



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:55 am GMT

PDB ID : 5C1A  
Title : p97-N750D/R753D/M757D/Q760D in complex with ATP-gamma-S  
Authors : Haenzelmann, P.; Schindelin, H.  
Deposited on : 2015-06-13  
Resolution : 3.80 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 : 1.7.2 (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

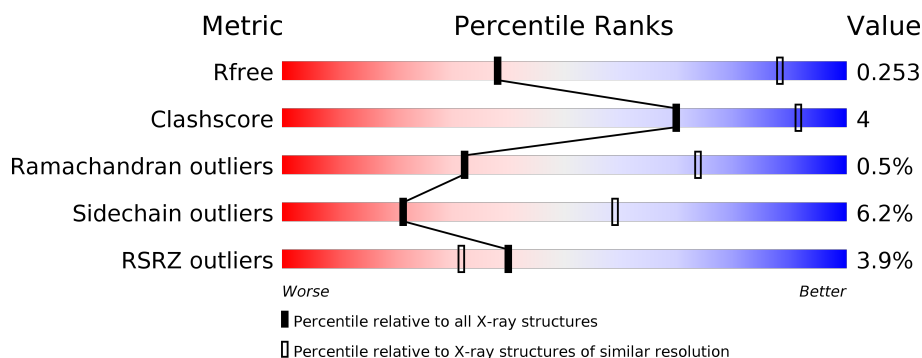
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

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	805	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	805	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	805	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	805	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	805	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	F	805	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	805	<div><div>2%</div><div><div></div><div></div><div></div></div><div>78%</div><div>13%</div><div>9%</div></div>
1	H	805	<div><div>3%</div><div><div></div><div></div><div></div></div><div>77%</div><div>12%</div><div>9%</div></div>
1	I	805	<div><div>4%</div><div><div></div><div></div><div></div></div><div>77%</div><div>13%</div><div>9%</div></div>
1	J	805	<div><div>4%</div><div><div></div><div></div><div></div></div><div>77%</div><div>13%</div><div>9%</div></div>
1	K	805	<div><div>5%</div><div><div></div><div></div><div></div></div><div>76%</div><div>15%</div><div>8%</div></div>
1	L	805	<div><div>3%</div><div><div></div><div></div><div></div></div><div>78%</div><div>13%</div><div>9%</div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 140261 atoms, of which 70187 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	735	Total	C	H	N	O	S	0	0	0
			11578	3616	5814	1019	1100	29			
1	B	735	Total	C	H	N	O	S	0	0	0
			11590	3623	5819	1019	1100	29			
1	C	735	Total	C	H	N	O	S	0	0	0
			11589	3623	5818	1019	1100	29			
1	D	735	Total	C	H	N	O	S	0	0	0
			11591	3623	5820	1019	1100	29			
1	E	735	Total	C	H	N	O	S	0	0	0
			11589	3623	5818	1019	1100	29			
1	F	735	Total	C	H	N	O	S	0	0	0
			11589	3623	5818	1019	1100	29			
1	G	735	Total	C	H	N	O	S	0	0	0
			11576	3616	5812	1019	1100	29			
1	H	735	Total	C	H	N	O	S	0	0	0
			11590	3623	5819	1019	1100	29			
1	I	735	Total	C	H	N	O	S	0	0	0
			11589	3623	5818	1019	1100	29			
1	J	735	Total	C	H	N	O	S	0	0	0
			11590	3623	5819	1019	1100	29			
1	K	744	Total	C	H	N	O	S	0	0	0
			11719	3663	5880	1029	1117	30			
1	L	735	Total	C	H	N	O	S	0	0	0
			11591	3623	5820	1019	1100	29			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	750	ASP	ASN	engineered mutation	UNP P55072
A	753	ASP	ARG	engineered mutation	UNP P55072
A	757	ASP	MET	engineered mutation	UNP P55072
A	760	ASP	GLN	engineered mutation	UNP P55072
B	750	ASP	ASN	engineered mutation	UNP P55072

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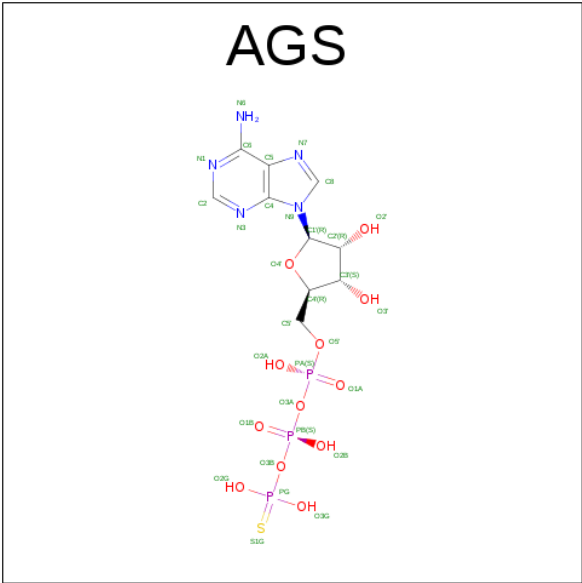
Chain	Residue	Modelled	Actual	Comment	Reference
B	753	ASP	ARG	engineered mutation	UNP P55072
B	757	ASP	MET	engineered mutation	UNP P55072
B	760	ASP	GLN	engineered mutation	UNP P55072
C	750	ASP	ASN	engineered mutation	UNP P55072
C	753	ASP	ARG	engineered mutation	UNP P55072
C	757	ASP	MET	engineered mutation	UNP P55072
C	760	ASP	GLN	engineered mutation	UNP P55072
D	750	ASP	ASN	engineered mutation	UNP P55072
D	753	ASP	ARG	engineered mutation	UNP P55072
D	757	ASP	MET	engineered mutation	UNP P55072
D	760	ASP	GLN	engineered mutation	UNP P55072
E	750	ASP	ASN	engineered mutation	UNP P55072
E	753	ASP	ARG	engineered mutation	UNP P55072
E	757	ASP	MET	engineered mutation	UNP P55072
E	760	ASP	GLN	engineered mutation	UNP P55072
F	750	ASP	ASN	engineered mutation	UNP P55072
F	753	ASP	ARG	engineered mutation	UNP P55072
F	757	ASP	MET	engineered mutation	UNP P55072
F	760	ASP	GLN	engineered mutation	UNP P55072
G	750	ASP	ASN	engineered mutation	UNP P55072
G	753	ASP	ARG	engineered mutation	UNP P55072
G	757	ASP	MET	engineered mutation	UNP P55072
G	760	ASP	GLN	engineered mutation	UNP P55072
H	750	ASP	ASN	engineered mutation	UNP P55072
H	753	ASP	ARG	engineered mutation	UNP P55072
H	757	ASP	MET	engineered mutation	UNP P55072
H	760	ASP	GLN	engineered mutation	UNP P55072
I	750	ASP	ASN	engineered mutation	UNP P55072
I	753	ASP	ARG	engineered mutation	UNP P55072
I	757	ASP	MET	engineered mutation	UNP P55072
I	760	ASP	GLN	engineered mutation	UNP P55072
J	750	ASP	ASN	engineered mutation	UNP P55072
J	753	ASP	ARG	engineered mutation	UNP P55072
J	757	ASP	MET	engineered mutation	UNP P55072
J	760	ASP	GLN	engineered mutation	UNP P55072
K	750	ASP	ASN	engineered mutation	UNP P55072
K	753	ASP	ARG	engineered mutation	UNP P55072
K	757	ASP	MET	engineered mutation	UNP P55072
K	760	ASP	GLN	engineered mutation	UNP P55072
L	750	ASP	ASN	engineered mutation	UNP P55072
L	753	ASP	ARG	engineered mutation	UNP P55072
L	757	ASP	MET	engineered mutation	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
L	760	ASP	GLN	engineered mutation	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	A	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	C	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	D	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	E	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	F	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	G	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	H	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	I	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	I	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	J	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	J	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	K	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	K	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	L	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		
2	L	1	Total	C	H	N	O	P	S	0	0
			44	10	13	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	2	Total	Mg	0	0
			2	2		
3	J	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	K	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		

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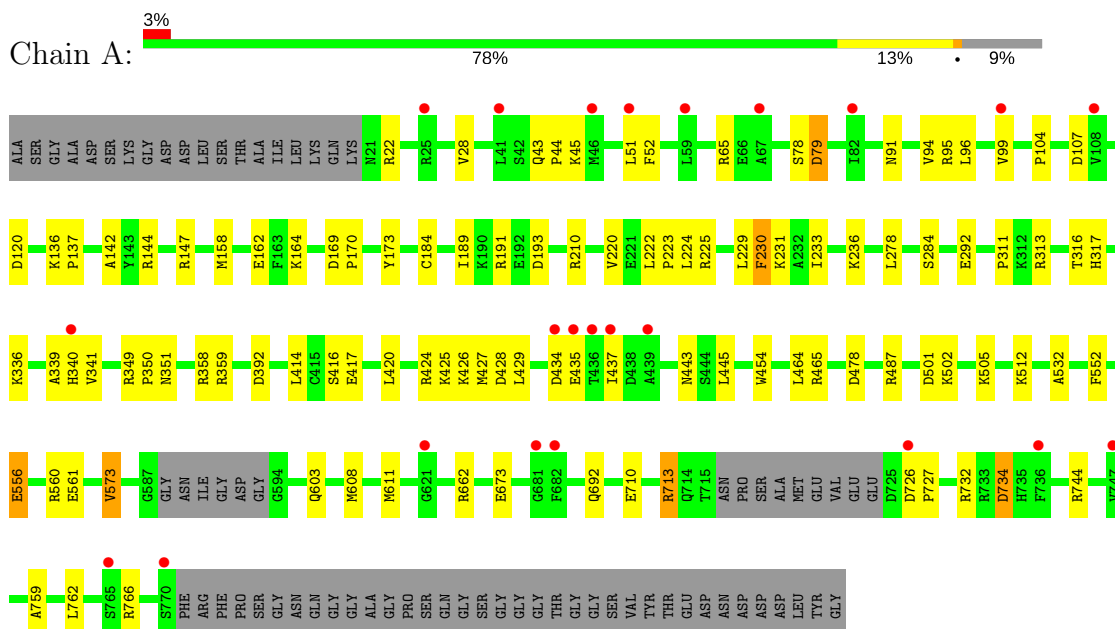
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	2	Total 2	Mg 2	0	0
3	B	2	Total 2	Mg 2	0	0
3	I	2	Total 2	Mg 2	0	0
3	C	2	Total 2	Mg 2	0	0
3	A	2	Total 2	Mg 2	0	0
3	L	2	Total 2	Mg 2	0	0
3	F	2	Total 2	Mg 2	0	0



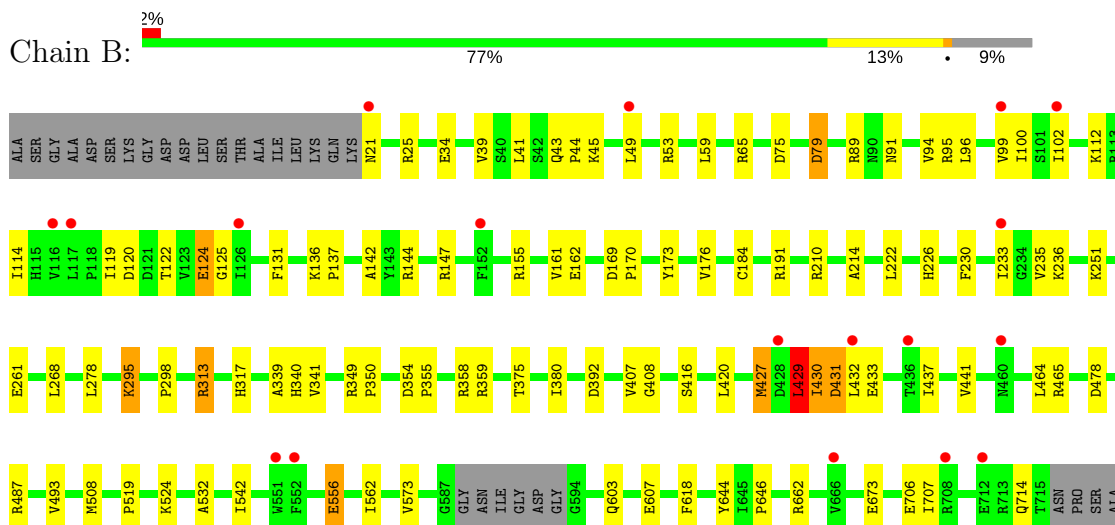
### 3 Residue-property plots

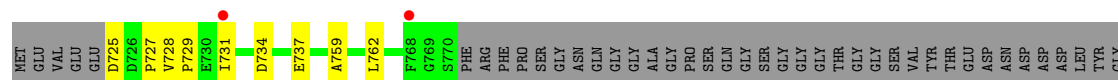
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Transitional endoplasmic reticulum ATPase

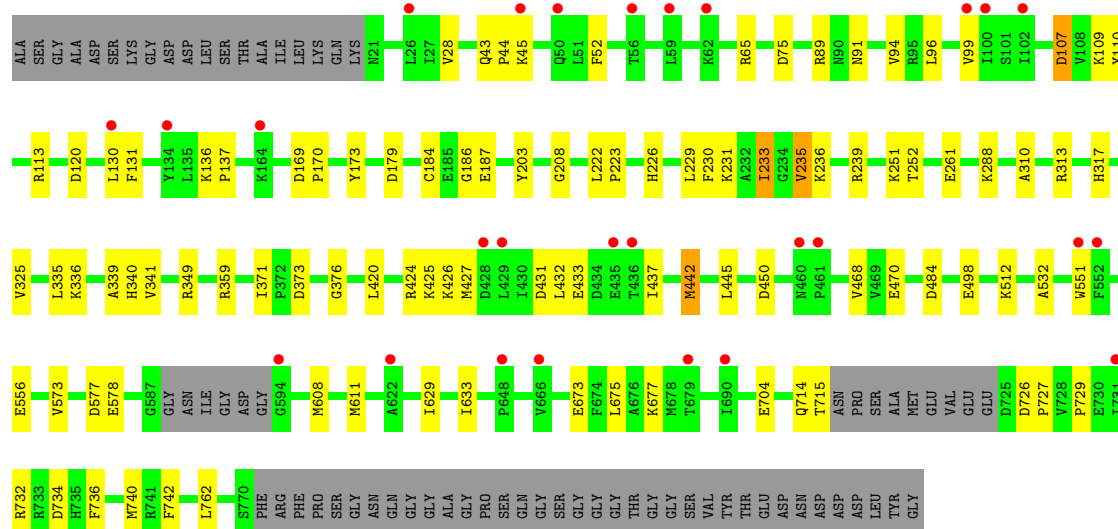
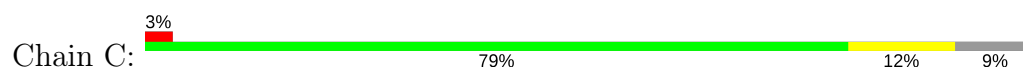


- Molecule 1: Transitional endoplasmic reticulum ATPase

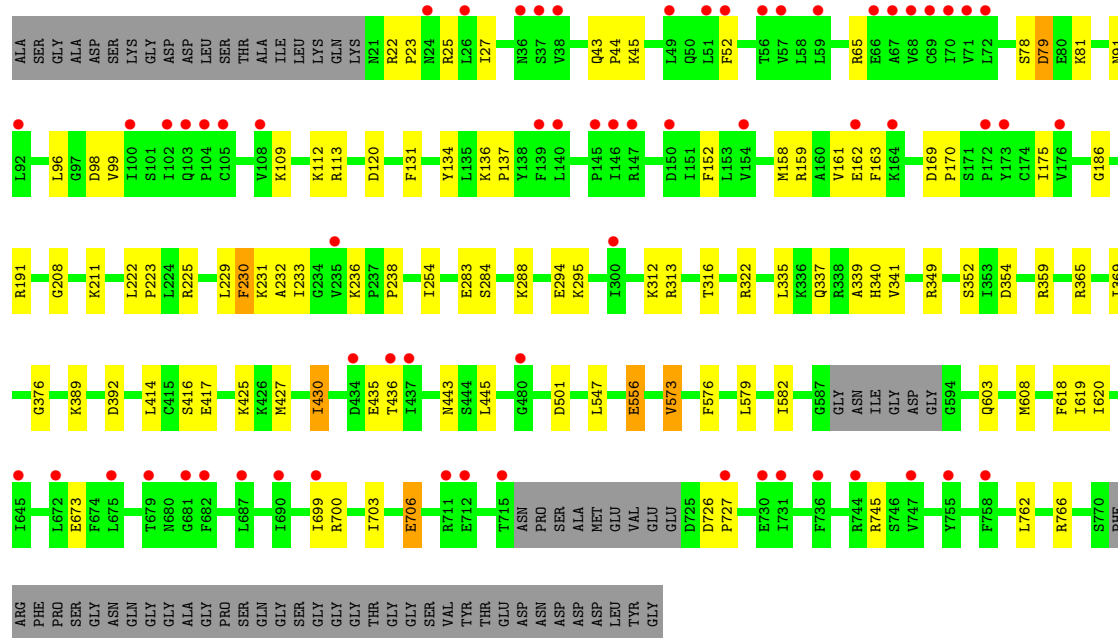
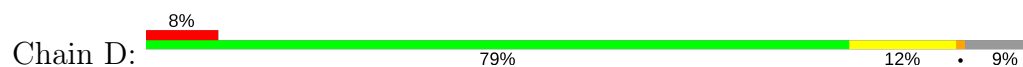




