:ARG:NE	2.53	0.41
1:G:176:VAL:HG13	1:G:176:VAL:O	2.20	0.41
1:C:320:VAL:HG22	1:C:323:ARG:NH2	2.36	0.41
1:F:35:ASP:HB3	1:F:38:VAL:CG1	2.49	0.41
1:D:324:ILE:HG22	1:D:325:VAL:N	2.36	0.41
1:L:113:ARG:HB3	1:L:169:ASP:HB2	2.01	0.41
1:B:90:ASN:O	1:B:93:ARG:NH1	2.54	0.41
1:B:321:GLU:OE1	1:F:322:ARG:CZ	2.68	0.41
1:H:193:ASP:N	1:H:193:ASP:OD1	2.53	0.41
1:B:118:PRO:HB2	1:B:123:VAL:HG11	2.02	0.41
1:K:176:VAL:HG13	1:K:176:VAL:O	2.21	0.41
1:D:115:HIS:HE1	1:D:185:GLU:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:ASN:O	1:G:93:ARG:NH1	2.54	0.41
1:F:134:TYR:O	1:F:137:PRO:HD2	2.21	0.41
1:C:43:GLN:N	1:C:44:PRO:HD2	2.35	0.41
1:L:252:THR:HA	1:L:302:PHE:CE2	2.56	0.41
1:G:131:PHE:CD1	1:G:131:PHE:C	2.94	0.41
1:K:348:ASN:HD22	1:K:348:ASN:N	2.19	0.41
1:A:176:VAL:O	1:A:176:VAL:HG13	2.20	0.41
1:H:176:VAL:HG13	1:H:176:VAL:O	2.21	0.41
1:B:176:VAL:HG13	1:B:176:VAL:O	2.20	0.41
1:G:212:GLN:O	1:G:216:ILE:HG12	2.21	0.41
1:L:35:ASP:HB3	1:L:38:VAL:CG1	2.50	0.41
1:H:35:ASP:HB3	1:H:38:VAL:CG1	2.49	0.41
1:A:113:ARG:HB3	1:A:169:ASP:HB2	2.03	0.41
1:I:274:ILE:HD13	1:I:274:ILE:HA	1.95	0.41
1:G:348:ASN:HB2	3:G:902:HOH:O	2.21	0.41
1:L:139:PHE:CD1	1:L:176:VAL:HG11	2.56	0.41
1:L:20:LYS:C	1:L:21:ASN:CG	2.79	0.41
1:A:320:VAL:HG22	1:A:323:ARG:NH2	2.35	0.41
1:L:222:LEU:N	1:L:223:PRO:HD2	2.35	0.41
1:I:206:ILE:HD13	1:I:254:ILE:HG12	2.03	0.41
1:D:37:SER:HA	3:D:914:HOH:O	2.21	0.41
1:K:297:ALA:HB1	1:K:298:PRO:HA	2.02	0.40
1:I:320:VAL:HG22	1:I:323:ARG:NH2	2.36	0.40
1:J:113:ARG:HB3	1:J:169:ASP:HB2	2.03	0.40
1:C:115:HIS:HE1	1:C:185:GLU:HB2	1.86	0.40
1:B:43:GLN:N	1:B:44:PRO:HD2	2.35	0.40
1:K:239:ARG:HD3	1:K:342:ILE:HG13	2.03	0.40
1:D:139:PHE:CD1	1:D:176:VAL:HG11	2.55	0.40
1:K:113:ARG:HB3	1:K:169:ASP:HB2	2.03	0.40
1:A:27:ILE:HA	1:A:98:ASP:O	2.22	0.40
1:I:228:ALA:CB	1:K:435:GLU:HG2	2.52	0.40
1:D:274:ILE:HD13	1:D:274:ILE:HA	1.95	0.40
1:K:351:ASN:HD22	1:K:351:ASN:N	2.19	0.40
1:D:320:VAL:HG22	1:D:323:ARG:NH2	2.36	0.40
1:J:35:ASP:HB3	1:J:38:VAL:CG1	2.50	0.40
1:K:327:GLN:HA	1:K:330:THR:HG22	2.03	0.40
1:B:131:PHE:CD1	1:B:131:PHE:C	2.94	0.40
1:L:274:ILE:HA	1:L:274:ILE:HD13	1.96	0.40
1:H:203:TYR:CD2	1:H:261:GLU:HG2	2.55	0.40
1:C:326:SER:HB3	1:E:276:SER:CB	2.45	0.40
1:A:139:PHE:CD1	1:A:176:VAL:HG11	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:GLY:N	2:C:800:ADP:O3B	2.44	0.40
1:K:249:THR:HA	1:K:407:VAL:HG22	2.04	0.40
1:A:197:SER:O	1:A:200:GLU:HB2	2.21	0.40
1:B:138:TYR:CE2	1:B:152:PHE:CD2	3.10	0.40
1:E:222:LEU:N	1:E:223:PRO:HD2	2.35	0.40
1:E:407:VAL:O	1:E:410:ASP:HB2	2.21	0.40
1:K:286:LEU:CD2	1:K:287:ARG:HH21	2.34	0.40
1:C:222:LEU:HD12	1:C:222:LEU:H	1.85	0.40
1:C:113:ARG:HB3	1:C:169:ASP:HB2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:404:HIS:CG	1:G:210:ARG:NH1[3_645]	1.92	0.28
1:B:52:PHE:CZ	1:I:49:LEU:O[4_455]	2.09	0.11

