



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:52 am GMT

PDB ID : 3ISS  
Title : Crystal structure of enolpyruvyl-UDP-GlcNAc synthase (MurA):UDP-N-acetyl-muramic acid:phosphite from Escherichia coli  
Authors : Jackson, S.G.; Zhang, F.; Chindemi, P.; Junop, M.S.; Berti, P.J.  
Deposited on : 2009-08-27  
Resolution : 2.50 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

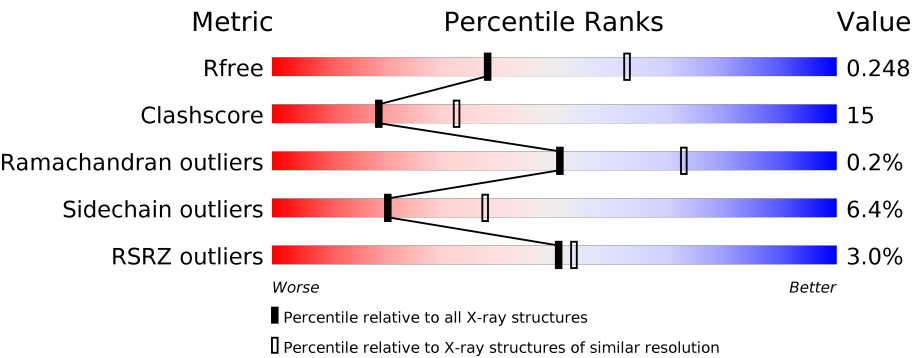
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	418	<div><div>%</div><div><div></div><div>79%</div><div>18%</div><div>.</div></div></div>
1	B	418	<div><div>5%</div><div><div></div><div>75%</div><div>23%</div><div>.</div></div></div>
1	C	418	<div><div></div><div><div></div><div>77%</div><div>21%</div><div>.</div></div></div>
1	D	418	<div><div></div><div><div></div><div>78%</div><div>20%</div><div>.</div></div></div>
1	E	418	<div><div>%</div><div><div></div><div>75%</div><div>22%</div><div>.</div></div></div>
1	F	418	<div><div>2%</div><div><div></div><div>74%</div><div>23%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	418	
1	H	418	
1	I	418	
1	J	418	
1	K	418	
1	L	418	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO3	A	501	-	-	-	X
2	PO3	C	502	-	-	-	X
2	PO3	D	503	-	-	-	X
2	PO3	E	504	-	-	-	X
2	PO3	I	509	-	-	-	X
2	PO3	J	510	-	-	-	X
2	PO3	K	511	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 39025 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 UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	B	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	C	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	D	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	E	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	F	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	G	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	H	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	I	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	J	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	K	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			
1	L	418	Total	C	N	O	S	0	0	0
			3133	1967	556	594	16			

There are 12 discrepancies between the modelled and reference sequences:

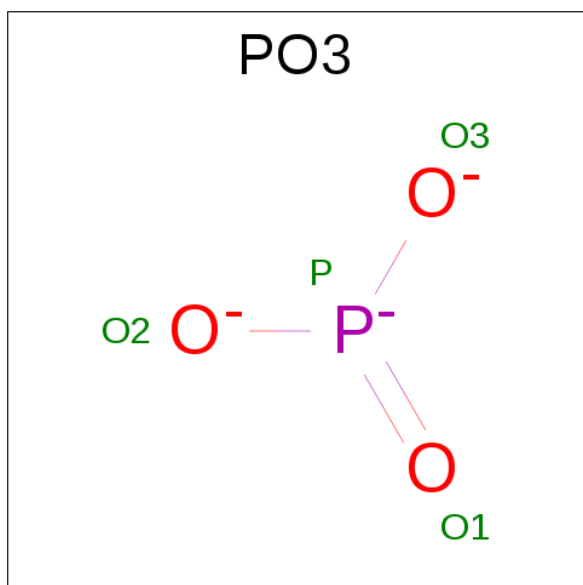
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ASP	ASN	ENGINEERED	UNP P0A749
B	67	ASP	ASN	ENGINEERED	UNP P0A749
C	67	ASP	ASN	ENGINEERED	UNP P0A749
D	67	ASP	ASN	ENGINEERED	UNP P0A749
E	67	ASP	ASN	ENGINEERED	UNP P0A749

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Chain	Residue	Modelled	Actual	Comment	Reference
F	67	ASP	ASN	ENGINEERED	UNP P0A749
G	67	ASP	ASN	ENGINEERED	UNP P0A749
H	67	ASP	ASN	ENGINEERED	UNP P0A749
I	67	ASP	ASN	ENGINEERED	UNP P0A749
J	67	ASP	ASN	ENGINEERED	UNP P0A749
K	67	ASP	ASN	ENGINEERED	UNP P0A749
L	67	ASP	ASN	ENGINEERED	UNP P0A749

- Molecule 2 is PHOSPHITE ION (three-letter code: PO3) (formula: O<sub>3</sub>P).



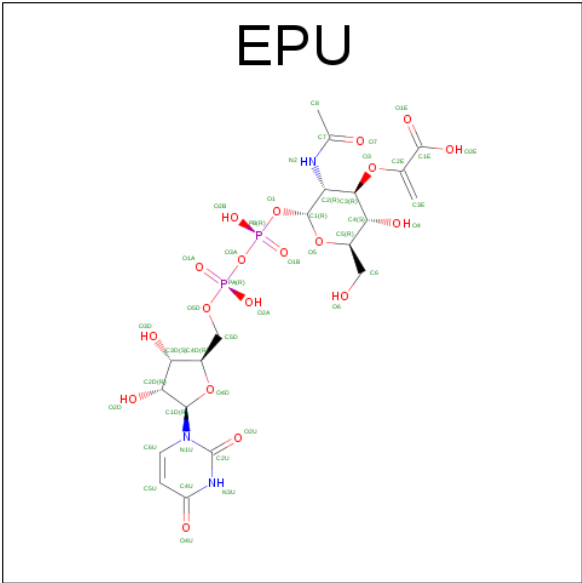
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			4	3	1		
2	B	1	Total	O	P	0	0
			4	3	1		
2	C	1	Total	O	P	0	0
			4	3	1		
2	D	1	Total	O	P	0	0
			4	3	1		
2	E	1	Total	O	P	0	0
			4	3	1		
2	F	1	Total	O	P	0	0
			4	3	1		
2	G	1	Total	O	P	0	0
			4	3	1		
2	H	1	Total	O	P	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	O	P	0	0
			4	3	1		
2	J	1	Total	O	P	0	0
			4	3	1		
2	K	1	Total	O	P	0	0
			4	3	1		
2	L	1	Total	O	P	0	0
			4	3	1		

- Molecule 3 is URIDINE-DIPHOSPHATE-2(N-ACETYLGUCOSAMINYL) BUTYRIC ACID (three-letter code: EPU) (formula: C<sub>20</sub>H<sub>29</sub>N<sub>3</sub>O<sub>19</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	B	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	C	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	D	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	E	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	F	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	G	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	I	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	J	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	K	1	Total	C	N	O	P	0	0
			44	20	3	19	2		
3	L	1	Total	C	N	O	P	0	0
			44	20	3	19	2		

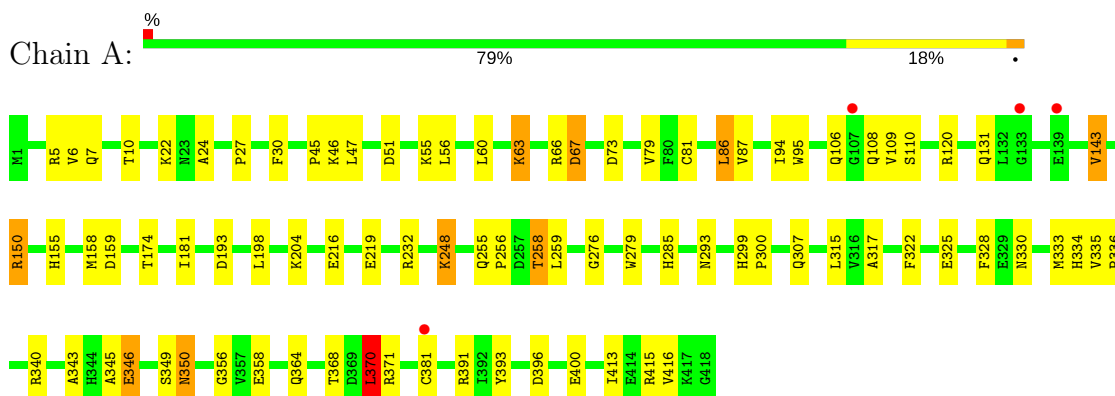
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	79	Total	O	0	0
			79	79		
4	B	63	Total	O	0	0
			63	63		
4	C	112	Total	O	0	0
			112	112		
4	D	106	Total	O	0	0
			106	106		
4	E	83	Total	O	0	0
			83	83		
4	F	69	Total	O	0	0
			69	69		
4	G	54	Total	O	0	0
			54	54		
4	H	84	Total	O	0	0
			84	84		
4	I	43	Total	O	0	0
			43	43		
4	J	55	Total	O	0	0
			55	55		
4	K	69	Total	O	0	0
			69	69		
4	L	36	Total	O	0	0
			36	36		

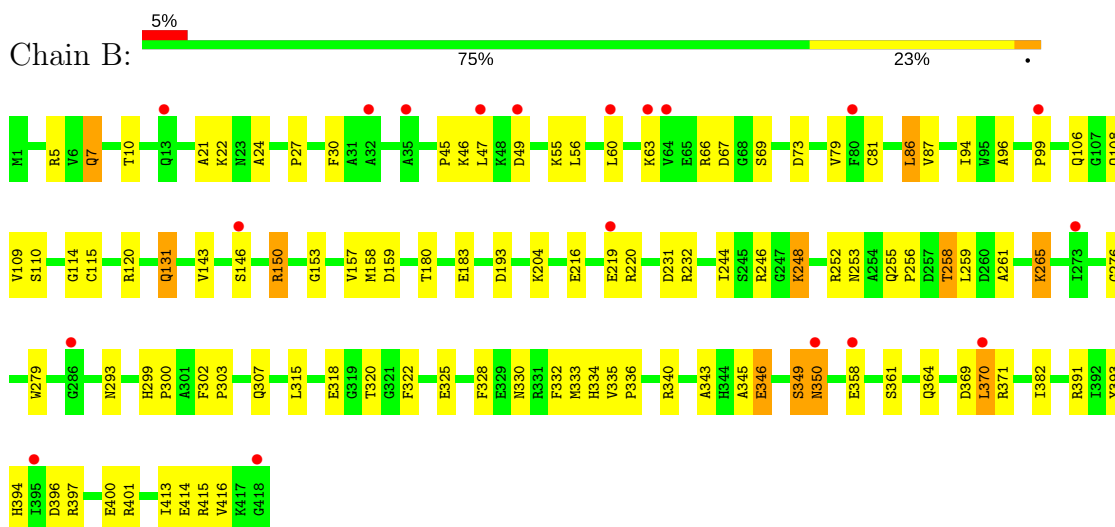
### 3 Residue-property plots

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.

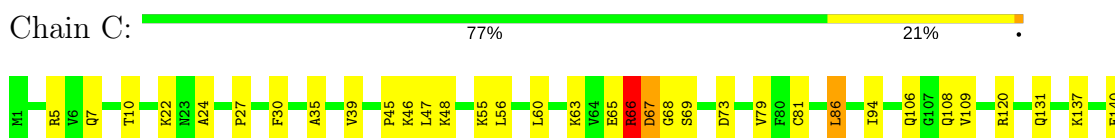
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



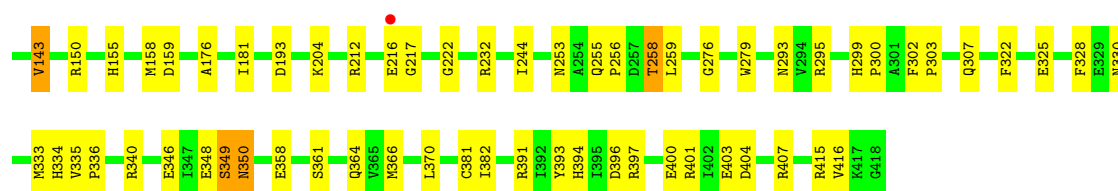
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

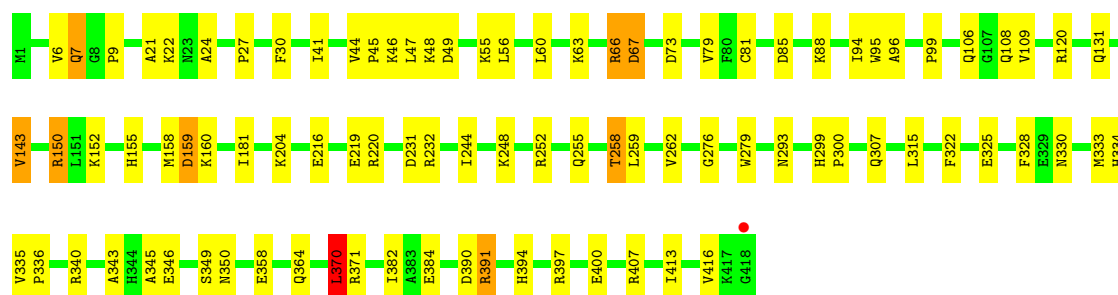






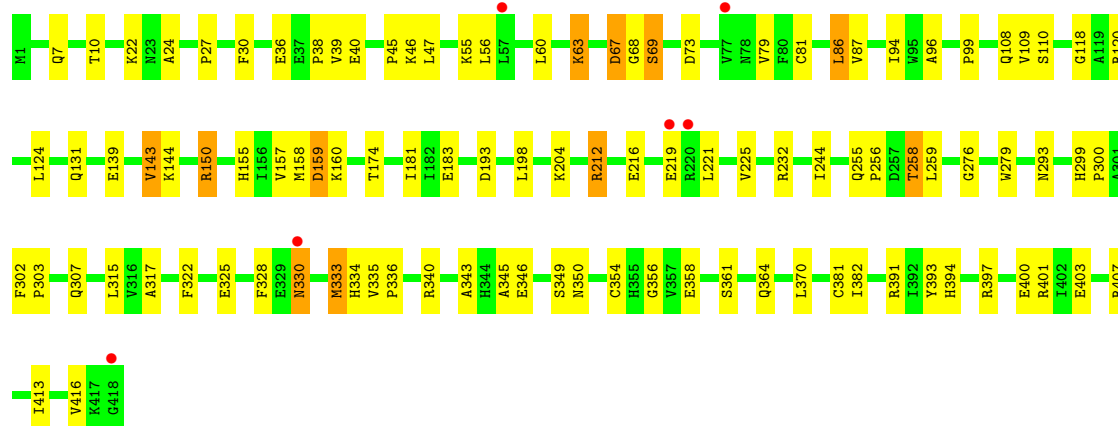
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain D: 78% 20%



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

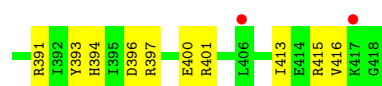
Chain E: 75% 22%



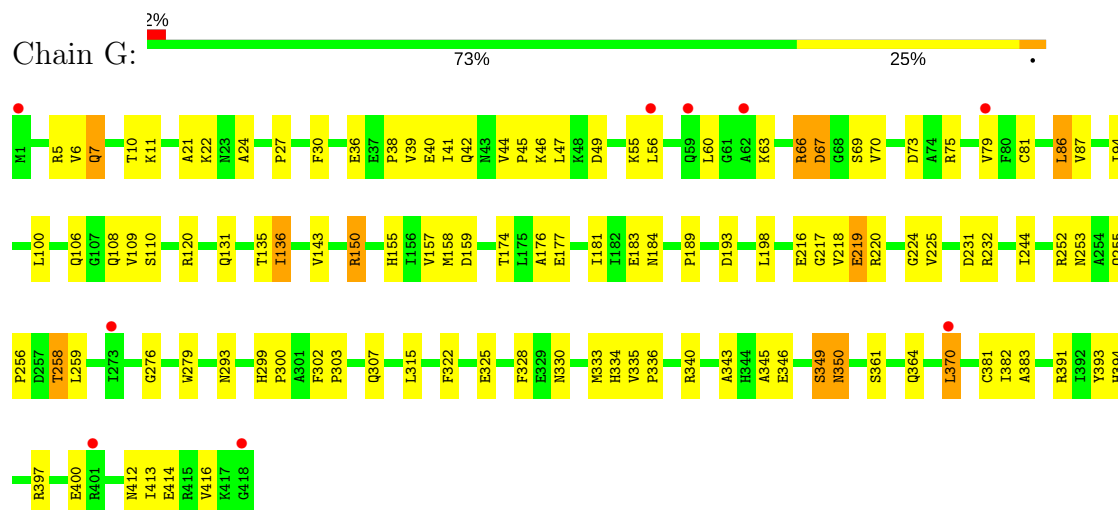
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

Chain F: 74% 23%

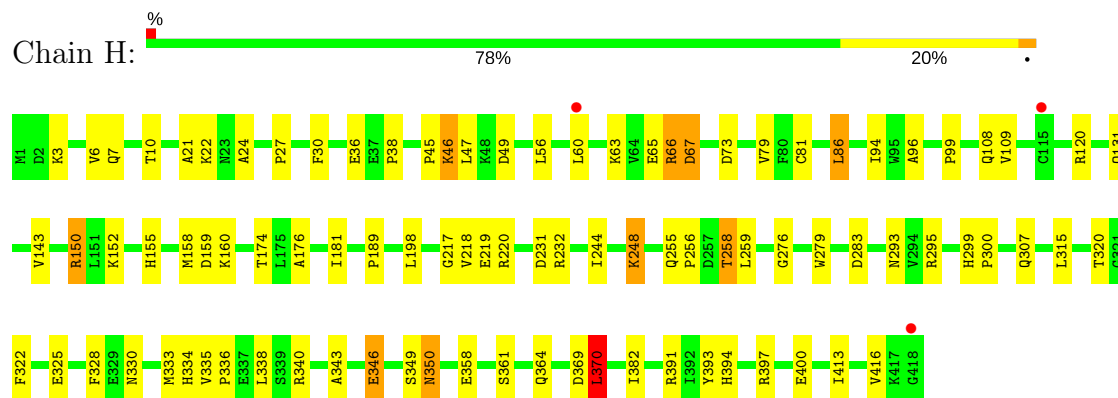




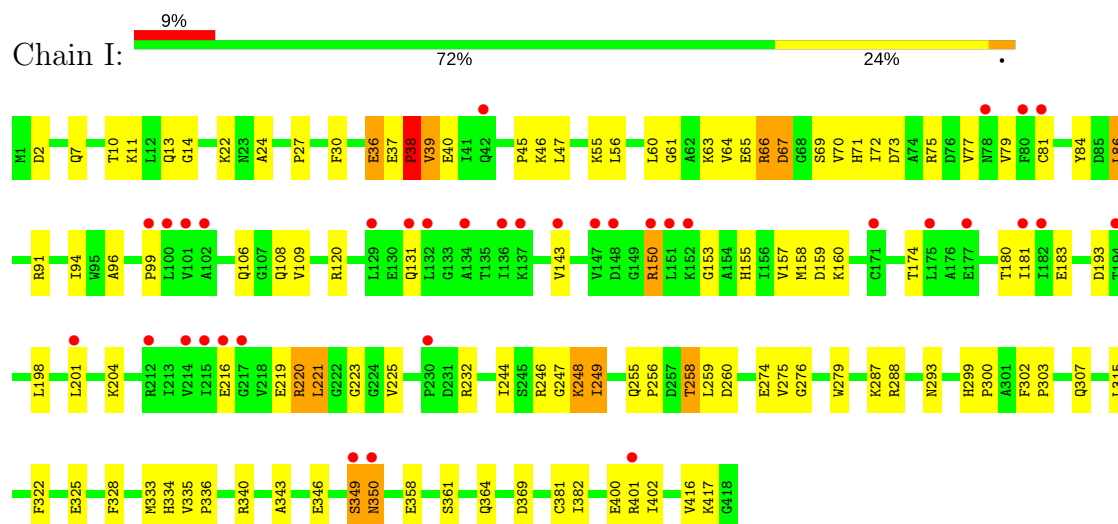
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