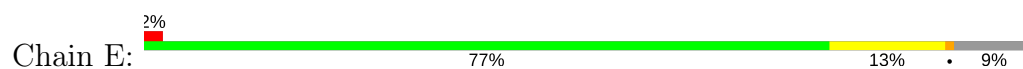
• Molecule 1: Transitional endoplasmic reticulum ATPase

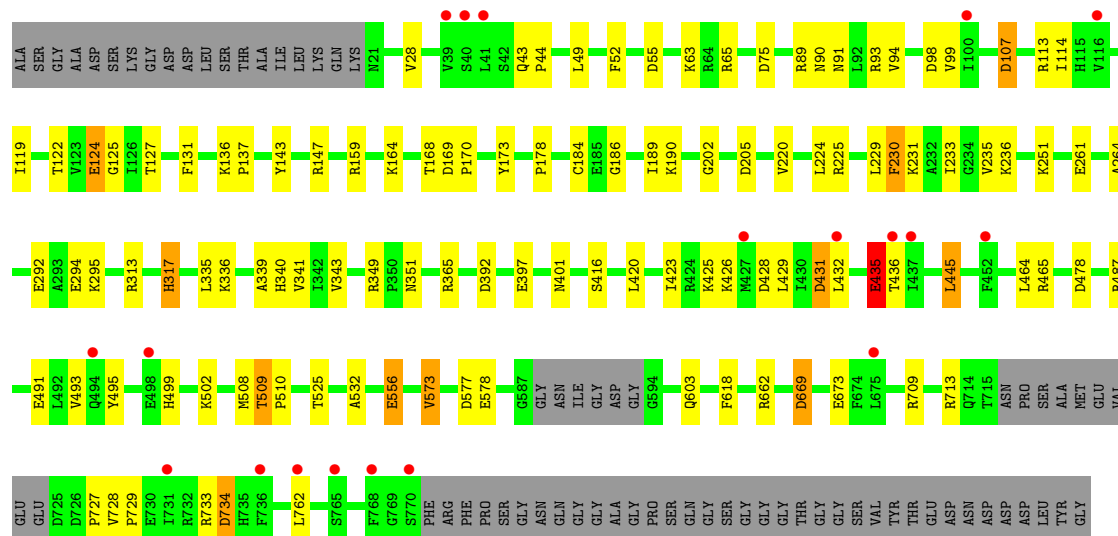


• Molecule 1: Transitional endoplasmic reticulum ATPase

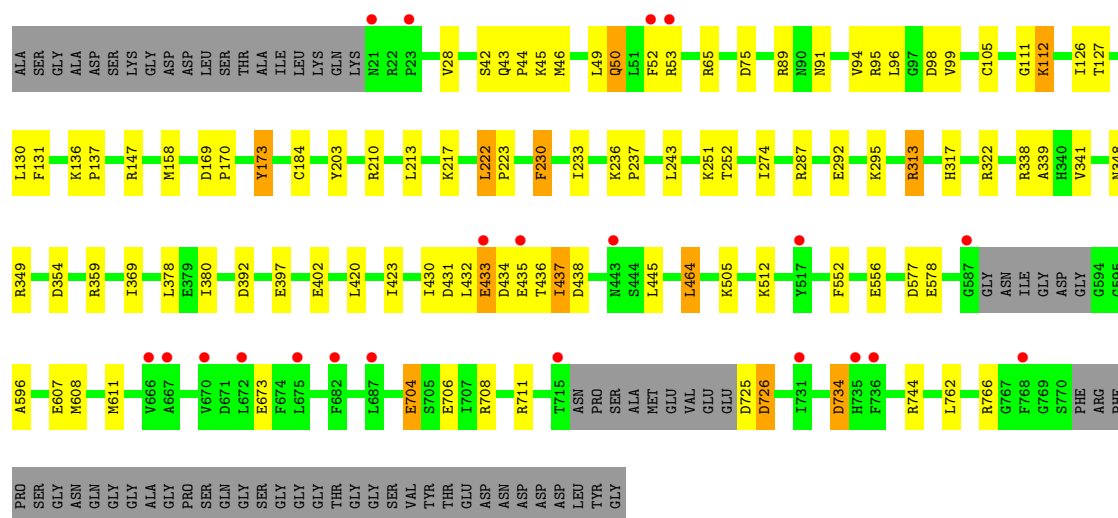
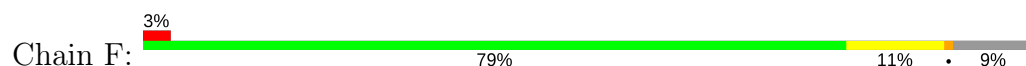


• Molecule 1: Transitional endoplasmic reticulum ATPase

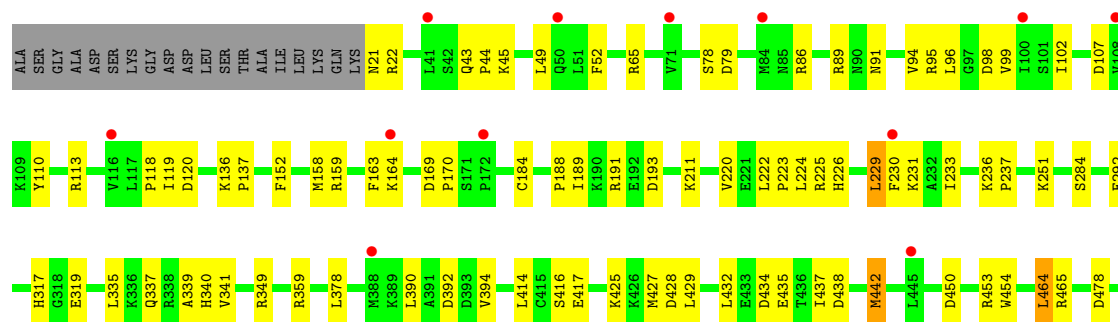
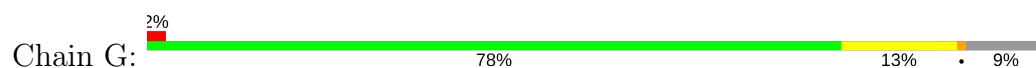


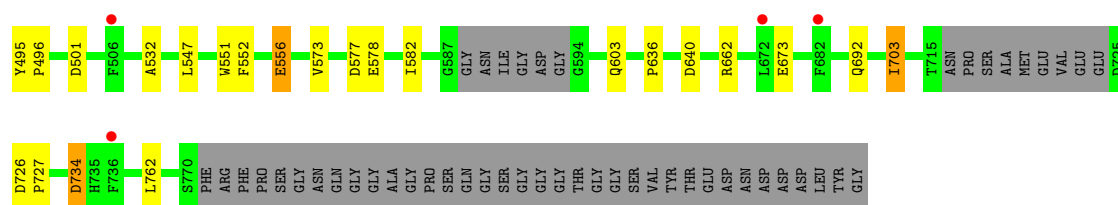


• Molecule 1: Transitional endoplasmic reticulum ATPase

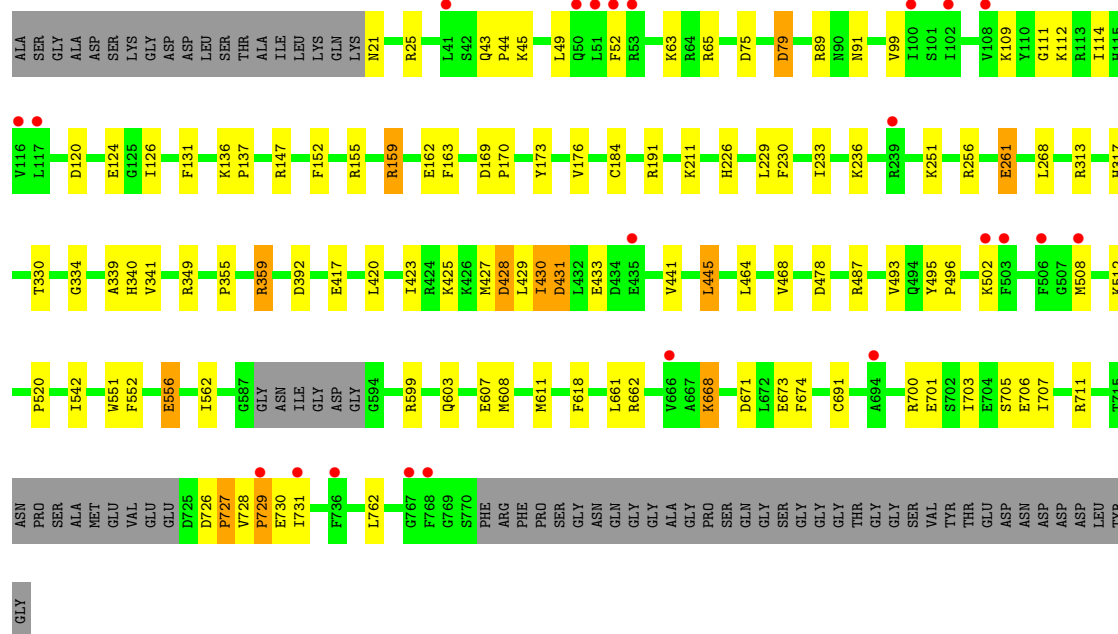
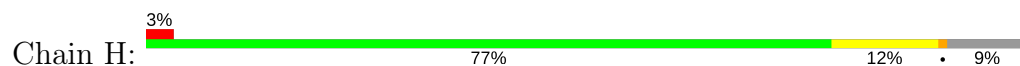


• Molecule 1: Transitional endoplasmic reticulum ATPase

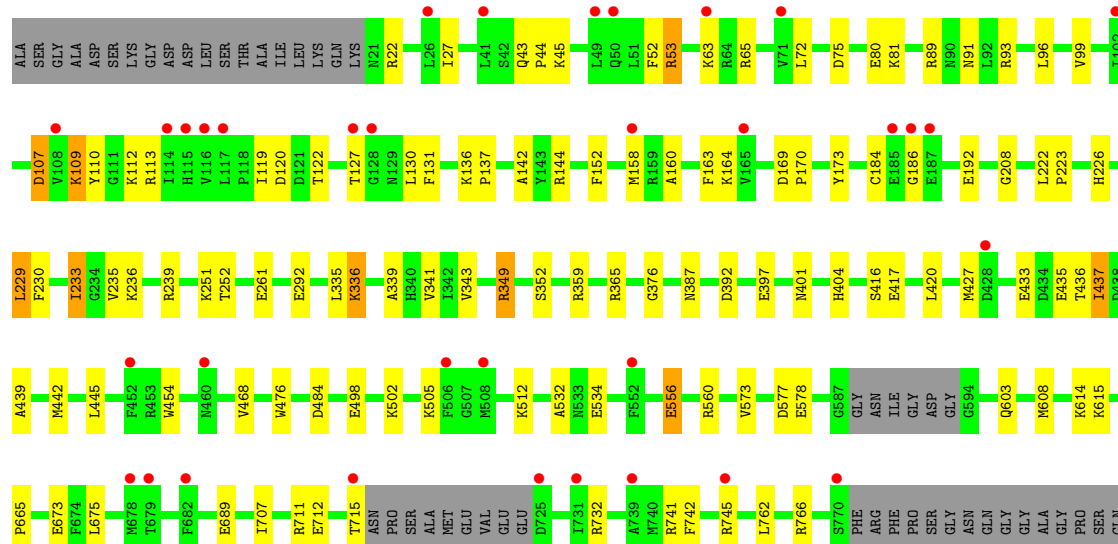




• Molecule 1: Transitional endoplasmic reticulum ATPase



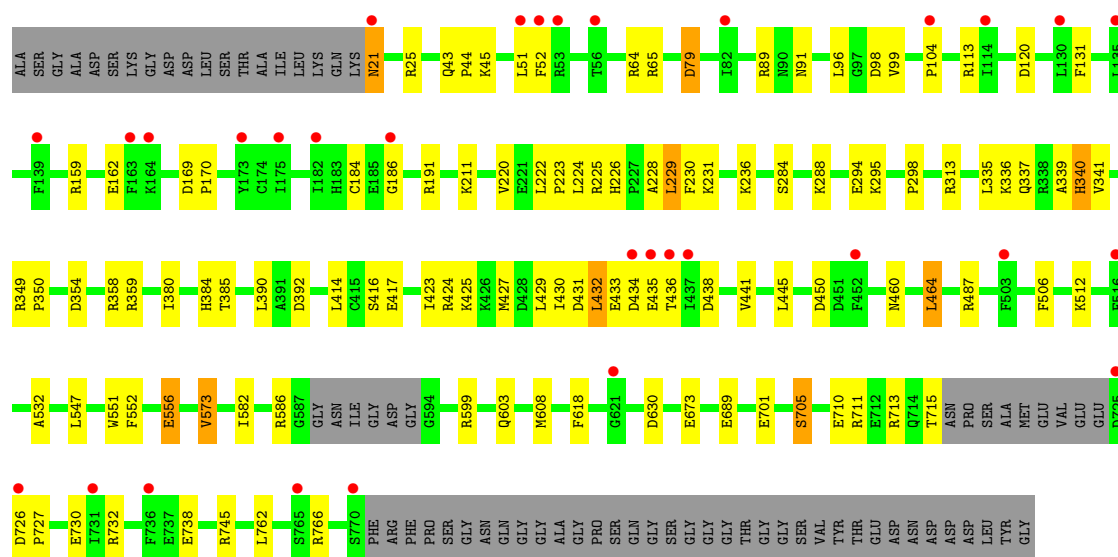
• Molecule 1: Transitional endoplasmic reticulum ATPase



GLY  
SER  
GLY  
GLY  
GLY  
THR  
GLY  
GLY  
SER  
SER  
VAL  
THR  
THR  
GLU  
ASP  
ASN  
ASP  
ASP  
ASP  
LEU  
TYR  
GLY

• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain J: 4% 77% 13% 9%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.67Å 145.47Å 251.40Å 90.00° 109.77° 90.00°	Depositor
Resolution (Å)	49.05 – 3.80 49.05 – 3.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.05-3.80) 98.7 (49.05-3.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.190 , 0.254 0.190 , 0.253	Depositor DCC
$R_{free}$ test set	6031 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	148.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 125.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	140261	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.29	0/5856	0.51	0/7906
1	B	0.30	0/5864	0.52	0/7917
1	C	0.29	0/5864	0.53	0/7917
1	D	0.27	0/5864	0.50	0/7917
1	E	0.30	0/5864	0.53	0/7917
1	F	0.30	0/5864	0.54	0/7917
1	G	0.29	0/5856	0.53	0/7906
1	H	0.29	0/5864	0.51	0/7917
1	I	0.28	0/5863	0.51	0/7913
1	J	0.29	0/5864	0.52	0/7917
1	K	0.30	0/5934	0.52	0/8014
1	L	0.29	0/5864	0.51	0/7917
All	All	0.29	0/70421	0.52	0/95075

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	B	429	LEU	Peptide
1	F	49	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	5764	5814	5812	48	0
1	B	5771	5819	5819	57	0
1	C	5771	5818	5818	44	0
1	D	5771	5820	5820	46	0
1	E	5771	5818	5818	53	0
1	F	5771	5818	5819	54	0
1	G	5764	5812	5811	52	0
1	H	5771	5819	5819	63	0
1	I	5771	5818	5818	51	0
1	J	5771	5819	5819	47	0
1	K	5839	5880	5879	67	0
1	L	5771	5820	5819	53	0
2	A	62	26	24	0	0
2	B	62	26	24	4	0
2	C	62	26	24	3	0
2	D	62	26	24	0	0
2	E	62	26	24	3	0
2	F	62	26	24	6	0
2	G	62	26	24	2	0
2	H	62	26	24	1	0
2	I	62	26	24	4	0
2	J	62	26	23	4	0
2	K	62	26	24	2	0
2	L	62	26	24	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
All	All	70074	70187	70158	595	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 4.