## 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	436/489 (89%)	419 (96%)	17 (4%)	0	100	100
1	B	437/489 (89%)	416 (95%)	21 (5%)	0	100	100
1	C	436/489 (89%)	418 (96%)	18 (4%)	0	100	100
1	D	437/489 (89%)	417 (95%)	20 (5%)	0	100	100
1	E	437/489 (89%)	418 (96%)	19 (4%)	0	100	100
1	F	436/489 (89%)	417 (96%)	19 (4%)	0	100	100
1	G	435/489 (89%)	418 (96%)	17 (4%)	0	100	100
1	H	436/489 (89%)	416 (95%)	19 (4%)	1 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	438/489 (90%)	418 (95%)	20 (5%)	0	100	100
1	J	443/489 (91%)	425 (96%)	18 (4%)	0	100	100
1	K	436/489 (89%)	398 (91%)	35 (8%)	3 (1%)	26	67
1	L	440/489 (90%)	419 (95%)	20 (4%)	1 (0%)	52	86
All	All	5247/5868 (89%)	4999 (95%)	243 (5%)	5 (0%)	56	89

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	23	PRO
1	K	241	ILE
1	K	277	LYS
1	K	359	ARG
1	H	106	PRO

### 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	375/418 (90%)	345 (92%)	30 (8%)	15	45
1	B	376/418 (90%)	346 (92%)	30 (8%)	15	45
1	C	375/418 (90%)	345 (92%)	30 (8%)	15	45
1	D	376/418 (90%)	345 (92%)	31 (8%)	14	44
1	E	376/418 (90%)	345 (92%)	31 (8%)	14	44
1	F	375/418 (90%)	343 (92%)	32 (8%)	13	42
1	G	374/418 (90%)	344 (92%)	30 (8%)	15	45
1	H	375/418 (90%)	344 (92%)	31 (8%)	14	43
1	I	377/418 (90%)	345 (92%)	32 (8%)	13	42
1	J	382/418 (91%)	349 (91%)	33 (9%)	13	41
1	K	375/418 (90%)	329 (88%)	46 (12%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	379/418 (91%)	349 (92%)	30 (8%)	15	46
All	All	4515/5016 (90%)	4129 (92%)	386 (8%)	13	42

All (386) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	33	ASN
1	A	56	THR
1	A	78	SER
1	A	96	LEU
1	A	109	LYS
1	A	127	THR
1	A	147	ARG
1	A	184	CYS
1	A	193	ASP
1	A	198	LEU
1	A	206	ILE
1	A	210	ARG
1	A	211	LYS
1	A	212	GLN
1	A	217	LYS
1	A	249	THR
1	A	256	ARG
1	A	288	LYS
1	A	313	ARG
1	A	314	GLU
1	A	315	LYS
1	A	322	ARG
1	A	324	ILE
1	A	327	GLN
1	A	335	LEU
1	A	338	ARG
1	A	375	THR
1	A	378	LEU
1	A	435	GLU
1	B	28	VAL
1	B	33	ASN
1	B	56	THR
1	B	96	LEU
1	B	109	LYS
1	B	127	THR

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Mol	Chain	Res	Type
1	B	147	ARG
1	B	184	CYS
1	B	193	ASP
1	B	199	ASN
1	B	206	ILE
1	B	210	ARG
1	B	211	LYS
1	B	212	GLN
1	B	217	LYS
1	B	249	THR
1	B	256	ARG
1	B	288	LYS
1	B	313	ARG
1	B	314	GLU
1	B	315	LYS
1	B	322	ARG
1	B	324	ILE
1	B	327	GLN
1	B	335	LEU
1	B	338	ARG
1	B	351	ASN
1	B	375	THR
1	B	378	LEU
1	B	435	GLU
1	C	28	VAL
1	C	33	ASN
1	C	56	THR
1	C	78	SER
1	C	96	LEU
1	C	109	LYS
1	C	127	THR
1	C	147	ARG
1	C	184	CYS
1	C	193	ASP
1	C	206	ILE
1	C	210	ARG
1	C	211	LYS
1	C	212	GLN
1	C	217	LYS
1	C	249	THR
1	C	256	ARG
1	C	288	LYS

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Mol	Chain	Res	Type
1	C	313	ARG
1	C	314	GLU
1	C	315	LYS
1	C	322	ARG
1	C	324	ILE
1	C	327	GLN
1	C	335	LEU
1	C	338	ARG
1	C	351	ASN
1	C	375	THR
1	C	378	LEU
1	C	435	GLU
1	D	22	ARG
1	D	28	VAL
1	D	33	ASN
1	D	56	THR
1	D	78	SER
1	D	96	LEU
1	D	109	LYS
1	D	147	ARG
1	D	184	CYS
1	D	193	ASP
1	D	206	ILE
1	D	210	ARG
1	D	211	LYS
1	D	212	GLN
1	D	217	LYS
1	D	249	THR
1	D	256	ARG
1	D	288	LYS
1	D	313	ARG
1	D	314	GLU
1	D	315	LYS
1	D	322	ARG
1	D	324	ILE
1	D	327	GLN
1	D	335	LEU
1	D	338	ARG
1	D	351	ASN
1	D	375	THR
1	D	378	LEU
1	D	435	GLU