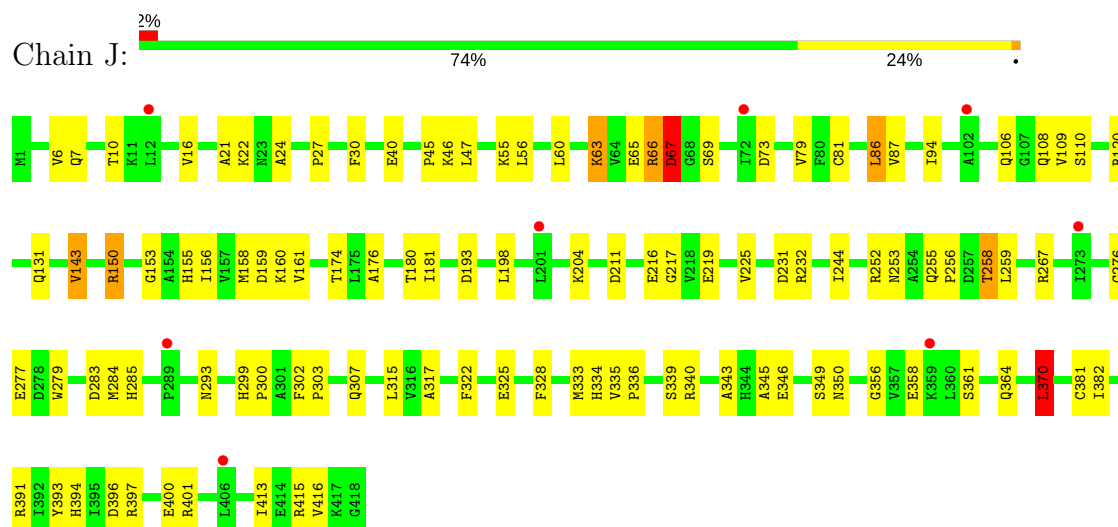
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



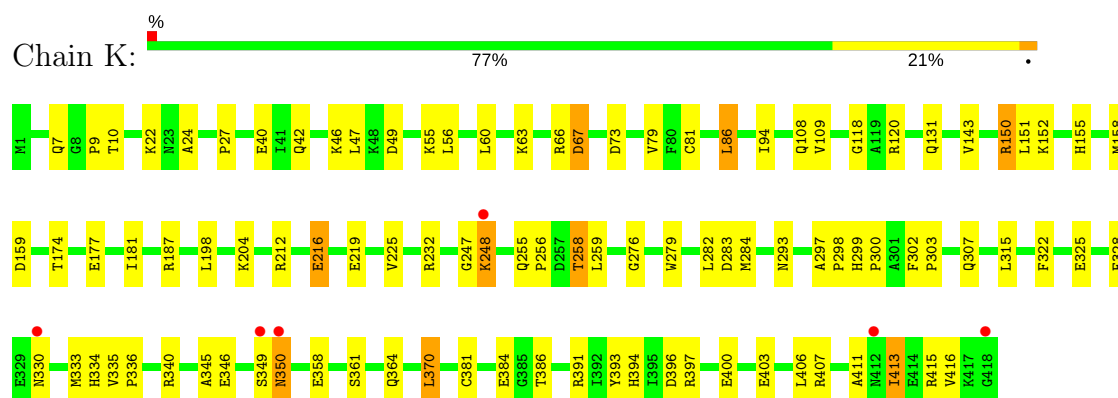
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



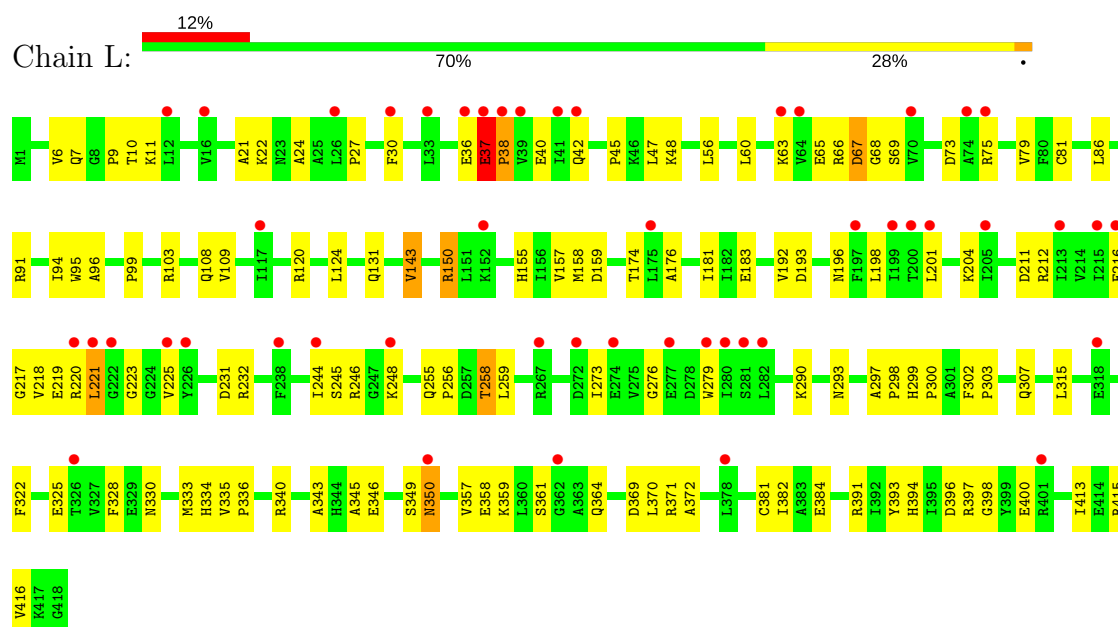
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.51Å 120.91Å 139.73Å 111.52° 104.44° 90.19°	Depositor
Resolution (Å)	47.48 – 2.50 47.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.48-2.50) 85.2 (47.48-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.222 , 0.254 0.210 , 0.248	Depositor DCC
$R_{free}$ test set	8363 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	39025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.08% 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: EPU, PO3

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	0.49	0/3176	0.61	1/4298 (0.0%)
1	B	0.51	1/3176 (0.0%)	0.60	3/4298 (0.1%)
1	C	0.54	0/3176	0.63	3/4298 (0.1%)
1	D	0.53	0/3176	0.62	2/4298 (0.0%)
1	E	0.51	0/3176	0.65	1/4298 (0.0%)
1	F	0.56	1/3176 (0.0%)	0.60	1/4298 (0.0%)
1	G	0.50	0/3176	0.62	2/4298 (0.0%)
1	H	0.53	0/3176	0.59	3/4298 (0.1%)
1	I	0.52	0/3176	0.59	1/4298 (0.0%)
1	J	0.48	0/3176	0.58	2/4298 (0.0%)
1	K	0.51	0/3176	0.59	2/4298 (0.0%)
1	L	0.52	0/3176	0.61	1/4298 (0.0%)
All	All	0.52	2/38112 (0.0%)	0.61	22/51576 (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	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	115	CYS	CB-SG	-5.21	1.73	1.81
1	B	115	CYS	C-N	-5.09	1.22	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	67	ASP	CB-CG-OD1	18.46	134.91	118.30
1	A	67	ASP	CB-CG-OD1	17.43	133.98	118.30
1	G	67	ASP	CB-CG-OD1	14.32	131.18	118.30
1	D	67	ASP	N-CA-CB	-14.03	85.34	110.60
1	C	67	ASP	N-CA-CB	-10.81	91.13	110.60
1	J	67	ASP	CB-CA-C	-7.38	95.64	110.40
1	C	67	ASP	CB-CA-C	-6.38	97.63	110.40
1	K	67	ASP	CB-CA-C	-5.97	98.47	110.40
1	L	37	GLU	C-N-CD	-5.92	107.58	120.60
1	I	369	ASP	CB-CA-C	5.82	122.04	110.40
1	C	68	GLY	N-CA-C	-5.80	98.61	113.10
1	H	370	LEU	CB-CA-C	-5.72	99.34	110.20
1	H	67	ASP	CB-CG-OD1	5.62	123.36	118.30
1	K	370	LEU	CB-CA-C	-5.45	99.84	110.20
1	H	67	ASP	CB-CA-C	-5.43	99.54	110.40
1	B	114	GLY	O-C-N	-5.39	114.07	122.70
1	B	115	CYS	O-C-N	-5.21	114.36	122.70
1	B	370	LEU	CB-CA-C	-5.10	100.50	110.20
1	D	370	LEU	CB-CA-C	-5.10	100.52	110.20
1	J	370	LEU	CB-CA-C	-5.08	100.54	110.20
1	F	370	LEU	CB-CA-C	-5.04	100.63	110.20
1	G	370	LEU	CB-CA-C	-5.03	100.64	110.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	66	ARG	Peptide
1	D	66	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	3133	0	3210	68	0
1	B	3133	0	3208	93	0
1	C	3133	0	3210	81	0
1	D	3133	0	3210	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3133	0	3210	90	0
1	F	3133	0	3210	103	0
1	G	3133	0	3210	106	0
1	H	3133	0	3210	88	0
1	I	3133	0	3210	107	0
1	J	3133	0	3210	92	0
1	K	3133	0	3210	123	0
1	L	3133	0	3210	122	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	1	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	1	0
3	A	44	0	26	0	0
3	B	44	0	26	1	0
3	C	44	0	26	2	0
3	D	44	0	26	0	0
3	E	44	0	26	2	0
3	F	44	0	26	3	0
3	G	44	0	26	0	0
3	H	44	0	26	3	0
3	I	44	0	26	1	0
3	J	44	0	26	1	0
3	K	44	0	26	0	0
3	L	44	0	26	2	0
4	A	79	0	0	7	0
4	B	63	0	0	14	0
4	C	112	0	0	11	0
4	D	106	0	0	5	0
4	E	83	0	0	2	0
4	F	69	0	0	7	0
4	G	54	0	0	15	0
4	H	84	0	0	9	0
4	I	43	0	0	10	0
4	J	55	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	69	0	0	12	0
4	L	36	0	0	8	0
All	All	39025	0	38830	1129	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 15.