All (595) 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:H:429:LEU:O	1:H:431:ASP:N	2.15	0.79
1:B:89:ARG:NH1	1:B:261:GLU:OE2	2.17	0.78
1:J:313:ARG:NE	1:J:354:ASP:OD2	2.19	0.75
1:B:429:LEU:O	1:B:431:ASP:N	2.21	0.74
1:H:65:ARG:NH1	1:H:91:ASN:O	2.20	0.73
1:B:124:GLU:OE2	1:C:231:LYS:NZ	2.21	0.73
1:G:434:ASP:OD2	1:H:226:HIS:ND1	2.21	0.73
1:J:745:ARG:O	1:K:764:GLN:NE2	2.21	0.73
1:K:709:ARG:NH1	1:K:720:MET:SD	2.62	0.73
1:L:65:ARG:NH1	1:L:91:ASN:O	2.22	0.73
2:E:902:AGS:O3G	1:F:766:ARG:NH1	2.21	0.73
1:A:502:LYS:NZ	1:F:706:GLU:OE2	2.22	0.73
1:K:355:PRO:O	1:K:359:ARG:NH1	2.22	0.72
1:G:692:GLN:NE2	1:H:508:MET:SD	2.64	0.71
1:K:417:GLU:OE1	1:L:365:ARG:NH2	2.24	0.70
1:D:162:GLU:OE1	1:D:191:ARG:NH2	2.25	0.70
1:G:339:ALA:O	1:G:341:VAL:N	2.25	0.70
1:K:339:ALA:O	1:K:341:VAL:N	2.25	0.70
1:J:417:GLU:OE1	1:K:365:ARG:NH2	2.25	0.70
1:A:339:ALA:O	1:A:341:VAL:N	2.25	0.69
1:A:744:ARG:NH2	1:B:759:ALA:O	2.25	0.69
1:B:65:ARG:NH1	1:B:91:ASN:O	2.25	0.68
1:D:706:GLU:OE2	1:E:502:LYS:NZ	2.26	0.68
1:E:65:ARG:NH1	1:E:91:ASN:O	2.26	0.68
1:G:65:ARG:NH1	1:G:91:ASN:O	2.26	0.68
1:F:65:ARG:NH1	1:F:91:ASN:O	2.27	0.68
1:E:89:ARG:NH1	1:E:261:GLU:OE2	2.27	0.67
1:D:313:ARG:NE	1:D:354:ASP:OD2	2.27	0.67
1:J:162:GLU:OE1	1:J:191:ARG:NH2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:673:GLU:N	1:E:673:GLU:OE1	2.27	0.66
1:C:107:ASP:N	1:C:107:ASP:OD1	2.25	0.66
1:G:465:ARG:NH2	1:H:607:GLU:OE1	2.29	0.66
1:H:417:GLU:OE1	1:I:365:ARG:NH2	2.29	0.66
1:L:734:ASP:OD1	1:L:734:ASP:N	2.29	0.65
1:E:317:HIS:O	1:F:322:ARG:NH2	2.29	0.64
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.80	0.64
1:H:339:ALA:O	1:H:341:VAL:N	2.31	0.64
1:C:673:GLU:OE1	1:C:673:GLU:N	2.31	0.64
1:J:339:ALA:O	1:J:341:VAL:N	2.31	0.64
1:F:339:ALA:O	1:F:341:VAL:N	2.32	0.63
1:K:79:ASP:N	1:K:79:ASP:OD1	2.29	0.63
1:F:46:MET:O	1:F:50:GLN:HA	1.99	0.63
1:A:79:ASP:N	1:A:79:ASP:OD1	2.29	0.62
1:C:339:ALA:O	1:C:341:VAL:N	2.32	0.62
1:H:552:PHE:O	1:H:599:ARG:NH2	2.32	0.62
1:K:478:ASP:OD1	1:K:662:ARG:NH2	2.32	0.62
1:J:294:GLU:OE2	1:J:337:GLN:NE2	2.32	0.62
1:G:49:LEU:HD21	1:G:102:ILE:HG23	1.81	0.62
1:K:65:ARG:NH1	1:K:91:ASN:O	2.32	0.62
1:G:673:GLU:OE1	1:G:673:GLU:N	2.33	0.62
1:J:79:ASP:OD1	1:J:79:ASP:N	2.29	0.62
1:F:512:LYS:NZ	1:F:608:MET:O	2.31	0.61
1:D:700:ARG:NE	1:E:491:GLU:OE2	2.34	0.61
1:L:673:GLU:N	1:L:673:GLU:OE1	2.33	0.61
1:B:350:PRO:O	1:B:358:ARG:NH2	2.34	0.61
1:L:432:LEU:O	1:L:434:ASP:N	2.34	0.61
2:G:902:AGS:O2B	2:G:902:AGS:O2G	2.18	0.60
1:J:701:GLU:O	1:J:705:SER:OG	2.19	0.60
1:F:673:GLU:N	1:F:673:GLU:OE1	2.35	0.60
1:I:65:ARG:NH1	1:I:91:ASN:O	2.35	0.60
1:A:759:ALA:O	1:F:744:ARG:NH1	2.34	0.60
1:F:251:LYS:NZ	2:F:901:AGS:O2B	2.34	0.60
1:H:162:GLU:OE1	1:H:191:ARG:NH2	2.34	0.60
1:J:98:ASP:OD1	1:J:225:ARG:NH1	2.33	0.60
1:E:339:ALA:O	1:E:341:VAL:N	2.34	0.60
1:K:512:LYS:NZ	1:K:611:MET:O	2.23	0.60
1:C:65:ARG:NH1	1:C:91:ASN:O	2.35	0.60
1:J:556:GLU:O	1:J:603:GLN:NE2	2.35	0.59
1:D:316:THR:O	1:D:322:ARG:NH2	2.35	0.59
1:I:251:LYS:NZ	2:I:901:AGS:O1B	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLU:N	1:A:673:GLU:OE1	2.35	0.59
1:H:478:ASP:OD1	1:H:662:ARG:NH2	2.35	0.59
1:D:79:ASP:OD1	1:D:79:ASP:N	2.32	0.59
1:L:339:ALA:O	1:L:341:VAL:N	2.36	0.59
1:L:251:LYS:NZ	2:L:901:AGS:O1B	2.36	0.59
1:K:98:ASP:OD1	1:K:225:ARG:NH2	2.35	0.58
1:D:339:ALA:O	1:D:341:VAL:N	2.36	0.58
1:F:313:ARG:NE	1:F:354:ASP:OD2	2.36	0.58
1:B:355:PRO:O	1:B:359:ARG:NH1	2.36	0.58
1:C:512:LYS:NZ	1:C:611:MET:O	2.35	0.58
1:C:251:LYS:NZ	2:C:901:AGS:O2B	2.36	0.58
2:J:902:AGS:O3G	1:K:766:ARG:NH1	2.36	0.57
1:A:434:ASP:OD2	1:B:226:HIS:ND1	2.37	0.57
1:A:222:LEU:HB2	1:A:223:PRO:HD3	1.87	0.57
1:B:673:GLU:OE1	1:B:673:GLU:N	2.35	0.57
1:H:701:GLU:O	1:H:705:SER:N	2.36	0.57
1:H:673:GLU:OE1	1:H:673:GLU:N	2.38	0.57
1:K:704:GLU:HA	1:K:707:ILE:HD11	1.87	0.57
1:B:124:GLU:OE1	1:B:125:GLY:N	2.38	0.56
1:K:724:GLU:O	1:K:726:ASP:N	2.39	0.56
1:K:119:ILE:O	1:K:122:THR:OG1	2.20	0.56
1:C:431:ASP:OD2	1:D:25:ARG:NH2	2.39	0.56
1:E:202:GLY:N	1:E:205:ASP:OD2	2.37	0.56
1:H:251:LYS:NZ	2:H:901:AGS:O1B	2.39	0.56
1:J:65:ARG:NH1	1:J:91:ASN:O	2.39	0.56
1:L:512:LYS:NZ	1:L:611:MET:O	2.31	0.56
1:J:701:GLU:OE1	1:J:732:ARG:NH2	2.38	0.56
1:E:556:GLU:O	1:E:603:GLN:NE2	2.38	0.56
1:E:124:GLU:OE1	1:E:125:GLY:N	2.40	0.55
1:D:294:GLU:OE2	1:D:337:GLN:NE2	2.39	0.55
1:K:673:GLU:OE1	1:K:673:GLU:N	2.39	0.55
1:B:79:ASP:OD1	1:B:79:ASP:N	2.40	0.55
1:B:313:ARG:NE	1:B:354:ASP:OD2	2.40	0.55
1:B:556:GLU:O	1:B:603:GLN:NE2	2.40	0.55
1:G:556:GLU:O	1:G:603:GLN:NE2	2.38	0.55
1:B:119:ILE:O	1:B:122:THR:OG1	2.24	0.55
1:I:673:GLU:N	1:I:673:GLU:OE1	2.39	0.55
1:F:423:ILE:HG12	1:F:445:LEU:HD21	1.89	0.55
1:H:706:GLU:OE1	1:I:502:LYS:NZ	2.39	0.55
1:I:512:LYS:NZ	1:I:608:MET:O	2.39	0.55
2:I:902:AGS:S1G	1:J:766:ARG:NH1	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:GLU:O	1:A:603:GLN:NE2	2.41	0.54
1:F:734:ASP:OD1	1:F:734:ASP:N	2.32	0.54
1:F:112:LYS:HB2	1:F:169:ASP:HB3	1.90	0.54
1:G:96:LEU:O	1:G:225:ARG:NH2	2.40	0.54
1:L:432:LEU:C	1:L:434:ASP:H	2.11	0.54
1:E:169:ASP:HB3	1:E:170:PRO:HD3	1.90	0.54
1:K:556:GLU:O	1:K:603:GLN:NE2	2.40	0.54
1:K:720:MET:SD	1:K:721:GLU:N	2.74	0.54
1:I:252:THR:OG1	2:I:901:AGS:O2B	2.25	0.53
1:A:734:ASP:OD1	1:A:734:ASP:N	2.30	0.53
1:H:726:ASP:N	1:H:727:PRO:HD3	2.23	0.53
1:J:464:LEU:H	1:J:464:LEU:HD12	1.72	0.53
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.91	0.53
1:C:736:PHE:O	1:C:740:MET:N	2.41	0.53
1:H:512:LYS:NZ	1:H:611:MET:O	2.40	0.53
1:A:478:ASP:OD1	1:A:662:ARG:NH2	2.40	0.53
1:B:162:GLU:OE1	1:B:191:ARG:NH2	2.41	0.53
1:H:79:ASP:N	1:H:79:ASP:OD1	2.39	0.53
1:J:284:SER:OG	1:J:288:LYS:NZ	2.41	0.53
1:I:339:ALA:O	1:I:341:VAL:N	2.42	0.53
1:D:389:LYS:HD3	1:D:443:ASN:O	2.08	0.52
1:K:191:ARG:NH1	1:K:195:GLU:O	2.41	0.52
1:D:673:GLU:OE1	1:D:673:GLU:N	2.42	0.52
1:C:252:THR:OG1	2:C:901:AGS:O1B	2.27	0.52
1:F:136:LYS:HB3	1:F:137:PRO:HD3	1.92	0.52
1:G:547:LEU:HD12	1:G:582:ILE:HD11	1.91	0.52
1:K:717:PRO:N	1:K:718:SER:HA	2.24	0.52
1:F:430:ILE:O	1:F:433:GLU:N	2.32	0.52
1:H:89:ARG:NH1	1:H:261:GLU:OE2	2.41	0.52
1:K:169:ASP:HB3	1:K:170:PRO:HD3	1.90	0.52
1:E:525:THR:OG1	1:E:577:ASP:OD2	2.28	0.52
1:F:512:LYS:NZ	1:F:611:MET:O	2.39	0.52
1:G:169:ASP:HB3	1:G:170:PRO:HD3	1.92	0.52
1:G:442:MET:HA	1:G:442:MET:CE	2.40	0.52
1:B:142:ALA:HB1	1:B:144:ARG:HG3	1.91	0.52
1:L:43:GLN:N	1:L:44:PRO:HD2	2.25	0.51
1:H:230:PHE:HA	1:H:233:ILE:HG22	1.92	0.51
1:K:509:THR:HG22	1:K:510:PRO:HD2	1.92	0.51
2:L:902:AGS:O1A	2:L:902:AGS:O2G	2.28	0.51
1:B:727:PRO:O	1:B:729:PRO:HD3	2.11	0.51
1:H:427:MET:HG2	1:H:427:MET:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:GLN:NE2	1:B:508:MET:SD	2.83	0.51
1:G:43:GLN:N	1:G:44:PRO:HD2	2.26	0.51
1:C:424:ARG:HG3	1:D:222:LEU:HD11	1.92	0.51
1:E:107:ASP:N	1:E:107:ASP:OD1	2.43	0.51
1:H:114:ILE:CD1	1:H:176:VAL:HG22	2.41	0.51
1:D:230:PHE:HA	1:D:233:ILE:HG22	1.92	0.51
1:B:478:ASP:OD1	1:B:662:ARG:NH2	2.44	0.51
1:L:434:ASP:C	1:L:436:THR:H	2.14	0.51
1:B:432:LEU:HD22	1:C:226:HIS:CE1	2.46	0.50
2:B:902:AGS:O2A	2:B:902:AGS:O2G	2.28	0.50
1:C:96:LEU:HD23	1:C:261:GLU:HG3	1.93	0.50
1:D:65:ARG:NH1	1:D:91:ASN:O	2.44	0.50
1:G:432:LEU:O	1:H:25:ARG:NH1	2.44	0.50
1:L:169:ASP:HB3	1:L:170:PRO:HD3	1.93	0.50
1:F:147:ARG:HG2	1:F:173:TYR:HB3	1.94	0.50
1:K:722:VAL:O	1:K:724:GLU:N	2.44	0.50
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.94	0.50
1:C:442:MET:CE	1:C:442:MET:HA	2.41	0.50
1:D:284:SER:OG	1:D:288:LYS:NZ	2.44	0.50
1:I:397:GLU:O	1:I:401:ASN:ND2	2.44	0.50
1:J:96:LEU:O	1:J:225:ARG:NH2	2.44	0.50
1:C:726:ASP:N	1:C:727:PRO:HD3	2.24	0.50
1:J:552:PHE:O	1:J:599:ARG:NH2	2.45	0.50
1:E:532:ALA:HB2	1:E:573:VAL:HG11	1.93	0.50
1:F:173:TYR:CD1	1:F:173:TYR:N	2.80	0.50
1:H:728:VAL:N	1:H:729:PRO:CD	2.75	0.50
1:L:441:VAL:O	1:L:444:SER:OG	2.26	0.50
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.94	0.50
1:E:43:GLN:N	1:E:44:PRO:HD2	2.27	0.50
1:H:169:ASP:HB3	1:H:170:PRO:HD3	1.92	0.50
1:H:728:VAL:O	1:H:730:GLU:N	2.45	0.49
1:J:551:TRP:CZ2	1:K:556:GLU:HG2	2.47	0.49
1:K:576:PHE:HB3	1:K:579:LEU:HD21	1.95	0.49
1:L:727:PRO:HB2	1:L:729:PRO:HD3	1.94	0.49
1:D:208:GLY:HA2	1:D:376:GLY:HA2	1.95	0.49
1:D:556:GLU:O	1:D:603:GLN:NE2	2.45	0.49
1:E:734:ASP:OD1	1:E:734:ASP:N	2.44	0.49
1:G:734:ASP:N	1:G:734:ASP:OD1	2.31	0.49
1:I:169:ASP:HB3	1:I:170:PRO:HD3	1.93	0.49
1:I:239:ARG:NH1	1:I:336:LYS:HD2	2.27	0.49
1:I:43:GLN:N	1:I:44:PRO:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:673:GLU:OE1	1:J:673:GLU:N	2.43	0.49
1:B:339:ALA:O	1:B:341:VAL:N	2.45	0.49
1:E:119:ILE:O	1:E:122:THR:OG1	2.30	0.49
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.93	0.49
1:B:734:ASP:N	1:B:734:ASP:OD1	2.42	0.49
1:L:147:ARG:HG2	1:L:173:TYR:HB3	1.95	0.49
1:F:432:LEU:C	1:F:434:ASP:H	2.16	0.49
1:I:89:ARG:NH1	1:I:261:GLU:OE1	2.45	0.49
1:K:230:PHE:HA	1:K:233:ILE:HG22	1.94	0.49
1:B:493:VAL:HG13	1:B:618:PHE:CD2	2.48	0.48
1:B:43:GLN:N	1:B:44:PRO:HD2	2.28	0.48