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Mol	Chain	Res	Type
1	D	460	ASN
1	E	28	VAL
1	E	33	ASN
1	E	56	THR
1	E	96	LEU
1	E	109	LYS
1	E	127	THR
1	E	147	ARG
1	E	184	CYS
1	E	193	ASP
1	E	200	GLU
1	E	206	ILE
1	E	210	ARG
1	E	211	LYS
1	E	212	GLN
1	E	217	LYS
1	E	249	THR
1	E	256	ARG
1	E	288	LYS
1	E	313	ARG
1	E	314	GLU
1	E	315	LYS
1	E	322	ARG
1	E	324	ILE
1	E	327	GLN
1	E	335	LEU
1	E	338	ARG
1	E	351	ASN
1	E	375	THR
1	E	378	LEU
1	E	435	GLU
1	E	460	ASN
1	F	28	VAL
1	F	33	ASN
1	F	56	THR
1	F	78	SER
1	F	96	LEU
1	F	107	ASP
1	F	109	LYS
1	F	147	ARG
1	F	184	CYS
1	F	193	ASP

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Mol	Chain	Res	Type
1	F	198	LEU
1	F	200	GLU
1	F	206	ILE
1	F	210	ARG
1	F	211	LYS
1	F	212	GLN
1	F	217	LYS
1	F	246	PRO
1	F	249	THR
1	F	256	ARG
1	F	288	LYS
1	F	313	ARG
1	F	314	GLU
1	F	315	LYS
1	F	322	ARG
1	F	324	ILE
1	F	335	LEU
1	F	338	ARG
1	F	351	ASN
1	F	375	THR
1	F	378	LEU
1	F	435	GLU
1	G	28	VAL
1	G	33	ASN
1	G	56	THR
1	G	78	SER
1	G	96	LEU
1	G	109	LYS
1	G	147	ARG
1	G	184	CYS
1	G	193	ASP
1	G	201	VAL
1	G	206	ILE
1	G	210	ARG
1	G	211	LYS
1	G	212	GLN
1	G	217	LYS
1	G	249	THR
1	G	256	ARG
1	G	288	LYS
1	G	313	ARG
1	G	314	GLU

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Mol	Chain	Res	Type
1	G	315	LYS
1	G	322	ARG
1	G	324	ILE
1	G	327	GLN
1	G	335	LEU
1	G	338	ARG
1	G	351	ASN
1	G	375	THR
1	G	378	LEU
1	G	435	GLU
1	H	28	VAL
1	H	33	ASN
1	H	56	THR
1	H	96	LEU
1	H	105	CYS
1	H	107	ASP
1	H	109	LYS
1	H	147	ARG
1	H	184	CYS
1	H	193	ASP
1	H	199	ASN
1	H	206	ILE
1	H	210	ARG
1	H	211	LYS
1	H	212	GLN
1	H	217	LYS
1	H	249	THR
1	H	256	ARG
1	H	288	LYS
1	H	313	ARG
1	H	314	GLU
1	H	315	LYS
1	H	322	ARG
1	H	324	ILE
1	H	327	GLN
1	H	335	LEU
1	H	338	ARG
1	H	351	ASN
1	H	375	THR
1	H	378	LEU
1	H	435	GLU
1	I	20	LYS

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Mol	Chain	Res	Type
1	I	22	ARG
1	I	28	VAL
1	I	33	ASN
1	I	56	THR
1	I	78	SER
1	I	96	LEU
1	I	109	LYS
1	I	147	ARG
1	I	184	CYS
1	I	193	ASP
1	I	200	GLU
1	I	206	ILE
1	I	210	ARG
1	I	211	LYS
1	I	212	GLN
1	I	217	LYS
1	I	249	THR
1	I	256	ARG
1	I	288	LYS
1	I	313	ARG
1	I	314	GLU
1	I	315	LYS
1	I	322	ARG
1	I	324	ILE
1	I	327	GLN
1	I	335	LEU
1	I	338	ARG
1	I	351	ASN
1	I	375	THR
1	I	378	LEU
1	I	435	GLU
1	J	18	LYS
1	J	20	LYS
1	J	21	ASN
1	J	28	VAL
1	J	33	ASN
1	J	56	THR
1	J	78	SER
1	J	96	LEU
1	J	109	LYS
1	J	127	THR
1	J	147	ARG

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Mol	Chain	Res	Type
1	J	184	CYS
1	J	193	ASP
1	J	196	GLU
1	J	206	ILE
1	J	210	ARG
1	J	211	LYS
1	J	212	GLN
1	J	217	LYS
1	J	249	THR
1	J	256	ARG
1	J	288	LYS
1	J	313	ARG
1	J	314	GLU
1	J	315	LYS
1	J	322	ARG
1	J	324	ILE
1	J	327	GLN
1	J	335	LEU
1	J	338	ARG
1	J	375	THR
1	J	378	LEU
1	J	435	GLU
1	K	28	VAL
1	K	33	ASN
1	K	56	THR
1	K	78	SER
1	K	96	LEU
1	K	109	LYS
1	K	127	THR
1	K	147	ARG
1	K	184	CYS
1	K	193	ASP
1	K	206	ILE
1	K	210	ARG
1	K	211	LYS
1	K	212	GLN
1	K	217	LYS
1	K	241	ILE
1	K	242	LEU
1	K	243	LEU
1	K	249	THR
1	K	256	ARG