All (1129) 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:248:LYS:CD	1:K:283:ASP:HA	1.32	1.55
1:K:248:LYS:HD2	1:K:283:ASP:CA	1.49	1.39
1:E:370:LEU:CD1	1:E:397:ARG:HB2	1.60	1.32
1:B:370:LEU:CD1	1:B:397:ARG:HB2	1.59	1.30
1:C:370:LEU:CD1	1:C:397:ARG:HB2	1.64	1.27
1:L:67:ASP:HB3	1:L:69:SER:O	1.33	1.27
1:D:370:LEU:CD1	1:D:397:ARG:HB2	1.64	1.26
1:J:370:LEU:CD1	1:J:397:ARG:HB2	1.66	1.25
1:K:370:LEU:CD1	1:K:397:ARG:HB2	1.65	1.24
1:G:370:LEU:CD1	1:G:397:ARG:HB2	1.66	1.24
1:F:370:LEU:CD1	1:F:397:ARG:HB2	1.69	1.22
1:H:370:LEU:CD1	1:H:397:ARG:HB2	1.70	1.21
1:L:370:LEU:CD1	1:L:397:ARG:HB2	1.73	1.18
1:I:37:GLU:CG	1:I:38:PRO:HD2	1.75	1.17
1:K:248:LYS:HA	1:K:248:LYS:HE3	1.18	1.13
1:K:248:LYS:HA	1:K:248:LYS:CE	1.61	1.12
1:I:37:GLU:HG3	1:I:38:PRO:HD2	1.20	1.10
1:E:403:GLU:HG3	4:E:756:HOH:O	1.50	1.09
1:I:248:LYS:O	1:I:249:ILE:HG22	1.54	1.08
1:I:37:GLU:HG3	1:I:38:PRO:CD	1.85	1.07
1:L:290:LYS:HB3	4:L:743:HOH:O	1.52	1.06
1:K:330:ASN:HB3	4:K:714:HOH:O	1.55	1.05
1:E:370:LEU:HD11	1:E:397:ARG:CB	1.87	1.04
1:G:370:LEU:HD11	1:G:397:ARG:CB	1.87	1.04
1:K:248:LYS:CA	1:K:248:LYS:HE3	1.89	1.03
1:E:370:LEU:HD11	1:E:397:ARG:HB2	1.37	1.01
1:K:370:LEU:HD11	1:K:397:ARG:HB2	1.41	1.01
1:C:370:LEU:HD11	1:C:397:ARG:HB2	1.42	1.00
1:B:370:LEU:HD11	1:B:397:ARG:CB	1.90	1.00
1:F:370:LEU:HD11	1:F:397:ARG:CB	1.92	1.00
1:B:370:LEU:CD1	1:B:397:ARG:CB	2.40	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:218:VAL:HG12	1:G:219:GLU:N	1.76	0.99
1:F:370:LEU:HD11	1:F:397:ARG:HB2	1.44	0.99
1:B:370:LEU:HD13	1:B:397:ARG:HB2	1.45	0.99
1:E:370:LEU:CD1	1:E:397:ARG:CB	2.41	0.98
1:C:370:LEU:HD11	1:C:397:ARG:CB	1.94	0.98
1:L:273:ILE:HB	4:L:704:HOH:O	1.63	0.98
1:K:152:LYS:HE2	1:K:177:GLU:OE1	1.63	0.97
1:J:370:LEU:HD11	1:J:397:ARG:CB	1.93	0.97
1:B:370:LEU:HD11	1:B:397:ARG:HB2	1.41	0.97
1:K:370:LEU:HD11	1:K:397:ARG:CB	1.95	0.97
1:D:370:LEU:HD11	1:D:397:ARG:CB	1.95	0.96
1:J:370:LEU:CD1	1:J:397:ARG:CB	2.44	0.96
1:H:370:LEU:HD11	1:H:397:ARG:CB	1.95	0.96
1:L:192:VAL:HG12	4:L:433:HOH:O	1.64	0.95
1:H:370:LEU:CD1	1:H:397:ARG:CB	2.43	0.95
1:G:370:LEU:CD1	1:G:397:ARG:CB	2.42	0.95
1:D:370:LEU:CD1	1:D:397:ARG:CB	2.45	0.94
1:L:48:LYS:HE2	4:L:761:HOH:O	1.68	0.93
1:G:370:LEU:HD11	1:G:397:ARG:HB2	1.44	0.93
1:F:391:ARG:NH1	1:F:393:TYR:HE2	1.66	0.93
1:C:370:LEU:HD13	1:C:397:ARG:HB2	1.48	0.93
1:L:370:LEU:HD11	1:L:397:ARG:CB	1.98	0.93
1:D:370:LEU:HD11	1:D:397:ARG:HB2	1.45	0.93
1:C:370:LEU:CD1	1:C:397:ARG:CB	2.45	0.93
1:E:370:LEU:HD13	1:E:397:ARG:HB2	1.49	0.92
1:D:370:LEU:HD13	1:D:397:ARG:HB2	1.47	0.92
1:K:370:LEU:CD1	1:K:397:ARG:CB	2.48	0.92
1:L:67:ASP:CB	1:L:69:SER:H	1.83	0.91
1:A:22:LYS:HE3	1:A:370:LEU:HD21	1.51	0.91
1:K:248:LYS:HD3	1:K:282:LEU:O	1.71	0.91
3:C:603:EPU:O4	3:C:603:EPU:HE31	1.69	0.91
1:L:370:LEU:CD1	1:L:397:ARG:CB	2.48	0.91
1:J:370:LEU:HD11	1:J:397:ARG:HB2	1.48	0.90
1:B:391:ARG:HD3	4:B:607:HOH:O	1.71	0.89
1:K:46:LYS:C	1:K:47:LEU:HD23	1.92	0.89
1:F:370:LEU:CD1	1:F:397:ARG:CB	2.47	0.89
1:J:370:LEU:HD13	1:J:397:ARG:HB2	1.52	0.89
1:I:37:GLU:CG	1:I:38:PRO:CD	2.47	0.88
1:B:246:ARG:HD2	4:B:786:HOH:O	1.73	0.88
1:K:370:LEU:HD13	1:K:397:ARG:HB2	1.54	0.87
1:B:131:GLN:HG2	4:B:720:HOH:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:391:ARG:NH1	1:F:393:TYR:CE2	2.42	0.87
1:G:5:ARG:HD2	1:G:414:GLU:OE2	1.73	0.87
1:E:330:ASN:HB3	1:H:330:ASN:CG	1.94	0.87
1:G:218:VAL:CG1	1:G:219:GLU:N	2.38	0.87
1:K:248:LYS:NZ	1:K:284:MET:HG2	1.89	0.87
1:H:370:LEU:HD13	1:H:397:ARG:HB2	1.55	0.87
1:H:370:LEU:HD11	1:H:397:ARG:HB2	1.55	0.86
1:E:330:ASN:HD22	1:E:330:ASN:N	1.72	0.86
1:K:247:GLY:O	1:K:248:LYS:CE	2.23	0.86
1:F:1:MET:HE1	1:F:391:ARG:NH1	1.90	0.86
1:J:293:ASN:CB	4:J:760:HOH:O	2.22	0.86
1:K:248:LYS:HE2	1:K:282:LEU:O	1.75	0.85
1:F:391:ARG:HH11	1:F:393:TYR:HE2	1.16	0.85
1:F:370:LEU:HD13	1:F:397:ARG:HB2	1.59	0.85
1:L:370:LEU:HD11	1:L:397:ARG:HB2	1.55	0.85
1:L:370:LEU:HD13	1:L:397:ARG:HB2	1.59	0.84
1:G:66:ARG:HG3	1:G:67:ASP:O	1.77	0.84
1:G:370:LEU:HD13	1:G:397:ARG:HB2	1.57	0.84
1:I:220:ARG:HG3	1:I:221:LEU:N	1.93	0.83
1:C:150:ARG:HB2	4:C:462:HOH:O	1.80	0.82
3:H:608:EPU:HE31	3:H:608:EPU:O4	1.79	0.82
1:K:150:ARG:HH12	1:K:219:GLU:HA	1.44	0.82
1:L:204:LYS:HD3	1:L:216:GLU:HB3	1.62	0.82
1:L:245:SER:O	1:L:246:ARG:HB2	1.80	0.82
1:J:66:ARG:HG3	1:J:67:ASP:O	1.81	0.81
1:E:400:GLU:O	1:E:401:ARG:HB2	1.79	0.81
1:L:232:ARG:HB3	1:L:258:THR:CG2	2.10	0.81
1:K:248:LYS:HD3	1:K:283:ASP:HA	1.60	0.81
1:L:204:LYS:HD3	1:L:216:GLU:CB	2.11	0.81
1:L:67:ASP:CG	1:L:69:SER:N	2.29	0.80
1:G:11:LYS:CE	4:G:796:HOH:O	2.29	0.80
1:G:11:LYS:HE3	4:G:796:HOH:O	1.80	0.80
1:I:232:ARG:HB3	1:I:258:THR:CG2	2.12	0.80
1:F:1:MET:HE1	1:F:391:ARG:HH12	1.43	0.79
1:I:293:ASN:ND2	1:I:322:PHE:H	1.79	0.79
1:E:330:ASN:ND2	1:E:330:ASN:N	2.30	0.79
1:G:232:ARG:HB3	1:G:258:THR:CG2	2.11	0.79
1:I:248:LYS:O	1:I:249:ILE:CG2	2.30	0.79
1:F:293:ASN:ND2	1:F:322:PHE:H	1.80	0.79
1:I:84:TYR:CE2	4:I:824:HOH:O	2.34	0.79
1:L:48:LYS:CE	4:L:761:HOH:O	2.26	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:37:GLU:HG2	1:I:38:PRO:HD2	1.61	0.79
1:D:232:ARG:HB3	1:D:258:THR:CG2	2.13	0.79
1:J:232:ARG:HB3	1:J:258:THR:CG2	2.13	0.79
1:C:293:ASN:ND2	1:C:322:PHE:H	1.80	0.78
1:H:232:ARG:HB3	1:H:258:THR:CG2	2.13	0.78
1:F:60:LEU:HA	1:F:79:VAL:HG13	1.66	0.78
1:G:218:VAL:CG1	1:G:219:GLU:H	1.95	0.78
1:L:36:GLU:O	1:L:37:GLU:HB3	1.81	0.78
1:B:232:ARG:HB3	1:B:258:THR:CG2	2.13	0.78
1:F:400:GLU:HG2	1:F:401:ARG:HG2	1.63	0.78
3:C:603:EPU:C3E	3:C:603:EPU:O4	2.32	0.78
1:J:66:ARG:C	1:J:67:ASP:O	2.14	0.78
1:H:293:ASN:ND2	1:H:322:PHE:H	1.81	0.77
1:L:36:GLU:O	1:L:37:GLU:CB	2.32	0.77
1:C:232:ARG:HB3	1:C:258:THR:CG2	2.15	0.77
1:A:120:ARG:HD2	4:A:780:HOH:O	1.84	0.77
1:A:232:ARG:HB3	1:A:258:THR:CG2	2.14	0.77
1:B:293:ASN:ND2	1:B:322:PHE:H	1.82	0.77
1:L:218:VAL:HG23	1:L:219:GLU:N	1.99	0.77
1:D:22:LYS:HE3	1:D:370:LEU:HD21	1.66	0.76
1:K:247:GLY:O	1:K:248:LYS:NZ	2.19	0.75
1:L:60:LEU:HA	1:L:79:VAL:HG13	1.68	0.75
1:G:293:ASN:ND2	1:G:322:PHE:H	1.84	0.75
1:H:3:LYS:HD2	4:H:498:HOH:O	1.86	0.75
1:J:66:ARG:O	1:J:67:ASP:O	2.03	0.75
1:L:357:VAL:HG12	1:L:358:GLU:N	2.02	0.75
1:A:232:ARG:HB3	1:A:258:THR:HG21	1.70	0.74
1:G:60:LEU:HA	1:G:79:VAL:HG13	1.69	0.74
1:B:22:LYS:HE3	1:B:370:LEU:HD21	1.68	0.74
1:K:248:LYS:CE	1:K:283:ASP:HA	2.17	0.74
1:A:293:ASN:ND2	1:A:322:PHE:H	1.86	0.74
1:K:248:LYS:CD	1:K:282:LEU:O	2.36	0.74
1:K:212:ARG:NH1	4:K:735:HOH:O	2.20	0.74
1:B:60:LEU:HA	1:B:79:VAL:HG13	1.69	0.74
1:C:60:LEU:HA	1:C:79:VAL:HG13	1.70	0.73
1:D:60:LEU:HA	1:D:79:VAL:HG13	1.70	0.73
1:F:232:ARG:HB3	1:F:258:THR:CG2	2.18	0.73
1:E:183:GLU:OE2	1:E:212:ARG:CZ	2.36	0.73
1:E:60:LEU:HA	1:E:79:VAL:HG13	1.70	0.73
1:K:232:ARG:HB3	1:K:258:THR:CG2	2.18	0.73
1:E:232:ARG:HB3	1:E:258:THR:CG2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ASN:ND2	1:D:322:PHE:H	1.85	0.73
1:A:60:LEU:HA	1:A:79:VAL:HG13	1.70	0.73
1:K:60:LEU:HA	1:K:79:VAL:HG13	1.70	0.73
1:A:368:THR:HB	4:A:556:HOH:O	1.89	0.73
1:L:232:ARG:HB3	1:L:258:THR:HG21	1.70	0.73
1:L:255:GLN:O	1:L:258:THR:HB	1.89	0.73
1:E:293:ASN:ND2	1:E:322:PHE:H	1.87	0.72
1:D:67:ASP:O	1:D:67:ASP:CG	2.24	0.72
1:F:255:GLN:O	1:F:258:THR:HB	1.89	0.72
1:H:232:ARG:HB3	1:H:258:THR:HG21	1.70	0.72
1:L:357:VAL:CG1	1:L:358:GLU:N	2.53	0.72
1:I:60:LEU:HA	1:I:79:VAL:HG13	1.70	0.72
1:K:248:LYS:CD	1:K:283:ASP:CA	2.28	0.72
1:I:84:TYR:HE2	4:I:824:HOH:O	1.68	0.72
1:J:293:ASN:ND2	1:J:322:PHE:H	1.88	0.72
1:F:296:THR:O	1:F:326:THR:HB	1.89	0.72
1:C:391:ARG:HG3	1:C:393:TYR:HE2	1.53	0.72
1:I:232:ARG:HB3	1:I:258:THR:HG21	1.70	0.71
1:D:232:ARG:HB3	1:D:258:THR:HG21	1.72	0.71
1:L:293:ASN:ND2	1:L:322:PHE:H	1.87	0.71
1:I:39:VAL:HG12	1:I:72:ILE:O	1.91	0.71
1:H:60:LEU:HA	1:H:79:VAL:HG13	1.71	0.71
1:L:67:ASP:CG	1:L:67:ASP:OXT	2.29	0.71
1:B:232:ARG:HB3	1:B:258:THR:HG21	1.72	0.71
1:J:24:ALA:O	1:J:27:PRO:HD2	1.90	0.71
1:J:255:GLN:O	1:J:258:THR:HB	1.91	0.71
1:F:326:THR:O	1:F:326:THR:CG2	2.39	0.71
1:J:66:ARG:HG3	1:J:67:ASP:N	2.06	0.71
1:B:255:GLN:O	1:B:258:THR:HB	1.90	0.71
1:B:5:ARG:HD2	1:B:414:GLU:OE2	1.90	0.71
1:I:248:LYS:C	1:I:249:ILE:CG2	2.59	0.71
1:A:5:ARG:HD3	4:A:420:HOH:O	1.90	0.70
1:C:232:ARG:HB3	1:C:258:THR:HG21	1.70	0.70
1:I:255:GLN:O	1:I:258:THR:HB	1.91	0.70
1:D:255:GLN:O	1:D:258:THR:HB	1.91	0.70
1:G:370:LEU:HD11	1:G:397:ARG:HB3	1.73	0.70
1:G:24:ALA:O	1:G:27:PRO:HD2	1.91	0.70
1:L:24:ALA:O	1:L:27:PRO:HD2	1.90	0.70
1:K:255:GLN:O	1:K:258:THR:HB	1.91	0.70
1:C:255:GLN:O	1:C:258:THR:HB	1.91	0.70
1:E:325:GLU:HG2	1:E:328:PHE:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:O	1:A:258:THR:HB	1.90	0.70
1:E:183:GLU:OE2	1:E:212:ARG:NH2	2.25	0.70
1:I:247:GLY:HA2	1:I:248:LYS:HE2	1.74	0.70
1:F:155:HIS:NE2	1:F:183:GLU:OE1	2.25	0.69
1:J:60:LEU:HA	1:J:79:VAL:HG13	1.73	0.69
1:K:248:LYS:HE3	1:K:248:LYS:N	2.06	0.69
1:G:232:ARG:HB3	1:G:258:THR:HG21	1.72	0.69
1:L:67:ASP:CB	1:L:69:SER:N	2.55	0.69
1:F:232:ARG:HB3	1:F:258:THR:HG21	1.73	0.69
1:K:247:GLY:C	1:K:248:LYS:HE3	2.12	0.69
1:I:220:ARG:CG	1:I:221:LEU:N	2.56	0.69
1:J:211:ASP:HB3	4:K:452:HOH:O	1.92	0.69
1:K:248:LYS:CE	1:K:282:LEU:O	2.40	0.69
1:K:340:ARG:NH1	1:K:364:GLN:O	2.25	0.69
1:H:293:ASN:HD22	1:H:322:PHE:H	1.39	0.69
1:E:232:ARG:HB3	1:E:258:THR:HG21	1.74	0.68
1:I:401:ARG:HA	4:I:436:HOH:O	1.92	0.68
1:F:88:LYS:NZ	4:F:637:HOH:O	2.20	0.68
1:K:232:ARG:HB3	1:K:258:THR:HG21	1.75	0.68
1:I:276:GLY:HA3	1:I:279:TRP:NE1	2.07	0.68
1:D:371:ARG:NH2	4:D:459:HOH:O	2.27	0.68
1:K:22:LYS:HE3	1:K:370:LEU:HD21	1.75	0.68
1:K:248:LYS:NZ	1:K:282:LEU:HD23	2.09	0.68
1:L:299:HIS:CG	1:L:300:PRO:HA	2.29	0.68
1:L:67:ASP:CG	1:L:69:SER:H	1.92	0.68
1:C:22:LYS:HE3	1:C:370:LEU:HD21	1.76	0.68
1:F:1:MET:CE	1:F:391:ARG:NH1	2.57	0.68
1:A:371:ARG:NH2	4:A:426:HOH:O	2.26	0.67
1:K:248:LYS:NZ	1:K:284:MET:N	2.42	0.67
1:A:46:LYS:NZ	1:A:67:ASP:OXT	2.25	0.67
1:K:293:ASN:ND2	1:K:322:PHE:H	1.92	0.67
1:H:22:LYS:HE3	1:H:370:LEU:HD21	1.77	0.67
1:J:232:ARG:HB3	1:J:258:THR:HG21	1.75	0.67
1:I:303:PRO:HA	4:I:419:HOH:O	1.94	0.67
1:G:255:GLN:O	1:G:258:THR:HB	1.94	0.67
1:J:22:LYS:HE3	1:J:370:LEU:HD21	1.77	0.67
1:C:401:ARG:HD2	1:C:404:ASP:OD2	1.95	0.67
1:J:293:ASN:HB2	4:J:760:HOH:O	1.88	0.66
1:G:325:GLU:HG2	1:G:328:PHE:O	1.95	0.66
1:H:255:GLN:O	1:H:258:THR:HB	1.95	0.66
1:B:246:ARG:CD	4:B:786:HOH:O	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:THR:O	1:F:326:THR:HG23	1.94	0.66
1:K:152:LYS:CE	1:K:177:GLU:OE1	2.40	0.66
1:K:66:ARG:HG3	1:K:67:ASP:O	1.96	0.66
1:F:293:ASN:HD22	1:F:322:PHE:H	1.43	0.66
1:H:325:GLU:HG2	1:H:328:PHE:O	1.96	0.66
1:A:24:ALA:O	1:A:27:PRO:HD2	1.96	0.66
1:K:247:GLY:O	1:K:248:LYS:HE3	1.94	0.66
1:B:370:LEU:HD11	1:B:397:ARG:C	2.17	0.66
1:I:401:ARG:CA	4:I:436:HOH:O	2.44	0.66
1:E:118:GLY:HA2	1:E:330:ASN:OD1	1.96	0.65
1:I:46:LYS:HG2	1:I:66:ARG:NH2	2.10	0.65
1:L:22:LYS:HE3	1:L:370:LEU:HD21	1.78	0.65
1:C:35:ALA:HB1	1:C:222:GLY:O	1.96	0.65
1:D:370:LEU:HD11	1:D:397:ARG:C	2.16	0.65
1:E:333:MET:O	1:E:336:PRO:HD2	1.97	0.65
1:K:248:LYS:HZ1	1:K:284:MET:HG2	1.61	0.65
1:F:299:HIS:CG	1:F:300:PRO:HA	2.31	0.65
1:G:333:MET:O	1:G:336:PRO:HD2	1.97	0.65
1:I:66:ARG:NH2	1:I:67:ASP:OD1	2.30	0.65
1:L:67:ASP:OD1	1:L:69:SER:N	2.30	0.65
1:C:403:GLU:HG3	4:C:463:HOH:O	1.98	0.64
1:C:108:GLN:NE2	4:C:444:HOH:O	2.30	0.64
1:E:255:GLN:O	1:E:258:THR:HB	1.97	0.64
1:E:330:ASN:H	1:E:330:ASN:ND2	1.94	0.64
1:K:63:LYS:HB2	1:K:73:ASP:HB3	1.79	0.64
1:J:299:HIS:CG	1:J:300:PRO:HA	2.33	0.64
1:C:330:ASN:O	1:C:330:ASN:ND2	2.30	0.64
1:F:88:LYS:CE	4:F:637:HOH:O	2.46	0.64
1:B:24:ALA:O	1:B:27:PRO:HD2	1.97	0.64
1:G:218:VAL:HG12	1:G:219:GLU:H	1.53	0.63
1:I:120:ARG:HD2	4:I:438:HOH:O	1.98	0.63
1:I:201:LEU:HB2	1:I:221:LEU:HD22	1.80	0.63
1:A:22:LYS:HE3	1:A:370:LEU:CD2	2.28	0.63
1:G:177:GLU:HG3	4:G:433:HOH:O	1.97	0.63
1:G:6:VAL:HG22	1:G:413:ILE:HG13	1.80	0.63
1:L:63:LYS:HB2	1:L:73:ASP:HB3	1.80	0.63
1:H:218:VAL:HG23	1:H:219:GLU:N	2.12	0.63
1:L:325:GLU:HG2	1:L:328:PHE:O	1.98	0.63
1:K:330:ASN:CB	4:K:714:HOH:O	2.26	0.63
1:K:276:GLY:HA3	1:K:279:TRP:NE1	2.14	0.63
1:D:63:LYS:HB2	1:D:73:ASP:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:248:LYS:HD2	1:K:283:ASP:CB	2.28	0.63
1:H:370:LEU:HD11	1:H:397:ARG:HB3	1.78	0.63
1:H:63:LYS:HB2	1:H:73:ASP:HB3	1.81	0.63
1:I:299:HIS:CG	1:I:300:PRO:HA	2.33	0.63
1:K:248:LYS:HE2	1:K:282:LEU:HD23	1.81	0.63
1:L:67:ASP:OD1	1:L:68:GLY:C	2.35	0.63
1:B:322:PHE:CE1	1:H:346:GLU:HG3	2.34	0.63
1:K:204:LYS:HD2	1:K:216:GLU:HG2	1.81	0.63
1:K:394:HIS:CE1	4:K:811:HOH:O	2.52	0.63
1:L:42:GLN:HA	1:L:69:SER:OG	1.99	0.63
1:G:299:HIS:CG	1:G:300:PRO:HA	2.33	0.62
1:C:340:ARG:NH1	1:C:364:GLN:O	2.32	0.62
1:B:46:LYS:NZ	4:B:434:HOH:O	2.29	0.62
1:J:267:ARG:NH1	4:J:697:HOH:O	2.29	0.62
1:K:325:GLU:HG2	1:K:328:PHE:O	1.99	0.62
1:E:330:ASN:HB3	1:H:330:ASN:ND2	2.14	0.62
1:K:299:HIS:CG	1:K:300:PRO:HA	2.34	0.62
1:B:276:GLY:HA3	1:B:279:TRP:NE1	2.15	0.62
1:B:299:HIS:CG	1:B:300:PRO:HA	2.35	0.62
1:G:63:LYS:HB2	1:G:73:ASP:HB3	1.80	0.62
1:K:248:LYS:HD2	1:K:283:ASP:HA	0.63	0.62
1:C:370:LEU:HD11	1:C:397:ARG:C	2.20	0.62
1:D:293:ASN:HD22	1:D:322:PHE:H	1.48	0.62
1:E:22:LYS:HE3	1:E:370:LEU:HD21	1.82	0.62
1:B:401:ARG:HG3	4:B:444:HOH:O	1.99	0.62
1:J:325:GLU:HG2	1:J:328:PHE:O	1.99	0.62
1:B:370:LEU:HD12	1:B:394:HIS:O	1.99	0.61
1:A:299:HIS:CG	1:A:300:PRO:HA	2.36	0.61
1:C:333:MET:O	1:C:336:PRO:HD2	2.00	0.61
1:J:120:ARG:HD2	4:J:673:HOH:O	1.99	0.61
1:B:333:MET:O	1:B:336:PRO:HD2	2.00	0.61
1:D:299:HIS:CG	1:D:300:PRO:HA	2.36	0.61
1:K:248:LYS:HZ3	1:K:284:MET:N	1.98	0.61
1:B:370:LEU:HD13	1:B:397:ARG:CB	2.21	0.61
1:E:299:HIS:CG	1:E:300:PRO:HA	2.35	0.61
1:L:150:ARG:NH2	1:L:218:VAL:O	2.31	0.61
1:A:120:ARG:HD3	1:A:328:PHE:CE1	2.36	0.61
1:E:24:ALA:O	1:E:27:PRO:HD2	2.00	0.61
1:F:63:LYS:HB2	1:F:73:ASP:HB3	1.83	0.61
1:B:346:GLU:HG3	1:H:322:PHE:CE1	2.36	0.60
1:F:248:LYS:HD3	1:F:283:ASP:CG	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:LYS:CD	4:G:796:HOH:O	2.48	0.60
1:D:160:LYS:HD2	1:F:295:ARG:HH21	1.65	0.60
1:K:403:GLU:HB2	1:K:413:ILE:HD13	1.82	0.60
1:J:276:GLY:HA3	1:J:279:TRP:NE1	2.17	0.60
1:J:63:LYS:HB2	1:J:73:ASP:HB3	1.83	0.60
1:J:161:VAL:HA	4:J:437:HOH:O	2.00	0.60
1:B:60:LEU:HA	1:B:79:VAL:CG1	2.31	0.60
1:C:330:ASN:CG	1:D:330:ASN:ND2	2.55	0.60
1:D:67:ASP:OD1	1:D:67:ASP:O	2.19	0.60
1:F:1:MET:HE3	1:F:391:ARG:NH2	2.17	0.60
1:G:42:GLN:NE2	4:G:420:HOH:O	2.33	0.60
1:C:325:GLU:HG2	1:C:328:PHE:O	2.01	0.60
1:E:47:LEU:HD21	1:E:400:GLU:N	2.17	0.60
1:G:340:ARG:NH1	1:G:364:GLN:O	2.35	0.60
1:G:44:VAL:O	1:G:66:ARG:NH2	2.31	0.60
1:J:333:MET:O	1:J:336:PRO:HD2	2.01	0.60
1:K:46:LYS:O	1:K:47:LEU:HD23	2.00	0.60
1:K:24:ALA:O	1:K:27:PRO:HD2	2.02	0.60
1:K:333:MET:O	1:K:336:PRO:HD2	2.02	0.60
1:F:276:GLY:HA3	1:F:279:TRP:NE1	2.17	0.60
1:G:177:GLU:N	4:G:433:HOH:O	2.34	0.60
1:G:299:HIS:ND1	1:G:300:PRO:HA	2.17	0.60
1:G:7:GLN:HB2	1:G:412:ASN:CG	2.22	0.60
1:I:333:MET:O	1:I:336:PRO:HD2	2.02	0.60
1:J:283:ASP:OD2	1:J:285:HIS:CE1	2.55	0.60
1:G:252:ARG:O	1:G:253:ASN:HB2	2.00	0.59
1:H:160:LYS:HE3	3:H:608:EPU:O2U	2.02	0.59
1:J:284:MET:O	1:J:285:HIS:C	2.40	0.59
1:J:370:LEU:HD11	1:J:397:ARG:HB3	1.82	0.59
1:C:258:THR:HG22	1:C:259:LEU:HG	1.84	0.59
1:J:370:LEU:HD11	1:J:397:ARG:C	2.22	0.59
1:L:36:GLU:O	1:L:37:GLU:CG	2.51	0.59
1:D:120:ARG:HD3	1:D:328:PHE:CE1	2.37	0.59
1:D:47:LEU:HD21	1:D:400:GLU:N	2.17	0.59
1:E:370:LEU:HD12	1:E:394:HIS:O	2.03	0.59
1:C:63:LYS:HB2	1:C:73:ASP:HB3	1.85	0.59
1:J:370:LEU:HD12	1:J:394:HIS:O	2.02	0.59
1:L:276:GLY:HA3	1:L:279:TRP:NE1	2.17	0.59
1:C:212:ARG:NH1	4:C:437:HOH:O	2.34	0.59
1:G:22:LYS:HE3	1:G:370:LEU:HD21	1.84	0.59
1:I:24:ALA:O	1:I:27:PRO:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:276:GLY:HA3	1:H:279:TRP:NE1	2.18	0.59
1:B:332:PHE:N	4:B:427:HOH:O	2.35	0.59
1:E:370:LEU:HD11	1:E:397:ARG:C	2.23	0.59
1:E:67:ASP:OD1	1:E:69:SER:N	2.36	0.59
1:I:61:GLY:O	1:I:77:VAL:HA	2.03	0.59
1:C:299:HIS:CG	1:C:300:PRO:HA	2.38	0.58
1:D:333:MET:O	1:D:336:PRO:HD2	2.03	0.58
1:F:370:LEU:HD11	1:F:397:ARG:HB3	1.81	0.58
1:F:60:LEU:HA	1:F:79:VAL:CG1	2.33	0.58
1:B:350:ASN:ND2	4:B:437:HOH:O	2.35	0.58
1:C:370:LEU:HD13	1:C:397:ARG:CB	2.27	0.58
1:K:391:ARG:HG3	1:K:393:TYR:HE2	1.68	0.58
1:A:63:LYS:HB2	1:A:73:ASP:HB3	1.85	0.58
1:F:47:LEU:HD21	1:F:400:GLU:N	2.18	0.58
1:G:383:ALA:HB3	4:G:511:HOH:O	2.02	0.58
1:J:391:ARG:HG3	1:J:393:TYR:CE2	2.38	0.58
1:D:370:LEU:HD12	1:D:394:HIS:O	2.03	0.58
1:J:391:ARG:HG3	1:J:393:TYR:HE2	1.68	0.58
1:B:63:LYS:HB2	1:B:73:ASP:HB3	1.85	0.58
1:C:295:ARG:NE	4:C:430:HOH:O	2.34	0.58
1:C:370:LEU:HD12	1:C:394:HIS:O	2.04	0.58
1:H:66:ARG:NE	1:H:67:ASP:O	2.36	0.58
1:I:293:ASN:HD22	1:I:322:PHE:H	1.51	0.58
1:K:42:GLN:NE2	4:K:434:HOH:O	2.36	0.58
