wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:04 PM BST

PDB ID	:	4AAQ
EMDB ID:	:	EMD-1998
Title	:	ATP-triggered molecular mechanics of the chaperonin GroEL
Authors	:	Clare, D.K.; Vasishtan, D.; Stagg, S.; Quispe, J.; Farr, G.W.; Topf, M.; Horwich, A.L.; Saibil, H.R.
Deposited on	:	2011-12-05
Resolution	:	8.00 Å(reported)
Based on PDB ID	:	1OEL

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

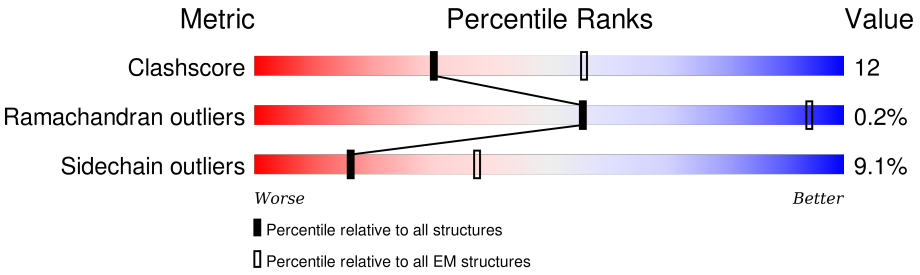
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	548	61% 27% 7%
1	B	548	60% 27% 7%
1	C	548	61% 26% 7%
1	D	548	60% 27% 8%
1	E	548	61% 27% 7%
1	F	548	61% 27% 7%
1	G	548	60% 27% 8%
1	H	548	78% 14%
1	I	548	78% 14%

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Mol	Chain	Length	Quality of chain
1	J	548	78% 14%
1	K	548	79% 14%
1	L	548	78% 14%
1	M	548	78% 14%
1	N	548	78% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	1526	-	-	X	-
3	PO4	B	1526	-	-	X	-
3	PO4	C	1527	-	-	X	-
3	PO4	D	1526	-	-	X	-
3	PO4	E	1526	-	-	X	-
3	PO4	F	1525	-	-	X	-
3	PO4	G	1525	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 54159 atoms, of which 84 are hydrogens and 0 are deuteriums.

In the tables below, 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 60 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	B	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	C	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	D	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	E	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	F	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	G	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	H	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	I	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	J	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	K	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	L	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	M	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		
1	N	524	Total	C	N	O	S	0	1
			3846	2391	665	770	20		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
B	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

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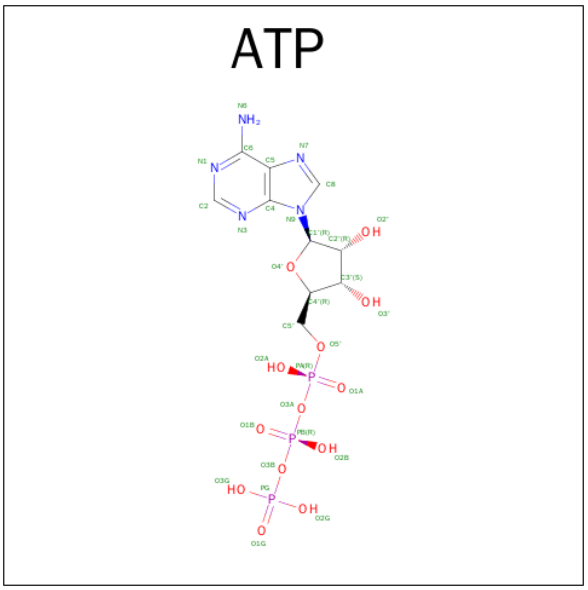
Chain	Residue	Modelled	Actual	Comment	Reference
C	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
D	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
E	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
F	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
G	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
H	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
I	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
J	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
K	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
L	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
M	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
N	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

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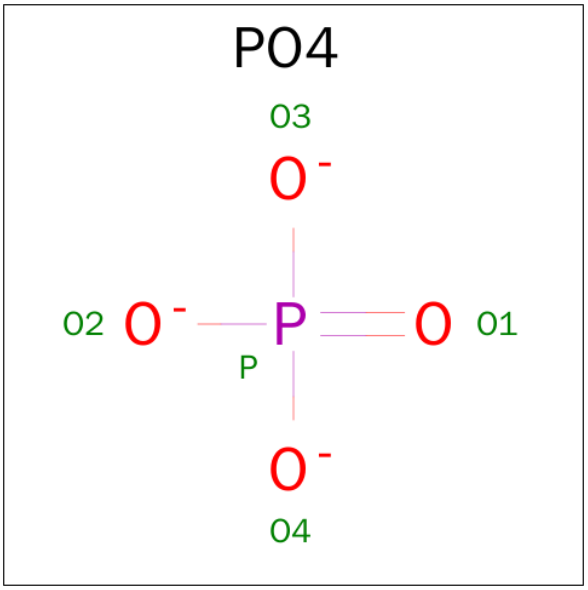
Mol	Chain	Residues	Atoms						AltConf
2	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
2	G	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	P	0
			1	1	
3	B	1	Total	P	0
			1	1	
3	C	1	Total	P	0
			1	1	
3	D	1	Total	P	0
			1	1	
3	E	1	Total	P	0
			1	1	
3	F	1	Total	P	0
			1	1	
3	G	1	Total	P	0
			1	1	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