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Mol	Chain	Res	Type
1	K	266	PHE
1	K	278	LEU
1	K	281	GLU
1	K	286	LEU
1	K	290	PHE
1	K	291	GLU
1	K	294	GLU
1	K	300	ILE
1	K	307	ASP
1	K	309	ILE
1	K	323	ARG
1	K	325	VAL
1	K	326	SER
1	K	330	THR
1	K	332	MET
1	K	335	LEU
1	K	340	HIS
1	K	348	ASN
1	K	349	ARG
1	K	351	ASN
1	K	353	ILE
1	K	363	PHE
1	K	366	GLU
1	K	375	THR
1	K	378	LEU
1	K	435	GLU
1	L	18	LYS
1	L	21	ASN
1	L	28	VAL
1	L	33	ASN
1	L	56	THR
1	L	96	LEU
1	L	109	LYS
1	L	147	ARG
1	L	184	CYS
1	L	193	ASP
1	L	198	LEU
1	L	206	ILE
1	L	210	ARG
1	L	211	LYS
1	L	212	GLN
1	L	217	LYS

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Mol	Chain	Res	Type
1	L	249	THR
1	L	256	ARG
1	L	288	LYS
1	L	313	ARG
1	L	314	GLU
1	L	315	LYS
1	L	322	ARG
1	L	324	ILE
1	L	335	LEU
1	L	338	ARG
1	L	351	ASN
1	L	375	THR
1	L	378	LEU
1	L	435	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	199	ASN
1	A	212	GLN
1	A	327	GLN
1	A	348	ASN
1	B	33	ASN
1	B	115	HIS
1	B	199	ASN
1	B	212	GLN
1	B	327	GLN
1	B	348	ASN
1	C	33	ASN
1	C	199	ASN
1	C	212	GLN
1	C	348	ASN
1	D	33	ASN
1	D	115	HIS
1	D	327	GLN
1	D	348	ASN
1	E	33	ASN
1	E	212	GLN
1	E	327	GLN
1	E	348	ASN
1	F	33	ASN

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Mol	Chain	Res	Type
1	F	115	HIS
1	F	183	HIS
1	F	212	GLN
1	F	348	ASN
1	G	212	GLN
1	G	327	GLN
1	G	348	ASN
1	H	33	ASN
1	H	212	GLN
1	H	327	GLN
1	H	348	ASN
1	I	33	ASN
1	I	327	GLN
1	I	348	ASN
1	J	33	ASN
1	J	212	GLN
1	J	317	HIS
1	J	327	GLN
1	J	348	ASN
1	K	33	ASN
1	K	348	ASN
1	K	351	ASN
1	L	33	ASN
1	L	50	GLN
1	L	212	GLN
1	L	327	GLN
1	L	348	ASN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

12 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$
2	ADP	A	800	-	22,29,29	0.91	1 (4%)	27,45,45	1.99	3 (11%)
2	ADP	B	800	-	22,29,29	0.99	1 (4%)	27,45,45	1.93	4 (14%)
2	ADP	C	800	-	22,29,29	0.97	1 (4%)	27,45,45	1.82	4 (14%)
2	ADP	D	800	-	22,29,29	1.03	1 (4%)	27,45,45	1.95	5 (18%)
2	ADP	E	800	-	22,29,29	0.96	1 (4%)	27,45,45	1.82	2 (7%)
2	ADP	F	800	-	22,29,29	0.98	1 (4%)	27,45,45	1.81	4 (14%)
2	ADP	G	800	-	22,29,29	0.98	1 (4%)	27,45,45	1.86	3 (11%)
2	ADP	H	800	-	22,29,29	0.89	1 (4%)	27,45,45	1.95	3 (11%)
2	ADP	I	800	-	22,29,29	0.96	2 (9%)	27,45,45	1.99	4 (14%)
2	ADP	J	800	-	22,29,29	1.10	1 (4%)	27,45,45	1.82	4 (14%)
2	ADP	K	800	-	22,29,29	0.85	1 (4%)	27,45,45	1.90	4 (14%)
2	ADP	L	800	-	22,29,29	0.99	1 (4%)	27,45,45	1.88	4 (14%)

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
2	ADP	A	800	-	-	0/12/32/32	0/3/3/3
2	ADP	B	800	-	-	0/12/32/32	0/3/3/3
2	ADP	C	800	-	-	0/12/32/32	0/3/3/3
2	ADP	D	800	-	-	0/12/32/32	0/3/3/3
2	ADP	E	800	-	-	0/12/32/32	0/3/3/3
2	ADP	F	800	-	-	0/12/32/32	0/3/3/3
2	ADP	G	800	-	-	0/12/32/32	0/3/3/3
2	ADP	H	800	-	-	0/12/32/32	0/3/3/3
2	ADP	I	800	-	-	0/12/32/32	0/3/3/3
2	ADP	J	800	-	-	0/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	K	800	-	-	0/12/32/32	0/3/3/3
2	ADP	L	800	-	-	0/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	800	ADP	C5-N7	-2.04	1.32	1.39
2	H	800	ADP	C5-C4	2.42	1.46	1.40
2	A	800	ADP	C5-C4	2.56	1.46	1.40
2	I	800	ADP	C5-C4	2.57	1.46	1.40
2	K	800	ADP	C5-C4	2.58	1.46	1.40
2	B	800	ADP	C5-C4	2.69	1.46	1.40
2	E	800	ADP	C5-C4	2.84	1.46	1.40
2	F	800	ADP	C5-C4	2.86	1.47	1.40
2	C	800	ADP	C5-C4	2.89	1.47	1.40
2	J	800	ADP	C5-C4	2.95	1.47	1.40
2	G	800	ADP	C5-C4	3.01	1.47	1.40
2	L	800	ADP	C5-C4	3.12	1.47	1.40
2	D	800	ADP	C5-C4	3.15	1.47	1.40