1:F:252:THR:OG1	2:F:901:AGS:O1B	2.31	0.48
1:G:222:LEU:HB2	1:G:223:PRO:HD3	1.94	0.48
1:K:493:VAL:HG13	1:K:618:PHE:CD2	2.48	0.48
1:L:439:ALA:O	1:L:443:ASN:N	2.41	0.48
1:C:233:ILE:HG22	1:C:235:VAL:H	1.77	0.48
1:E:431:ASP:OD1	1:E:432:LEU:N	2.46	0.48
1:I:107:ASP:OD1	1:I:107:ASP:N	2.46	0.48
1:J:120:ASP:OD1	1:J:120:ASP:N	2.46	0.48
1:E:499:HIS:HB3	1:E:502:LYS:HG3	1.96	0.48
1:J:222:LEU:HB2	1:J:223:PRO:HD3	1.95	0.48
1:K:43:GLN:N	1:K:44:PRO:HD2	2.28	0.48
1:K:75:ASP:N	1:K:75:ASP:OD1	2.47	0.48
1:E:233:ILE:HG23	1:E:235:VAL:H	1.78	0.48
1:G:478:ASP:OD1	1:G:662:ARG:NH2	2.44	0.48
1:L:51:LEU:HD21	1:L:104:PRO:HB3	1.95	0.48
1:G:464:LEU:H	1:G:464:LEU:HD12	1.79	0.48
1:A:142:ALA:HB1	1:A:144:ARG:HG3	1.95	0.48
1:C:75:ASP:OD1	1:C:75:ASP:N	2.46	0.48
1:F:437:ILE:N	1:F:437:ILE:HD13	2.29	0.48
1:E:230:PHE:HA	1:E:233:ILE:HG22	1.96	0.48
1:H:43:GLN:N	1:H:44:PRO:HD2	2.28	0.48
1:K:136:LYS:HB3	1:K:137:PRO:HD3	1.96	0.48
1:I:136:LYS:HB3	1:I:137:PRO:HD3	1.96	0.48
1:E:147:ARG:HG2	1:E:173:TYR:HB3	1.96	0.47
1:J:169:ASP:HB3	1:J:170:PRO:HD3	1.95	0.47
1:B:112:LYS:HB2	1:B:169:ASP:HB3	1.96	0.47
1:F:169:ASP:HB3	1:F:170:PRO:HD3	1.95	0.47
1:A:43:GLN:N	1:A:44:PRO:HD2	2.30	0.47
1:D:27:ILE:HB	1:D:81:LYS:HG2	1.97	0.47
1:E:397:GLU:O	1:E:401:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:PHE:HA	1:F:233:ILE:HG22	1.96	0.47
1:G:136:LYS:HB3	1:G:137:PRO:HD3	1.96	0.47
2:L:902:AGS:O2B	2:L:902:AGS:O2G	2.33	0.47
1:B:120:ASP:N	1:B:120:ASP:OD1	2.47	0.47
1:D:152:PHE:CZ	1:D:163:PHE:HB2	2.49	0.47
1:D:96:LEU:O	1:D:225:ARG:NH2	2.47	0.47
1:G:726:ASP:N	1:G:727:PRO:HD3	2.29	0.47
1:E:75:ASP:N	1:E:75:ASP:OD1	2.45	0.47
1:F:432:LEU:O	1:F:434:ASP:N	2.48	0.47
1:A:512:LYS:NZ	1:A:611:MET:O	2.38	0.47
1:E:220:VAL:CG1	1:E:224:LEU:HD22	2.43	0.47
1:H:430:ILE:HG23	1:H:431:ASP:N	2.30	0.47
1:I:158:MET:HE1	1:I:445:LEU:HD13	1.97	0.47
1:K:435:GLU:HG3	1:K:436:THR:H	1.79	0.47
1:D:547:LEU:HD12	1:D:582:ILE:HD11	1.97	0.47
1:F:725:ASP:O	1:F:726:ASP:HB2	2.15	0.47
1:A:311:PRO:HD2	1:A:316:THR:HG22	1.97	0.47
2:C:902:AGS:S1G	1:D:766:ARG:NH1	2.88	0.47
1:E:709:ARG:HH22	1:E:727:PRO:HB3	1.80	0.47
1:H:493:VAL:HG13	1:H:618:PHE:CD2	2.50	0.47
1:K:698:ALA:HB1	1:K:731:ILE:HG22	1.95	0.47
1:C:310:ALA:HA	1:C:325:VAL:HG22	1.97	0.47
1:G:577:ASP:OD1	1:G:578:GLU:N	2.48	0.47
1:G:703:ILE:HG22	1:H:502:LYS:HD2	1.97	0.47
1:F:434:ASP:C	1:F:436:THR:H	2.17	0.47
1:G:94:VAL:HG13	1:G:98:ASP:HB2	1.97	0.47
1:I:119:ILE:O	1:I:122:THR:OG1	2.32	0.47
1:J:21:ASN:OD1	1:J:21:ASN:N	2.48	0.47
1:F:75:ASP:OD1	1:F:75:ASP:N	2.47	0.46
1:J:512:LYS:NZ	1:J:608:MET:O	2.42	0.46
1:L:75:ASP:OD1	1:L:75:ASP:N	2.49	0.46
1:E:224:LEU:HD23	1:E:264:ALA:HB2	1.97	0.46
1:F:43:GLN:N	1:F:44:PRO:HD2	2.31	0.46
1:G:79:ASP:N	1:G:79:ASP:OD1	2.48	0.46
1:H:556:GLU:O	1:H:603:GLN:NE2	2.48	0.46
1:H:668:LYS:HE3	1:H:668:LYS:HA	1.98	0.46
1:K:435:GLU:CG	1:K:436:THR:H	2.28	0.46
1:D:312:LYS:N	1:D:352:SER:O	2.49	0.46
1:D:417:GLU:OE1	1:E:365:ARG:NH2	2.49	0.46
1:L:437:ILE:N	1:L:437:ILE:HD13	2.30	0.46
1:G:233:ILE:HD13	1:L:442:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:LYS:HE2	1:C:426:LYS:HE2	1.98	0.46
1:E:465:ARG:NH2	1:F:607:GLU:OE2	2.49	0.46
1:I:142:ALA:HB1	1:I:144:ARG:HG3	1.97	0.46
1:D:576:PHE:HB3	1:D:579:LEU:HD21	1.98	0.46
1:F:111:GLY:HA2	1:F:170:PRO:HG2	1.97	0.46
1:F:378:LEU:HD13	1:F:397:GLU:HA	1.97	0.46
1:F:89:ARG:NH1	1:F:96:LEU:HD21	2.31	0.46
1:I:75:ASP:N	1:I:75:ASP:OD1	2.49	0.46
1:A:158:MET:SD	1:B:233:ILE:HD11	2.56	0.46
1:H:112:LYS:HB2	1:H:169:ASP:HB3	1.98	0.46
1:K:716:ASN:C	1:K:718:SER:HA	2.35	0.46
1:F:348:ASN:ND2	2:F:901:AGS:S1G	2.89	0.46
1:G:95:ARG:HB2	1:G:225:ARG:NH2	2.30	0.46
1:I:96:LEU:HD23	1:I:261:GLU:HG3	1.98	0.46
1:H:703:ILE:HG22	1:H:707:ILE:HD12	1.98	0.46
1:J:43:GLN:N	1:J:44:PRO:HD2	2.31	0.46
1:A:28:VAL:HG21	1:A:94:VAL:HG11	1.96	0.46
1:D:231:LYS:HG2	1:D:232:ALA:N	2.30	0.46
1:J:350:PRO:O	1:J:358:ARG:NH2	2.49	0.46
2:K:902:AGS:O2G	2:K:902:AGS:O2B	2.33	0.46
1:F:577:ASP:OD1	1:F:578:GLU:N	2.48	0.46
1:K:152:PHE:CZ	1:K:163:PHE:HB2	2.51	0.46
1:A:136:LYS:HB3	1:A:137:PRO:CD	2.46	0.45
1:D:136:LYS:HB3	1:D:137:PRO:HD3	1.98	0.45
1:L:136:LYS:HB3	1:L:137:PRO:HD3	1.98	0.45
1:A:164:LYS:HE2	1:A:189:ILE:CD1	2.46	0.45
1:B:532:ALA:HB2	1:B:573:VAL:HG11	1.98	0.45
1:H:147:ARG:HG2	1:H:173:TYR:HB3	1.98	0.45
1:D:43:GLN:N	1:D:44:PRO:HD2	2.31	0.45
1:E:28:VAL:HG21	1:E:94:VAL:HG11	1.98	0.45
1:G:251:LYS:N	2:G:901:AGS:O1B	2.46	0.45
1:I:63:LYS:HD3	1:I:93:ARG:HG3	1.97	0.45
1:E:423:ILE:HG12	1:E:445:LEU:HD11	1.98	0.45
1:F:251:LYS:NZ	2:F:901:AGS:S1G	2.89	0.45
1:L:373:ASP:HB3	1:L:470:GLU:HB3	1.99	0.45
1:B:437:ILE:HG12	1:C:229:LEU:CD1	2.47	0.45
1:D:134:TYR:CD2	1:D:161:VAL:HG11	2.51	0.45
1:G:152:PHE:CZ	1:G:163:PHE:HB2	2.51	0.45
1:H:551:TRP:CZ2	1:I:556:GLU:HG2	2.52	0.45
1:L:703:ILE:O	1:L:707:ILE:HG13	2.17	0.45
1:B:41:LEU:HD11	1:B:102:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ASP:OD1	1:B:75:ASP:N	2.49	0.45
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.52	0.45
1:C:43:GLN:N	1:C:44:PRO:HD2	2.31	0.45
1:E:136:LYS:HB3	1:E:137:PRO:HD3	1.98	0.45
1:G:164:LYS:HE2	1:G:189:ILE:CD1	2.47	0.45
1:G:442:MET:SD	1:H:233:ILE:HD13	2.56	0.45
1:K:707:ILE:O	1:K:711:ARG:HG3	2.16	0.45
1:L:231:LYS:O	1:L:231:LYS:HD2	2.17	0.45
1:B:114:ILE:CD1	1:B:176:VAL:HG22	2.46	0.45
1:D:169:ASP:HB3	1:D:170:PRO:HD3	1.98	0.45
1:E:98:ASP:OD1	1:E:225:ARG:NH2	2.49	0.45
1:H:423:ILE:O	1:H:427:MET:N	2.49	0.45
1:A:532:ALA:HB2	1:A:573:VAL:HG11	1.99	0.45
1:C:136:LYS:HB3	1:C:137:PRO:HD3	1.98	0.45
1:E:509:THR:HG22	1:E:510:PRO:HD2	1.99	0.45
1:F:222:LEU:HB3	1:F:223:PRO:HD3	1.98	0.45
1:H:728:VAL:N	1:H:729:PRO:HD2	2.32	0.45
1:J:89:ARG:NH1	1:J:96:LEU:HD21	2.31	0.45
1:A:230:PHE:HA	1:A:233:ILE:HG22	1.98	0.45
1:H:430:ILE:HG23	1:H:431:ASP:H	1.82	0.45
1:J:532:ALA:HB2	1:J:573:VAL:HG11	1.99	0.45
1:L:310:ALA:HA	1:L:325:VAL:HG22	1.97	0.45
1:E:143:TYR:CE1	1:E:178:PRO:HD3	2.52	0.45
1:E:294:GLU:HG3	1:E:339:ALA:HB3	1.99	0.45
1:K:230:PHE:CZ	1:K:237:PRO:HB3	2.52	0.45
1:C:512:LYS:NZ	1:C:608:MET:O	2.46	0.44
1:H:551:TRP:CE2	1:I:556:GLU:HG2	2.51	0.44
1:L:120:ASP:N	1:L:120:ASP:OD1	2.50	0.44
1:A:220:VAL:CG1	1:A:224:LEU:HD12	2.47	0.44
1:E:669:ASP:OD1	1:E:733:ARG:NH1	2.50	0.44
1:F:42:SER:O	1:F:46:MET:N	2.44	0.44
1:G:390:LEU:HD23	1:G:394:VAL:HG11	1.99	0.44
1:L:126:ILE:CD1	1:L:159:ARG:HD3	2.48	0.44
1:L:438:ASP:OD1	1:L:438:ASP:N	2.51	0.44
1:L:439:ALA:HA	1:L:442:MET:HB3	1.99	0.44
1:B:430:ILE:HD11	1:B:441:VAL:HG11	1.99	0.44
1:H:542:ILE:HD13	1:H:562:ILE:HD13	1.98	0.44
1:A:424:ARG:HG3	1:B:222:LEU:HD22	1.99	0.44
1:B:298:PRO:HA	1:B:340:HIS:O	2.17	0.44
1:I:484:ASP:N	1:I:484:ASP:OD1	2.51	0.44
1:G:120:ASP:N	1:G:120:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:532:ALA:HB2	1:G:573:VAL:HG11	1.98	0.44
1:J:51:LEU:CD2	1:J:104:PRO:HB3	2.47	0.44
1:I:404:HIS:NE2	1:I:468:VAL:HG21	2.32	0.44
1:J:431:ASP:HA	1:J:434:ASP:HB2	1.98	0.44
1:B:89:ARG:CZ	1:B:96:LEU:HD21	2.48	0.44
1:H:75:ASP:OD1	1:H:75:ASP:N	2.49	0.44
1:I:160:ALA:HB2	1:I:387:ASN:HD21	1.82	0.44
1:A:120:ASP:OD1	1:A:120:ASP:N	2.51	0.44
1:B:644:TYR:CE2	1:B:646:PRO:HB3	2.52	0.44
1:D:112:LYS:HB2	1:D:169:ASP:HB3	1.99	0.44
1:G:89:ARG:NH1	1:G:96:LEU:HD21	2.32	0.44
1:H:727:PRO:HB2	1:H:729:PRO:CD	2.48	0.44
1:K:734:ASP:OD1	1:K:734:ASP:N	2.50	0.44
1:C:89:ARG:NH1	1:C:96:LEU:HD21	2.32	0.44
1:D:222:LEU:HB2	1:D:223:PRO:HD3	1.99	0.44
1:D:699:ILE:O	1:D:703:ILE:HD12	2.18	0.44
1:F:173:TYR:HD1	1:F:173:TYR:N	2.15	0.44
1:C:484:ASP:OD1	1:C:484:ASP:N	2.51	0.43
1:E:425:LYS:HE3	1:E:426:LYS:HE2	2.00	0.43
1:F:105:CYS:SG	1:F:173:TYR:HE2	2.41	0.43
1:L:185:GLU:O	1:L:187:GLU:N	2.51	0.43
1:L:501:ASP:OD1	1:L:502:LYS:N	2.51	0.43
1:B:122:THR:HB	1:B:161:VAL:HA	2.00	0.43
1:A:465:ARG:NH2	1:B:607:GLU:OE1	2.51	0.43
1:F:552:PHE:CE1	1:F:596:ALA:HB2	2.53	0.43
1:G:450:ASP:OD1	1:G:453:ARG:NH1	2.51	0.43
1:I:222:LEU:HB3	1:I:223:PRO:HD3	2.00	0.43
1:K:532:ALA:HB2	1:K:573:VAL:HG11	2.00	0.43
1:K:744:ARG:NH2	1:L:763:GLN:OE1	2.51	0.43
1:A:65:ARG:NH1	1:A:91:ASN:O	2.44	0.43
1:D:703:ILE:HD13	1:E:495:TYR:CE2	2.54	0.43
1:H:512:LYS:NZ	1:H:608:MET:O	2.43	0.43
1:J:726:ASP:N	1:J:727:PRO:HD3	2.33	0.43
1:K:124:GLU:OE1	1:K:125:GLY:N	2.51	0.43
1:K:158:MET:HB2	1:L:233:ILE:HD11	2.01	0.43
1:L:539:PHE:CE2	1:L:541:SER:HB2	2.53	0.43
1:B:542:ILE:HD13	1:B:562:ILE:HD13	2.01	0.43
1:D:22:ARG:HB3	1:D:23:PRO:HD2	1.99	0.43
1:E:478:ASP:OD2	1:E:662:ARG:NH2	2.51	0.43
1:F:438:ASP:OD1	1:F:438:ASP:N	2.51	0.43
1:I:233:ILE:HG22	1:I:235:VAL:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:902:AGS:O2B	2:J:902:AGS:O2G	2.35	0.43
1:E:493:VAL:HG13	1:E:618:PHE:CD2	2.53	0.43
1:I:208:GLY:HA2	1:I:376:GLY:HA2	2.00	0.43
1:K:385:THR:HB	1:K:390:LEU:HD11	2.01	0.43
1:K:126:ILE:HG21	1:K:439:ALA:HB2	1.99	0.43
1:L:28:VAL:HG21	1:L:94:VAL:HG11	2.00	0.43
1:C:136:LYS:HB3	1:C:137:PRO:CD	2.48	0.43
1:F:94:VAL:HG13	1:F:98:ASP:HB2	2.01	0.43
1:I:707:ILE:O	1:I:711:ARG:HG3	2.18	0.43