1:B:322:PHE:HE1	1:H:346:GLU:HG3	1.68	0.58
1:C:293:ASN:HD22	1:C:322:PHE:H	1.49	0.58
1:C:60:LEU:HA	1:C:79:VAL:CG1	2.34	0.58
1:F:371:ARG:NH2	4:F:427:HOH:O	2.36	0.58
1:G:276:GLY:HA3	1:G:279:TRP:NE1	2.19	0.58
1:I:64:VAL:HA	1:I:71:HIS:O	2.03	0.58
1:K:248:LYS:CE	1:K:282:LEU:HD23	2.33	0.58
1:E:67:ASP:OD1	1:E:68:GLY:C	2.37	0.58
3:F:606:EPU:O4	3:F:606:EPU:HE31	2.03	0.58
1:H:333:MET:O	1:H:336:PRO:HD2	2.04	0.58
1:H:370:LEU:HD11	1:H:397:ARG:C	2.24	0.58
1:K:47:LEU:HD23	1:K:47:LEU:N	2.16	0.58
1:C:276:GLY:HA3	1:C:279:TRP:NE1	2.18	0.58
1:A:333:MET:O	1:A:336:PRO:HD2	2.03	0.57
1:L:36:GLU:O	1:L:37:GLU:HG2	2.04	0.57
1:A:66:ARG:NH2	1:A:67:ASP:OD1	2.30	0.57
1:L:370:LEU:HD11	1:L:397:ARG:C	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ARG:NE	4:B:786:HOH:O	2.37	0.57
1:C:391:ARG:HG3	1:C:393:TYR:CE2	2.37	0.57
1:G:60:LEU:HA	1:G:79:VAL:CG1	2.34	0.57
1:B:22:LYS:HE3	1:B:370:LEU:CD2	2.34	0.57
1:J:66:ARG:CG	1:J:67:ASP:O	2.50	0.57
1:L:370:LEU:HD11	1:L:397:ARG:HB3	1.84	0.57
1:H:299:HIS:CG	1:H:300:PRO:HA	2.39	0.57
1:L:258:THR:HG22	1:L:259:LEU:HG	1.86	0.57
1:E:370:LEU:HD11	1:E:397:ARG:HB3	1.83	0.57
1:F:340:ARG:NH1	1:F:364:GLN:O	2.37	0.57
1:A:325:GLU:HG2	1:A:328:PHE:O	2.05	0.57
1:A:391:ARG:HG3	1:A:393:TYR:CE2	2.39	0.57
1:C:24:ALA:O	1:C:27:PRO:HD2	2.04	0.57
1:G:46:LYS:HA	1:G:66:ARG:HH12	1.70	0.57
1:H:94:ILE:HA	1:H:109:VAL:HG11	1.87	0.57
1:D:22:LYS:HE3	1:D:370:LEU:CD2	2.34	0.57
1:I:258:THR:HG22	1:I:259:LEU:HG	1.87	0.57
1:L:120:ARG:HD3	1:L:328:PHE:CE1	2.40	0.57
1:L:219:GLU:O	1:L:220:ARG:HG3	2.05	0.56
1:B:391:ARG:HG3	1:B:393:TYR:CE2	2.40	0.56
1:I:60:LEU:HA	1:I:79:VAL:CG1	2.36	0.56
1:A:391:ARG:HG3	1:A:393:TYR:HE2	1.69	0.56
1:J:47:LEU:HD21	1:J:400:GLU:N	2.20	0.56
1:K:391:ARG:HG3	1:K:393:TYR:CE2	2.40	0.56
1:E:63:LYS:HB2	1:E:73:ASP:HB3	1.88	0.56
1:I:246:ARG:HG2	1:I:287:LYS:O	2.05	0.56
1:L:60:LEU:HA	1:L:79:VAL:CG1	2.35	0.56
1:G:293:ASN:HD22	1:G:322:PHE:H	1.51	0.56
1:A:293:ASN:HD22	1:A:322:PHE:H	1.54	0.56
1:A:60:LEU:HA	1:A:79:VAL:CG1	2.36	0.56
1:F:333:MET:O	1:F:336:PRO:HD2	2.05	0.56
1:H:120:ARG:HD3	1:H:328:PHE:HE1	1.71	0.56
1:G:391:ARG:HG3	1:G:393:TYR:HE2	1.71	0.55
1:H:60:LEU:HA	1:H:79:VAL:CG1	2.36	0.55
1:I:36:GLU:HG3	1:I:221:LEU:O	2.06	0.55
1:L:47:LEU:HD21	1:L:400:GLU:N	2.21	0.55
1:B:325:GLU:HG2	1:B:328:PHE:O	2.06	0.55
1:K:120:ARG:HD3	1:K:328:PHE:CE1	2.41	0.55
1:K:370:LEU:HD11	1:K:397:ARG:C	2.27	0.55
1:F:330:ASN:HB3	1:G:330:ASN:ND2	2.22	0.55
1:J:299:HIS:ND1	1:J:300:PRO:HA	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ALA:O	1:D:27:PRO:HD2	2.06	0.55
1:K:248:LYS:HG3	1:K:283:ASP:OD1	2.06	0.55
1:A:47:LEU:HD21	1:A:400:GLU:N	2.22	0.55
1:I:11:LYS:HE2	1:I:248:LYS:HE3	1.87	0.55
1:C:46:LYS:O	1:C:47:LEU:HD23	2.06	0.55
1:E:293:ASN:HD22	1:E:322:PHE:H	1.52	0.55
1:G:370:LEU:HD12	1:G:394:HIS:O	2.07	0.55
1:A:46:LYS:CE	1:A:67:ASP:OXT	2.55	0.55
1:F:1:MET:HE3	1:F:391:ARG:CZ	2.37	0.55
1:H:299:HIS:ND1	1:H:300:PRO:HA	2.21	0.55
1:L:38:PRO:O	1:L:223:GLY:HA3	2.07	0.55
1:D:60:LEU:HA	1:D:79:VAL:CG1	2.36	0.55
1:F:94:ILE:HA	1:F:109:VAL:HG11	1.89	0.55
1:K:60:LEU:HA	1:K:79:VAL:CG1	2.36	0.55
1:C:45:PRO:HB2	1:C:47:LEU:HG	1.89	0.55
1:D:407:ARG:HG3	4:D:423:HOH:O	2.06	0.55
1:D:45:PRO:HB2	1:D:47:LEU:HG	1.89	0.55
1:K:247:GLY:O	1:K:248:LYS:HG2	2.06	0.55
1:K:248:LYS:NZ	1:K:284:MET:H	2.03	0.55
1:L:211:ASP:N	1:L:211:ASP:OD1	2.33	0.55
1:B:299:HIS:ND1	1:B:300:PRO:HA	2.22	0.55
1:I:325:GLU:HG2	1:I:328:PHE:O	2.07	0.55
1:K:370:LEU:HD12	1:K:394:HIS:O	2.07	0.55
1:G:39:VAL:HG23	1:G:224:GLY:O	2.08	0.54
1:A:258:THR:HG22	1:A:259:LEU:HG	1.89	0.54
1:L:45:PRO:HB2	1:L:47:LEU:HG	1.89	0.54
1:L:75:ARG:HA	1:L:103:ARG:HH22	1.71	0.54
1:B:369:ASP:C	1:B:369:ASP:OD1	2.45	0.54
1:D:22:LYS:CE	1:D:370:LEU:HD21	2.37	0.54
1:J:60:LEU:HA	1:J:79:VAL:CG1	2.37	0.54
1:H:47:LEU:HD21	1:H:400:GLU:N	2.22	0.54
1:A:276:GLY:HA3	1:A:279:TRP:NE1	2.23	0.54
1:F:258:THR:HG22	1:F:259:LEU:HG	1.89	0.54
1:F:120:ARG:HD3	1:F:328:PHE:HE1	1.71	0.54
1:K:94:ILE:HA	1:K:109:VAL:HG11	1.90	0.54
1:B:391:ARG:HG3	1:B:393:TYR:HE2	1.70	0.54
1:G:370:LEU:HD11	1:G:397:ARG:C	2.28	0.54
1:C:120:ARG:HD3	1:C:328:PHE:CE1	2.43	0.54
1:D:325:GLU:HG2	1:D:328:PHE:O	2.07	0.54
1:E:60:LEU:HA	1:E:79:VAL:CG1	2.36	0.54
3:H:608:EPU:C3E	3:H:608:EPU:O4	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ILE:HA	1:B:109:VAL:HG11	1.90	0.54
1:D:94:ILE:HA	1:D:109:VAL:HG11	1.89	0.54
1:E:94:ILE:HA	1:E:109:VAL:HG11	1.89	0.54
1:G:24:ALA:C	1:G:27:PRO:HD2	2.28	0.54
1:J:66:ARG:HG3	1:J:67:ASP:C	2.28	0.54
1:L:11:LYS:HD2	1:L:246:ARG:O	2.07	0.54
1:B:46:LYS:O	1:B:47:LEU:HD23	2.08	0.54
1:F:150:ARG:HH22	1:F:219:GLU:HA	1.73	0.54
1:G:94:ILE:HA	1:G:109:VAL:HG11	1.89	0.54
1:I:299:HIS:ND1	1:I:300:PRO:HA	2.22	0.54
1:D:220:ARG:HD2	4:D:733:HOH:O	2.08	0.53
1:I:13:GLN:HA	1:I:249:ILE:HG22	1.89	0.53
1:I:47:LEU:HD21	1:I:400:GLU:N	2.23	0.53
1:J:258:THR:HG22	1:J:259:LEU:HG	1.89	0.53
1:L:218:VAL:HG23	1:L:219:GLU:H	1.74	0.53
1:A:120:ARG:HD3	1:A:328:PHE:HE1	1.73	0.53
1:B:370:LEU:HD11	1:B:397:ARG:HB3	1.87	0.53
1:B:47:LEU:HD21	1:B:400:GLU:N	2.23	0.53
1:L:150:ARG:HH12	1:L:219:GLU:HA	1.74	0.53
1:G:120:ARG:HD3	1:G:328:PHE:CE1	2.43	0.53
1:G:36:GLU:OE1	1:G:220:ARG:CZ	2.56	0.53
1:I:276:GLY:HA3	1:I:279:TRP:CD1	2.43	0.53
1:L:244:ILE:HD12	1:L:382:ILE:HD13	1.89	0.53
1:D:258:THR:HG22	1:D:259:LEU:HG	1.90	0.53
1:D:120:ARG:HD3	1:D:328:PHE:HE1	1.73	0.53
1:G:150:ARG:NH2	4:G:752:HOH:O	2.41	0.53
1:I:335:VAL:HB	1:I:336:PRO:HD3	1.90	0.53
1:A:94:ILE:HA	1:A:109:VAL:HG11	1.91	0.53
1:B:146:SER:HB2	4:B:452:HOH:O	2.09	0.53
1:F:325:GLU:HG2	1:F:328:PHE:O	2.07	0.53
1:B:150:ARG:HH12	1:B:219:GLU:HA	1.73	0.53
1:C:244:ILE:HD12	1:C:382:ILE:HD13	1.90	0.53
1:D:276:GLY:HA3	1:D:279:TRP:NE1	2.24	0.53
1:F:285:HIS:CE1	1:H:152:LYS:HZ3	2.26	0.53
1:G:218:VAL:HG12	1:G:220:ARG:H	1.73	0.53
1:H:24:ALA:O	1:H:27:PRO:HD2	2.08	0.53
1:H:370:LEU:HD13	1:H:397:ARG:CB	2.26	0.53
1:H:391:ARG:HG3	1:H:393:TYR:CE2	2.44	0.53
1:L:67:ASP:HB2	1:L:69:SER:H	1.67	0.53
1:B:22:LYS:CE	1:B:370:LEU:HD21	2.38	0.53
1:H:3:LYS:CE	4:H:498:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:LEU:HD22	1:G:343:ALA:HB1	1.91	0.52
1:H:45:PRO:HB2	1:H:47:LEU:HG	1.91	0.52
1:K:212:ARG:NH2	4:K:738:HOH:O	2.40	0.52
1:K:299:HIS:ND1	1:K:300:PRO:HA	2.23	0.52
1:K:152:LYS:HD3	1:K:177:GLU:HB2	1.92	0.52
1:A:120:ARG:CD	4:A:780:HOH:O	2.51	0.52
1:E:299:HIS:ND1	1:E:300:PRO:HA	2.23	0.52
1:F:22:LYS:HE3	1:F:370:LEU:HD21	1.92	0.52
1:K:258:THR:HG22	1:K:259:LEU:HG	1.90	0.52
1:L:24:ALA:C	1:L:27:PRO:HD2	2.30	0.52
1:B:293:ASN:HD22	1:B:322:PHE:H	1.55	0.52
1:F:370:LEU:HD11	1:F:397:ARG:C	2.30	0.52
1:F:66:ARG:HB3	1:F:70:VAL:HG22	1.91	0.52
1:G:391:ARG:HG3	1:G:393:TYR:CE2	2.44	0.52
1:H:120:ARG:HD3	1:H:328:PHE:CE1	2.44	0.52
1:J:24:ALA:C	1:J:27:PRO:HD2	2.29	0.52
1:B:120:ARG:HD3	1:B:328:PHE:CE1	2.45	0.52
1:L:192:VAL:C	4:L:433:HOH:O	2.48	0.52
1:C:330:ASN:CG	1:C:330:ASN:O	2.48	0.52
1:E:391:ARG:HG3	1:E:393:TYR:CE2	2.44	0.52
1:F:38:PRO:O	1:F:223:GLY:HA3	2.09	0.52
1:G:47:LEU:HD21	1:G:400:GLU:N	2.24	0.52
1:H:258:THR:HG22	1:H:259:LEU:HG	1.92	0.52
1:J:46:LYS:HZ3	1:J:67:ASP:HB2	1.75	0.52
1:K:276:GLY:HA3	1:K:279:TRP:CE2	2.45	0.52
1:L:299:HIS:ND1	1:L:300:PRO:HA	2.24	0.52
1:B:244:ILE:HD12	1:B:382:ILE:HD13	1.92	0.52
1:C:334:HIS:H	1:C:334:HIS:CD2	2.28	0.52
1:J:370:LEU:HD13	1:J:397:ARG:CB	2.27	0.52
1:G:120:ARG:HD3	1:G:328:PHE:HE1	1.75	0.52
1:L:219:GLU:O	1:L:220:ARG:CG	2.58	0.52
1:A:46:LYS:O	1:A:47:LEU:HD23	2.10	0.52
1:F:299:HIS:ND1	1:F:300:PRO:HA	2.24	0.52
1:G:176:ALA:C	4:G:433:HOH:O	2.49	0.51
1:J:16:VAL:HB	4:J:425:HOH:O	2.09	0.51
1:K:120:ARG:HD3	1:K:328:PHE:HE1	1.74	0.51
1:L:196:ASN:ND2	4:L:433:HOH:O	2.43	0.51
1:L:333:MET:O	1:L:336:PRO:HD2	2.10	0.51
1:C:10:THR:HG21	4:C:476:HOH:O	2.10	0.51
1:A:346:GLU:HG3	1:E:322:PHE:HE1	1.76	0.51
1:H:369:ASP:HB2	4:H:449:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:276:GLY:HA3	1:I:279:TRP:CE2	2.46	0.51
1:J:46:LYS:NZ	1:J:67:ASP:OXT	2.43	0.51
1:H:340:ARG:NH1	1:H:364:GLN:O	2.43	0.51
1:L:201:LEU:CB	1:L:221:LEU:HD23	2.41	0.51
1:L:335:VAL:HB	1:L:336:PRO:HD3	1.91	0.51
1:C:66:ARG:HE	1:C:67:ASP:HB3	1.75	0.51
1:F:36:GLU:O	1:F:75:ARG:HG2	2.11	0.51
1:E:330:ASN:HB3	1:H:330:ASN:OD1	2.10	0.51
1:I:120:ARG:HD3	1:I:328:PHE:CE1	2.45	0.51
1:E:276:GLY:HA3	1:E:279:TRP:NE1	2.26	0.51
1:F:88:LYS:HE2	4:F:637:HOH:O	2.10	0.51
1:G:150:ARG:HH22	1:G:219:GLU:HA	1.76	0.51
1:H:370:LEU:HD12	1:H:394:HIS:O	2.11	0.51
1:I:204:LYS:HB2	1:I:216:GLU:HB3	1.92	0.51
1:I:94:ILE:HA	1:I:109:VAL:HG11	1.92	0.51
1:K:22:LYS:HE3	1:K:370:LEU:CD2	2.41	0.51
1:C:47:LEU:HD21	1:C:400:GLU:N	2.25	0.51
1:D:150:ARG:HH22	1:D:219:GLU:HA	1.75	0.51
1:E:325:GLU:CG	1:E:328:PHE:O	2.58	0.51
1:I:350:ASN:H	1:I:350:ASN:HD22	1.58	0.51
1:L:193:ASP:HA	4:L:433:HOH:O	2.10	0.51
1:L:391:ARG:HG3	1:L:393:TYR:CE2	2.45	0.51
1:A:340:ARG:NH1	1:A:364:GLN:O	2.44	0.51
1:B:258:THR:HG22	1:B:259:LEU:HG	1.92	0.51
1:F:120:ARG:HD3	1:F:328:PHE:CE1	2.46	0.51
1:G:177:GLU:CA	4:G:433:HOH:O	2.57	0.51
1:E:258:THR:HG22	1:E:259:LEU:HG	1.92	0.51
1:F:335:VAL:HB	1:F:336:PRO:HD3	1.93	0.51
1:I:66:ARG:HD2	1:I:70:VAL:HG22	1.92	0.51
1:L:204:LYS:HD3	1:L:216:GLU:CG	2.40	0.51
1:L:94:ILE:HA	1:L:109:VAL:HG11	1.93	0.51
1:E:391:ARG:HG3	1:E:393:TYR:HE2	1.76	0.51
1:H:150:ARG:HH22	1:H:219:GLU:HA	1.75	0.51
1:B:276:GLY:HA3	1:B:279:TRP:CE2	2.46	0.50
1:E:120:ARG:HD3	1:E:328:PHE:HE1	1.76	0.50
1:K:22:LYS:CE	1:K:370:LEU:HD21	2.41	0.50
1:B:66:ARG:O	1:B:67:ASP:OXT	2.30	0.50
1:I:340:ARG:NH1	1:I:364:GLN:O	2.44	0.50
1:J:340:ARG:NH1	1:J:364:GLN:O	2.45	0.50
1:L:334:HIS:H	1:L:334:HIS:CD2	2.29	0.50
1:K:248:LYS:HZ2	1:K:284:MET:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:10:THR:HG22	1:G:381:CYS:O	2.11	0.50
1:G:66:ARG:O	1:G:67:ASP:O	2.30	0.50
1:J:293:ASN:HB3	4:J:760:HOH:O	2.02	0.50
1:A:334:HIS:H	1:A:334:HIS:CD2	2.29	0.50
1:I:220:ARG:HG3	1:I:221:LEU:H	1.74	0.50
1:I:334:HIS:H	1:I:334:HIS:CD2	2.28	0.50
1:L:37:GLU:O	1:L:37:GLU:HG3	2.10	0.50
1:D:252:ARG:NH2	4:D:428:HOH:O	2.43	0.50
1:F:325:GLU:CG	1:F:328:PHE:O	2.59	0.50
1:G:66:ARG:HB2	1:G:70:VAL:HG22	1.94	0.50
1:H:276:GLY:HA3	1:H:279:TRP:CE2	2.46	0.50
1:H:391:ARG:HG3	1:H:393:TYR:HE2	1.77	0.50
1:H:3:LYS:NZ	4:H:498:HOH:O	2.25	0.50
1:J:276:GLY:HA3	1:J:279:TRP:CE2	2.47	0.50
1:C:120:ARG:HD2	4:C:797:HOH:O	2.11	0.50
1:C:391:ARG:CG	1:C:393:TYR:CE2	2.95	0.50
1:D:155:HIS:HD2	1:D:181:ILE:HB	1.77	0.50
1:D:262:VAL:HG23	4:D:422:HOH:O	2.11	0.50
1:F:1:MET:CE	1:F:391:ARG:CZ	2.89	0.50
1:F:24:ALA:O	1:F:27:PRO:HD2	2.12	0.50
1:H:150:ARG:HH12	1:H:219:GLU:HA	1.77	0.50
1:I:10:THR:HG22	1:I:381:CYS:O	2.12	0.50
1:J:94:ILE:HA	1:J:109:VAL:HG11	1.93	0.50
1:L:42:GLN:HG2	1:L:69:SER:OG	2.12	0.50
1:F:45:PRO:HB2	1:F:47:LEU:HG	1.92	0.50
1:I:66:ARG:O	1:I:67:ASP:OXT	2.29	0.50
1:D:244:ILE:HD12	1:D:382:ILE:HD13	1.93	0.50
1:E:22:LYS:HE3	1:E:370:LEU:CD2	2.42	0.50
1:F:66:ARG:O	1:F:67:ASP:O	2.30	0.50
1:C:94:ILE:HA	1:C:109:VAL:HG11	1.93	0.49
1:F:276:GLY:HA3	1:F:279:TRP:CE2	2.47	0.49
1:G:218:VAL:HG13	1:G:219:GLU:H	1.74	0.49
1:H:176:ALA:O	1:H:217:GLY:HA3	2.12	0.49
1:H:46:LYS:O	1:H:47:LEU:HD23	2.12	0.49
1:I:66:ARG:O	1:I:67:ASP:C	2.50	0.49
1:K:293:ASN:HD22	1:K:322:PHE:H	1.58	0.49
1:K:56:LEU:HB2	1:K:86:LEU:CD2	2.42	0.49
1:L:276:GLY:HA3	1:L:279:TRP:CE2	2.47	0.49
1:G:276:GLY:HA3	1:G:279:TRP:CE2	2.47	0.49
1:I:275:VAL:O	1:I:275:VAL:HG23	2.11	0.49
1:I:37:GLU:HB3	1:I:223:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:370:LEU:HD12	1:L:394:HIS:O	2.12	0.49
1:A:56:LEU:HB2	1:A:86:LEU:CD2	2.43	0.49
1:B:346:GLU:HG3	1:H:322:PHE:HE1	1.76	0.49
1:C:370:LEU:HD11	1:C:397:ARG:HB3	1.90	0.49
1:G:184:ASN:ND2	4:G:421:HOH:O	2.45	0.49
1:L:370:LEU:HD13	1:L:397:ARG:CB	2.32	0.49
1:E:120:ARG:HD3	1:E:328:PHE:CE1	2.47	0.49
1:F:350:ASN:ND2	1:F:350:ASN:H	2.11	0.49
1:E:370:LEU:HD13	1:E:397:ARG:CB	2.26	0.49
1:A:87:VAL:HG21	1:A:110:SER:HB3	1.94	0.49
1:K:174:THR:HG21	1:K:198:LEU:HD13	1.94	0.49
1:K:248:LYS:HG3	1:K:283:ASP:CG	2.33	0.49
1:K:364:GLN:HB3	4:K:451:HOH:O	2.12	0.49
1:K:10:THR:HG22	1:K:381:CYS:O	2.13	0.49
1:J:335:VAL:HB	1:J:336:PRO:HD3	1.94	0.49
1:D:334:HIS:CD2	1:D:334:HIS:H	2.31	0.49
1:E:45:PRO:HB2	1:E:47:LEU:HG	1.95	0.49
1:I:2:ASP:OD1	1:I:417:LYS:CD	2.61	0.49
1:B:334:HIS:H	1:B:334:HIS:CD2	2.29	0.49
1:C:276:GLY:HA3	1:C:279:TRP:CE2	2.48	0.49
1:D:299:HIS:ND1	1:D:300:PRO:HA	2.28	0.49
1:F:96:ALA:O	1:F:99:PRO:HD2	2.13	0.49
1:G:334:HIS:CD2	1:G:334:HIS:H	2.29	0.49
1:J:22:LYS:CE	1:J:370:LEU:HD21	2.43	0.49
1:L:256:PRO:C	1:L:258:THR:H	2.16	0.49
1:H:67:ASP:C	1:H:67:ASP:OD1	2.51	0.49
1:K:152:LYS:CD	1:K:177:GLU:OE1	2.61	0.49
1:K:187:ARG:NH2	4:K:452:HOH:O	2.34	0.49
1:B:24:ALA:C	1:B:27:PRO:HD2	2.32	0.48
1:E:36:GLU:HG3	1:E:221:LEU:O	2.13	0.48
1:E:340:ARG:NH1	1:E:364:GLN:O	2.46	0.48
1:E:10:THR:HG22	1:E:381:CYS:O	2.13	0.48
1:G:46:LYS:HA	1:G:66:ARG:NH1	2.27	0.48
1:H:66:ARG:HG3	1:H:67:ASP:O	2.13	0.48
1:A:299:HIS:ND1	1:A:300:PRO:HA	2.28	0.48
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.94	0.48
1:J:150:ARG:HH12	1:J:219:GLU:HA	1.77	0.48
1:L:174:THR:HG21	1:L:198:LEU:HD13	1.95	0.48
1:K:24:ALA:C	1:K:27:PRO:HD2	2.33	0.48
1:A:24:ALA:C	1:A:27:PRO:HD2	2.34	0.48
1:D:109:VAL:O	1:D:143:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:LEU:HB2	1:G:86:LEU:CD2	2.43	0.48
1:L:22:LYS:HE3	1:L:370:LEU:CD2	2.43	0.48
1:L:96:ALA:O	1:L:99:PRO:HD2	2.13	0.48
1:A:45:PRO:HB2	1:A:47:LEU:HG	1.96	0.48
1:C:348:GLU:HG3	1:F:322:PHE:CE2	2.49	0.48
1:D:370:LEU:HD13	1:D:397:ARG:CB	2.26	0.48
1:J:315:LEU:HD22	1:J:343:ALA:HB1	1.96	0.48
1:H:56:LEU:HB2	1:H:86:LEU:CD2	2.43	0.48
1:I:81:CYS:HA	1:I:108:GLN:O	2.14	0.48
1:I:66:ARG:CB	1:I:70:VAL:HG22	2.43	0.48
1:K:204:LYS:CD	1:K:216:GLU:HG2	2.44	0.48
1:K:248:LYS:HE2	1:K:282:LEU:C	2.34	0.48
1:H:3:LYS:CD	4:H:498:HOH:O	2.53	0.48
1:I:63:LYS:HB2	1:I:73:ASP:HB3	1.95	0.48
1:L:109:VAL:O	1:L:143:VAL:HG13	2.14	0.48
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.96	0.48
1:F:370:LEU:HD12	1:F:394:HIS:O	2.13	0.48
1:I:350:ASN:H	1:I:350:ASN:ND2	2.12	0.48
1:J:160:LYS:HE3	3:J:610:EPU:O2U	2.12	0.48
1:L:30:PHE:HE1	1:L:56:LEU:HD23	1.78	0.48
1:L:340:ARG:NH1	1:L:364:GLN:O	2.47	0.48
1:A:150:ARG:HH22	1:A:219:GLU:HA	1.79	0.48
1:A:315:LEU:HD22	1:A:343:ALA:HB1	1.96	0.48
1:C:22:LYS:HE3	1:C:370:LEU:CD2	2.41	0.48
1:B:400:GLU:HG3	4:B:444:HOH:O	2.13	0.47
1:D:46:LYS:NZ	1:D:67:ASP:O	2.33	0.47
1:F:350:ASN:HD22	1:F:350:ASN:H	1.59	0.47
1:E:124:LEU:HB2	3:E:605:EPU:O4U	2.14	0.47
1:E:150:ARG:HH22	1:E:219:GLU:HA	1.78	0.47
1:F:160:LYS:HE3	3:F:606:EPU:O2U	2.14	0.47
1:G:335:VAL:HB	1:G:336:PRO:HD3	1.96	0.47
1:G:370:LEU:HD13	1:G:397:ARG:CB	2.29	0.47
1:I:201:LEU:CB	1:I:221:LEU:HD22	2.43	0.47
1:B:315:LEU:HD22	1:B:343:ALA:HB1	1.96	0.47
1:D:150:ARG:HH12	1:D:219:GLU:HA	1.78	0.47
1:I:36:GLU:O	1:I:75:ARG:HG2	2.14	0.47
1:L:22:LYS:CE	1:L:370:LEU:HD21	2.44	0.47
1:L:396:ASP:OD2	1:L:415:ARG:NH2	2.46	0.47
1:E:30:PHE:HE1	1:E:56:LEU:HD23	1.80	0.47
1:F:155:HIS:HD2	1:F:181:ILE:HB	1.80	0.47
1:F:302:PHE:HA	1:F:303:PRO:HD3	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:22:LYS:HE3	1:J:370:LEU:CD2	2.43	0.47
1:K:22:LYS:HE2	1:K:49:ASP:OD2	2.15	0.47
1:K:334:HIS:H	1:K:334:HIS:CD2	2.31	0.47
1:L:155:HIS:HD2	1:L:181:ILE:HB	1.79	0.47
1:E:24:ALA:C	1:E:27:PRO:HD2	2.34	0.47
1:J:401:ARG:NH2	4:J:438:HOH:O	2.47	0.47
1:L:6:VAL:HG22	1:L:413:ILE:HG13	1.95	0.47
1:B:340:ARG:NH1	1:B:364:GLN:O	2.47	0.47
1:E:22:LYS:CE	1:E:370:LEU:HD21	2.45	0.47
1:E:46:LYS:O	1:E:47:LEU:HD23	2.15	0.47
1:J:334:HIS:H	1:J:334:HIS:CD2	2.32	0.47
1:K:248:LYS:HD2	1:K:283:ASP:C	2.26	0.47
1:L:315:LEU:HD21	1:L:345:ALA:HB2	1.95	0.47
1:L:315:LEU:HD22	1:L:343:ALA:HB1	1.97	0.47
1:B:45:PRO:HB2	1:B:47:LEU:HG	1.97	0.47
1:E:334:HIS:H	1:E:334:HIS:CD2	2.31	0.47
1:F:244:ILE:HD12	1:F:382:ILE:HD13	1.96	0.47
1:L:302:PHE:HA	1:L:303:PRO:HD3	1.75	0.47
1:C:299:HIS:ND1	1:C:300:PRO:HA	2.30	0.47
1:C:350:ASN:HD22	1:C:350:ASN:H	1.63	0.47
1:E:150:ARG:HH12	1:E:219:GLU:HA	1.79	0.47
1:H:232:ARG:HD3	1:H:258:THR:HG23	1.96	0.47
1:C:253:ASN:OD1	4:C:484:HOH:O	2.20	0.47
1:C:256:PRO:C	1:C:258:THR:H	2.18	0.47
1:C:330:ASN:ND2	1:D:330:ASN:ND2	2.63	0.47
1:D:335:VAL:HB	1:D:336:PRO:HD3	1.96	0.47
1:E:204:LYS:HB2	1:E:216:GLU:HB3	1.97	0.47
1:G:41:ILE:O	1:G:69:SER:HB3	2.15	0.47
1:I:248:LYS:C	1:I:249:ILE:HG23	2.35	0.47
1:K:403:GLU:CB	1:K:413:ILE:HD13	2.45	0.47
1:A:256:PRO:C	1:A:258:THR:H	2.17	0.47
1:B:87:VAL:HG21	1:B:110:SER:HB3	1.95	0.47
1:D:159:ASP:OD1	1:F:265:LYS:NZ	2.47	0.47
1:F:81:CYS:HA	1:F:108:GLN:O	2.15	0.47
1:H:65:GLU:OE2	4:H:446:HOH:O	2.20	0.47
1:E:335:VAL:HB	1:E:336:PRO:HD3	1.96	0.47
1:K:232:ARG:HD3	1:K:258:THR:HG23	1.97	0.47
1:G:21:ALA:HA	1:G:231:ASP:HB2	1.97	0.46