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	800	ADP	N3-C2-N1	-8.01	122.76	128.89
2	A	800	ADP	N3-C2-N1	-7.81	122.91	128.89
2	I	800	ADP	N3-C2-N1	-7.78	122.94	128.89
2	B	800	ADP	N3-C2-N1	-7.36	123.26	128.89
2	L	800	ADP	N3-C2-N1	-7.35	123.26	128.89
2	D	800	ADP	N3-C2-N1	-7.09	123.46	128.89
2	G	800	ADP	N3-C2-N1	-7.03	123.51	128.89
2	E	800	ADP	N3-C2-N1	-6.84	123.66	128.89
2	C	800	ADP	N3-C2-N1	-6.79	123.70	128.89
2	J	800	ADP	N3-C2-N1	-6.79	123.70	128.89
2	K	800	ADP	N3-C2-N1	-6.60	123.84	128.89
2	F	800	ADP	N3-C2-N1	-6.59	123.85	128.89
2	E	800	ADP	PA-O3A-PB	-3.88	119.66	132.67
2	D	800	ADP	PA-O3A-PB	-3.86	119.72	132.67
2	J	800	ADP	PA-O3A-PB	-3.84	119.80	132.67
2	F	800	ADP	PA-O3A-PB	-3.80	119.93	132.67
2	A	800	ADP	PA-O3A-PB	-3.65	120.42	132.67
2	B	800	ADP	PA-O3A-PB	-3.62	120.52	132.67
2	K	800	ADP	C4-C5-N7	-3.56	106.20	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	800	ADP	PA-O3A-PB	-3.40	121.27	132.67
2	H	800	ADP	PA-O3A-PB	-3.37	121.37	132.67
2	K	800	ADP	PA-O3A-PB	-3.33	121.50	132.67
2	G	800	ADP	PA-O3A-PB	-3.19	121.96	132.67
2	C	800	ADP	PA-O3A-PB	-3.16	122.06	132.67
2	L	800	ADP	PA-O3A-PB	-3.15	122.11	132.67
2	G	800	ADP	C4-C5-N7	-3.01	106.71	109.48
2	C	800	ADP	C4-C5-N7	-2.92	106.80	109.48
2	I	800	ADP	C4-C5-N7	-2.84	106.87	109.48
2	B	800	ADP	C4-C5-N7	-2.74	106.96	109.48
2	D	800	ADP	C4-C5-N7	-2.72	106.98	109.48
2	F	800	ADP	C4-C5-N7	-2.68	107.01	109.48
2	A	800	ADP	C4-C5-N7	-2.46	107.22	109.48
2	H	800	ADP	C4-C5-N7	-2.25	107.41	109.48
2	J	800	ADP	C4-C5-N7	-2.23	107.43	109.48
2	L	800	ADP	C4-C5-N7	-2.13	107.52	109.48
2	L	800	ADP	C2-N1-C6	2.03	122.40	118.77
2	J	800	ADP	O2B-PB-O1B	2.05	117.19	110.58
2	K	800	ADP	O3B-PB-O2B	2.07	115.28	107.38
2	F	800	ADP	O2B-PB-O1B	2.09	117.30	110.58
2	C	800	ADP	O2B-PB-O1B	2.12	117.40	110.58
2	I	800	ADP	O2B-PB-O1B	2.14	117.47	110.58
2	B	800	ADP	O2B-PB-O1B	2.18	117.59	110.58
2	D	800	ADP	C2-N1-C6	2.23	122.75	118.77
2	D	800	ADP	O2B-PB-O1B	2.40	118.31	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	ADP	2	0
2	B	800	ADP	2	0
2	C	800	ADP	4	0
2	D	800	ADP	2	0
2	E	800	ADP	2	0
2	F	800	ADP	3	0
2	G	800	ADP	2	0
2	H	800	ADP	3	0
2	I	800	ADP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	800	ADP	2	0
2	K	800	ADP	3	0
2	L	800	ADP	4	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	438/489 (89%)	0.31	37 (8%) 14 7	71, 120, 172, 275	0
1	B	439/489 (89%)	-0.02	19 (4%) 39 23	57, 92, 153, 208	0
1	C	438/489 (89%)	0.20	31 (7%) 19 10	76, 120, 177, 233	0
1	D	439/489 (89%)	0.25	35 (7%) 15 8	60, 115, 176, 280	0
1	E	439/489 (89%)	0.54	58 (13%) 4 2	66, 132, 211, 261	0
1	F	438/489 (89%)	0.00	17 (3%) 43 25	60, 95, 169, 215	0
1	G	437/489 (89%)	0.25	31 (7%) 19 10	60, 111, 169, 221	0
1	H	438/489 (89%)	0.08	20 (4%) 36 21	60, 105, 163, 233	0
1	I	440/489 (89%)	0.26	33 (7%) 17 9	61, 122, 182, 285	0
1	J	445/489 (91%)	0.00	18 (4%) 42 25	50, 93, 153, 238	0
1	K	438/489 (89%)	0.83	87 (19%) 1 1	64, 142, 208, 239	0
1	L	442/489 (90%)	0.41	44 (9%) 9 5	76, 139, 204, 287	0
All	All	5271/5868 (89%)	0.26	430 (8%) 14 7	50, 115, 188, 287	0