1:K:707:ILE:HD12	1:K:707:ILE:N	2.34	0.43
1:B:427:MET:CG	1:B:432:LEU:HD21	2.48	0.43
1:J:586:ARG:NH1	1:J:630:ASP:OD2	2.46	0.43
1:K:220:VAL:CG1	1:K:224:LEU:HD22	2.48	0.43
1:L:117:LEU:HD21	1:L:185:GLU:H	1.84	0.43
1:A:426:LYS:HG3	1:A:445:LEU:CD1	2.49	0.43
1:F:230:PHE:CZ	1:F:237:PRO:HB3	2.54	0.43
1:I:349:ARG:HG3	1:I:352:SER:CB	2.49	0.43
1:I:532:ALA:HB2	1:I:573:VAL:HG11	1.99	0.43
1:B:519:PRO:O	1:B:524:LYS:NZ	2.51	0.43
1:C:120:ASP:N	1:C:120:ASP:OD1	2.52	0.43
1:D:427:MET:HG2	1:D:430:ILE:HG22	2.00	0.43
1:F:136:LYS:HB3	1:F:137:PRO:CD	2.49	0.43
1:F:28:VAL:HG21	1:F:94:VAL:HG11	2.01	0.43
1:H:423:ILE:HG12	1:H:445:LEU:HD21	2.01	0.43
1:E:114:ILE:HG12	1:E:168:THR:HG22	2.01	0.42
1:A:233:ILE:HD11	1:F:158:MET:HB2	2.00	0.42
1:F:704:GLU:O	1:F:708:ARG:HG3	2.19	0.42
1:J:226:HIS:HB3	1:J:229:LEU:HG	2.00	0.42
1:K:90:ASN:O	1:K:93:ARG:NH1	2.50	0.42
1:L:380:ILE:HD12	2:L:901:AGS:N1	2.34	0.42
1:B:295:LYS:HA	1:B:295:LYS:HE3	2.00	0.42
1:C:373:ASP:HB3	1:C:470:GLU:HB3	2.00	0.42
1:A:766:ARG:NH1	2:F:902:AGS:O3G	2.50	0.42
1:I:560:ARG:HG3	1:I:603:GLN:HE21	1.84	0.42
1:L:703:ILE:HD12	1:L:704:GLU:N	2.33	0.42
1:A:51:LEU:HD21	1:A:104:PRO:HG3	2.01	0.42
1:A:556:GLU:OE1	1:A:560:ARG:NH1	2.51	0.42
1:C:371:ILE:HD11	1:C:468:VAL:HG22	2.01	0.42
1:G:49:LEU:HG	1:G:49:LEU:O	2.19	0.42
1:H:542:ILE:HD12	1:H:562:ILE:HG21	2.01	0.42
1:I:226:HIS:HB3	1:I:229:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:577:ASP:OD1	1:I:578:GLU:N	2.49	0.42
1:H:520:PRO:HB3	1:I:766:ARG:NH1	2.35	0.42
1:J:424:ARG:HG3	1:K:222:LEU:HD11	2.02	0.42
1:L:123:VAL:HA	1:L:126:ILE:HG13	2.01	0.42
1:D:608:MET:HG2	1:D:619:ILE:HD13	2.01	0.42
1:E:251:LYS:NZ	2:E:901:AGS:S1G	2.93	0.42
1:H:126:ILE:HG13	1:H:159:ARG:HD2	2.01	0.42
1:I:164:LYS:NZ	1:I:192:GLU:OE1	2.50	0.42
1:J:423:ILE:HD11	1:K:233:ILE:CD1	2.49	0.42
1:K:317:HIS:O	1:L:322:ARG:NH2	2.50	0.42
1:L:514:VAL:HG11	1:L:643:ILE:HD12	2.00	0.42
1:B:210:ARG:O	1:B:214:ALA:N	2.49	0.42
1:C:96:LEU:HD22	1:C:96:LEU:N	2.34	0.42
1:I:53:ARG:HB2	1:I:72:LEU:HD23	2.01	0.42
1:A:96:LEU:O	1:A:225:ARG:NH2	2.53	0.42
1:C:222:LEU:HB3	1:C:223:PRO:HD3	2.02	0.42
1:E:727:PRO:O	1:E:729:PRO:HD3	2.18	0.42
1:G:158:MET:SD	1:H:233:ILE:HD11	2.59	0.42
1:G:119:ILE:HG21	1:G:191:ARG:HG2	2.01	0.42
1:J:433:GLU:O	1:J:433:GLU:HG3	2.19	0.42
1:K:397:GLU:O	1:K:401:ASN:ND2	2.52	0.42
1:E:90:ASN:O	1:E:93:ARG:NH1	2.52	0.42
1:G:136:LYS:HB3	1:G:137:PRO:CD	2.49	0.42
1:H:52:PHE:CD1	1:H:52:PHE:N	2.87	0.42
1:H:671:ASP:HB3	1:H:674:PHE:HB3	2.02	0.42
1:K:89:ARG:NH1	1:K:261:GLU:OE2	2.51	0.42
1:K:434:ASP:O	1:K:435:GLU:CG	2.68	0.42
1:L:108:VAL:HG11	1:L:175:ILE:HG13	2.02	0.42
1:L:635:ARG:NH1	1:L:636:PRO:O	2.53	0.42
1:E:63:LYS:HG2	1:E:63:LYS:O	2.20	0.42
1:F:127:THR:HG22	1:F:437:ILE:HB	2.02	0.42
1:G:110:TYR:CD1	1:G:110:TYR:N	2.88	0.42
1:J:710:GLU:OE2	1:J:713:ARG:NH2	2.52	0.42
1:B:407:VAL:CG1	1:B:408:GLY:N	2.83	0.42
1:D:109:LYS:O	1:D:175:ILE:N	2.43	0.42
1:F:203:TYR:CE2	1:F:217:LYS:HD3	2.54	0.42
1:G:429:LEU:HD12	1:G:429:LEU:H	1.84	0.42
1:H:427:MET:O	1:H:428:ASP:C	2.57	0.42
1:I:335:LEU:HD11	1:I:343:VAL:CG2	2.49	0.42
1:I:437:ILE:N	1:I:437:ILE:CD1	2.82	0.42
1:A:726:ASP:N	1:A:727:PRO:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:ASP:OD1	1:D:225:ARG:NH1	2.37	0.42
1:E:164:LYS:HD3	1:E:189:ILE:HD11	2.02	0.42
1:H:120:ASP:N	1:H:120:ASP:OD1	2.53	0.42
1:J:298:PRO:HA	1:J:340:HIS:O	2.20	0.42
1:C:734:ASP:N	1:C:734:ASP:OD1	2.53	0.41
1:E:251:LYS:NZ	2:E:901:AGS:O2B	2.52	0.41
1:F:464:LEU:H	1:F:464:LEU:HD12	1.85	0.41
1:A:28:VAL:HG21	1:A:94:VAL:CG1	2.50	0.41
1:D:501:ASP:N	1:D:501:ASP:OD1	2.53	0.41
1:E:335:LEU:HD11	1:E:343:VAL:CG2	2.49	0.41
1:H:330:THR:O	1:H:334:GLY:N	2.52	0.41
1:K:542:ILE:CD1	1:K:562:ILE:HG21	2.50	0.41
1:K:695:CYS:SG	1:L:506:PHE:HB3	2.60	0.41
1:B:136:LYS:HB3	1:B:137:PRO:HD3	2.02	0.41
1:C:28:VAL:HG21	1:C:94:VAL:HG11	2.02	0.41
1:D:120:ASP:OD1	1:D:120:ASP:N	2.53	0.41
1:H:728:VAL:O	1:H:729:PRO:C	2.59	0.41
1:J:380:ILE:HG23	2:J:901:AGS:C2	2.50	0.41
1:K:438:ASP:OD1	1:K:438:ASP:N	2.53	0.41
1:A:95:ARG:HB2	1:A:225:ARG:NH2	2.35	0.41
1:A:501:ASP:N	1:A:501:ASP:OD1	2.53	0.41
1:C:208:GLY:HA2	1:C:376:GLY:HA2	2.02	0.41
1:C:442:MET:HA	1:C:442:MET:HE2	2.02	0.41
1:D:726:ASP:N	1:D:727:PRO:HD3	2.34	0.41
1:G:501:ASP:N	1:G:501:ASP:OD1	2.52	0.41
1:H:495:TYR:N	1:H:496:PRO:HD2	2.35	0.41
1:L:226:HIS:HB3	1:L:229:LEU:HG	2.03	0.41
1:A:512:LYS:NZ	1:A:608:MET:O	2.44	0.41
1:A:94:VAL:HG12	1:A:95:ARG:N	2.35	0.41
1:C:532:ALA:HB2	1:C:573:VAL:HG11	2.03	0.41
1:C:577:ASP:OD1	1:C:578:GLU:N	2.52	0.41
1:G:220:VAL:CG1	1:G:224:LEU:HD12	2.51	0.41
1:H:63:LYS:HG2	1:H:63:LYS:O	2.20	0.41
1:I:27:ILE:HB	1:I:81:LYS:HG2	2.02	0.41
1:C:727:PRO:C	1:C:729:PRO:HD3	2.41	0.41
1:E:577:ASP:OD1	1:E:578:GLU:N	2.52	0.41
1:G:118:PRO:HG2	1:G:188:PRO:HB3	2.03	0.41
1:G:226:HIS:HB3	1:G:229:LEU:HG	2.00	0.41
1:G:417:GLU:HG3	1:G:454:TRP:HZ3	1.85	0.41
1:H:152:PHE:CZ	1:H:163:PHE:HB2	2.56	0.41
1:J:385:THR:HB	1:J:390:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:204:ASP:N	1:L:204:ASP:OD1	2.54	0.41
1:D:158:MET:HE2	1:E:235:VAL:HG21	2.03	0.41
1:D:254:ILE:HD12	1:D:369:ILE:HD13	2.03	0.41
1:F:94:VAL:HG12	1:F:95:ARG:N	2.35	0.41
1:I:136:LYS:HB3	1:I:137:PRO:CD	2.51	0.41
1:J:220:VAL:CG1	1:J:224:LEU:HD12	2.50	0.41
1:K:122:THR:HB	1:K:161:VAL:HA	2.01	0.41
1:L:123:VAL:O	1:L:126:ILE:N	2.50	0.41
1:L:726:ASP:N	1:L:727:PRO:HD3	2.35	0.41
1:A:417:GLU:HG3	1:A:454:TRP:HZ3	1.86	0.41
1:A:710:GLU:HA	1:A:713:ARG:HD3	2.02	0.41
1:C:110:TYR:N	1:C:110:TYR:CD1	2.89	0.41
1:I:127:THR:O	1:I:439:ALA:N	2.46	0.41
1:I:417:GLU:HG3	1:I:454:TRP:HZ3	1.85	0.41
1:K:389:LYS:HD3	1:K:443:ASN:O	2.21	0.41
1:L:136:LYS:HB3	1:L:137:PRO:CD	2.51	0.41
1:B:147:ARG:HG2	1:B:173:TYR:HB3	2.01	0.41
1:B:725:ASP:C	1:B:727:PRO:HD3	2.41	0.41
1:C:629:ILE:HG12	1:C:633:ILE:HD12	2.02	0.41
1:F:243:LEU:HD22	1:F:369:ILE:HD11	2.03	0.41
1:F:380:ILE:HD12	2:F:901:AGS:N1	2.36	0.41
1:J:438:ASP:HB3	1:J:441:VAL:HB	2.03	0.41
1:J:547:LEU:HD12	1:J:582:ILE:HD11	2.03	0.41
1:K:283:GLU:OE1	1:K:323:ARG:NH1	2.53	0.41
1:A:162:GLU:OE1	1:A:191:ARG:NH2	2.54	0.41
1:A:350:PRO:O	1:A:358:ARG:NH2	2.53	0.41
1:B:59:LEU:HD22	1:B:100:ILE:HD13	2.02	0.41
1:D:573:VAL:HG23	1:D:620:ILE:HD13	2.03	0.41
1:G:495:TYR:N	1:G:496:PRO:HD2	2.36	0.41
1:A:147:ARG:HG2	1:A:173:TYR:HB3	2.03	0.41
1:B:251:LYS:NZ	2:B:901:AGS:O2B	2.51	0.41
1:G:390:LEU:HD12	1:G:390:LEU:N	2.36	0.41
1:G:86:ARG:HG3	1:G:89:ARG:NH1	2.36	0.41
1:I:158:MET:N	1:I:387:ASN:O	2.53	0.41
1:K:251:LYS:NZ	2:K:901:AGS:O1B	2.53	0.41
1:A:429:LEU:HD12	1:A:429:LEU:H	1.85	0.40
1:B:94:VAL:HG12	1:B:95:ARG:N	2.36	0.40
1:D:238:PRO:HB3	1:D:365:ARG:HE	1.86	0.40
1:E:435:GLU:CG	1:E:436:THR:H	2.35	0.40
1:G:636:PRO:HA	1:G:640:ASP:HB3	2.03	0.40
1:I:476:TRP:NE1	1:I:534:GLU:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:665:PRO:HD2	1:J:506:PHE:HA	2.04	0.40
1:J:432:LEU:HG	1:K:25:ARG:NH1	2.35	0.40
1:L:701:GLU:OE2	1:L:735:HIS:NE2	2.43	0.40
1:C:432:LEU:HG	1:C:433:GLU:N	2.36	0.40
1:H:661:LEU:HD21	1:H:691:CYS:SG	2.61	0.40
1:J:228:ALA:HA	1:J:231:LYS:HD3	2.04	0.40
1:J:384:HIS:HE1	2:J:901:AGS:N3	2.20	0.40
1:K:147:ARG:HG2	1:K:173:TYR:HB3	2.03	0.40
1:K:191:ARG:NH2	1:K:197:SER:HA	2.36	0.40
1:L:89:ARG:NH1	1:L:96:LEU:HD21	2.35	0.40
1:A:420:LEU:HD22	1:B:222:LEU:HD23	2.02	0.40
1:G:230:PHE:CE1	1:G:237:PRO:HB3	2.57	0.40
1:H:111:GLY:HA2	1:H:170:PRO:HG2	2.03	0.40
1:H:355:PRO:O	1:H:359:ARG:NH1	2.55	0.40
1:H:430:ILE:HD11	1:H:441:VAL:HG11	2.04	0.40
1:I:152:PHE:CZ	1:I:163:PHE:HB2	2.56	0.40
1:I:335:LEU:HD11	1:I:343:VAL:HG23	2.03	0.40
1:K:136:LYS:HB3	1:K:137:PRO:CD	2.52	0.40
1:K:22:ARG:CG	1:K:23:PRO:HD2	2.52	0.40
1:B:39:VAL:HG11	1:B:59:LEU:HD11	2.03	0.40
1:B:408:GLY:HA3	2:B:901:AGS:N7	2.37	0.40
1:H:136:LYS:HB3	1:H:137:PRO:HD3	2.03	0.40
1:I:120:ASP:N	1:I:120:ASP:OD1	2.54	0.40
1:L:220:VAL:CG1	1:L:224:LEU:HD12	2.52	0.40
1:L:430:ILE:HD12	1:L:430:ILE:N	2.37	0.40
1:B:380:ILE:HD12	2:B:901:AGS:C6	2.52	0.40
1:C:239:ARG:NH1	1:C:335:LEU:O	2.55	0.40
1:E:52:PHE:HD1	1:E:55:ASP:OD1	2.05	0.40
1:G:335:LEU:C	1:G:337:GLN:N	2.74	0.40
1:I:109:LYS:HD2	1:I:110:TYR:N	2.36	0.40
2:I:902:AGS:O2A	2:I:902:AGS:O2G	2.40	0.40
1:K:33:ASN:ND2	1:K:38:VAL:HG11	2.36	0.40
1:K:74:ASP:OD2	1:K:83:ARG:NE	2.48	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	729/805 (91%)	705 (97%)	23 (3%)	1 (0%)	55	88
1	B	729/805 (91%)	703 (96%)	23 (3%)	3 (0%)	38	77
1	C	729/805 (91%)	704 (97%)	23 (3%)	2 (0%)	44	81
1	D	729/805 (91%)	707 (97%)	20 (3%)	2 (0%)	44	81
1	E	729/805 (91%)	704 (97%)	20 (3%)	5 (1%)	25	68
1	F	729/805 (91%)	703 (96%)	22 (3%)	4 (0%)	32	73
1	G	729/805 (91%)	706 (97%)	22 (3%)	1 (0%)	55	88
1	H	729/805 (91%)	702 (96%)	21 (3%)	6 (1%)	22	65
1	I	727/805 (90%)	705 (97%)	21 (3%)	1 (0%)	55	88
1	J	729/805 (91%)	707 (97%)	20 (3%)	2 (0%)	44	81
1	K	740/805 (92%)	700 (95%)	27 (4%)	13 (2%)	10	50
1	L	729/805 (91%)	706 (97%)	18 (2%)	5 (1%)	25	68
All	All	8757/9660 (91%)	8452 (96%)	260 (3%)	45 (0%)	32	73