1:G:174:THR:HG21	1:G:198:LEU:HD13	1.98	0.46
1:L:21:ALA:HA	1:L:231:ASP:HB2	1.95	0.46
1:E:108:GLN:HG3	1:E:144:LYS:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ALA:HA	1:E:157:VAL:HG11	1.97	0.46
1:E:174:THR:HG21	1:E:198:LEU:HD13	1.98	0.46
1:H:22:LYS:HE2	1:H:49:ASP:OD2	2.15	0.46
1:K:407:ARG:NH1	1:K:413:ILE:O	2.48	0.46
1:L:357:VAL:HG12	1:L:359:LYS:N	2.29	0.46
1:C:204:LYS:HB2	1:C:216:GLU:HB3	1.98	0.46
1:E:315:LEU:HD22	1:E:343:ALA:HB1	1.97	0.46
1:F:56:LEU:HB2	1:F:86:LEU:CD2	2.46	0.46
1:G:258:THR:HG22	1:G:259:LEU:HG	1.97	0.46
1:H:22:LYS:HE3	1:H:370:LEU:CD2	2.45	0.46
1:H:340:ARG:NH2	4:H:453:HOH:O	2.25	0.46
1:I:303:PRO:HA	4:I:643:HOH:O	2.15	0.46
1:B:150:ARG:HH22	1:B:219:GLU:HA	1.79	0.46
1:F:187:ARG:NH1	4:F:454:HOH:O	2.32	0.46
1:J:120:ARG:HD3	1:J:328:PHE:CE1	2.51	0.46
1:B:30:PHE:HE1	1:B:56:LEU:HD23	1.80	0.46
1:D:66:ARG:O	1:D:66:ARG:HG3	2.15	0.46
1:C:56:LEU:HB2	1:C:86:LEU:CD2	2.46	0.46
1:E:56:LEU:HB2	1:E:86:LEU:CD2	2.45	0.46
1:J:106:GLN:HE21	1:J:108:GLN:HE22	1.63	0.46
1:K:386:THR:HB	4:K:436:HOH:O	2.16	0.46
1:B:56:LEU:HB2	1:B:86:LEU:CD2	2.44	0.46
1:C:120:ARG:HD3	1:C:328:PHE:HE1	1.79	0.46
1:C:10:THR:HG22	1:C:381:CYS:O	2.16	0.46
1:G:45:PRO:HB2	1:G:47:LEU:HG	1.97	0.46
1:H:155:HIS:HD2	1:H:181:ILE:HB	1.81	0.46
1:I:201:LEU:O	1:I:221:LEU:HD23	2.16	0.46
1:K:248:LYS:CG	1:K:283:ASP:OD1	2.63	0.46
1:A:10:THR:HG22	1:A:381:CYS:O	2.15	0.46
1:E:315:LEU:HD21	1:E:345:ALA:HB2	1.98	0.46
1:F:174:THR:HG21	1:F:198:LEU:HD13	1.98	0.46
1:H:299:HIS:O	4:H:447:HOH:O	2.21	0.46
1:H:315:LEU:HD22	1:H:343:ALA:HB1	1.97	0.46
1:E:139:GLU:CG	1:E:144:LYS:HD2	2.46	0.46
1:I:402:ILE:N	4:I:436:HOH:O	2.38	0.46
1:A:396:ASP:OD2	1:A:415:ARG:NH2	2.47	0.45
1:G:22:LYS:HE3	1:G:370:LEU:CD2	2.47	0.45
1:K:335:VAL:HB	1:K:336:PRO:HD3	1.98	0.45
1:B:265:LYS:NZ	1:E:159:ASP:OD1	2.50	0.45
1:C:106:GLN:HE21	1:C:108:GLN:HE22	1.64	0.45
1:C:155:HIS:HD2	1:C:181:ILE:HB	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:LYS:HB2	1:F:216:GLU:HB3	1.99	0.45
1:F:370:LEU:HD13	1:F:397:ARG:CB	2.35	0.45
1:G:75:ARG:NH1	4:G:813:HOH:O	2.23	0.45
1:J:285:HIS:N	4:J:444:HOH:O	2.48	0.45
1:B:302:PHE:HA	1:B:303:PRO:HD3	1.75	0.45
1:E:118:GLY:CA	1:E:330:ASN:OD1	2.64	0.45
1:F:150:ARG:HH12	1:F:219:GLU:HA	1.81	0.45
1:G:7:GLN:HB2	1:G:412:ASN:ND2	2.30	0.45
1:H:350:ASN:H	1:H:350:ASN:HD22	1.64	0.45
1:I:45:PRO:HB2	1:I:47:LEU:HG	1.97	0.45
1:J:256:PRO:C	1:J:258:THR:H	2.19	0.45
1:J:302:PHE:HA	1:J:303:PRO:HD3	1.77	0.45
1:L:120:ARG:HD3	1:L:328:PHE:HE1	1.80	0.45
1:A:315:LEU:HD21	1:A:345:ALA:HB2	1.98	0.45
1:C:24:ALA:C	1:C:27:PRO:HD2	2.36	0.45
1:E:276:GLY:HA3	1:E:279:TRP:CE2	2.51	0.45
1:F:248:LYS:HD3	1:F:283:ASP:OD2	2.17	0.45
1:F:24:ALA:C	1:F:27:PRO:HD2	2.37	0.45
1:F:10:THR:HG22	1:F:381:CYS:O	2.16	0.45
1:H:334:HIS:H	1:H:334:HIS:CD2	2.35	0.45
1:I:37:GLU:HG2	1:I:38:PRO:CD	2.35	0.45
1:B:396:ASP:OD2	1:B:415:ARG:NH2	2.50	0.45
1:E:109:VAL:O	1:E:143:VAL:HG13	2.15	0.45
1:F:66:ARG:CB	1:F:70:VAL:HG22	2.45	0.45
1:G:67:ASP:OXT	1:G:67:ASP:OD1	2.34	0.45
1:I:150:ARG:HH12	1:I:219:GLU:HA	1.81	0.45
1:I:2:ASP:OD1	1:I:417:LYS:HD3	2.17	0.45
1:B:320:THR:HG21	1:H:320:THR:HG21	1.98	0.45
1:G:155:HIS:HD2	1:G:181:ILE:HB	1.81	0.45
1:H:325:GLU:CG	1:H:328:PHE:O	2.65	0.45
1:K:66:ARG:NE	1:K:67:ASP:O	2.50	0.45
1:A:330:ASN:HB3	1:B:330:ASN:ND2	2.31	0.45
1:D:204:LYS:HB2	1:D:216:GLU:HB3	1.99	0.45
1:D:21:ALA:HA	1:D:231:ASP:HB2	1.98	0.45
1:F:330:ASN:ND2	1:G:330:ASN:HB3	2.32	0.45
1:L:37:GLU:HA	1:L:38:PRO:HA	1.69	0.45
1:B:220:ARG:HA	4:B:487:HOH:O	2.15	0.45
1:B:232:ARG:HD3	1:B:258:THR:HG23	1.99	0.45
1:B:369:ASP:OD1	1:B:371:ARG:N	2.43	0.45
1:D:390:ASP:O	1:D:391:ARG:CB	2.63	0.45
1:J:252:ARG:O	1:J:253:ASN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:38:PRO:O	1:L:223:GLY:CA	2.65	0.45
1:E:160:LYS:HE3	3:E:605:EPU:O2U	2.17	0.45
1:H:295:ARG:NE	4:H:451:HOH:O	2.50	0.45
1:I:260:ASP:HB2	4:I:820:HOH:O	2.17	0.45
1:I:56:LEU:HB2	1:I:86:LEU:CD2	2.47	0.45
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.99	0.45
1:H:350:ASN:ND2	1:H:350:ASN:H	2.15	0.45
1:I:219:GLU:CG	1:I:219:GLU:O	2.65	0.45
1:I:275:VAL:O	1:I:275:VAL:CG2	2.65	0.45
1:L:81:CYS:HA	1:L:108:GLN:O	2.17	0.45
1:E:67:ASP:CG	1:E:69:SER:N	2.70	0.44
1:A:150:ARG:HH12	1:A:219:GLU:HA	1.83	0.44
1:J:81:CYS:HA	1:J:108:GLN:O	2.17	0.44
1:J:204:LYS:HB2	1:J:216:GLU:HB3	1.98	0.44
1:J:244:ILE:HD12	1:J:382:ILE:HD13	1.99	0.44
1:K:118:GLY:HA3	4:K:446:HOH:O	2.17	0.44
1:D:276:GLY:HA3	1:D:279:TRP:CE2	2.52	0.44
1:B:248:LYS:HB2	1:B:248:LYS:HE3	1.46	0.44
1:E:256:PRO:C	1:E:258:THR:H	2.21	0.44
1:G:177:GLU:HA	4:G:433:HOH:O	2.17	0.44
1:L:10:THR:HG22	1:L:381:CYS:O	2.18	0.44
1:A:6:VAL:HG22	1:A:413:ILE:HG13	1.98	0.44
1:C:22:LYS:CE	1:C:370:LEU:HD21	2.45	0.44
1:G:349:SER:HB3	1:G:350:ASN:H	1.61	0.44
1:H:6:VAL:HG22	1:H:413:ILE:HG13	1.99	0.44
1:I:24:ALA:C	1:I:27:PRO:HD2	2.37	0.44
1:B:204:LYS:HB2	1:B:216:GLU:HB3	1.99	0.44
1:B:256:PRO:C	1:B:258:THR:H	2.20	0.44
1:C:5:ARG:NH1	4:C:428:HOH:O	2.50	0.44
1:I:256:PRO:C	1:I:258:THR:H	2.20	0.44
1:J:150:ARG:HH22	1:J:219:GLU:HA	1.82	0.44
1:J:87:VAL:HG21	1:J:110:SER:HB3	2.00	0.44
1:K:151:LEU:C	1:K:152:LYS:HG2	2.38	0.44
1:K:155:HIS:HD2	1:K:181:ILE:HB	1.82	0.44
1:L:219:GLU:C	1:L:220:ARG:HG3	2.38	0.44
1:L:391:ARG:HG3	1:L:393:TYR:HE2	1.83	0.44
1:B:22:LYS:HE2	1:B:49:ASP:OD2	2.17	0.44
1:F:256:PRO:C	1:F:258:THR:H	2.21	0.44
1:F:46:LYS:O	1:F:47:LEU:HD23	2.18	0.44
1:I:155:HIS:HD2	1:I:181:ILE:HB	1.82	0.44
1:K:47:LEU:HD21	1:K:400:GLU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ALA:C	1:D:27:PRO:HD2	2.38	0.44
1:L:27:PRO:HG3	1:L:95:TRP:CH2	2.53	0.44
1:A:285:HIS:HB3	1:D:152:LYS:CD	2.47	0.44
1:B:81:CYS:HA	1:B:108:GLN:O	2.18	0.44
1:C:396:ASP:OD2	1:C:415:ARG:NH2	2.49	0.44
1:D:96:ALA:O	1:D:99:PRO:HD2	2.18	0.44
1:E:302:PHE:HA	1:E:303:PRO:HD3	1.73	0.44
1:H:81:CYS:HA	1:H:108:GLN:O	2.18	0.44
1:L:176:ALA:O	1:L:217:GLY:HA3	2.18	0.44
1:L:357:VAL:CG1	1:L:358:GLU:H	2.27	0.44
1:A:155:HIS:HD2	1:A:181:ILE:HB	1.82	0.43
1:A:219:GLU:HG2	1:A:219:GLU:O	2.17	0.43
1:D:85:ASP:HA	1:D:88:LYS:HE2	1.99	0.43
1:G:256:PRO:C	1:G:258:THR:H	2.21	0.43
1:K:256:PRO:C	1:K:258:THR:H	2.20	0.43
1:L:350:ASN:HD22	1:L:350:ASN:H	1.66	0.43
1:B:96:ALA:O	1:B:99:PRO:HD2	2.18	0.43
1:G:66:ARG:C	1:G:67:ASP:O	2.55	0.43
1:H:24:ALA:C	1:H:27:PRO:HD2	2.37	0.43
1:J:10:THR:HG22	1:J:381:CYS:O	2.18	0.43
1:K:302:PHE:HA	1:K:303:PRO:HD3	1.78	0.43
1:L:183:GLU:OE2	1:L:212:ARG:CZ	2.65	0.43
1:L:350:ASN:ND2	1:L:350:ASN:H	2.16	0.43
1:C:350:ASN:H	1:C:350:ASN:ND2	2.15	0.43
1:D:340:ARG:NH1	1:D:364:GLN:O	2.51	0.43
1:F:396:ASP:OD2	1:F:415:ARG:NH2	2.49	0.43
1:I:46:LYS:O	1:I:47:LEU:HD23	2.17	0.43
1:L:371:ARG:NH1	1:L:398:GLY:O	2.51	0.43
1:A:109:VAL:O	1:A:143:VAL:HG13	2.19	0.43
1:A:317:ALA:O	1:A:356:GLY:HA3	2.18	0.43
1:F:334:HIS:H	1:F:334:HIS:CD2	2.36	0.43
1:G:244:ILE:HD12	1:G:382:ILE:HD13	2.00	0.43
1:I:40:GLU:HB3	1:I:225:VAL:HG22	1.99	0.43
1:J:315:LEU:HD21	1:J:345:ALA:HB2	1.99	0.43
1:L:219:GLU:HG2	1:L:220:ARG:HG3	2.00	0.43
1:L:293:ASN:HD22	1:L:322:PHE:H	1.63	0.43
1:A:22:LYS:HB2	1:A:47:LEU:HD12	2.00	0.43
1:D:6:VAL:HG22	1:D:413:ILE:HG13	1.99	0.43
1:E:87:VAL:HG21	1:E:110:SER:HB3	2.00	0.43
1:G:46:LYS:HE2	1:G:67:ASP:OD1	2.18	0.43
1:I:11:LYS:HE2	1:I:248:LYS:CE	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:GLY:O	1:I:249:ILE:HB	2.19	0.43
1:I:276:GLY:CA	1:I:279:TRP:CE2	3.01	0.43
1:I:91:ARG:HG2	2:I:509:PO3:O1	2.19	0.43
1:J:45:PRO:HB2	1:J:47:LEU:HG	2.00	0.43
1:D:81:CYS:HA	1:D:108:GLN:O	2.17	0.43
1:D:9:PRO:HD3	1:D:384:GLU:HA	2.00	0.43
1:G:41:ILE:HG22	1:G:44:VAL:CG2	2.49	0.43
1:H:30:PHE:HE1	1:H:56:LEU:HD23	1.83	0.43
1:H:36:GLU:OE1	1:H:220:ARG:NH2	2.51	0.43
1:I:30:PHE:HE1	1:I:56:LEU:HD23	1.82	0.43
1:H:256:PRO:C	1:H:258:THR:H	2.21	0.43
1:J:176:ALA:O	1:J:217:GLY:HA3	2.19	0.43
1:J:174:THR:HG21	1:J:198:LEU:HD13	2.00	0.43
1:J:396:ASP:OD2	1:J:415:ARG:NH2	2.51	0.43
1:L:232:ARG:HD3	1:L:258:THR:HG23	2.00	0.43
1:C:407:ARG:NH1	4:C:463:HOH:O	2.38	0.43
1:F:6:VAL:HG22	1:F:413:ILE:HG13	2.01	0.43
1:F:27:PRO:HG3	1:F:95:TRP:CH2	2.54	0.43
1:H:335:VAL:HB	1:H:336:PRO:HD3	2.00	0.43
1:J:283:ASP:OD1	1:J:284:MET:N	2.52	0.43
1:K:248:LYS:HZ3	1:K:282:LEU:HD23	1.80	0.43
1:B:350:ASN:ND2	1:B:350:ASN:H	2.16	0.43
1:F:42:GLN:HG2	1:F:69:SER:OG	2.19	0.43
1:G:81:CYS:HA	1:G:108:GLN:O	2.18	0.43
1:G:40:GLU:HB3	1:G:225:VAL:HG22	2.01	0.43
1:G:22:LYS:HE2	1:G:49:ASP:OD2	2.19	0.43
1:K:67:ASP:OD1	1:K:67:ASP:C	2.57	0.43
1:L:124:LEU:HB2	3:L:612:EPU:O4U	2.19	0.43
1:A:276:GLY:HA3	1:A:279:TRP:CE2	2.53	0.43
1:A:30:PHE:HE1	1:A:56:LEU:HD23	1.84	0.43
1:D:315:LEU:HD22	1:D:343:ALA:HB1	2.00	0.43
1:I:120:ARG:HD3	1:I:328:PHE:HE1	1.84	0.43
1:F:315:LEU:HD22	1:F:343:ALA:HB1	1.99	0.42
1:F:391:ARG:NH1	1:F:393:TYR:OH	2.52	0.42
1:J:56:LEU:HB2	1:J:86:LEU:CD2	2.48	0.42
1:K:297:ALA:HB1	1:K:298:PRO:CD	2.49	0.42
1:F:333:MET:HG3	4:F:442:HOH:O	2.18	0.42
1:G:30:PHE:HE1	1:G:56:LEU:HD23	1.84	0.42
1:G:5:ARG:HB3	1:G:414:GLU:HG3	2.00	0.42
1:H:21:ALA:HA	1:H:231:ASP:HB2	2.01	0.42
1:H:232:ARG:CB	1:H:258:THR:CG2	2.90	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244:ILE:HD12	1:H:382:ILE:HD13	2.01	0.42
1:I:66:ARG:HB2	1:I:70:VAL:HG22	2.00	0.42
1:K:258:THR:HG21	4:K:442:HOH:O	2.19	0.42
1:K:350:ASN:H	1:K:350:ASN:ND2	2.17	0.42
1:E:81:CYS:HA	1:E:108:GLN:O	2.18	0.42
1:E:244:ILE:HD12	1:E:382:ILE:HD13	2.00	0.42
1:F:232:ARG:CB	1:F:258:THR:CG2	2.93	0.42
1:I:302:PHE:HA	1:I:303:PRO:HD3	1.80	0.42
1:I:37:GLU:CG	1:I:38:PRO:N	2.82	0.42
1:I:96:ALA:O	1:I:99:PRO:HD2	2.19	0.42
1:J:6:VAL:HG22	1:J:413:ILE:HG13	2.01	0.42
1:L:91:ARG:HD2	2:L:512:PO3:O1	2.18	0.42
1:A:232:ARG:CB	1:A:258:THR:CG2	2.94	0.42
1:F:41:ILE:O	1:F:69:SER:HA	2.19	0.42
1:G:315:LEU:HD21	1:G:345:ALA:HB2	2.01	0.42
1:G:87:VAL:HG21	1:G:110:SER:HB3	2.00	0.42
1:K:81:CYS:HA	1:K:108:GLN:O	2.19	0.42
1:D:315:LEU:HD21	1:D:345:ALA:HB2	2.00	0.42
1:K:396:ASP:OD2	1:K:415:ARG:NH2	2.52	0.42
1:B:315:LEU:HD21	1:B:345:ALA:HB2	2.02	0.42
1:B:370:LEU:HD11	1:B:397:ARG:CA	2.45	0.42
1:G:157:VAL:HA	1:G:183:GLU:HB2	2.01	0.42
1:H:338:LEU:HA	1:H:338:LEU:HD23	1.88	0.42
1:J:153:GLY:HA2	1:J:180:THR:OG1	2.19	0.42
1:K:406:LEU:C	1:K:411:ALA:HB3	2.40	0.42
1:A:350:ASN:HD22	1:A:350:ASN:H	1.68	0.42
1:A:27:PRO:HG3	1:A:95:TRP:CH2	2.54	0.42
1:C:366:MET:O	4:C:436:HOH:O	2.22	0.42
1:E:370:LEU:HD11	1:E:397:ARG:CA	2.48	0.42
1:G:106:GLN:HE21	1:G:108:GLN:HE22	1.67	0.42
1:G:176:ALA:O	1:G:217:GLY:HA3	2.18	0.42
1:I:219:GLU:O	1:I:219:GLU:HG2	2.20	0.42
1:I:244:ILE:HD12	1:I:382:ILE:HD13	2.02	0.42
1:I:247:GLY:CA	1:I:248:LYS:HE2	2.46	0.42
1:J:40:GLU:HB3	1:J:225:VAL:HG22	2.01	0.42
1:K:370:LEU:HD11	1:K:397:ARG:HB3	1.91	0.42
1:L:204:LYS:HD3	1:L:216:GLU:HG2	2.00	0.42
1:C:391:ARG:CG	1:C:393:TYR:HE2	2.24	0.42
1:G:11:LYS:HD3	4:G:796:HOH:O	2.16	0.42
1:C:81:CYS:HA	1:C:108:GLN:O	2.20	0.42
1:D:7:GLN:HA	1:D:7:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:PHE:HA	1:G:303:PRO:HD3	1.82	0.42
1:I:153:GLY:HA2	1:I:180:THR:OG1	2.20	0.42
1:I:246:ARG:HH21	1:I:288:ARG:HD2	1.83	0.42
1:K:350:ASN:H	1:K:350:ASN:HD22	1.68	0.42
1:A:174:THR:HG21	1:A:198:LEU:HD13	2.02	0.42
1:C:67:ASP:HB2	1:C:69:SER:O	2.20	0.42
3:F:606:EPU:C3E	3:F:606:EPU:O4	2.67	0.42
1:G:135:THR:C	1:G:136:ILE:HG12	2.40	0.42
1:G:46:LYS:CE	1:G:67:ASP:OD1	2.67	0.42
1:H:248:LYS:HE3	1:H:283:ASP:OD2	2.20	0.42
1:I:315:LEU:HD22	1:I:343:ALA:HB1	2.02	0.42
1:B:350:ASN:HD22	1:B:350:ASN:H	1.68	0.41
1:F:267:ARG:NH1	4:F:432:HOH:O	2.51	0.41
1:C:348:GLU:CG	1:F:322:PHE:CE2	3.03	0.41
1:G:189:PRO:HD3	1:G:299:HIS:CD2	2.54	0.41
1:J:317:ALA:O	1:J:356:GLY:HA3	2.20	0.41
1:K:247:GLY:O	1:K:248:LYS:CG	2.68	0.41
1:D:94:ILE:HD12	1:D:109:VAL:HG11	2.01	0.41
1:I:160:LYS:HE3	3:I:609:EPU:O2U	2.20	0.41
1:I:22:LYS:HB2	1:I:47:LEU:HD12	2.02	0.41
1:K:330:ASN:HB3	1:L:330:ASN:ND2	2.35	0.41
1:K:9:PRO:HD3	1:K:384:GLU:HA	2.03	0.41
1:A:46:LYS:HE2	4:A:436:HOH:O	2.20	0.41
1:E:354:CYS:O	4:E:425:HOH:O	2.22	0.41
1:F:391:ARG:NH1	1:F:393:TYR:CZ	2.87	0.41
1:J:156:ILE:HA	4:J:534:HOH:O	2.20	0.41
1:A:81:CYS:HA	1:A:108:GLN:O	2.19	0.41
1:E:155:HIS:HD2	1:E:181:ILE:HB	1.84	0.41
1:A:346:GLU:HG3	1:E:322:PHE:CE1	2.53	0.41
1:I:106:GLN:HE21	1:I:108:GLN:HE22	1.68	0.41
1:B:318:GLU:OE2	4:B:814:HOH:O	2.21	0.41
1:C:109:VAL:O	1:C:143:VAL:HG13	2.21	0.41
1:D:66:ARG:O	1:D:67:ASP:OXT	2.39	0.41
1:F:109:VAL:O	1:F:143:VAL:HG13	2.20	0.41
1:F:349:SER:HB3	1:F:350:ASN:H	1.71	0.41
1:K:40:GLU:HB3	1:K:225:VAL:HG22	2.02	0.41
1:C:349:SER:HB3	1:C:350:ASN:H	1.66	0.41
1:F:30:PHE:HE1	1:F:56:LEU:HD23	1.86	0.41
1:I:350:ASN:N	1:I:350:ASN:HD22	2.18	0.41
1:J:21:ALA:HA	1:J:231:ASP:HB2	2.02	0.41
1:L:297:ALA:HB1	1:L:298:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:369:ASP:HB3	1:L:372:ALA:HB3	2.03	0.41
1:L:94:ILE:HD12	1:L:109:VAL:HG11	2.03	0.41
1:D:232:ARG:HD3	1:D:258:THR:HG23	2.02	0.41
1:E:317:ALA:O	1:E:356:GLY:HA3	2.20	0.41
1:I:349:SER:HB3	1:I:350:ASN:H	1.65	0.41
1:J:109:VAL:O	1:J:143:VAL:HG13	2.20	0.41
1:L:40:GLU:HB3	1:L:225:VAL:HG22	2.03	0.41
1:B:157:VAL:HA	1:B:183:GLU:HB2	2.03	0.41
1:B:370:LEU:HD23	3:B:602:EPU:O2E	2.21	0.41
1:C:176:ALA:O	1:C:217:GLY:HA3	2.21	0.41
1:C:330:ASN:CG	1:D:330:ASN:HD22	2.24	0.41
1:G:100:LEU:HA	1:G:100:LEU:HD23	1.89	0.41
1:G:232:ARG:HD3	1:G:258:THR:HG23	2.03	0.41
1:H:22:LYS:CE	1:H:370:LEU:HD21	2.47	0.41
1:I:401:ARG:N	4:I:436:HOH:O	2.52	0.41
1:J:336:PRO:O	1:J:339:SER:HB2	2.20	0.41
1:C:30:PHE:HE1	1:C:56:LEU:HD23	1.85	0.41
1:G:412:ASN:HA	4:G:426:HOH:O	2.21	0.41
1:I:150:ARG:HH22	1:I:219:GLU:HA	1.85	0.41
1:L:201:LEU:HB2	1:L:221:LEU:HD23	2.03	0.41
1:L:357:VAL:HG12	1:L:359:LYS:H	1.85	0.41
1:A:106:GLN:HE21	1:A:108:GLN:HE22	1.69	0.41
1:A:204:LYS:HB2	1:A:216:GLU:HB3	2.03	0.41
1:B:153:GLY:HA2	1:B:180:THR:OG1	2.21	0.41
1:E:139:GLU:HG2	1:E:144:LYS:HD2	2.03	0.41
1:F:330:ASN:CG	1:G:330:ASN:CG	2.79	0.41
1:H:370:LEU:CD1	1:H:397:ARG:HB3	2.39	0.41
1:H:96:ALA:O	1:H:99:PRO:HD2	2.21	0.41
1:J:293:ASN:HD22	1:J:322:PHE:H	1.62	0.41
1:A:248:LYS:HE2	1:A:248:LYS:HB2	1.78	0.41
1:B:7:GLN:NE2	4:B:449:HOH:O	2.54	0.41
1:D:248:LYS:HB2	1:D:248:LYS:HE3	1.90	0.41
1:D:370:LEU:HD11	1:D:397:ARG:CA	2.49	0.41
1:F:315:LEU:HD21	1:F:345:ALA:HB2	2.03	0.41
1:H:189:PRO:HD3	1:H:299:HIS:CD2	2.56	0.41
1:I:157:VAL:HA	1:I:183:GLU:HB2	2.03	0.41
1:J:155:HIS:HD2	1:J:181:ILE:HB	1.85	0.41
1:J:325:GLU:CG	1:J:328:PHE:O	2.67	0.41
1:K:297:ALA:HB1	1:K:298:PRO:HD2	2.03	0.41
1:K:330:ASN:ND2	1:L:330:ASN:HB3	2.36	0.41
1:L:9:PRO:HD3	1:L:384:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:612:EPU:O1B	3:L:612:EPU:O2A	2.37	0.41
1:J:30:PHE:HE1	1:J:56:LEU:HD23	1.86	0.40
1:D:106:GLN:HE21	1:D:108:GLN:HE22	1.69	0.40
1:D:27:PRO:HG3	1:D:95:TRP:CH2	2.56	0.40
1:D:30:PHE:HE1	1:D:56:LEU:HD23	1.86	0.40
1:E:96:ALA:O	1:E:99:PRO:HD2	2.20	0.40
1:H:174:THR:HG21	1:H:198:LEU:HD13	2.04	0.40
1:K:247:GLY:O	1:K:248:LYS:CD	2.69	0.40
1:K:315:LEU:HD21	1:K:345:ALA:HB2	2.03	0.40
1:L:30:PHE:CE1	1:L:56:LEU:HD23	2.56	0.40
1:A:51:ASP:OD1	4:A:434:HOH:O	2.22	0.40
1:B:21:ALA:HA	1:B:231:ASP:HB2	2.02	0.40
1:B:252:ARG:O	1:B:253:ASN:HB2	2.21	0.40
1:E:40:GLU:HB3	1:E:225:VAL:HG22	2.03	0.40
1:E:403:GLU:OE2	1:J:277:GLU:OE2	2.39	0.40
1:F:100:LEU:HA	1:F:100:LEU:HD23	1.93	0.40
1:I:174:THR:HG21	1:I:198:LEU:HD13	2.03	0.40
1:L:157:VAL:HA	1:L:183:GLU:HB2	2.04	0.40
1:B:106:GLN:HE21	1:B:108:GLN:HE22	1.69	0.40
1:B:349:SER:HB3	1:B:350:ASN:H	1.70	0.40
1:D:22:LYS:HE2	1:D:49:ASP:OD2	2.22	0.40
1:F:9:PRO:HD3	1:F:384:GLU:HA	2.02	0.40
1:J:277:GLU:CG	4:J:783:HOH:O	2.70	0.40
1:J:391:ARG:CG	1:J:393:TYR:CE2	3.04	0.40
1:J:46:LYS:HZ1	1:J:67:ASP:HB3	1.87	0.40
1:B:120:ARG:HD3	1:B:328:PHE:HE1	1.83	0.40
1:C:302:PHE:HA	1:C:303:PRO:HD3	1.73	0.40
1:C:350:ASN:HD22	1:C:350:ASN:N	2.19	0.40
1:D:41:ILE:HG22	1:D:44:VAL:CG2	2.51	0.40
1:E:407:ARG:NH1	1:E:413:ILE:O	2.54	0.40
1:E:47:LEU:HA	1:E:47:LEU:HD23	1.81	0.40
1:K:248:LYS:HD2	1:K:284:MET:N	2.35	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	414/418 (99%)	403 (97%)	10 (2%)	1 (0%)	51	73
1	B	414/418 (99%)	404 (98%)	10 (2%)	0	100	100
1	C	414/418 (99%)	401 (97%)	13 (3%)	0	100	100
1	D	414/418 (99%)	404 (98%)	9 (2%)	1 (0%)	51	73
1	E	414/418 (99%)	403 (97%)	11 (3%)	0	100	100
1	F	414/418 (99%)	404 (98%)	10 (2%)	0	100	100
1	G	414/418 (99%)	402 (97%)	12 (3%)	0	100	100
1	H	414/418 (99%)	403 (97%)	10 (2%)	1 (0%)	51	73
1	I	414/418 (99%)	399 (96%)	13 (3%)	2 (0%)	32	53
1	J	414/418 (99%)	404 (98%)	9 (2%)	1 (0%)	51	73
1	K	414/418 (99%)	403 (97%)	11 (3%)	0	100	100
1	L	414/418 (99%)	400 (97%)	12 (3%)	2 (0%)	32	53
All	All	4968/5016 (99%)	4830 (97%)	130 (3%)	8 (0%)	51	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	37	GLU
1	L	38	PRO
1	A	370	LEU
1	H	370	LEU
1	I	38	PRO
1	J	370	LEU
1	D	370	LEU
1	I	39	VAL