All (430) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	279	ALA	8.7
1	I	432	LEU	8.6
1	D	433	GLU	7.8
1	E	279	ALA	7.5
1	K	432	LEU	7.5
1	E	432	LEU	7.3
1	I	436	THR	7.2
1	K	284	SER	7.0
1	E	113	ARG	6.8
1	E	435	GLU	6.4
1	K	460	ASN	6.4

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Mol	Chain	Res	Type	RSRZ
1	G	434	ASP	5.9
1	K	109	LYS	5.8
1	L	187	GLU	5.8
1	I	437	ILE	5.7
1	K	279	ALA	5.7
1	H	435	GLU	5.7
1	E	166	VAL	5.7
1	K	194	GLU	5.6
1	L	432	LEU	5.5
1	F	317	HIS	5.5
1	A	435	GLU	5.3
1	K	278	LEU	5.2
1	J	436	THR	5.2
1	I	433	GLU	5.1
1	I	431	ASP	5.1
1	A	433	GLU	5.1
1	C	435	GLU	5.1
1	C	317	HIS	5.0
1	E	433	GLU	5.0
1	C	193	ASP	4.9
1	K	338	ARG	4.9
1	D	360	PHE	4.9
1	K	339	ALA	4.9
1	B	338	ARG	4.9
1	E	461	PRO	4.9
1	E	112	LYS	4.8
1	G	435	GLU	4.8
1	D	279	ALA	4.8
1	K	434	ASP	4.8
1	E	194	GLU	4.8
1	L	172	PRO	4.7
1	L	64	ARG	4.7
1	D	432	LEU	4.7
1	J	337	GLN	4.7
1	F	319	GLU	4.7
1	G	143	TYR	4.7
1	L	173	TYR	4.7
1	H	75	ASP	4.7
1	K	64	ARG	4.6
1	E	109	LYS	4.6
1	G	64	ARG	4.6
1	K	280	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	K	317	HIS	4.5
1	G	337	GLN	4.5
1	I	428	ASP	4.4
1	K	352	SER	4.4
1	K	350	PRO	4.4
1	B	337	GLN	4.4
1	J	434	ASP	4.4
1	K	173	TYR	4.4
1	K	349	ARG	4.4
1	L	63	LYS	4.4
1	K	340	HIS	4.3
1	J	433	GLU	4.3
1	K	436	THR	4.3
1	J	461	PRO	4.3
1	I	279	ALA	4.3
1	D	434	ASP	4.3
1	F	337	GLN	4.3
1	K	277	LYS	4.2
1	L	101	SER	4.2
1	L	21	ASN	4.2
1	B	53	ARG	4.2
1	K	193	ASP	4.2
1	G	338	ARG	4.2
1	E	193	ASP	4.1
1	L	53	ARG	4.1
1	L	244	TYR	4.1
1	K	112	LYS	4.1
1	L	429	LEU	4.1
1	D	50	GLN	4.0
1	E	75	ASP	4.0
1	K	63	LYS	4.0
1	E	280	GLY	4.0
1	K	286	LEU	4.0
1	E	108	VAL	4.0
1	A	345	ALA	3.9
1	H	459	SER	3.9
1	J	239	ARG	3.9
1	G	63	LYS	3.9
1	I	109	LYS	3.9
1	E	317	HIS	3.9
1	A	338	ARG	3.9
1	C	141	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	K	140	LEU	3.9
1	K	141	GLU	3.8
1	K	163	PHE	3.8
1	L	181	VAL	3.8
1	I	34	GLU	3.8
1	A	75	ASP	3.8
1	I	52	PHE	3.7
1	K	108	VAL	3.7
1	A	344	MET	3.7
1	J	317	HIS	3.7
1	K	128	GLY	3.7
1	A	76	THR	3.7
1	K	185	GLU	3.6
1	L	278	LEU	3.6
1	E	107	ASP	3.6
1	I	434	ASP	3.6
1	A	113	ARG	3.6
1	E	34	GLU	3.6
1	A	434	ASP	3.6
1	G	440	GLU	3.6
1	K	360	PHE	3.6
1	G	34	GLU	3.6
1	A	194	GLU	3.6
1	C	338	ARG	3.6
1	C	401	ASN	3.6
1	I	194	GLU	3.5
1	C	128	GLY	3.5
1	A	337	GLN	3.5
1	D	143	TYR	3.5
1	F	279	ALA	3.5
1	C	434	ASP	3.5
1	E	314	GLU	3.5
1	I	349	ARG	3.5
1	L	194	GLU	3.4
1	K	333	ASP	3.4
1	I	459	SER	3.4
1	G	109	LYS	3.4
1	H	350	PRO	3.4
1	H	63	LYS	3.4
1	K	244	TYR	3.4
1	B	434	ASP	3.4
1	I	187	GLU	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	337	GLN	3.4
1	H	279	ALA	3.4
1	K	117	LEU	3.4
1	A	437	ILE	3.4
1	D	22	ARG	3.4
1	D	317	HIS	3.4
1	J	462	SER	3.3
1	K	179	ASP	3.3
1	K	62	LYS	3.3
1	D	278	LEU	3.3
1	I	318	GLY	3.3
1	K	342	ILE	3.3
1	E	136	LYS	3.3
1	K	355	PRO	3.3