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	430	ILE
1	B	431	ASP
1	B	728	VAL
1	D	186	GLY
1	E	435	GLU
1	F	433	GLU
1	F	726	ASP
1	H	428	ASP
1	H	430	ILE
1	H	431	ASP
1	H	729	PRO
1	K	435	GLU

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Mol	Chain	Res	Type
1	K	723	GLU
1	K	724	GLU
1	K	725	ASP
1	L	433	GLU
1	A	340	HIS
1	E	728	VAL
1	F	50	GLN
1	F	435	GLU
1	J	186	GLY
1	K	707	ILE
1	K	729	PRO
1	L	435	GLU
1	D	340	HIS
1	E	431	ASP
1	H	727	PRO
1	J	340	HIS
1	K	340	HIS
1	K	717	PRO
1	G	340	HIS
1	K	431	ASP
1	L	340	HIS
1	C	340	HIS
1	E	340	HIS
1	H	340	HIS
1	K	186	GLY
1	K	720	MET
1	K	727	PRO
1	L	186	GLY
1	L	23	PRO
1	E	186	GLY
1	I	186	GLY
1	C	186	GLY
1	K	726	ASP

### 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	627/677 (93%)	584 (93%)	43 (7%)	18	56
1	B	628/677 (93%)	591 (94%)	37 (6%)	23	60
1	C	628/677 (93%)	589 (94%)	39 (6%)	21	59
1	D	628/677 (93%)	597 (95%)	31 (5%)	29	65
1	E	628/677 (93%)	590 (94%)	38 (6%)	22	60
1	F	628/677 (93%)	592 (94%)	36 (6%)	24	62
1	G	627/677 (93%)	588 (94%)	39 (6%)	21	59
1	H	628/677 (93%)	593 (94%)	35 (6%)	25	62
1	I	628/677 (93%)	583 (93%)	45 (7%)	17	54
1	J	628/677 (93%)	583 (93%)	45 (7%)	17	54
1	K	636/677 (94%)	594 (93%)	42 (7%)	19	57
1	L	628/677 (93%)	594 (95%)	34 (5%)	26	63
All	All	7542/8124 (93%)	7078 (94%)	464 (6%)	21	59

All (464) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	45	LYS
1	A	52	PHE
1	A	78	SER
1	A	79	ASP
1	A	99	VAL
1	A	107	ASP
1	A	184	CYS
1	A	193	ASP
1	A	210	ARG
1	A	229	LEU
1	A	230	PHE
1	A	231	LYS
1	A	236	LYS
1	A	278	LEU
1	A	284	SER
1	A	292	GLU
1	A	313	ARG
1	A	317	HIS
1	A	336	LYS
1	A	349	ARG
1	A	351	ASN

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Mol	Chain	Res	Type
1	A	359	ARG
1	A	392	ASP
1	A	414	LEU
1	A	416	SER
1	A	425	LYS
1	A	427	MET
1	A	428	ASP
1	A	435	GLU
1	A	437	ILE
1	A	443	ASN
1	A	464	LEU
1	A	487	ARG
1	A	505	LYS
1	A	552	PHE
1	A	556	GLU
1	A	561	GLU
1	A	573	VAL
1	A	713	ARG
1	A	732	ARG
1	A	734	ASP
1	A	762	LEU
1	B	21	ASN
1	B	25	ARG
1	B	34	GLU
1	B	45	LYS
1	B	49	LEU
1	B	53	ARG
1	B	79	ASP
1	B	99	VAL
1	B	124	GLU
1	B	131	PHE
1	B	155	ARG
1	B	184	CYS
1	B	235	VAL
1	B	236	LYS
1	B	268	LEU
1	B	278	LEU
1	B	295	LYS
1	B	313	ARG
1	B	317	HIS
1	B	349	ARG
1	B	375	THR

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Mol	Chain	Res	Type
1	B	392	ASP
1	B	416	SER
1	B	420	LEU
1	B	427	MET
1	B	429	LEU
1	B	433	GLU
1	B	464	LEU
1	B	465	ARG
1	B	487	ARG
1	B	556	GLU
1	B	706	GLU
1	B	707	ILE
1	B	714	GLN
1	B	731	ILE
1	B	737	GLU
1	B	762	LEU
1	C	45	LYS
1	C	52	PHE
1	C	99	VAL
1	C	107	ASP
1	C	109	LYS
1	C	113	ARG
1	C	130	LEU
1	C	131	PHE
1	C	173	TYR
1	C	179	ASP
1	C	184	CYS
1	C	187	GLU
1	C	230	PHE
1	C	233	ILE
1	C	235	VAL
1	C	236	LYS
1	C	288	LYS
1	C	313	ARG
1	C	317	HIS
1	C	336	LYS
1	C	349	ARG
1	C	359	ARG
1	C	420	LEU
1	C	427	MET
1	C	437	ILE
1	C	442	MET

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Mol	Chain	Res	Type
1	C	445	LEU
1	C	450	ASP
1	C	498	GLU
1	C	551	TRP
1	C	556	GLU
1	C	675	LEU
1	C	677	LYS
1	C	704	GLU
1	C	714	GLN
1	C	715	THR
1	C	732	ARG
1	C	742	PHE
1	C	762	LEU
1	D	45	LYS
1	D	52	PHE
1	D	78	SER
1	D	79	ASP
1	D	99	VAL
1	D	113	ARG
1	D	131	PHE
1	D	159	ARG
1	D	211	LYS
1	D	229	LEU
1	D	230	PHE
1	D	236	LYS
1	D	283	GLU
1	D	295	LYS
1	D	335	LEU
1	D	349	ARG
1	D	359	ARG
1	D	392	ASP
1	D	414	LEU
1	D	416	SER
1	D	425	LYS
1	D	430	ILE
1	D	435	GLU
1	D	436	THR
1	D	445	LEU
1	D	556	GLU
1	D	573	VAL
1	D	618	PHE
1	D	706	GLU

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Mol	Chain	Res	Type
1	D	745	ARG
1	D	762	LEU
1	E	49	LEU
1	E	99	VAL
1	E	107	ASP
1	E	113	ARG
1	E	124	GLU
1	E	127	THR
1	E	131	PHE
1	E	159	ARG
1	E	184	CYS
1	E	190	LYS
1	E	229	LEU
1	E	230	PHE
1	E	231	LYS
1	E	236	LYS
1	E	292	GLU
1	E	295	LYS
1	E	313	ARG
1	E	317	HIS
1	E	336	LYS
1	E	349	ARG
1	E	351	ASN
1	E	392	ASP
1	E	416	SER
1	E	420	LEU
1	E	428	ASP
1	E	429	LEU
1	E	435	GLU
1	E	445	LEU
1	E	464	LEU
1	E	487	ARG
1	E	508	MET
1	E	509	THR
1	E	556	GLU
1	E	573	VAL
1	E	669	ASP
1	E	713	ARG
1	E	734	ASP
1	E	762	LEU
1	F	45	LYS
1	F	52	PHE

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Mol	Chain	Res	Type
1	F	53	ARG
1	F	99	VAL
1	F	112	LYS
1	F	126	ILE
1	F	130	LEU
1	F	131	PHE
1	F	173	TYR
1	F	184	CYS
1	F	210	ARG
1	F	213	LEU
1	F	222	LEU
1	F	230	PHE
1	F	236	LYS
1	F	274	ILE
1	F	287	ARG
1	F	292	GLU
1	F	295	LYS
1	F	313	ARG
1	F	317	HIS
1	F	338	ARG
1	F	349	ARG
1	F	359	ARG
1	F	392	ASP
1	F	402	GLU
1	F	420	LEU
1	F	431	ASP
1	F	437	ILE
1	F	464	LEU
1	F	505	LYS
1	F	556	GLU
1	F	704	GLU
1	F	711	ARG
1	F	734	ASP
1	F	762	LEU
1	G	21	ASN
1	G	22	ARG
1	G	45	LYS
1	G	52	PHE
1	G	78	SER
1	G	99	VAL
1	G	107	ASP
1	G	113	ARG

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Mol	Chain	Res	Type
1	G	159	ARG
1	G	184	CYS
1	G	193	ASP
1	G	211	LYS
1	G	229	LEU
1	G	231	LYS
1	G	236	LYS
1	G	284	SER
1	G	292	GLU
1	G	317	HIS
1	G	319	GLU
1	G	349	ARG
1	G	359	ARG
1	G	378	LEU
1	G	392	ASP
1	G	414	LEU
1	G	416	SER
1	G	425	LYS
1	G	427	MET
1	G	428	ASP
1	G	435	GLU
1	G	437	ILE
1	G	438	ASP
1	G	442	MET
1	G	464	LEU
1	G	551	TRP
1	G	552	PHE
1	G	556	GLU
1	G	703	ILE
1	G	734	ASP
1	G	762	LEU
1	H	21	ASN
1	H	45	LYS
1	H	49	LEU
1	H	79	ASP
1	H	99	VAL
1	H	109	LYS
1	H	124	GLU
1	H	131	PHE
1	H	155	ARG
1	H	159	ARG
1	H	184	CYS

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Mol	Chain	Res	Type
1	H	211	LYS
1	H	229	LEU
1	H	236	LYS
1	H	256	ARG
1	H	261	GLU
1	H	268	LEU
1	H	313	ARG
1	H	317	HIS
1	H	349	ARG
1	H	359	ARG
1	H	392	ASP
1	H	420	LEU
1	H	425	LYS
1	H	433	GLU
1	H	445	LEU
1	H	464	LEU
1	H	468	VAL
1	H	487	ARG
1	H	556	GLU
1	H	668	LYS
1	H	700	ARG
1	H	711	ARG
1	H	731	ILE
1	H	762	LEU
1	I	22	ARG
1	I	45	LYS
1	I	52	PHE
1	I	53	ARG
1	I	80	GLU
1	I	99	VAL
1	I	107	ASP
1	I	109	LYS
1	I	112	LYS
1	I	113	ARG
1	I	130	LEU
1	I	131	PHE
1	I	173	TYR
1	I	184	CYS
1	I	229	LEU
1	I	230	PHE
1	I	233	ILE
1	I	236	LYS

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Mol	Chain	Res	Type
1	I	292	GLU
1	I	336	LYS
1	I	349	ARG
1	I	359	ARG
1	I	392	ASP
1	I	416	SER
1	I	420	LEU
1	I	427	MET
1	I	433	GLU
1	I	435	GLU
1	I	436	THR
1	I	437	ILE
1	I	442	MET
1	I	498	GLU
1	I	505	LYS
1	I	556	GLU
1	I	614	LYS
1	I	615	LYS
1	I	675	LEU
1	I	689	GLU
1	I	712	GLU
1	I	715	THR
1	I	732	ARG
1	I	741	ARG
1	I	742	PHE
1	I	745	ARG
1	I	762	LEU
1	J	21	ASN
1	J	25	ARG
1	J	45	LYS
1	J	52	PHE
1	J	64	ARG
1	J	79	ASP
1	J	99	VAL
1	J	113	ARG
1	J	131	PHE
1	J	159	ARG
1	J	184	CYS
1	J	211	LYS
1	J	229	LEU
1	J	230	PHE
1	J	236	LYS

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Mol	Chain	Res	Type
1	J	295	LYS
1	J	335	LEU
1	J	336	LYS
1	J	349	ARG
1	J	359	ARG
1	J	392	ASP
1	J	414	LEU
1	J	416	SER
1	J	425	LYS
1	J	427	MET
1	J	429	LEU
1	J	430	ILE
1	J	432	LEU
1	J	435	GLU
1	J	436	THR
1	J	445	LEU
1	J	450	ASP
1	J	460	ASN
1	J	464	LEU
1	J	487	ARG
1	J	556	GLU
1	J	573	VAL
1	J	618	PHE
1	J	689	GLU
1	J	705	SER
1	J	711	ARG
1	J	715	THR
1	J	730	GLU
1	J	738	GLU
1	J	762	LEU
1	K	22	ARG
1	K	49	LEU
1	K	64	ARG
1	K	79	ASP
1	K	90	ASN
1	K	99	VAL
1	K	109	LYS
1	K	113	ARG
1	K	124	GLU
1	K	127	THR
1	K	131	PHE
1	K	132	GLU

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Mol	Chain	Res	Type
1	K	190	LYS
1	K	191	ARG
1	K	236	LYS
1	K	261	GLU
1	K	313	ARG
1	K	349	ARG
1	K	392	ASP
1	K	416	SER
1	K	420	LEU
1	K	425	LYS
1	K	428	ASP
1	K	429	LEU
1	K	435	GLU
1	K	445	LEU
1	K	464	LEU
1	K	468	VAL
1	K	477	GLU
1	K	487	ARG
1	K	509	THR
1	K	556	GLU
1	K	573	VAL
1	K	669	ASP
1	K	700	ARG
1	K	707	ILE
1	K	722	VAL
1	K	723	GLU
1	K	732	ARG
1	K	734	ASP
1	K	762	LEU
1	K	768	PHE
1	L	22	ARG
1	L	45	LYS
1	L	52	PHE
1	L	53	ARG
1	L	99	VAL
1	L	126	ILE
1	L	131	PHE
1	L	141	GLU
1	L	173	TYR
1	L	184	CYS
1	L	187	GLU
1	L	190	LYS

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Mol	Chain	Res	Type
1	L	222	LEU
1	L	230	PHE
1	L	236	LYS
1	L	274	ILE
1	L	287	ARG
1	L	319	GLU
1	L	336	LYS
1	L	338	ARG
1	L	349	ARG
1	L	359	ARG
1	L	401	ASN
1	L	402	GLU
1	L	420	LEU
1	L	431	ASP
1	L	442	MET
1	L	464	LEU
1	L	465	ARG
1	L	505	LYS
1	L	556	GLU
1	L	675	LEU
1	L	734	ASP
1	L	762	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	406	HIS
1	I	340	HIS

### 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

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 for Mogul analysis.

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	AGS	A	901	3	26,33,33	1.51	7 (26%)	22,52,52	2.41	3 (13%)
2	AGS	A	902	3	26,33,33	1.37	6 (23%)	22,52,52	2.41	4 (18%)
2	AGS	B	901	3	26,33,33	1.39	5 (19%)	22,52,52	2.33	3 (13%)
2	AGS	B	902	3	26,33,33	1.40	6 (23%)	22,52,52	2.52	4 (18%)
2	AGS	C	901	3	26,33,33	1.39	6 (23%)	22,52,52	2.44	3 (13%)
2	AGS	C	902	3	26,33,33	1.40	6 (23%)	22,52,52	2.37	3 (13%)
2	AGS	D	901	3	26,33,33	1.40	6 (23%)	22,52,52	2.40	3 (13%)
2	AGS	D	902	3	26,33,33	1.39	5 (19%)	22,52,52	2.39	3 (13%)
2	AGS	E	901	3	26,33,33	1.52	7 (26%)	22,52,52	2.42	4 (18%)
2	AGS	E	902	3	26,33,33	1.38	4 (15%)	22,52,52	2.28	3 (13%)
2	AGS	F	901	3	26,33,33	1.38	5 (19%)	22,52,52	2.43	3 (13%)
2	AGS	F	902	3	26,33,33	1.35	6 (23%)	22,52,52	2.54	4 (18%)
2	AGS	G	901	3	26,33,33	1.45	7 (26%)	22,52,52	2.47	3 (13%)
2	AGS	G	902	3	26,33,33	1.41	6 (23%)	22,52,52	2.47	4 (18%)
2	AGS	H	901	3	26,33,33	1.41	6 (23%)	22,52,52	2.38	4 (18%)
2	AGS	H	902	3	26,33,33	1.33	5 (19%)	22,52,52	2.49	4 (18%)
2	AGS	I	901	3	26,33,33	1.40	6 (23%)	22,52,52	2.32	4 (18%)
2	AGS	I	902	3	26,33,33	1.41	5 (19%)	22,52,52	2.41	4 (18%)
2	AGS	J	901	3	26,33,33	1.49	6 (23%)	22,52,52	2.40	5 (22%)
2	AGS	J	902	3	26,33,33	1.31	5 (19%)	22,52,52	2.59	2 (9%)
2	AGS	K	901	3	26,33,33	1.44	6 (23%)	22,52,52	2.38	4 (18%)
2	AGS	K	902	3	26,33,33	1.42	5 (19%)	22,52,52	2.47	4 (18%)
2	AGS	L	901	3	26,33,33	1.42	6 (23%)	22,52,52	2.55	3 (13%)
2	AGS	L	902	3	26,33,33	1.37	6 (23%)	22,52,52	2.48	3 (13%)

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	AGS	A	901	3	-	0/17/38/38	0/3/3/3
2	AGS	A	902	3	-	0/17/38/38	0/3/3/3
2	AGS	B	901	3	-	0/17/38/38	0/3/3/3
2	AGS	B	902	3	-	0/17/38/38	0/3/3/3
2	AGS	C	901	3	-	0/17/38/38	0/3/3/3
2	AGS	C	902	3	-	0/17/38/38	0/3/3/3
2	AGS	D	901	3	-	0/17/38/38	0/3/3/3
2	AGS	D	902	3	-	0/17/38/38	0/3/3/3
2	AGS	E	901	3	-	0/17/38/38	0/3/3/3
2	AGS	E	902	3	-	0/17/38/38	0/3/3/3
2	AGS	F	901	3	-	0/17/38/38	0/3/3/3
2	AGS	F	902	3	-	0/17/38/38	0/3/3/3
2	AGS	G	901	3	-	0/17/38/38	0/3/3/3
2	AGS	G	902	3	-	0/17/38/38	0/3/3/3
2	AGS	H	901	3	-	0/17/38/38	0/3/3/3
2	AGS	H	902	3	-	0/17/38/38	0/3/3/3
2	AGS	I	901	3	-	0/17/38/38	0/3/3/3
2	AGS	I	902	3	-	0/17/38/38	0/3/3/3
2	AGS	J	901	3	-	0/17/38/38	0/3/3/3
2	AGS	J	902	3	-	0/17/38/38	0/3/3/3
2	AGS	K	901	3	-	0/17/38/38	0/3/3/3
2	AGS	K	902	3	-	0/17/38/38	0/3/3/3
2	AGS	L	901	3	-	0/17/38/38	0/3/3/3
2	AGS	L	902	3	-	0/17/38/38	0/3/3/3