### 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	331/331 (100%)	312 (94%)	19 (6%)	24	44
1	B	331/331 (100%)	309 (93%)	22 (7%)	19	36
1	C	331/331 (100%)	309 (93%)	22 (7%)	19	36
1	D	331/331 (100%)	315 (95%)	16 (5%)	30	53
1	E	331/331 (100%)	307 (93%)	24 (7%)	16	31
1	F	331/331 (100%)	309 (93%)	22 (7%)	19	36
1	G	331/331 (100%)	310 (94%)	21 (6%)	21	38
1	H	331/331 (100%)	311 (94%)	20 (6%)	22	41
1	I	331/331 (100%)	303 (92%)	28 (8%)	12	23
1	J	331/331 (100%)	309 (93%)	22 (7%)	19	36
1	K	331/331 (100%)	312 (94%)	19 (6%)	24	44
1	L	331/331 (100%)	311 (94%)	20 (6%)	22	41
All	All	3972/3972 (100%)	3717 (94%)	255 (6%)	20	38

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	55	LYS
1	A	63	LYS
1	A	86	LEU
1	A	131	GLN
1	A	143	VAL
1	A	150	ARG
1	A	158	MET
1	A	159	ASP
1	A	193	ASP
1	A	248	LYS
1	A	258	THR
1	A	307	GLN
1	A	346	GLU
1	A	349	SER
1	A	350	ASN
1	A	358	GLU
1	A	370	LEU
1	A	416	VAL
1	B	7	GLN
1	B	10	THR
1	B	55	LYS