1	K	320	VAL	3.3
1	C	319	GLU	3.3
1	F	435	GLU	3.3
1	E	62	LYS	3.3
1	G	155	HIS	3.3
1	K	190	LYS	3.3
1	D	64	ARG	3.3
1	L	404	HIS	3.2
1	K	267	PHE	3.2
1	A	358	ARG	3.2
1	I	338	ARG	3.2
1	B	109	LYS	3.2
1	K	172	PRO	3.2
1	C	64	ARG	3.2
1	E	103	GLN	3.2
1	E	110	TYR	3.2
1	E	63	LYS	3.2
1	K	107	ASP	3.2
1	L	193	ASP	3.2
1	K	191	ARG	3.1
1	D	140	LEU	3.1
1	G	52	PHE	3.1
1	B	435	GLU	3.1
1	E	189	ILE	3.1
1	K	298	PRO	3.1
1	E	190	LYS	3.1
1	A	34	GLU	3.1
1	L	338	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	232	ALA	3.1
1	A	294	GLU	3.1
1	A	343	VAL	3.1
1	L	185	GLU	3.1
1	A	234	GLY	3.1
1	K	345	ALA	3.0
1	I	32	ILE	3.0
1	K	268	LEU	3.0
1	D	128	GLY	3.0
1	G	186	GLY	3.0
1	G	187	GLU	3.0
1	J	63	LYS	3.0
1	L	435	GLU	3.0
1	C	231	LYS	3.0
1	B	72	LEU	3.0
1	D	280	GLY	3.0
1	K	143	TYR	3.0
1	L	317	HIS	3.0
1	B	21	ASN	3.0
1	F	128	GLY	3.0
1	K	33	ASN	3.0
1	K	76	THR	2.9
1	I	141	GLU	2.9
1	D	63	LYS	2.9
1	A	62	LYS	2.9
1	L	20	LYS	2.9
1	D	343	VAL	2.9
1	F	436	THR	2.9
1	E	179	ASP	2.9
1	D	436	THR	2.9
1	B	350	PRO	2.9
1	K	295	LYS	2.9
1	D	281	GLU	2.9
1	F	336	LYS	2.9
1	K	106	PRO	2.9
1	F	404	HIS	2.9
1	L	183	HIS	2.9
1	H	434	ASP	2.8
1	H	280	GLY	2.8
1	K	428	ASP	2.8
1	C	63	LYS	2.8
1	K	186	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	392	ASP	2.8
1	K	313	ARG	2.8
1	L	188	PRO	2.8
1	F	63	LYS	2.8
1	H	427	MET	2.8
1	C	433	GLU	2.8
1	L	62	LYS	2.8
1	E	127	THR	2.8
1	K	187	GLU	2.8
1	E	143	TYR	2.8
1	C	169	ASP	2.8
1	D	34	GLU	2.7
1	L	125	GLY	2.7
1	B	433	GLU	2.7
1	C	404	HIS	2.7
1	H	317	HIS	2.7
1	I	140	LEU	2.7
1	E	129	ASN	2.7
1	A	106	PRO	2.7
1	K	32	ILE	2.7
1	K	151	ILE	2.7
1	G	33	ASN	2.7
1	L	19	GLN	2.7
1	K	358	ARG	2.7
1	A	60	LYS	2.7
1	L	427	MET	2.7
1	J	432	LEU	2.7
1	E	244	TYR	2.7
1	F	294	GLU	2.7
1	A	239	ARG	2.7
1	L	199	ASN	2.6
1	E	312	LYS	2.6
1	L	113	ARG	2.6
1	K	152	PHE	2.6
1	I	64	ARG	2.6
1	K	75	ASP	2.6
1	K	287	ARG	2.6
1	B	404	HIS	2.6
1	L	186	GLY	2.6
1	K	113	ARG	2.6
1	L	428	ASP	2.6
1	K	282	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	32	ILE	2.6
1	E	32	ILE	2.6
1	A	438	ASP	2.6
1	A	278	LEU	2.6
1	E	80	GLU	2.6
1	I	193	ASP	2.6
1	C	244	TYR	2.5
1	C	127	THR	2.5
1	H	109	LYS	2.5
1	E	140	LEU	2.5
1	K	274	ILE	2.5
1	E	436	THR	2.5
1	B	349	ARG	2.5
1	D	52	PHE	2.5
1	E	173	TYR	2.5
1	K	110	TYR	2.5
1	K	328	LEU	2.5
1	K	319	GLU	2.5
1	H	338	ARG	2.5
1	E	350	PRO	2.5
1	A	404	HIS	2.5
1	E	195	GLU	2.5
1	G	193	ASP	2.5
1	K	326	SER	2.5
1	C	278	LEU	2.5
1	F	34	GLU	2.5
1	K	361	GLY	2.5
1	C	72	LEU	2.4
1	E	169	ASP	2.4
1	E	141	GLU	2.4
1	I	360	PHE	2.4
1	K	150	ASP	2.4
1	B	140	LEU	2.4
1	I	169	ASP	2.4
1	D	319	GLU	2.4
1	A	459	SER	2.4
1	H	172	PRO	2.4
1	B	173	TYR	2.4
1	G	140	LEU	2.4
1	E	247	PRO	2.4
1	D	336	LYS	2.4
1	C	336	LYS	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	106	PRO	2.4
1	D	194	GLU	2.4
1	E	128	GLY	2.4
1	K	351	ASN	2.4