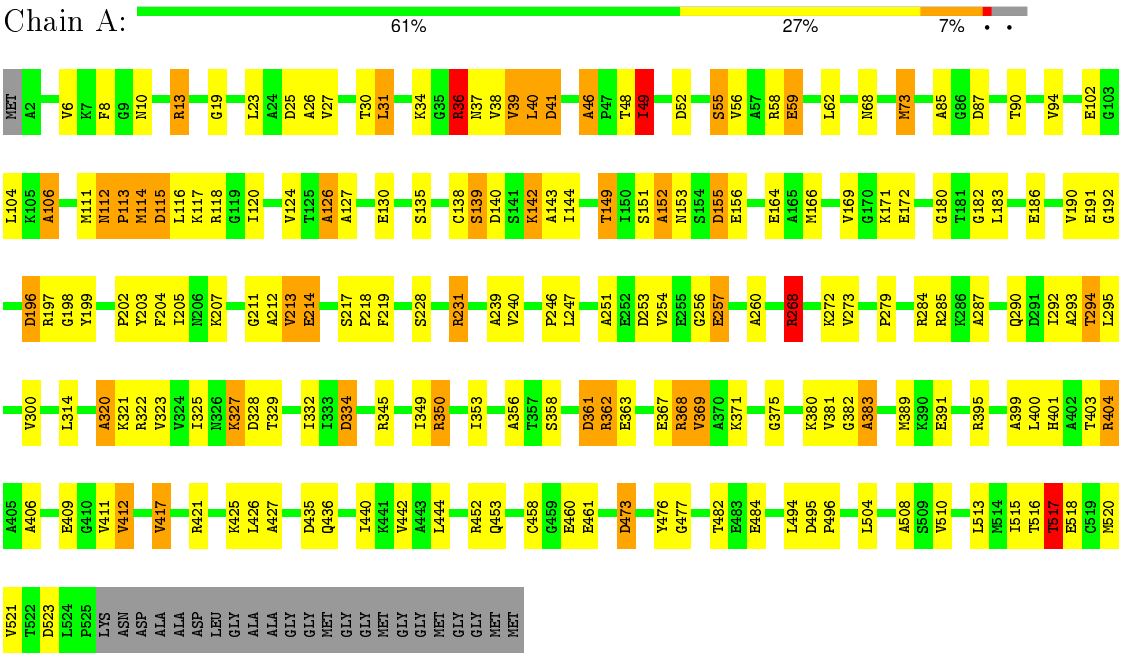
Mol	Chain	Residues	Atoms	AltConf
4	G	1	Total Mg 1 1	0
4	D	1	Total Mg 1 1	0
4	E	1	Total Mg 1 1	0
4	B	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	A	1	Total Mg 1 1	0
4	F	1	Total Mg 1 1	0

3 Residue-property plots (i)

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

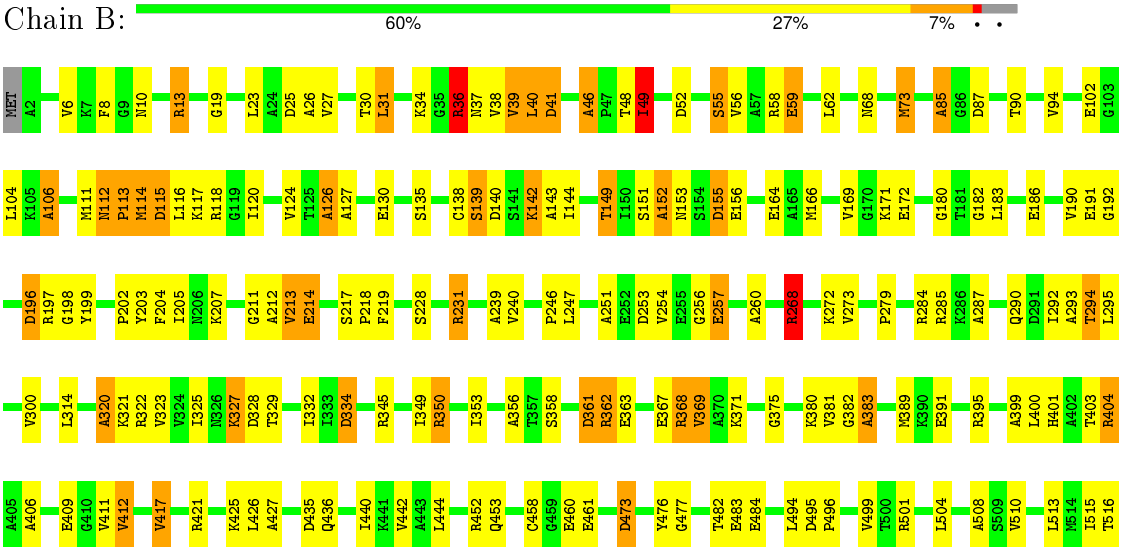
- Molecule 1: 60 KDA CHAPERONIN

Chain A:



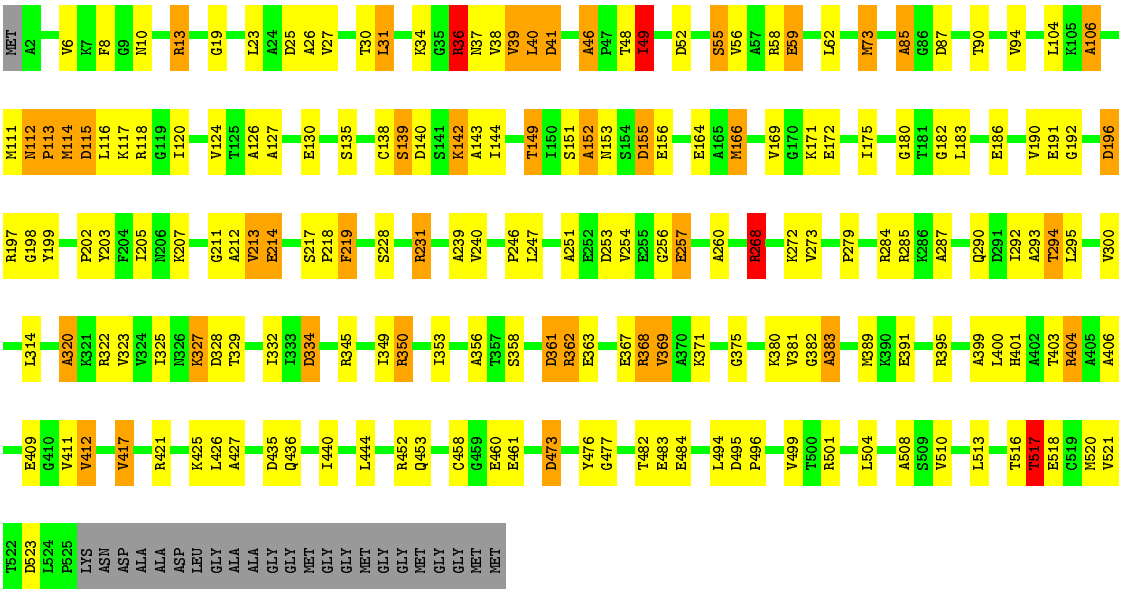
- Molecule 1: 60 KDA CHAPERONIN

Chain B:



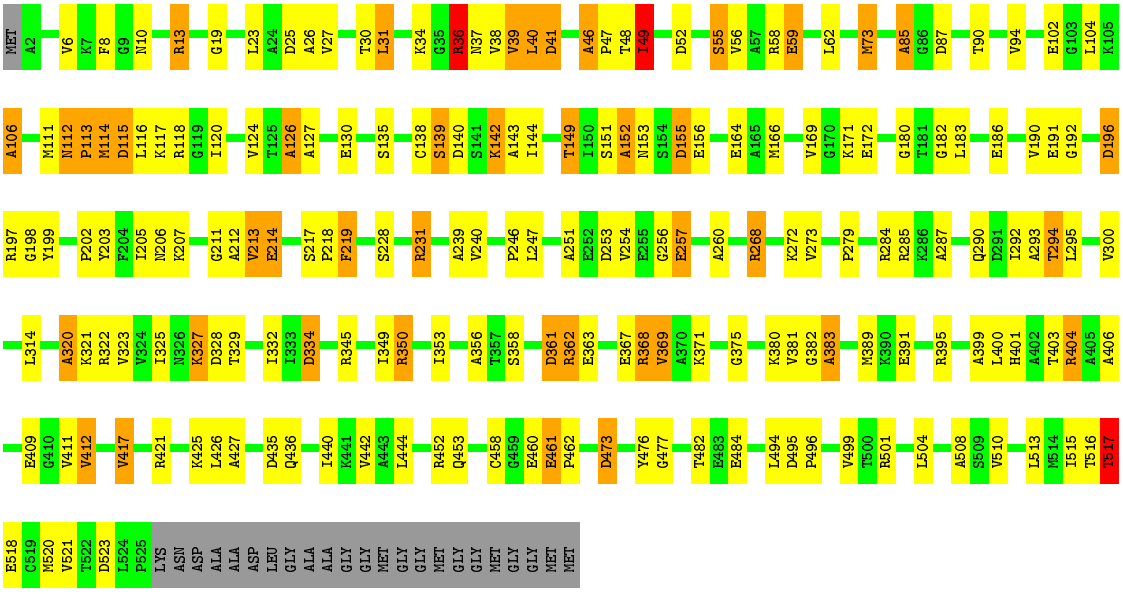
• Molecule 1: 60 KDA CHAPERONIN

Chain C:



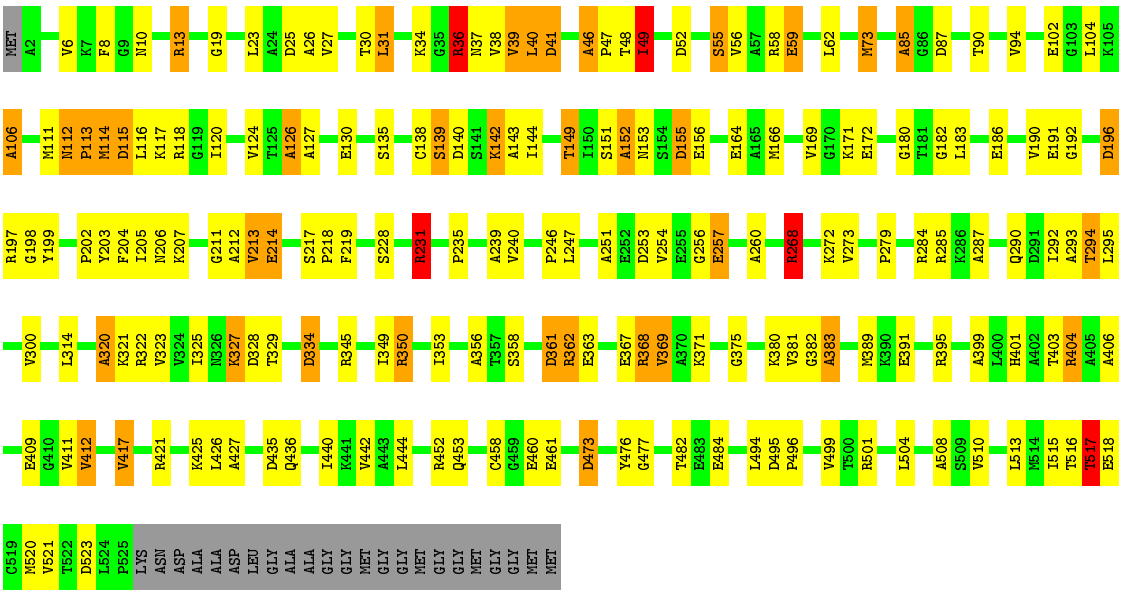
• Molecule 1: 60 KDA CHAPERONIN

Chain D:



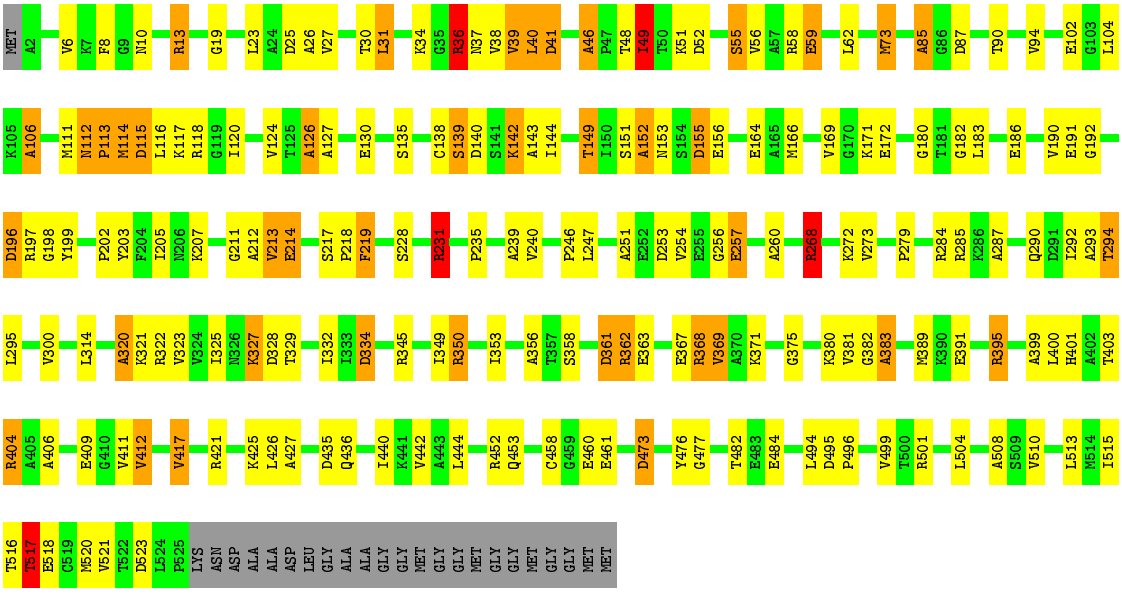
• Molecule 1: 60 KDA CHAPERONIN

Chain E:



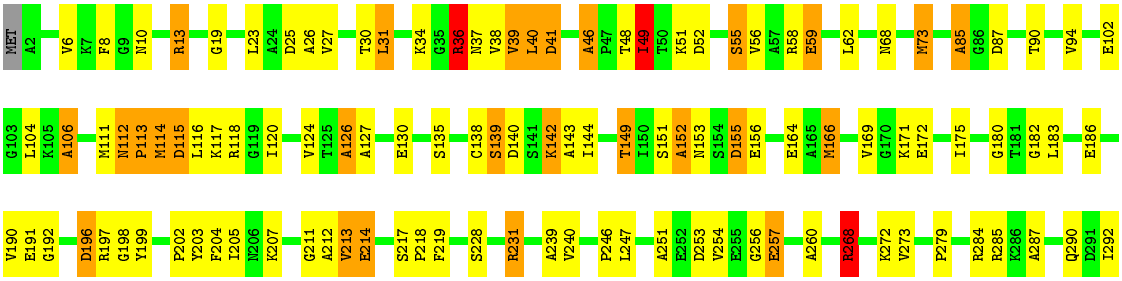
• Molecule 1: 60 KDA CHAPERONIN

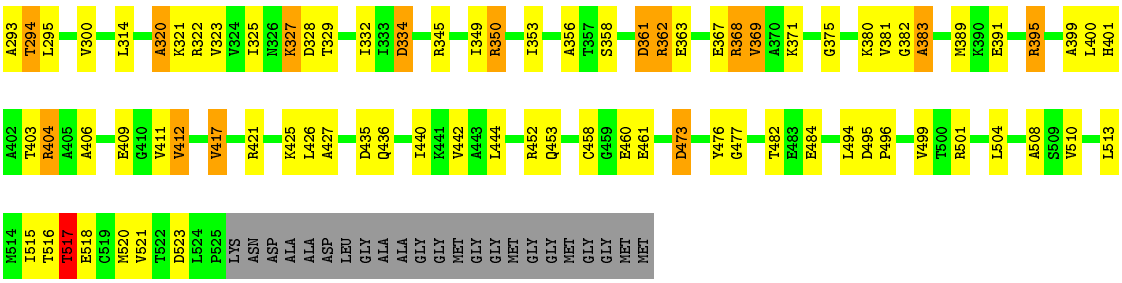
Chain F:



• Molecule 1: 60 KDA CHAPERONIN

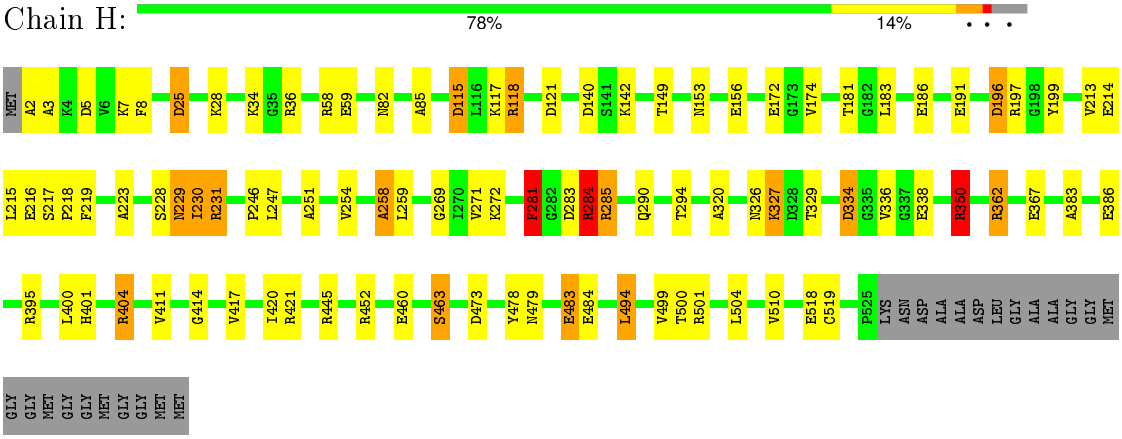
Chain G:





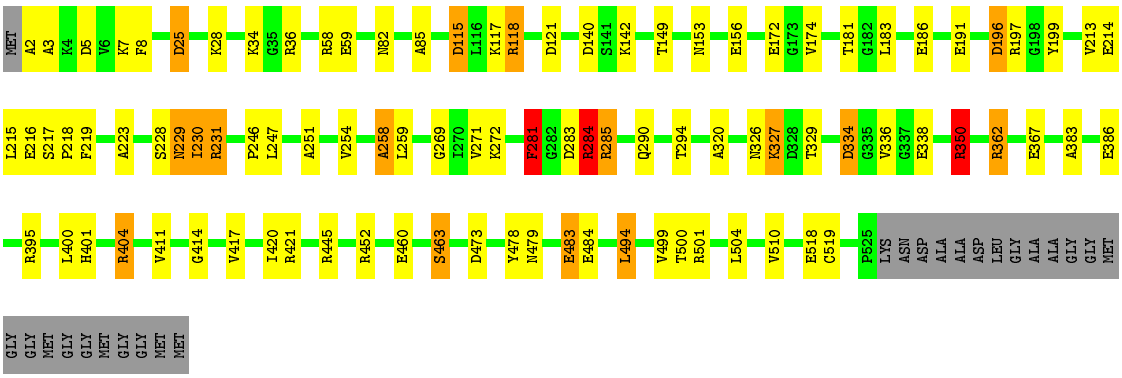
• Molecule 1: 60 KDA CHAPERONIN

Chain H:



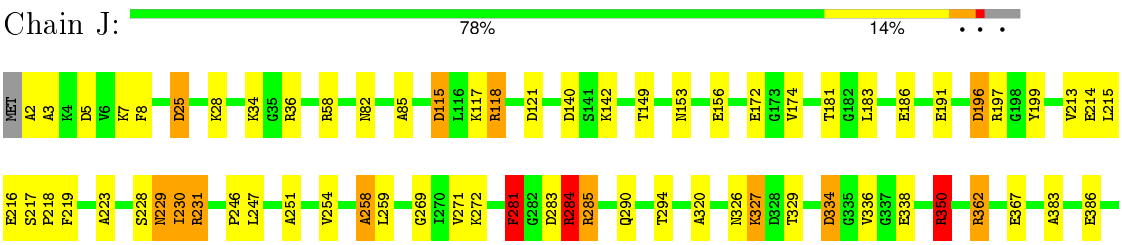
• Molecule 1: 60 KDA CHAPERONIN

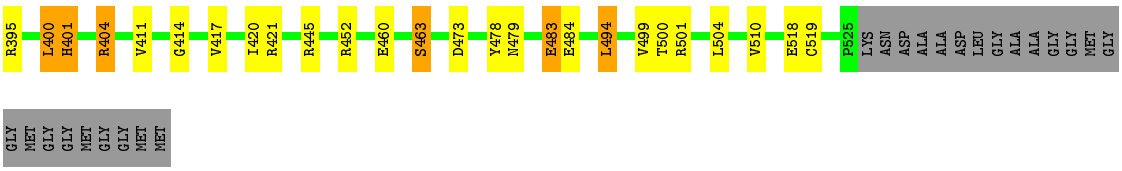
Chain I:



• Molecule 1: 60 KDA CHAPERONIN

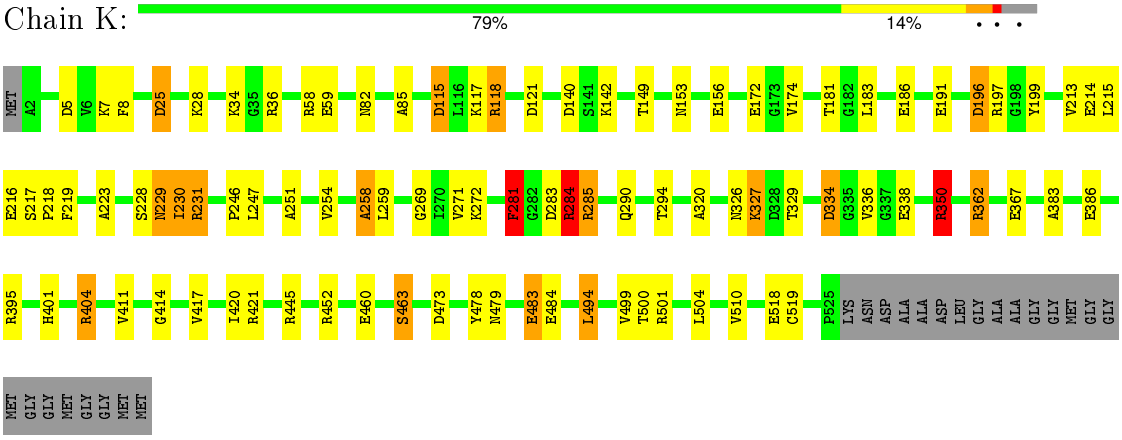
Chain J:





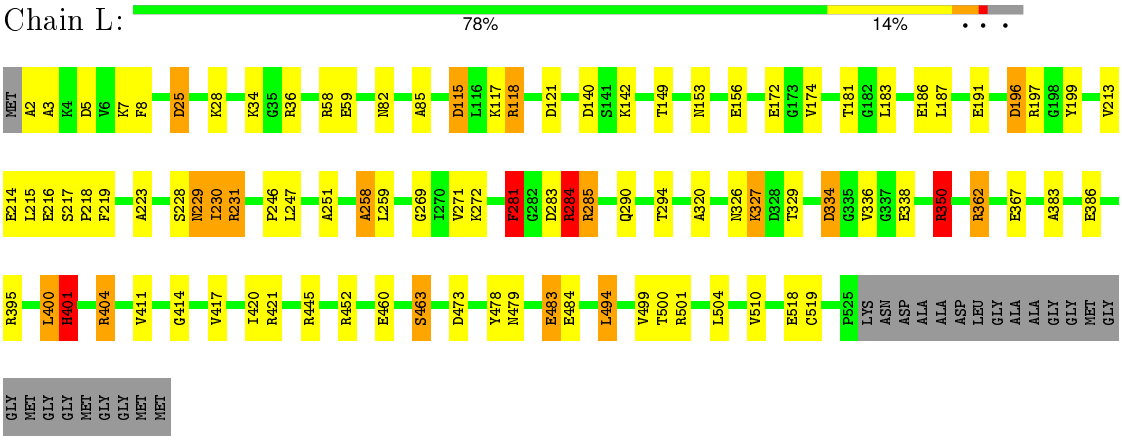
• Molecule 1: 60 KDA CHAPERONIN

Chain K:



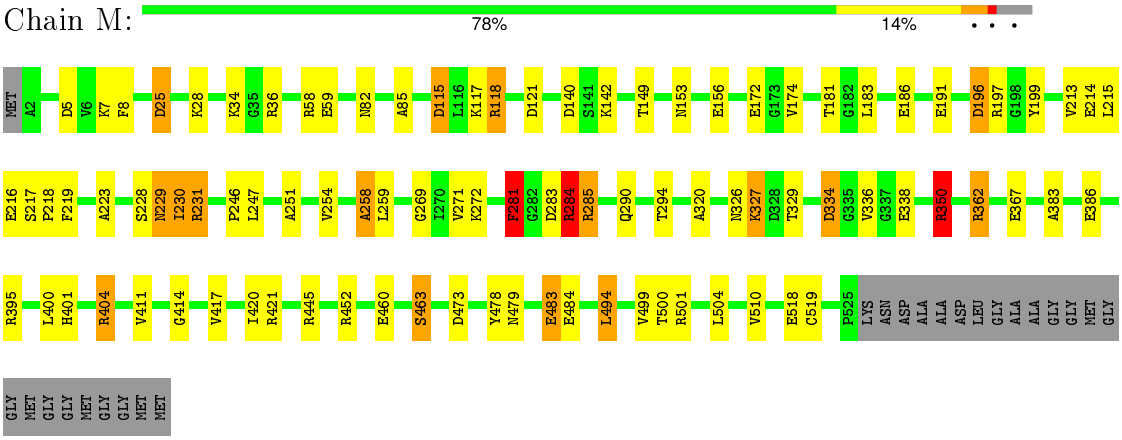
• Molecule 1: 60 KDA CHAPERONIN

Chain L:



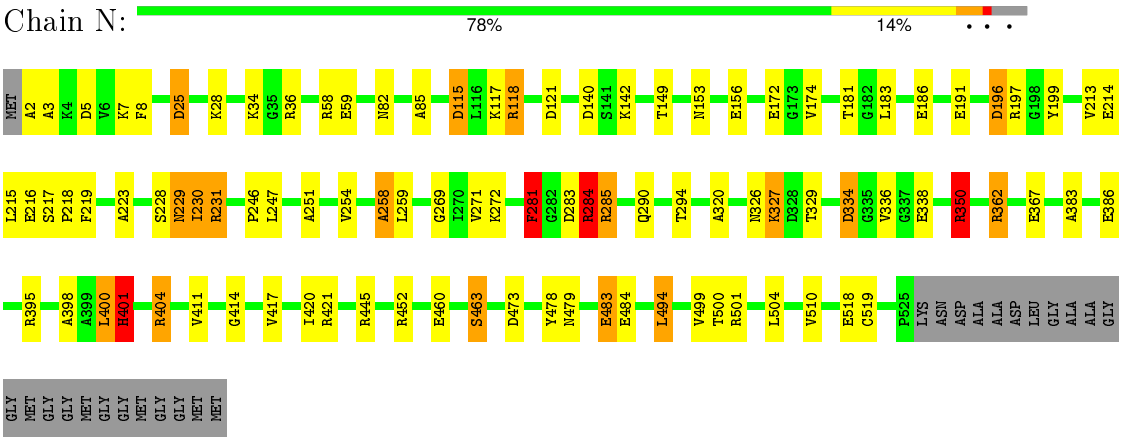
• Molecule 1: 60 KDA CHAPERONIN

Chain M:



- Molecule 1: 60 KDA CHAPERONIN

Chain N:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE WAS PHASE FLIPPED	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	15	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 4K CCD CAMERA	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MG, ATP