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	901	AGS	O2'-C2'	-2.70	1.36	1.43
2	E	901	AGS	O2'-C2'	-2.57	1.37	1.43
2	A	901	AGS	O2'-C2'	-2.55	1.37	1.43
2	F	901	AGS	O2'-C2'	-2.52	1.37	1.43
2	I	902	AGS	O2'-C2'	-2.50	1.37	1.43
2	K	902	AGS	C2'-C3'	-2.50	1.46	1.53
2	K	902	AGS	O2'-C2'	-2.50	1.37	1.43
2	B	902	AGS	C2'-C3'	-2.48	1.46	1.53
2	B	902	AGS	O2'-C2'	-2.45	1.37	1.43
2	L	902	AGS	O2'-C2'	-2.44	1.37	1.43
2	A	902	AGS	O2'-C2'	-2.42	1.37	1.43
2	G	902	AGS	O2'-C2'	-2.40	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	AGS	O2'-C2'	-2.39	1.37	1.43
2	C	902	AGS	O2'-C2'	-2.37	1.37	1.43
2	L	901	AGS	O2'-C2'	-2.37	1.37	1.43
2	D	901	AGS	O2'-C2'	-2.37	1.37	1.43
2	G	901	AGS	O2'-C2'	-2.37	1.37	1.43
2	B	901	AGS	O2'-C2'	-2.37	1.37	1.43
2	H	901	AGS	O2'-C2'	-2.35	1.37	1.43
2	I	901	AGS	O2'-C2'	-2.34	1.37	1.43
2	K	901	AGS	O2'-C2'	-2.33	1.37	1.43
2	A	901	AGS	O3'-C3'	-2.31	1.37	1.43
2	G	902	AGS	C2'-C3'	-2.31	1.47	1.53
2	C	902	AGS	C2'-C3'	-2.30	1.47	1.53
2	E	901	AGS	C2'-C3'	-2.30	1.47	1.53
2	J	901	AGS	C2'-C3'	-2.30	1.47	1.53
2	D	902	AGS	O2'-C2'	-2.29	1.37	1.43
2	H	901	AGS	O3'-C3'	-2.28	1.37	1.43
2	C	901	AGS	C2'-C3'	-2.28	1.47	1.53
2	E	901	AGS	O3'-C3'	-2.27	1.37	1.43
2	F	902	AGS	O2'-C2'	-2.26	1.37	1.43
2	H	902	AGS	O2'-C2'	-2.25	1.37	1.43
2	L	901	AGS	O3'-C3'	-2.25	1.37	1.43
2	K	901	AGS	O3'-C3'	-2.25	1.37	1.43
2	K	902	AGS	O3'-C3'	-2.24	1.37	1.43
2	G	901	AGS	O3'-C3'	-2.23	1.37	1.43
2	L	902	AGS	C2'-C3'	-2.22	1.47	1.53
2	F	901	AGS	O3'-C3'	-2.20	1.37	1.43
2	L	901	AGS	C2'-C3'	-2.19	1.47	1.53
2	B	902	AGS	O3'-C3'	-2.19	1.37	1.43
2	G	901	AGS	C2'-C3'	-2.19	1.47	1.53
2	F	902	AGS	C2'-C3'	-2.19	1.47	1.53
2	H	901	AGS	C2'-C3'	-2.19	1.47	1.53
2	D	901	AGS	C2'-C3'	-2.18	1.47	1.53
2	H	902	AGS	C2'-C3'	-2.18	1.47	1.53
2	B	901	AGS	O3'-C3'	-2.18	1.37	1.43
2	J	901	AGS	O3'-C3'	-2.15	1.38	1.43
2	I	901	AGS	C2'-C3'	-2.15	1.47	1.53
2	F	901	AGS	C2'-C3'	-2.14	1.47	1.53
2	C	901	AGS	O3'-C3'	-2.13	1.38	1.43
2	L	902	AGS	O3'-C3'	-2.13	1.38	1.43
2	I	902	AGS	O3'-C3'	-2.12	1.38	1.43
2	A	902	AGS	O3'-C3'	-2.11	1.38	1.43
2	E	902	AGS	O2'-C2'	-2.11	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	902	AGS	O3'-C3'	-2.11	1.38	1.43
2	G	902	AGS	O3'-C3'	-2.09	1.38	1.43
2	A	901	AGS	C2'-C3'	-2.09	1.47	1.53
2	D	902	AGS	O3'-C3'	-2.08	1.38	1.43
2	J	902	AGS	O2'-C2'	-2.07	1.38	1.43
2	H	902	AGS	O3'-C3'	-2.07	1.38	1.43
2	A	901	AGS	C2'-C1'	-2.07	1.50	1.53
2	D	901	AGS	O3'-C3'	-2.06	1.38	1.43
2	K	901	AGS	C2'-C3'	-2.06	1.48	1.53
2	G	901	AGS	C2'-C1'	-2.05	1.50	1.53
2	A	902	AGS	C2'-C3'	-2.05	1.48	1.53
2	F	902	AGS	O3'-C3'	-2.03	1.38	1.43
2	I	901	AGS	O3'-C3'	-2.03	1.38	1.43
2	E	901	AGS	C2'-C1'	-2.02	1.50	1.53
2	J	902	AGS	O3'-C3'	-2.01	1.38	1.43
2	B	902	AGS	PG-S1G	2.01	1.94	1.90
2	L	902	AGS	PG-S1G	2.09	1.94	1.90
2	A	902	AGS	PG-S1G	2.10	1.94	1.90
2	C	902	AGS	PG-S1G	2.21	1.94	1.90
2	L	901	AGS	PG-S1G	2.26	1.94	1.90
2	J	902	AGS	PG-S1G	2.35	1.95	1.90
2	I	901	AGS	C6-N6	2.35	1.43	1.34
2	I	902	AGS	PG-S1G	2.36	1.95	1.90
2	D	902	AGS	PG-S1G	2.36	1.95	1.90
2	J	901	AGS	C6-N6	2.39	1.43	1.34
2	A	901	AGS	C6-N6	2.41	1.44	1.34
2	B	901	AGS	C6-N6	2.42	1.44	1.34
2	G	902	AGS	PG-S1G	2.44	1.95	1.90
2	F	901	AGS	C6-N6	2.46	1.44	1.34
2	G	901	AGS	C6-N6	2.48	1.44	1.34
2	C	901	AGS	C6-N6	2.49	1.44	1.34
2	B	901	AGS	PG-S1G	2.49	1.95	1.90
2	J	902	AGS	C6-N6	2.50	1.44	1.34
2	K	902	AGS	C6-N6	2.50	1.44	1.34
2	J	901	AGS	PG-S1G	2.50	1.95	1.90
2	K	901	AGS	C6-N6	2.50	1.44	1.34
2	E	901	AGS	C6-N6	2.51	1.44	1.34
2	K	901	AGS	PG-S1G	2.52	1.95	1.90
2	H	901	AGS	C6-N6	2.53	1.44	1.34
2	F	902	AGS	PG-S1G	2.54	1.95	1.90
2	L	901	AGS	C6-N6	2.54	1.44	1.34
2	D	901	AGS	PG-S1G	2.55	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	901	AGS	PG-S1G	2.56	1.95	1.90
2	A	901	AGS	PG-S1G	2.58	1.95	1.90
2	F	902	AGS	C6-N6	2.58	1.44	1.34
2	L	902	AGS	C6-N6	2.58	1.44	1.34
2	E	902	AGS	C6-N6	2.59	1.44	1.34
2	D	901	AGS	C6-N6	2.59	1.44	1.34
2	A	902	AGS	C6-N6	2.59	1.44	1.34
2	C	902	AGS	C6-N6	2.61	1.44	1.34
2	B	902	AGS	C6-N6	2.62	1.44	1.34
2	G	902	AGS	C6-N6	2.64	1.44	1.34
2	I	902	AGS	C6-N6	2.65	1.44	1.34
2	H	902	AGS	C6-N6	2.65	1.45	1.34
2	C	901	AGS	PG-S1G	2.65	1.95	1.90
2	G	901	AGS	PG-S1G	2.67	1.95	1.90
2	D	902	AGS	C6-N6	2.68	1.45	1.34
2	I	901	AGS	PG-S1G	2.74	1.95	1.90
2	B	902	AGS	C2-N3	2.75	1.36	1.32
2	C	901	AGS	C2-N3	2.78	1.36	1.32
2	E	902	AGS	PG-S1G	2.79	1.95	1.90
2	G	901	AGS	C2-N3	2.79	1.36	1.32
2	K	902	AGS	C2-N3	2.79	1.36	1.32
2	I	901	AGS	C2-N3	2.82	1.36	1.32
2	E	901	AGS	PG-S1G	2.87	1.96	1.90
2	J	901	AGS	C2-N3	2.91	1.37	1.32
2	F	901	AGS	C2-N3	2.91	1.37	1.32
2	A	902	AGS	C2-N3	2.95	1.37	1.32
2	B	901	AGS	C2-N3	3.00	1.37	1.32
2	L	901	AGS	C2-N3	3.02	1.37	1.32
2	A	901	AGS	C2-N3	3.03	1.37	1.32
2	K	901	AGS	C2-N3	3.04	1.37	1.32
2	H	901	AGS	C2-N3	3.07	1.37	1.32
2	J	902	AGS	C2-N3	3.07	1.37	1.32
2	G	902	AGS	C2-N3	3.09	1.37	1.32
2	E	901	AGS	C2-N3	3.09	1.37	1.32
2	L	902	AGS	C2-N3	3.11	1.37	1.32
2	D	901	AGS	C2-N3	3.12	1.37	1.32
2	H	902	AGS	C2-N3	3.15	1.37	1.32
2	C	902	AGS	C2-N3	3.24	1.37	1.32
2	F	902	AGS	C2-N3	3.24	1.37	1.32
2	D	902	AGS	C2-N3	3.28	1.37	1.32
2	E	902	AGS	C2-N3	3.35	1.37	1.32
2	I	902	AGS	C2-N3	3.37	1.37	1.32

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	902	AGS	N3-C2-N1	-10.51	119.70	128.86
2	J	902	AGS	N3-C2-N1	-10.41	119.79	128.86
2	L	901	AGS	N3-C2-N1	-10.31	119.88	128.86
2	B	902	AGS	N3-C2-N1	-10.21	119.96	128.86
2	G	901	AGS	N3-C2-N1	-10.19	119.98	128.86
2	L	902	AGS	N3-C2-N1	-10.11	120.06	128.86
2	H	902	AGS	N3-C2-N1	-10.09	120.07	128.86
2	C	902	AGS	N3-C2-N1	-10.02	120.13	128.86
2	G	902	AGS	N3-C2-N1	-10.01	120.14	128.86
2	A	902	AGS	N3-C2-N1	-10.01	120.14	128.86
2	I	902	AGS	N3-C2-N1	-10.00	120.15	128.86
2	K	902	AGS	N3-C2-N1	-9.97	120.18	128.86
2	A	901	AGS	N3-C2-N1	-9.94	120.20	128.86
2	E	901	AGS	N3-C2-N1	-9.92	120.22	128.86
2	D	901	AGS	N3-C2-N1	-9.91	120.22	128.86
2	K	901	AGS	N3-C2-N1	-9.82	120.31	128.86
2	D	902	AGS	N3-C2-N1	-9.80	120.32	128.86
2	J	901	AGS	N3-C2-N1	-9.77	120.35	128.86
2	F	901	AGS	N3-C2-N1	-9.70	120.41	128.86
2	C	901	AGS	N3-C2-N1	-9.63	120.47	128.86
2	I	901	AGS	N3-C2-N1	-9.57	120.53	128.86
2	E	902	AGS	N3-C2-N1	-9.46	120.62	128.86
2	H	901	AGS	N3-C2-N1	-9.39	120.68	128.86
2	B	901	AGS	N3-C2-N1	-9.19	120.86	128.86
2	J	902	AGS	PB-O3B-PG	-4.87	116.60	132.35
2	B	901	AGS	PB-O3B-PG	-4.18	118.84	132.35
2	L	901	AGS	PB-O3B-PG	-4.14	118.97	132.35
2	C	901	AGS	PB-O3B-PG	-4.14	118.98	132.35
2	H	901	AGS	PB-O3B-PG	-4.06	119.24	132.35
2	B	902	AGS	PB-O3B-PG	-4.02	119.37	132.35
2	G	902	AGS	PB-O3B-PG	-4.01	119.39	132.35
2	K	902	AGS	PB-O3B-PG	-3.85	119.90	132.35
2	H	902	AGS	PB-O3B-PG	-3.84	119.94	132.35
2	L	902	AGS	PB-O3B-PG	-3.83	119.98	132.35
2	D	902	AGS	PB-O3B-PG	-3.75	120.24	132.35
2	G	901	AGS	PB-O3B-PG	-3.67	120.50	132.35
2	F	901	AGS	PB-O3B-PG	-3.58	120.78	132.35
2	A	901	AGS	PB-O3B-PG	-3.58	120.78	132.35
2	K	901	AGS	PB-O3B-PG	-3.46	121.18	132.35
2	D	901	AGS	PB-O3B-PG	-3.28	121.76	132.35
2	I	901	AGS	PB-O3B-PG	-3.12	122.26	132.35
2	E	901	AGS	PB-O3B-PG	-3.09	122.38	132.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	902	AGS	PB-O3B-PG	-3.00	122.66	132.35
2	A	902	AGS	PB-O3B-PG	-2.97	122.76	132.35
2	J	901	AGS	PB-O3B-PG	-2.95	122.83	132.35
2	I	902	AGS	PB-O3B-PG	-2.92	122.91	132.35
2	E	902	AGS	PB-O3B-PG	-2.85	123.15	132.35
2	C	902	AGS	PB-O3B-PG	-2.78	123.36	132.35
2	H	901	AGS	C4-C5-N7	-2.55	106.94	109.41
2	L	902	AGS	C4-C5-N7	-2.51	106.98	109.41
2	E	902	AGS	C4-C5-N7	-2.48	107.02	109.41
2	A	902	AGS	C4-C5-N7	-2.41	107.08	109.41
2	K	902	AGS	C4-C5-N7	-2.39	107.10	109.41
2	D	901	AGS	C4-C5-N7	-2.32	107.16	109.41
2	H	902	AGS	C4-C5-N7	-2.26	107.22	109.41
2	B	902	AGS	C4-C5-N7	-2.26	107.23	109.41
2	D	902	AGS	C4-C5-N7	-2.21	107.28	109.41
2	K	901	AGS	C4-C5-N7	-2.20	107.28	109.41
2	J	901	AGS	C4-C5-N7	-2.19	107.30	109.41
2	I	902	AGS	C4-C5-N7	-2.16	107.32	109.41
2	B	901	AGS	C4-C5-N7	-2.13	107.35	109.41
2	G	902	AGS	C4-C5-N7	-2.11	107.37	109.41
2	I	901	AGS	C4-C5-N7	-2.09	107.39	109.41
2	C	902	AGS	C4-C5-N7	-2.08	107.40	109.41
2	J	901	AGS	C4'-O4'-C1'	-2.08	107.56	109.77
2	F	902	AGS	C4-C5-N7	-2.05	107.42	109.41
2	E	901	AGS	C4-C5-N7	-2.00	107.48	109.41
2	H	902	AGS	O4'-C4'-C3'	2.08	109.30	105.17
2	K	901	AGS	O4'-C4'-C3'	2.11	109.35	105.17
2	A	902	AGS	O4'-C4'-C3'	2.11	109.35	105.17
2	B	902	AGS	O4'-C4'-C3'	2.14	109.42	105.17
2	G	902	AGS	O4'-C4'-C3'	2.15	109.44	105.17
2	I	902	AGS	O4'-C4'-C3'	2.16	109.46	105.17
2	F	902	AGS	O4'-C4'-C3'	2.21	109.55	105.17
2	C	901	AGS	O4'-C4'-C3'	2.32	109.78	105.17
2	K	902	AGS	O4'-C4'-C3'	2.32	109.78	105.17
2	H	901	AGS	O4'-C4'-C3'	2.34	109.81	105.17
2	A	901	AGS	O4'-C4'-C3'	2.37	109.87	105.17
2	L	901	AGS	O4'-C4'-C3'	2.39	109.93	105.17
2	F	901	AGS	O4'-C4'-C3'	2.43	110.00	105.17
2	G	901	AGS	O4'-C4'-C3'	2.45	110.05	105.17
2	J	901	AGS	O4'-C4'-C3'	2.60	110.34	105.17
2	I	901	AGS	O4'-C4'-C3'	2.62	110.37	105.17
2	E	901	AGS	O4'-C4'-C3'	2.71	110.56	105.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	AGS	3	0
2	B	902	AGS	1	0
2	C	901	AGS	2	0
2	C	902	AGS	1	0
2	E	901	AGS	2	0
2	E	902	AGS	1	0
2	F	901	AGS	5	0
2	F	902	AGS	1	0
2	G	901	AGS	1	0
2	G	902	AGS	1	0
2	H	901	AGS	1	0
2	I	901	AGS	2	0
2	I	902	AGS	2	0
2	J	901	AGS	2	0
2	J	902	AGS	2	0
2	K	901	AGS	1	0
2	K	902	AGS	1	0
2	L	901	AGS	2	0
2	L	902	AGS	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	728:VAL	C	729:PRO	N	3.06