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Mol	Chain	Res	Type
1	B	69	SER
1	B	86	LEU
1	B	131	GLN
1	B	143	VAL
1	B	150	ARG
1	B	158	MET
1	B	159	ASP
1	B	193	ASP
1	B	248	LYS
1	B	258	THR
1	B	265	LYS
1	B	307	GLN
1	B	346	GLU
1	B	349	SER
1	B	350	ASN
1	B	358	GLU
1	B	361	SER
1	B	413	ILE
1	B	416	VAL
1	C	7	GLN
1	C	39	VAL
1	C	48	LYS
1	C	55	LYS
1	C	65	GLU
1	C	66	ARG
1	C	86	LEU
1	C	131	GLN
1	C	137	LYS
1	C	140	GLU
1	C	143	VAL
1	C	158	MET
1	C	159	ASP
1	C	193	ASP
1	C	258	THR
1	C	307	GLN
1	C	346	GLU
1	C	349	SER
1	C	350	ASN
1	C	358	GLU
1	C	361	SER
1	C	416	VAL
1	D	7	GLN

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Mol	Chain	Res	Type
1	D	48	LYS
1	D	55	LYS
1	D	131	GLN
1	D	143	VAL
1	D	150	ARG
1	D	158	MET
1	D	159	ASP
1	D	258	THR
1	D	307	GLN
1	D	346	GLU
1	D	349	SER
1	D	350	ASN
1	D	358	GLU
1	D	391	ARG
1	D	416	VAL
1	E	7	GLN
1	E	38	PRO
1	E	39	VAL
1	E	55	LYS
1	E	63	LYS
1	E	69	SER
1	E	86	LEU
1	E	131	GLN
1	E	143	VAL
1	E	150	ARG
1	E	158	MET
1	E	159	ASP
1	E	193	ASP
1	E	212	ARG
1	E	258	THR
1	E	307	GLN
1	E	330	ASN
1	E	333	MET
1	E	346	GLU
1	E	349	SER
1	E	350	ASN
1	E	358	GLU
1	E	361	SER
1	E	416	VAL
1	F	7	GLN
1	F	38	PRO
1	F	55	LYS

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Mol	Chain	Res	Type
1	F	67	ASP
1	F	86	LEU
1	F	131	GLN
1	F	143	VAL
1	F	150	ARG
1	F	158	MET
1	F	159	ASP
1	F	183	GLU
1	F	258	THR
1	F	265	LYS
1	F	295	ARG
1	F	307	GLN
1	F	326	THR
1	F	346	GLU
1	F	349	SER
1	F	350	ASN
1	F	358	GLU
1	F	361	SER
1	F	416	VAL
1	G	7	GLN
1	G	38	PRO
1	G	55	LYS
1	G	66	ARG
1	G	86	LEU
1	G	131	GLN
1	G	136	ILE
1	G	143	VAL
1	G	150	ARG
1	G	158	MET
1	G	159	ASP
1	G	193	ASP
1	G	216	GLU
1	G	219	GLU
1	G	258	THR
1	G	307	GLN
1	G	346	GLU
1	G	349	SER
1	G	350	ASN
1	G	361	SER
1	G	416	VAL
1	H	7	GLN
1	H	10	THR

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Mol	Chain	Res	Type
1	H	38	PRO
1	H	46	LYS
1	H	66	ARG
1	H	86	LEU
1	H	131	GLN
1	H	143	VAL
1	H	150	ARG
1	H	158	MET
1	H	159	ASP
1	H	248	LYS
1	H	258	THR
1	H	307	GLN
1	H	346	GLU
1	H	349	SER
1	H	350	ASN
1	H	358	GLU
1	H	361	SER
1	H	416	VAL
1	I	7	GLN
1	I	36	GLU
1	I	38	PRO
1	I	55	LYS
1	I	65	GLU
1	I	66	ARG
1	I	67	ASP
1	I	69	SER
1	I	86	LEU
1	I	131	GLN
1	I	143	VAL
1	I	150	ARG
1	I	158	MET
1	I	159	ASP
1	I	193	ASP
1	I	220	ARG
1	I	221	LEU
1	I	248	LYS
1	I	249	ILE
1	I	258	THR
1	I	274	GLU
1	I	307	GLN
1	I	346	GLU
1	I	349	SER

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Mol	Chain	Res	Type
1	I	350	ASN
1	I	358	GLU
1	I	361	SER
1	I	416	VAL
1	J	7	GLN
1	J	55	LYS
1	J	63	LYS
1	J	65	GLU
1	J	66	ARG
1	J	67	ASP
1	J	69	SER
1	J	86	LEU
1	J	131	GLN
1	J	143	VAL
1	J	150	ARG
1	J	158	MET
1	J	159	ASP
1	J	193	ASP
1	J	258	THR
1	J	307	GLN
1	J	346	GLU
1	J	349	SER
1	J	350	ASN
1	J	358	GLU
1	J	361	SER
1	J	416	VAL
1	K	7	GLN
1	K	55	LYS
1	K	86	LEU
1	K	131	GLN
1	K	143	VAL
1	K	150	ARG
1	K	158	MET
1	K	159	ASP
1	K	216	GLU
1	K	248	LYS
1	K	258	THR
1	K	307	GLN
1	K	346	GLU
1	K	349	SER
1	K	350	ASN
1	K	358	GLU

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Mol	Chain	Res	Type
1	K	361	SER
1	K	413	ILE
1	K	416	VAL
1	L	7	GLN
1	L	37	GLU
1	L	65	GLU
1	L	66	ARG
1	L	67	ASP
1	L	86	LEU
1	L	131	GLN
1	L	143	VAL
1	L	150	ARG
1	L	158	MET
1	L	159	ASP
1	L	221	LEU
1	L	248	LYS
1	L	258	THR
1	L	307	GLN
1	L	346	GLU
1	L	349	SER
1	L	350	ASN
1	L	361	SER
1	L	416	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	42	GLN
1	A	59	GLN
1	A	106	GLN
1	A	155	HIS
1	A	184	ASN
1	A	293	ASN
1	A	334	HIS
1	A	344	HIS
1	A	350	ASN
1	B	7	GLN
1	B	42	GLN
1	B	59	GLN
1	B	106	GLN
1	B	184	ASN

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Mol	Chain	Res	Type
1	B	293	ASN
1	B	334	HIS
1	B	344	HIS
1	B	350	ASN
1	C	7	GLN
1	C	42	GLN
1	C	59	GLN
1	C	106	GLN
1	C	155	HIS
1	C	184	ASN
1	C	293	ASN
1	C	330	ASN
1	C	334	HIS
1	C	344	HIS
1	C	350	ASN
1	D	7	GLN
1	D	42	GLN
1	D	59	GLN
1	D	71	HIS
1	D	106	GLN
1	D	155	HIS
1	D	184	ASN
1	D	293	ASN
1	D	330	ASN
1	D	334	HIS
1	D	350	ASN
1	E	42	GLN
1	E	59	GLN
1	E	106	GLN
1	E	184	ASN
1	E	293	ASN
1	E	330	ASN
1	E	334	HIS
1	E	344	HIS
1	E	350	ASN
1	F	7	GLN
1	F	42	GLN
1	F	59	GLN
1	F	71	HIS
1	F	106	GLN
1	F	184	ASN
1	F	293	ASN

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Mol	Chain	Res	Type
1	F	334	HIS
1	F	344	HIS
1	F	350	ASN
1	G	7	GLN
1	G	42	GLN
1	G	59	GLN
1	G	106	GLN
1	G	155	HIS
1	G	184	ASN
1	G	293	ASN
1	G	334	HIS
1	G	344	HIS
1	G	350	ASN
1	H	7	GLN
1	H	59	GLN
1	H	106	GLN
1	H	155	HIS
1	H	184	ASN
1	H	293	ASN
1	H	334	HIS
1	H	350	ASN
1	I	7	GLN
1	I	42	GLN
1	I	59	GLN
1	I	106	GLN
1	I	155	HIS
1	I	184	ASN
1	I	293	ASN
1	I	334	HIS
1	I	344	HIS
1	I	350	ASN
1	J	7	GLN
1	J	42	GLN
1	J	59	GLN
1	J	106	GLN
1	J	184	ASN
1	J	293	ASN
1	J	334	HIS
1	J	344	HIS
1	J	350	ASN
1	K	7	GLN
1	K	42	GLN

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Mol	Chain	Res	Type
1	K	59	GLN
1	K	106	GLN
1	K	184	ASN
1	K	293	ASN
1	K	334	HIS
1	K	344	HIS
1	K	350	ASN
1	K	364	GLN
1	L	7	GLN
1	L	42	GLN
1	L	59	GLN
1	L	106	GLN
1	L	155	HIS
1	L	184	ASN
1	L	293	ASN
1	L	334	HIS
1	L	350	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

24 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	PO3	A	501	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	A	601	-	36,46,46	2.24	10 (27%)	44,69,69	2.04	8 (18%)
2	PO3	B	502	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	B	602	-	36,46,46	2.11	3 (8%)	44,69,69	2.03	8 (18%)
2	PO3	C	502	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	C	603	-	36,46,46	2.20	11 (30%)	44,69,69	2.09	8 (18%)
2	PO3	D	503	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	D	604	-	36,46,46	2.12	10 (27%)	44,69,69	2.48	11 (25%)
2	PO3	E	504	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	E	605	-	36,46,46	2.19	7 (19%)	44,69,69	1.92	12 (27%)
2	PO3	F	506	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	F	606	-	36,46,46	2.19	14 (38%)	44,69,69	2.00	9 (20%)
2	PO3	G	507	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	G	607	-	36,46,46	2.05	6 (16%)	44,69,69	2.05	9 (20%)
2	PO3	H	508	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	H	608	-	36,46,46	2.02	7 (19%)	44,69,69	2.13	8 (18%)
2	PO3	I	509	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	I	609	-	36,46,46	2.29	10 (27%)	44,69,69	2.13	12 (27%)
2	PO3	J	510	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	J	610	-	36,46,46	2.21	9 (25%)	44,69,69	2.35	12 (27%)
2	PO3	K	511	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	K	611	-	36,46,46	2.15	5 (13%)	44,69,69	2.07	10 (22%)
2	PO3	L	512	-	0,3,3	0.00	-	0,3,3	0.00	-
3	EPU	L	612	-	36,46,46	2.13	8 (22%)	44,69,69	2.06	9 (20%)

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	PO3	A	501	-	-	0/0/0/0	0/0/0/0
3	EPU	A	601	-	-	0/24/71/71	0/3/3/3
2	PO3	B	502	-	-	0/0/0/0	0/0/0/0
3	EPU	B	602	-	-	0/24/71/71	0/3/3/3
2	PO3	C	502	-	-	0/0/0/0	0/0/0/0
3	EPU	C	603	-	-	0/24/71/71	0/3/3/3
2	PO3	D	503	-	-	0/0/0/0	0/0/0/0
3	EPU	D	604	-	-	0/24/71/71	0/3/3/3
2	PO3	E	504	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPU	E	605	-	-	0/24/71/71	0/3/3/3
2	PO3	F	506	-	-	0/0/0/0	0/0/0/0
3	EPU	F	606	-	-	0/24/71/71	0/3/3/3
2	PO3	G	507	-	-	0/0/0/0	0/0/0/0
3	EPU	G	607	-	-	0/24/71/71	0/3/3/3
2	PO3	H	508	-	-	0/0/0/0	0/0/0/0
3	EPU	H	608	-	-	0/24/71/71	0/3/3/3
2	PO3	I	509	-	-	0/0/0/0	0/0/0/0
3	EPU	I	609	-	-	0/24/71/71	0/3/3/3
2	PO3	J	510	-	-	0/0/0/0	0/0/0/0
3	EPU	J	610	-	-	0/24/71/71	0/3/3/3
2	PO3	K	511	-	-	0/0/0/0	0/0/0/0
3	EPU	K	611	-	-	0/24/71/71	0/3/3/3
2	PO3	L	512	-	-	0/0/0/0	0/0/0/0
3	EPU	L	612	-	-	0/24/71/71	0/3/3/3

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	EPU	O3-C3	-4.34	1.38	1.44
3	F	606	EPU	O3-C3	-4.18	1.38	1.44
3	B	602	EPU	O3-C3	-4.15	1.38	1.44
3	I	609	EPU	PB-O1	-3.69	1.51	1.60
3	A	601	EPU	C6U-N1U	-3.68	1.30	1.35
3	I	609	EPU	C6U-N1U	-3.61	1.30	1.35
3	I	609	EPU	O3-C3	-3.60	1.39	1.44
3	B	602	EPU	C6U-N1U	-3.59	1.30	1.35
3	K	611	EPU	C6U-N1U	-3.58	1.30	1.35
3	E	605	EPU	O3-C3	-3.44	1.39	1.44
3	J	610	EPU	C6U-N1U	-3.44	1.31	1.35
3	C	603	EPU	C6U-N1U	-3.26	1.31	1.35
3	F	606	EPU	C6U-N1U	-3.24	1.31	1.35
3	A	601	EPU	PB-O1	-3.22	1.52	1.60
3	H	608	EPU	C2U-N3U	-3.21	1.31	1.38
3	D	604	EPU	O3-C3	-3.20	1.39	1.44
3	A	601	EPU	O3-C3	-3.19	1.39	1.44
3	H	608	EPU	C6U-N1U	-3.17	1.31	1.35
3	J	610	EPU	O3-C3	-3.16	1.40	1.44
3	L	612	EPU	C6U-N1U	-3.14	1.31	1.35
3	L	612	EPU	C3-C2	-3.08	1.47	1.53
3	E	605	EPU	C6U-N1U	-3.06	1.31	1.35
3	L	612	EPU	O3-C3	-3.03	1.40	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	611	EPU	O3-C3	-2.97	1.40	1.44
3	D	604	EPU	C2U-N3U	-2.95	1.32	1.38
3	E	605	EPU	C2U-N3U	-2.93	1.32	1.38
3	F	606	EPU	C2D-C1D	-2.91	1.49	1.53
3	G	607	EPU	C6U-N1U	-2.90	1.31	1.35
3	I	609	EPU	C2U-N3U	-2.89	1.32	1.38
3	C	603	EPU	C2U-N3U	-2.84	1.32	1.38
3	J	610	EPU	C3-C2	-2.75	1.48	1.53
3	J	610	EPU	C2U-N3U	-2.73	1.32	1.38
3	A	601	EPU	C2U-N3U	-2.73	1.32	1.38
3	D	604	EPU	C6U-N1U	-2.72	1.32	1.35
3	G	607	EPU	C2U-N3U	-2.72	1.32	1.38
3	F	606	EPU	PB-O2B	-2.61	1.42	1.55
3	F	606	EPU	PB-O1	-2.59	1.54	1.60
3	L	612	EPU	C2U-N3U	-2.59	1.33	1.38
3	F	606	EPU	C2U-N3U	-2.54	1.33	1.38
3	H	608	EPU	O3-C3	-2.52	1.40	1.44
3	J	610	EPU	C2D-C1D	-2.51	1.49	1.53
3	D	604	EPU	O5-C5	-2.50	1.38	1.44
3	H	608	EPU	PB-O1	-2.49	1.54	1.60
3	F	606	EPU	O4D-C4D	-2.44	1.39	1.45
3	I	609	EPU	PA-O2A	-2.40	1.43	1.55
3	D	604	EPU	PB-O2B	-2.38	1.43	1.55
3	K	611	EPU	C3-C2	-2.38	1.48	1.53
3	E	605	EPU	C3D-C2D	-2.37	1.47	1.53
3	H	608	EPU	C2D-C1D	-2.32	1.50	1.53
3	L	612	EPU	C3D-C2D	-2.29	1.47	1.53
3	H	608	EPU	PB-O2B	-2.27	1.43	1.55
3	F	606	EPU	C1-C2	-2.26	1.49	1.53
3	D	604	EPU	PA-O2A	-2.24	1.43	1.55
3	C	603	EPU	PB-O2B	-2.24	1.43	1.55
3	G	607	EPU	PB-O1	-2.23	1.55	1.60
3	C	603	EPU	PB-O1	-2.21	1.55	1.60
3	E	605	EPU	C2D-C1D	-2.18	1.50	1.53
3	A	601	EPU	PA-O2A	-2.18	1.44	1.55
3	C	603	EPU	C3-C2	-2.16	1.49	1.53
3	I	609	EPU	O4D-C4D	-2.16	1.40	1.45
3	L	612	EPU	C2D-C1D	-2.16	1.50	1.53
3	A	601	EPU	PB-O2B	-2.15	1.44	1.55
3	C	603	EPU	O7-C7	-2.15	1.18	1.23
3	D	604	EPU	PA-O1A	-2.14	1.42	1.50
3	F	606	EPU	C4-C5	-2.13	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	603	EPU	C4-C5	-2.12	1.48	1.53
3	A	601	EPU	C2D-C1D	-2.11	1.50	1.53
3	F	606	EPU	PB-O1B	-2.10	1.43	1.50
3	I	609	EPU	PB-O2B	-2.10	1.44	1.55
3	G	607	EPU	PB-O2B	-2.10	1.44	1.55
3	I	609	EPU	C3-C2	-2.10	1.49	1.53
3	A	601	EPU	PA-O1A	-2.09	1.43	1.50
3	E	605	EPU	PA-O2A	-2.09	1.44	1.55
3	F	606	EPU	PA-O2A	-2.09	1.44	1.55
3	C	603	EPU	PA-O2A	-2.09	1.44	1.55
3	I	609	EPU	C2D-C1D	-2.09	1.50	1.53
3	C	603	EPU	C2D-C1D	-2.09	1.50	1.53
3	J	610	EPU	C1-C2	-2.09	1.49	1.53
3	D	604	EPU	O7-C7	-2.08	1.18	1.23
3	J	610	EPU	O5-C5	-2.07	1.39	1.44
3	F	606	EPU	C3D-C2D	-2.07	1.47	1.53
3	A	601	EPU	O4D-C4D	-2.07	1.40	1.45
3	F	606	EPU	O7-C7	-2.06	1.18	1.23
3	D	604	EPU	C3D-C2D	-2.06	1.48	1.53
3	J	610	EPU	C2-N2	-2.05	1.42	1.45
3	L	612	EPU	O4D-C4D	-2.03	1.40	1.45
3	K	611	EPU	PA-O2A	-2.02	1.45	1.55
3	G	607	EPU	O3-C2E	2.02	1.43	1.36
3	F	606	EPU	C3E-C2E	7.97	1.49	1.33
3	H	608	EPU	C3E-C2E	8.20	1.50	1.33
3	C	603	EPU	C3E-C2E	8.21	1.50	1.33
3	D	604	EPU	C3E-C2E	8.65	1.51	1.33
3	G	607	EPU	C3E-C2E	8.72	1.51	1.33
3	L	612	EPU	C3E-C2E	8.90	1.51	1.33
3	A	601	EPU	C3E-C2E	8.93	1.51	1.33
3	I	609	EPU	C3E-C2E	8.93	1.51	1.33
3	B	602	EPU	C3E-C2E	8.99	1.51	1.33
3	J	610	EPU	C3E-C2E	9.04	1.51	1.33
3	E	605	EPU	C3E-C2E	9.15	1.52	1.33
3	K	611	EPU	C3E-C2E	9.16	1.52	1.33