1	B	23	PRO	2.4
1	E	349	ARG	2.4
1	E	181	VAL	2.4
1	H	231	LYS	2.4
1	I	190	LYS	2.4
1	A	436	THR	2.4
1	H	179	ASP	2.4
1	I	317	HIS	2.4
1	L	140	LEU	2.3
1	G	128	GLY	2.3
1	E	278	LEU	2.3
1	K	330	THR	2.3
1	A	185	GLU	2.3
1	D	155	HIS	2.3
1	K	359	ARG	2.3
1	L	117	LEU	2.3
1	E	192	GLU	2.3
1	A	33	ASN	2.3
1	L	150	ASP	2.3
1	E	316	THR	2.3
1	L	431	ASP	2.3
1	K	285	ASN	2.3
1	D	338	ARG	2.3
1	E	231	LYS	2.3
1	C	239	ARG	2.3
1	L	196	GLU	2.3
1	E	117	LEU	2.3
1	E	438	ASP	2.3
1	K	431	ASP	2.3
1	C	33	ASN	2.3
1	L	155	HIS	2.3
1	K	34	GLU	2.3
1	L	436	THR	2.3
1	D	349	ARG	2.3
1	E	172	PRO	2.3
1	I	172	PRO	2.3
1	C	279	ALA	2.3
1	C	460	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	K	192	GLU	2.3
1	F	338	ARG	2.3
1	C	210	ARG	2.2
1	L	46	MET	2.2
1	L	52	PHE	2.2
1	G	231	LYS	2.2
1	G	405	GLY	2.2
1	F	428	ASP	2.2
1	H	345	ALA	2.2
1	K	281	GLU	2.2
1	J	338	ARG	2.2
1	K	306	LEU	2.2
1	E	313	ARG	2.2
1	K	327	GLN	2.2
1	E	434	ASP	2.2
1	F	323	ARG	2.2
1	G	53	ARG	2.2
1	I	239	ARG	2.2
1	K	291	GLU	2.2
1	C	431	ASP	2.2
1	D	342	ILE	2.2
1	G	141	GLU	2.2
1	C	428	ASP	2.2
1	K	160	ALA	2.2
1	J	437	ILE	2.2
1	J	141	GLU	2.2
1	A	140	LEU	2.2
1	G	443	ASN	2.2
1	I	244	TYR	2.2
1	L	33	ASN	2.2
1	D	239	ARG	2.2
1	H	22	ARG	2.2
1	G	124	GLU	2.2
1	D	345	ALA	2.2
1	H	315	LYS	2.1
1	K	52	PHE	2.1
1	A	280	GLY	2.1
1	C	343	VAL	2.1
1	K	72	LEU	2.1
1	K	344	MET	2.1
1	C	312	LYS	2.1
1	C	75	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	69	CYS	2.1
1	H	278	LEU	2.1
1	A	52	PHE	2.1
1	A	281	GLU	2.1
1	C	167	GLU	2.1
1	E	24	ASN	2.1
1	B	432	LEU	2.1
1	J	404	HIS	2.1
1	D	53	ARG	2.1
1	A	193	ASP	2.1
1	B	75	ASP	2.1
1	J	360	PHE	2.1
1	D	344	MET	2.1
1	L	366	GLU	2.1
1	L	104	PRO	2.1
1	I	429	LEU	2.1
1	L	108	VAL	2.1
1	A	143	TYR	2.1
1	I	179	ASP	2.1
1	I	314	GLU	2.1
1	F	432	LEU	2.1
1	K	297	ALA	2.1
1	B	52	PHE	2.1
1	A	317	HIS	2.1
1	D	179	ASP	2.1
1	I	117	LEU	2.1
1	E	239	ARG	2.1
1	J	190	LYS	2.0
1	J	435	GLU	2.0
1	E	64	ARG	2.0
1	G	346	ALA	2.0
1	A	61	GLY	2.0
1	A	432	LEU	2.0
1	D	429	LEU	2.0
1	E	360	PHE	2.0
1	J	231	LYS	2.0
1	F	280	GLY	2.0
1	D	187	GLU	2.0
1	B	340	HIS	2.0
1	G	317	HIS	2.0
1	E	145	PRO	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	B	800	27/27	0.96	0.17	-0.12	71,74,79,84	0
2	ADP	K	800	27/27	0.94	0.17	-0.18	95,102,110,112	0
2	ADP	L	800	27/27	0.95	0.16	-0.22	87,90,104,111	0
2	ADP	G	800	27/27	0.96	0.16	-0.26	79,86,95,96	0
2	ADP	I	800	27/27	0.95	0.17	-0.27	78,82,88,90	0
2	ADP	D	800	27/27	0.96	0.15	-0.37	73,76,82,84	0
2	ADP	F	800	27/27	0.97	0.14	-0.55	76,78,82,83	0
2	ADP	C	800	27/27	0.97	0.14	-0.55	87,91,101,105	0
2	ADP	A	800	27/27	0.96	0.15	-0.57	75,81,95,99	0
2	ADP	H	800	27/27	0.97	0.14	-0.62	74,77,88,97	0
2	ADP	E	800	27/27	0.97	0.12	-0.86	75,83,94,97	0
2	ADP	J	800	27/27	0.98	0.12	-0.92	59,64,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.