## 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	735/805 (91%)	0.27	23 (3%)	49	39	104, 177, 239, 332	0
1	B	735/805 (91%)	0.25	20 (2%)	55	44	101, 170, 246, 376	0
1	C	735/805 (91%)	0.30	27 (3%)	42	34	112, 181, 249, 329	0
1	D	735/805 (91%)	0.46	63 (8%)	11	9	118, 195, 263, 337	0
1	E	735/805 (91%)	0.22	19 (2%)	56	46	105, 173, 252, 352	0
1	F	735/805 (91%)	0.21	21 (2%)	52	42	98, 170, 249, 333	0
1	G	735/805 (91%)	0.24	16 (2%)	62	53	104, 173, 246, 315	0
1	H	735/805 (91%)	0.28	23 (3%)	49	39	104, 178, 245, 307	0
1	I	735/805 (91%)	0.33	34 (4%)	33	26	115, 185, 262, 351	0
1	J	735/805 (91%)	0.29	31 (4%)	37	29	109, 179, 240, 435	0
1	K	744/805 (92%)	0.35	43 (5%)	24	18	98, 173, 255, 362	0
1	L	735/805 (91%)	0.25	23 (3%)	49	39	100, 170, 243, 341	0
All	All	8829/9660 (91%)	0.29	343 (3%)	40	32	98, 177, 250, 435	0

All (343) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	770	SER	8.4
1	J	435	GLU	7.7
1	K	21	ASN	6.3
1	A	434	ASP	5.9
1	C	435	GLU	5.4
1	B	436	THR	5.0
1	J	434	ASP	4.8
1	J	436	THR	4.8
1	C	436	THR	4.7
1	K	427	MET	4.6
1	B	432	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	L	134	TYR	4.5
1	J	437	ILE	4.5
1	J	725	ASP	4.4
1	D	146	ILE	4.4
1	D	108	VAL	4.3
1	D	26	LEU	4.3
1	C	99	VAL	4.2
1	C	62	LYS	4.2
1	C	100	ILE	4.1
1	D	736	PHE	4.1
1	F	667	ALA	4.1
1	A	770	SER	4.1
1	I	745	ARG	4.0
1	G	108	VAL	4.0
1	H	435	GLU	4.0
1	L	726	ASP	4.0
1	D	69	CYS	3.9
1	J	726	ASP	3.9
1	C	552	PHE	3.9
1	H	116	VAL	3.9
1	B	21	ASN	3.9
1	K	24	ASN	3.9
1	I	116	VAL	3.9
1	F	23	PRO	3.8
1	I	63	LYS	3.8
1	F	433	GLU	3.8
1	D	49	LEU	3.8
1	G	736	PHE	3.8
1	L	162	GLU	3.7
1	L	176	VAL	3.7
1	B	117	LEU	3.7
1	K	23	PRO	3.7
1	A	340	HIS	3.6
1	L	116	VAL	3.6
1	E	736	PHE	3.6
1	C	460	ASN	3.6
1	D	434	ASP	3.6
1	K	134	TYR	3.5
1	K	116	VAL	3.5
1	B	428	ASP	3.5
1	I	679	THR	3.5
1	E	770	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	26	LEU	3.5
1	D	92	LEU	3.5
1	D	56	THR	3.5
1	K	102	ILE	3.5
1	D	731	ILE	3.4
1	I	731	ILE	3.4
1	D	235	VAL	3.4
1	E	40	SER	3.4
1	D	105	CYS	3.4
1	F	435	GLU	3.4
1	K	722	VAL	3.3
1	D	164	LYS	3.3
1	J	52	PHE	3.3
1	I	186	GLY	3.3
1	L	119	ILE	3.3
1	D	100	ILE	3.3
1	I	770	SER	3.3
1	A	621	GLY	3.3
1	J	135	LEU	3.2
1	D	672	LEU	3.2
1	D	51	LEU	3.2
1	B	731	ILE	3.2
1	D	71	VAL	3.2
1	D	681	GLY	3.1
1	I	127	THR	3.1
1	F	666	VAL	3.1
1	H	51	LEU	3.1
1	E	768	PHE	3.1
1	D	37	SER	3.1
1	K	176	VAL	3.1
1	L	164	LYS	3.1
1	A	67	ALA	3.1
1	I	508	MET	3.0
1	K	117	LEU	3.0
1	K	51	LEU	3.0
1	D	67	ALA	3.0
1	K	53	ARG	3.0
1	B	126	ILE	3.0
1	B	666	VAL	3.0
1	D	437	ILE	3.0
1	D	712	GLU	3.0
1	E	437	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	102	ILE	2.9
1	A	41	LEU	2.9
1	J	164	LYS	2.9
1	D	59	LEU	2.9
1	B	152	PHE	2.9
1	A	435	GLU	2.9
1	D	70	ILE	2.9
1	D	682	PHE	2.9
1	A	82	ILE	2.9
1	J	186	GLY	2.9
1	K	118	PRO	2.9
1	K	426	LYS	2.8
1	H	731	ILE	2.8
1	E	427	MET	2.8
1	H	102	ILE	2.8
1	I	26	LEU	2.8
1	I	552	PHE	2.8
1	C	731	ILE	2.8
1	K	164	LYS	2.8
1	C	45	LYS	2.8
1	L	133	VAL	2.8
1	E	436	THR	2.8
1	C	164	LYS	2.8
1	E	494	GLN	2.8
1	E	432	LEU	2.8
1	K	718	SER	2.8
1	B	116	VAL	2.7
1	D	730	GLU	2.7
1	L	725	ASP	2.7
1	L	730	GLU	2.7
1	D	758	PHE	2.7
1	K	135	LEU	2.7
1	D	139	PHE	2.7
1	K	726	ASP	2.7
1	A	682	PHE	2.7
1	B	712	GLU	2.7
1	D	679	THR	2.7
1	K	25	ARG	2.7
1	K	166	VAL	2.7
1	A	437	ILE	2.7
1	J	56	THR	2.7
1	I	739	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	116	VAL	2.7
1	K	708	ARG	2.6
1	I	428	ASP	2.6
1	F	731	ILE	2.6
1	K	100	ILE	2.6
1	F	53	ARG	2.6
1	L	37	SER	2.6
1	H	768	PHE	2.6
1	H	694	ALA	2.6
1	J	182	ILE	2.6
1	E	675	LEU	2.6
1	A	46	MET	2.6
1	A	51	LEU	2.6
1	D	645	ILE	2.6
1	G	682	PHE	2.6
1	C	429	LEU	2.6
1	I	678	MET	2.6
1	K	39	VAL	2.6
1	D	104	PRO	2.6
1	G	41	LEU	2.6
1	L	115	HIS	2.6
1	G	164	LYS	2.6
1	L	36	ASN	2.6
1	B	233	ILE	2.6
1	D	103	GLN	2.6
1	H	100	ILE	2.6
1	D	480	GLY	2.6
1	K	70	ILE	2.6
1	D	38	VAL	2.6
1	D	154	VAL	2.6
1	I	71	VAL	2.5
1	K	99	VAL	2.5
1	C	594	GLY	2.5
1	K	139	PHE	2.5
1	K	719	ALA	2.5
1	E	39	VAL	2.5
1	C	134	TYR	2.5
1	J	53	ARG	2.5
1	A	765	SER	2.5
1	B	99	VAL	2.5
1	J	21	ASN	2.5
1	L	165	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	269	ILE	2.5
1	B	460	ASN	2.5
1	J	139	PHE	2.5
1	E	762	LEU	2.5
1	K	506	PHE	2.5
1	F	736	PHE	2.5
1	K	725	ASP	2.5
1	E	498	GLU	2.5
1	I	682	PHE	2.5
1	H	503	PHE	2.5
1	F	670	VAL	2.5
1	I	165	VAL	2.5
1	B	552	PHE	2.5
1	B	708	ARG	2.5
1	F	52	PHE	2.5
1	K	71	VAL	2.4
1	G	172	PRO	2.4
1	J	516	PHE	2.4
1	D	57	VAL	2.4
1	F	768	PHE	2.4
1	K	56	THR	2.4
1	H	41	LEU	2.4
1	I	114	ILE	2.4
1	E	731	ILE	2.4
1	D	68	VAL	2.4
1	L	715	THR	2.4
1	K	720	MET	2.4
1	C	622	ALA	2.4
1	H	729	PRO	2.4
1	I	452	PHE	2.4
1	D	72	LEU	2.4
1	D	36	ASN	2.4
1	C	130	LEU	2.4
1	J	51	LEU	2.4
1	D	66	GLU	2.4
1	K	716	ASN	2.4
1	K	103	GLN	2.3
1	G	672	LEU	2.3
1	H	666	VAL	2.3
1	A	726	ASP	2.3
1	E	765	SER	2.3
1	L	710	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	140	LEU	2.3
1	I	108	VAL	2.3
1	K	717	PRO	2.3
1	I	115	HIS	2.3
1	G	388	MET	2.3
1	H	506	PHE	2.3
1	C	428	ASP	2.3
1	I	725	ASP	2.3
1	H	239	ARG	2.3
1	H	767	GLY	2.3
1	L	166	VAL	2.3
1	C	56	THR	2.3
1	I	506	PHE	2.3
1	D	755	TYR	2.3
1	C	50	GLN	2.3
1	D	102	ILE	2.3
1	G	445	LEU	2.3
1	I	41	LEU	2.3
1	I	102	ILE	2.3
1	I	185	GLU	2.3
1	B	768	PHE	2.3
1	A	108	VAL	2.3
1	D	687	LEU	2.3
1	D	173	TYR	2.3
1	D	145	PRO	2.2
1	F	443	ASN	2.2
1	I	460	ASN	2.2
1	A	681	GLY	2.2
1	J	452	PHE	2.2
1	D	715	THR	2.2
1	C	648	PRO	2.2
1	B	551	TRP	2.2
1	D	162	GLU	2.2
1	D	747	VAL	2.2
1	G	100	ILE	2.2
1	L	130	LEU	2.2
1	C	59	LEU	2.2
1	D	675	LEU	2.2
1	J	82	ILE	2.2
1	H	53	ARG	2.2
1	J	104	PRO	2.2
1	A	747	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	114	ILE	2.2
1	K	723	GLU	2.2
1	D	24	ASN	2.2
1	K	104	PRO	2.2
1	A	25	ARG	2.2
1	I	128	GLY	2.2
1	K	114	ILE	2.2
1	K	130	LEU	2.2
1	A	59	LEU	2.2
1	A	436	THR	2.2
1	H	736	PHE	2.2
1	K	505	LYS	2.2
1	F	735	HIS	2.2
1	A	99	VAL	2.2
1	D	744	ARG	2.2
1	E	41	LEU	2.2
1	H	50	GLN	2.2
1	B	49	LEU	2.2
1	C	666	VAL	2.2
1	I	49	LEU	2.2
1	C	690	ILE	2.2
1	C	679	THR	2.2
1	F	517	TYR	2.2
1	D	150	ASP	2.1
1	A	736	PHE	2.1
1	E	452	PHE	2.1
1	J	736	PHE	2.1
1	H	502	LYS	2.1
1	L	224	LEU	2.1
1	J	163	PHE	2.1
1	I	187	GLU	2.1
1	G	50	GLN	2.1
1	L	229	LEU	2.1
1	D	172	PRO	2.1
1	G	71	VAL	2.1
1	C	461	PRO	2.1
1	F	715	THR	2.1
1	F	21	ASN	2.1
1	J	130	LEU	2.1
1	L	117	LEU	2.1
1	J	765	SER	2.1
1	D	300	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	731	ILE	2.1
1	I	715	THR	2.1
1	K	721	GLU	2.1
1	G	230	PHE	2.1
1	D	436	THR	2.1
1	F	675	LEU	2.1
1	H	52	PHE	2.1
1	J	173	TYR	2.1
1	I	50	GLN	2.1
1	D	52	PHE	2.1
1	D	711	ARG	2.0
1	L	708	ARG	2.0
1	D	176	VAL	2.0
1	I	117	LEU	2.0
1	F	587	GLY	2.0
1	G	84	MET	2.0
1	H	117	LEU	2.0
1	A	439	ALA	2.0
1	B	102	ILE	2.0
1	C	551	TRP	2.0
1	D	690	ILE	2.0
1	E	100	ILE	2.0
1	G	116	VAL	2.0
1	H	108	VAL	2.0
1	J	621	GLY	2.0
1	D	699	ILE	2.0
1	D	727	PRO	2.0
1	F	682	PHE	2.0
1	F	687	LEU	2.0
1	G	506	PHE	2.0
1	D	147	ARG	2.0
1	J	175	ILE	2.0
1	K	714	GLN	2.0
1	I	158	MET	2.0
1	F	672	LEU	2.0
1	K	57	VAL	2.0
1	J	503	PHE	2.0
1	H	508	MET	2.0

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

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

## 6.3 Carbohydrates

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	AGS	K	902	31/31	0.91	0.30	0.55	96,121,149,154	0
2	AGS	F	901	31/31	0.92	0.31	0.49	94,131,160,160	0
2	AGS	I	902	31/31	0.86	0.31	0.35	125,150,180,187	0
2	AGS	G	902	31/31	0.88	0.32	0.34	112,139,179,187	0
2	AGS	L	901	31/31	0.95	0.29	0.32	102,132,160,173	0
2	AGS	F	902	31/31	0.85	0.30	0.23	122,150,185,190	0
2	AGS	B	901	31/31	0.92	0.32	0.12	102,131,160,170	0
2	AGS	E	902	31/31	0.82	0.30	0.09	102,148,179,184	0
2	AGS	J	902	31/31	0.91	0.27	-0.03	99,140,168,181	0
2	AGS	J	901	31/31	0.92	0.29	-0.05	111,139,167,210	0
2	AGS	G	901	31/31	0.93	0.27	-0.06	104,134,164,210	0
2	AGS	L	902	31/31	0.91	0.27	-0.08	112,136,166,169	0
2	AGS	D	901	31/31	0.93	0.27	-0.15	103,137,166,208	0
2	AGS	A	901	31/31	0.96	0.29	-0.19	102,125,153,197	0
2	AGS	C	902	31/31	0.90	0.28	-0.21	105,140,172,196	0
2	AGS	B	902	31/31	0.93	0.28	-0.26	101,128,152,156	0
2	AGS	H	901	31/31	0.94	0.30	-0.32	105,133,162,165	0
2	AGS	C	901	31/31	0.95	0.27	-0.34	105,138,166,177	0
2	AGS	K	901	31/31	0.96	0.27	-0.39	100,132,164,172	0
3	MG	H	903	1/1	0.98	0.33	-0.47	132,132,132,132	0
2	AGS	D	902	31/31	0.89	0.25	-0.47	111,144,182,204	0
2	AGS	H	902	31/31	0.90	0.25	-0.54	110,139,165,169	0
2	AGS	A	902	31/31	0.91	0.24	-0.55	120,142,172,177	0
2	AGS	I	901	31/31	0.93	0.26	-0.60	105,131,158,186	0
2	AGS	E	901	31/31	0.93	0.25	-0.67	105,131,164,179	0
3	MG	J	903	1/1	0.84	0.72	-	105,105,105,105	0
3	MG	I	904	1/1	0.97	0.41	-	145,145,145,145	0
3	MG	E	903	1/1	0.97	0.26	-	113,113,113,113	0
3	MG	B	903	1/1	0.98	0.38	-	113,113,113,113	0
3	MG	E	904	1/1	0.96	0.33	-	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	F	903	1/1	0.97	0.39	-	94,94,94,94	0
3	MG	G	903	1/1	0.94	0.63	-	113,113,113,113	0
3	MG	L	904	1/1	0.95	0.50	-	115,115,115,115	0
3	MG	K	903	1/1	0.99	0.33	-	112,112,112,112	0
3	MG	C	904	1/1	0.99	0.38	-	137,137,137,137	0
3	MG	A	904	1/1	0.95	0.24	-	128,128,128,128	0
3	MG	G	904	1/1	0.97	0.58	-	119,119,119,119	0
3	MG	J	904	1/1	0.98	0.38	-	112,112,112,112	0
3	MG	F	904	1/1	0.90	0.59	-	149,149,149,149	0
3	MG	H	904	1/1	0.90	0.48	-	134,134,134,134	0
3	MG	B	904	1/1	0.98	0.53	-	114,114,114,114	0
3	MG	A	903	1/1	0.95	0.51	-	110,110,110,110	0
3	MG	L	903	1/1	0.94	0.31	-	117,117,117,117	0
3	MG	C	903	1/1	0.91	0.38	-	94,94,94,94	0
3	MG	D	904	1/1	0.97	0.34	-	127,127,127,127	0
3	MG	D	903	1/1	0.92	0.49	-	122,122,122,122	0
3	MG	I	903	1/1	0.96	0.32	-	138,138,138,138	0
3	MG	K	904	1/1	0.99	0.38	-	99,99,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.