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	608	EPU	C1E-C2E-C3E	-8.98	104.31	121.07
3	G	607	EPU	C1E-C2E-C3E	-8.63	104.96	121.07
3	D	604	EPU	C1E-C2E-C3E	-8.13	105.90	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	EPU	C1E-C2E-C3E	-7.74	106.63	121.07
3	L	612	EPU	C1E-C2E-C3E	-7.31	107.42	121.07
3	J	610	EPU	C1E-C2E-C3E	-7.18	107.67	121.07
3	D	604	EPU	O5-C1-O1	-6.45	102.94	111.36
3	K	611	EPU	C1E-C2E-C3E	-6.37	109.18	121.07
3	C	603	EPU	C3-C2-N2	-6.36	99.82	111.00
3	I	609	EPU	O5-C1-O1	-6.31	103.12	111.36
3	F	606	EPU	C1E-C2E-C3E	-6.29	109.34	121.07
3	E	605	EPU	C1E-C2E-C3E	-6.19	109.52	121.07
3	C	603	EPU	C1E-C2E-C3E	-5.68	110.47	121.07
3	J	610	EPU	O5-C1-O1	-5.52	104.15	111.36
3	A	601	EPU	C1E-C2E-C3E	-5.32	111.13	121.07
3	A	601	EPU	C3-C2-N2	-5.24	101.78	111.00
3	I	609	EPU	C1E-C2E-C3E	-5.16	111.44	121.07
3	I	609	EPU	C3-C2-N2	-5.13	101.98	111.00
3	J	610	EPU	C3-C2-N2	-5.00	102.21	111.00
3	A	601	EPU	O5-C1-O1	-4.95	104.90	111.36
3	K	611	EPU	O5-C1-O1	-4.82	105.07	111.36
3	L	612	EPU	C3-C2-N2	-4.48	103.13	111.00
3	D	604	EPU	C1-O5-C5	-4.23	105.74	113.72
3	F	606	EPU	C3-C2-N2	-4.11	103.77	111.00
3	G	607	EPU	C3-C2-N2	-4.07	103.85	111.00
3	K	611	EPU	C3-C2-N2	-4.04	103.90	111.00
3	L	612	EPU	O5-C1-O1	-4.02	106.11	111.36
3	D	604	EPU	O5-C1-C2	-3.82	102.82	110.65
3	E	605	EPU	C3-C2-N2	-3.56	104.75	111.00
3	L	612	EPU	O3D-C3D-C2D	-3.46	100.74	111.83
3	D	604	EPU	C3-C2-N2	-3.43	104.96	111.00
3	D	604	EPU	C3-C4-C5	-3.33	102.53	109.67
3	I	609	EPU	C6-C5-C4	-3.28	105.33	113.00
3	A	601	EPU	C6-C5-C4	-3.19	105.53	113.00
3	F	606	EPU	O5-C1-C2	-3.11	104.28	110.65
3	I	609	EPU	O6-C6-C5	-3.05	101.07	111.34
3	E	605	EPU	O5-C1-C2	-3.04	104.43	110.65
3	J	610	EPU	O3D-C3D-C4D	-3.01	102.29	111.09
3	H	608	EPU	C3-C2-N2	-2.91	105.88	111.00
3	C	603	EPU	O4-C4-C3	-2.91	103.26	109.87
3	J	610	EPU	O6-C6-C5	-2.77	102.03	111.34
3	E	605	EPU	O3D-C3D-C2D	-2.74	103.06	111.83
3	J	610	EPU	C6-C5-C4	-2.74	106.60	113.00
3	C	603	EPU	C2-N2-C7	-2.71	116.33	123.19
3	G	607	EPU	O5-C1-O1	-2.71	107.83	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	606	EPU	O5-C1-O1	-2.67	107.88	111.36
3	C	603	EPU	O5-C1-C2	-2.65	105.23	110.65
3	L	612	EPU	C6-C5-C4	-2.63	106.85	113.00
3	K	611	EPU	O5-C1-C2	-2.62	105.28	110.65
3	L	612	EPU	C1-C2-N2	-2.60	106.63	111.03
3	H	608	EPU	C1-C2-N2	-2.59	106.65	111.03
3	B	602	EPU	C3-C2-N2	-2.53	106.54	111.00
3	A	601	EPU	O6-C6-C5	-2.53	102.82	111.34
3	J	610	EPU	C2-N2-C7	-2.47	116.94	123.19
3	E	605	EPU	O2D-C2D-C3D	-2.44	104.01	111.83
3	F	606	EPU	C1-C2-C3	-2.38	105.42	109.87
3	A	601	EPU	O4-C4-C3	-2.33	104.57	109.87
3	F	606	EPU	O3D-C3D-C2D	-2.31	104.42	111.83
3	G	607	EPU	C1-C2-N2	-2.29	107.16	111.03
3	G	607	EPU	O3A-PB-O1	-2.27	97.98	102.05
3	H	608	EPU	O4-C4-C3	-2.25	104.75	109.87
3	E	605	EPU	C2-N2-C7	-2.23	117.53	123.19
3	D	604	EPU	O2D-C2D-C3D	-2.23	104.68	111.83
3	J	610	EPU	O5D-PA-O1A	-2.21	100.34	109.25
3	B	602	EPU	C2-N2-C7	-2.20	117.61	123.19
3	I	609	EPU	O3D-C3D-C2D	-2.20	104.77	111.83
3	E	605	EPU	O3A-PB-O1	-2.19	98.13	102.05
3	I	609	EPU	O4-C4-C3	-2.19	104.88	109.87
3	D	604	EPU	O6-C6-C5	-2.19	103.97	111.34
3	L	612	EPU	O6-C6-C5	-2.18	104.00	111.34
3	B	602	EPU	O3D-C3D-C2D	-2.17	104.87	111.83
3	B	602	EPU	O5-C1-O1	-2.14	108.57	111.36
3	H	608	EPU	O5-C1-C2	-2.13	106.29	110.65
3	K	611	EPU	C2-N2-C7	-2.11	117.85	123.19
3	J	610	EPU	O3A-PB-O1	-2.09	98.32	102.05
3	I	609	EPU	C1-O5-C5	-2.08	109.80	113.72
3	C	603	EPU	O5-C1-O1	-2.08	108.65	111.36
3	I	609	EPU	C2-N2-C7	-2.07	117.95	123.19
3	G	607	EPU	O2D-C2D-C3D	-2.05	105.25	111.83
3	A	601	EPU	C2-N2-C7	-2.05	117.99	123.19
3	I	609	EPU	O4D-C4D-C5D	-2.02	102.57	109.40
3	D	604	EPU	O3D-C3D-C2D	-2.02	105.35	111.83
3	K	611	EPU	C5U-C4U-N3U	-2.01	118.32	123.12
3	J	610	EPU	O2A-PA-O1A	2.03	122.78	112.28
3	E	605	EPU	O1-C1-C2	2.04	112.09	108.40
3	I	609	EPU	O4D-C1D-N1U	2.05	112.18	108.08
3	G	607	EPU	O2B-PB-O1B	2.06	122.92	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	EPU	O2A-PA-O1A	2.07	122.98	112.28
3	E	605	EPU	O5-C5-C6	2.07	111.38	106.41
3	K	611	EPU	O4-C4-C5	2.10	114.57	109.28
3	E	605	EPU	O2A-PA-O1A	2.19	123.64	112.28
3	F	606	EPU	C2D-C3D-C4D	2.27	107.04	102.62
3	H	608	EPU	C4D-O4D-C1D	2.35	112.27	109.77
3	E	605	EPU	O2B-PB-O1B	2.36	124.48	112.28
3	G	607	EPU	O3-C3-C2	2.36	112.53	107.98
3	K	611	EPU	O2A-PA-O1A	2.42	124.79	112.28
3	K	611	EPU	C4D-O4D-C1D	2.59	112.53	109.77
3	C	603	EPU	C8-C7-N2	2.72	121.02	116.11
3	F	606	EPU	C4D-O4D-C1D	2.75	112.69	109.77
3	B	602	EPU	C4D-O4D-C1D	2.78	112.73	109.77
3	H	608	EPU	O3-C3-C2	2.79	113.36	107.98
3	L	612	EPU	O3A-PB-O1	2.91	107.24	102.05
3	D	604	EPU	C1-C2-N2	3.28	116.58	111.03
3	J	610	EPU	C4D-O4D-C1D	3.67	113.67	109.77
3	L	612	EPU	C4U-N3U-C2U	4.83	118.28	114.13
3	G	607	EPU	C4U-N3U-C2U	5.13	118.53	114.13
3	E	605	EPU	C4U-N3U-C2U	5.25	118.64	114.13
3	I	609	EPU	C4U-N3U-C2U	5.32	118.70	114.13
3	A	601	EPU	C4U-N3U-C2U	5.64	118.97	114.13
3	C	603	EPU	C4U-N3U-C2U	5.85	119.16	114.13
3	F	606	EPU	C4U-N3U-C2U	6.18	119.44	114.13
3	H	608	EPU	C4U-N3U-C2U	6.36	119.59	114.13
3	B	602	EPU	C4U-N3U-C2U	6.63	119.82	114.13
3	J	610	EPU	C4U-N3U-C2U	6.79	119.96	114.13
3	K	611	EPU	C4U-N3U-C2U	7.04	120.18	114.13
3	D	604	EPU	C4U-N3U-C2U	7.20	120.32	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	EPU	1	0
3	C	603	EPU	2	0
3	E	605	EPU	2	0
3	F	606	EPU	3	0
3	H	608	EPU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	509	PO3	1	0
3	I	609	EPU	1	0
3	J	610	EPU	1	0
2	L	512	PO3	1	0
3	L	612	EPU	2	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	418/418 (100%)	-0.12	4 (0%) 82 83	36, 55, 83, 120	0
1	B	418/418 (100%)	0.28	19 (4%) 34 36	37, 67, 100, 186	0
1	C	418/418 (100%)	-0.23	1 (0%) 94 95	26, 48, 71, 116	0
1	D	418/418 (100%)	-0.28	1 (0%) 94 95	30, 48, 72, 118	0
1	E	418/418 (100%)	-0.09	6 (1%) 75 76	32, 52, 77, 143	0
1	F	418/418 (100%)	-0.02	8 (1%) 67 69	33, 55, 85, 127	0
1	G	418/418 (100%)	0.08	9 (2%) 62 64	34, 61, 98, 147	0
1	H	418/418 (100%)	-0.18	3 (0%) 87 88	32, 51, 69, 132	0
1	I	418/418 (100%)	0.34	36 (8%) 11 11	38, 71, 118, 170	0
1	J	418/418 (100%)	0.05	8 (1%) 67 69	34, 64, 97, 128	0
1	K	418/418 (100%)	-0.08	6 (1%) 75 76	29, 53, 79, 169	0
1	L	418/418 (100%)	0.62	49 (11%) 5 4	42, 81, 129, 203	0
All	All	5016/5016 (100%)	0.03	150 (2%) 51 53	26, 57, 99, 203	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	418	GLY	8.9
1	L	222	GLY	7.0
1	L	221	LEU	6.6
1	L	215	ILE	6.1
1	I	215	ILE	6.0
1	I	81	CYS	5.7
1	B	418	GLY	5.4
1	I	216	GLU	5.3
1	E	418	GLY	5.2
1	L	39	VAL	5.0
1	I	177	GLU	4.9

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Mol	Chain	Res	Type	RSRZ
1	I	136	ILE	4.9
1	D	418	GLY	4.7
1	I	152	LYS	4.4
1	K	418	GLY	4.3
1	I	99	PRO	4.2
1	G	418	GLY	4.2
1	J	201	LEU	4.2
1	I	134	ALA	4.2
1	I	181	ILE	4.0
1	F	225	VAL	3.9
1	L	63	LYS	3.9
1	L	41	ILE	3.9
1	L	199	ILE	3.8
1	L	12	LEU	3.6
1	L	75	ARG	3.5
1	I	148	ASP	3.5
1	L	216	GLU	3.5
1	L	197	PHE	3.4
1	G	401	ARG	3.4
1	B	395	ILE	3.4
1	G	1	MET	3.4
1	L	225	VAL	3.4
1	J	359	LYS	3.3
1	L	279	TRP	3.3
1	B	47	LEU	3.3
1	I	147	VAL	3.3
1	I	132	LEU	3.2
1	B	273	ILE	3.2
1	E	57	LEU	3.2
1	G	59	GLN	3.2
1	B	146	SER	3.2
1	E	77	VAL	3.1
1	L	37	GLU	3.1
1	G	56	LEU	3.1
1	K	248	LYS	3.1
1	L	401	ARG	3.1
1	L	30	PHE	3.1
1	K	349	SER	3.1
1	J	273	ILE	3.0
1	L	282	LEU	3.0
1	J	72	ILE	3.0
1	L	277	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	175	LEU	3.0
1	L	213	ILE	3.0
1	B	370	LEU	2.9
1	F	72	ILE	2.9
1	I	349	SER	2.9
1	L	201	LEU	2.9
1	K	330	ASN	2.9
1	G	273	ILE	2.8
1	H	60	LEU	2.8
1	J	12	LEU	2.8
1	L	64	VAL	2.7
1	I	350	ASN	2.7
1	K	412	ASN	2.7
1	L	200	THR	2.7
1	L	26	LEU	2.7
1	I	217	GLY	2.7
1	L	205	ILE	2.7
1	B	80	PHE	2.7
1	F	53	SER	2.7
1	E	330	ASN	2.7
1	I	102	ALA	2.7
1	I	194	THR	2.7
1	B	219	GLU	2.7
1	B	49	ASP	2.6
1	A	133	GLY	2.6
1	E	220	ARG	2.6
1	I	137	LYS	2.6
1	L	267	ARG	2.6
1	I	143	VAL	2.6
1	B	60	LEU	2.6
1	K	350	ASN	2.6
1	B	35	ALA	2.5
1	B	32	ALA	2.5
1	A	139	GLU	2.5
1	B	286	GLY	2.5
1	B	358	GLU	2.5
1	I	230	PRO	2.5
1	L	226	TYR	2.5
1	I	171	CYS	2.5
1	F	115	CYS	2.5
1	A	107	GLY	2.5
1	B	13	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	272	ASP	2.5
1	B	99	PRO	2.5
1	F	221	LEU	2.4
1	L	238	PHE	2.4
1	G	79	VAL	2.4
1	L	16	VAL	2.4
1	J	289	PRO	2.4
1	I	131	GLN	2.4
1	L	326	THR	2.4
1	L	281	SER	2.4
1	L	362	GLY	2.4
1	I	401	ARG	2.4
1	I	201	LEU	2.4
1	B	64	VAL	2.3
1	I	42	GLN	2.3
1	I	78	ASN	2.3
1	F	406	LEU	2.3
1	I	175	LEU	2.3
1	I	80	PHE	2.3
1	G	62	ALA	2.3
1	H	115	CYS	2.3
1	I	129	LEU	2.3
1	L	378	LEU	2.3
1	L	36	GLU	2.3
1	L	33	LEU	2.3
1	L	42	GLN	2.2
1	L	152	LYS	2.2
1	L	117	ILE	2.2
1	I	151	LEU	2.2
1	L	38	PRO	2.2
1	F	243	ALA	2.2
1	L	350	ASN	2.2
1	C	216	GLU	2.2
1	B	350	ASN	2.1
1	E	219	GLU	2.1
1	G	370	LEU	2.1
1	L	318	GLU	2.1
1	B	63	LYS	2.1
1	I	214	VAL	2.1
1	L	70	VAL	2.1
1	L	274	GLU	2.1
1	L	248	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	74	ALA	2.1
1	L	220	ARG	2.1
1	L	244	ILE	2.1
1	F	417	LYS	2.1
1	J	102	ALA	2.0
1	I	182	ILE	2.0
1	I	101	VAL	2.0
1	L	280	ILE	2.0
1	A	381	CYS	2.0
1	I	150	ARG	2.0
1	I	212	ARG	2.0
1	I	100	LEU	2.0
1	J	406	LEU	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	PO3	C	502	4/4	0.97	0.28	5.83	59,66,66,70	0
2	PO3	I	509	4/4	0.98	0.24	3.46	49,72,72,87	0
2	PO3	J	510	4/4	0.98	0.23	3.45	53,65,65,68	0
2	PO3	K	511	4/4	0.94	0.32	2.96	56,69,71,79	0
2	PO3	E	504	4/4	0.96	0.23	2.81	58,64,65,68	0
2	PO3	A	501	4/4	0.92	0.27	2.74	65,66,69,73	0
2	PO3	D	503	4/4	0.92	0.22	2.22	52,56,65,67	0
2	PO3	H	508	4/4	0.94	0.25	1.78	54,56,57,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO3	L	512	4/4	0.94	0.23	1.52	68,73,83,85	0
2	PO3	F	506	4/4	0.97	0.24	1.43	71,73,76,77	0
2	PO3	G	507	4/4	0.97	0.20	1.33	50,53,55,58	0
3	EPU	I	609	44/44	0.92	0.17	0.16	55,65,70,74	0
2	PO3	B	502	4/4	0.89	0.16	-0.11	61,70,74,81	0
3	EPU	G	607	44/44	0.95	0.17	-0.20	39,50,58,65	0
3	EPU	C	603	44/44	0.97	0.13	-0.41	33,41,49,61	0
3	EPU	F	606	44/44	0.95	0.14	-0.42	33,41,52,67	0
3	EPU	H	608	44/44	0.96	0.14	-0.47	37,50,61,63	0
3	EPU	A	601	44/44	0.96	0.15	-0.49	38,51,59,63	0
3	EPU	B	602	44/44	0.95	0.14	-0.54	43,51,59,68	0
3	EPU	L	612	44/44	0.96	0.15	-0.56	56,64,70,77	0
3	EPU	J	610	44/44	0.96	0.13	-0.77	42,48,54,61	0
3	EPU	D	604	44/44	0.95	0.12	-0.84	32,43,53,59	0
3	EPU	K	611	44/44	0.96	0.13	-0.92	33,44,52,69	0
3	EPU	E	605	44/44	0.97	0.13	-0.93	34,42,56,62	0

## 6.5 Other polymers

There are no such residues in this entry.