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	1.79	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	B	1.79	4/3873 (0.1%)	1.57	90/5229 (1.7%)
1	C	1.79	4/3873 (0.1%)	1.57	87/5229 (1.7%)
1	D	1.79	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	E	1.80	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	F	1.79	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	G	1.79	4/3873 (0.1%)	1.57	89/5229 (1.7%)
1	H	0.70	2/3873 (0.1%)	1.09	22/5229 (0.4%)
1	I	0.68	2/3873 (0.1%)	1.09	22/5229 (0.4%)
1	J	0.74	2/3873 (0.1%)	1.11	24/5229 (0.5%)
1	K	0.69	1/3873 (0.0%)	1.10	23/5229 (0.4%)
1	L	0.74	1/3873 (0.0%)	1.12	28/5229 (0.5%)
1	M	0.68	1/3873 (0.0%)	1.12	27/5229 (0.5%)
1	N	0.81	2/3873 (0.1%)	1.10	23/5229 (0.4%)
All	All	1.37	39/54222 (0.1%)	1.36	791/73206 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	9
1	C	0	10
1	D	0	10
1	E	0	9
1	F	0	10
1	G	0	9
1	H	0	10
1	I	0	10

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	10
1	K	0	10
1	L	0	11
1	M	0	10
1	N	0	11
All	All	0	138

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	36	ARG	CZ-NH1	91.40	2.51	1.33
1	G	36	ARG	CZ-NH1	91.28	2.51	1.33
1	B	36	ARG	CZ-NH1	91.26	2.51	1.33
1	F	36	ARG	CZ-NH1	91.25	2.51	1.33
1	D	36	ARG	CZ-NH1	91.20	2.51	1.33
1	C	36	ARG	CZ-NH1	91.16	2.51	1.33
1	A	36	ARG	CZ-NH1	91.00	2.51	1.33
1	N	400	LEU	C-N	21.68	1.83	1.34
1	L	400	LEU	C-N	19.10	1.77	1.34
1	N	401	HIS	C-N	-18.91	0.90	1.34
1	J	400	LEU	C-N	16.74	1.72	1.34
1	H	401	HIS	C-N	11.32	1.60	1.34
1	A	401	HIS	C-N	10.23	1.57	1.34
1	K	401	HIS	C-N	-10.22	1.10	1.34
1	G	401	HIS	C-N	10.10	1.57	1.34
1	B	401	HIS	C-N	10.02	1.57	1.34
1	F	401	HIS	C-N	9.94	1.56	1.34
1	C	401	HIS	C-N	9.72	1.56	1.34
1	E	401	HIS	C-N	9.57	1.56	1.34
1	D	401	HIS	C-N	9.54	1.55	1.34
1	F	36	ARG	CD-NE	9.10	1.61	1.46
1	C	36	ARG	CD-NE	9.09	1.61	1.46
1	A	36	ARG	CD-NE	9.04	1.61	1.46
1	B	36	ARG	CD-NE	9.02	1.61	1.46
1	D	36	ARG	CD-NE	9.00	1.61	1.46
1	E	36	ARG	CD-NE	9.00	1.61	1.46
1	G	36	ARG	CD-NE	8.96	1.61	1.46
1	J	401	HIS	C-N	-8.68	1.14	1.34
1	I	401	HIS	C-N	5.77	1.47	1.34
1	H	400	LEU	C-N	5.70	1.47	1.34
1	I	400	LEU	C-N	5.62	1.47	1.34
1	M	400	LEU	C-N	5.23	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	517	THR	CA-CB	5.14	1.66	1.53
1	G	517	THR	CA-CB	5.13	1.66	1.53
1	C	517	THR	CA-CB	5.11	1.66	1.53
1	A	517	THR	CA-CB	5.11	1.66	1.53
1	E	517	THR	CA-CB	5.11	1.66	1.53
1	B	517	THR	CA-CB	5.09	1.66	1.53
1	D	517	THR	CA-CB	5.09	1.66	1.53

All (791) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	36	ARG	NE-CZ-NH1	22.64	131.62	120.30
1	D	36	ARG	NE-CZ-NH1	22.58	131.59	120.30
1	G	36	ARG	NE-CZ-NH1	22.57	131.58	120.30
1	C	36	ARG	NE-CZ-NH1	22.51	131.56	120.30
1	A	36	ARG	NE-CZ-NH1	22.48	131.54	120.30
1	B	36	ARG	NE-CZ-NH1	22.45	131.52	120.30
1	E	36	ARG	NE-CZ-NH1	22.44	131.52	120.30
1	E	36	ARG	NH1-CZ-NH2	-13.84	104.18	119.40
1	B	36	ARG	CD-NE-CZ	13.81	142.94	123.60
1	F	36	ARG	NH1-CZ-NH2	-13.79	104.23	119.40
1	G	36	ARG	NH1-CZ-NH2	-13.78	104.24	119.40
1	G	36	ARG	CD-NE-CZ	13.77	142.87	123.60
1	A	36	ARG	CD-NE-CZ	13.76	142.86	123.60
1	D	36	ARG	NH1-CZ-NH2	-13.75	104.28	119.40
1	D	36	ARG	CD-NE-CZ	13.74	142.84	123.60
1	A	36	ARG	NH1-CZ-NH2	-13.74	104.28	119.40
1	B	36	ARG	NH1-CZ-NH2	-13.74	104.29	119.40
1	F	36	ARG	CD-NE-CZ	13.73	142.83	123.60
1	E	36	ARG	CD-NE-CZ	13.72	142.81	123.60
1	C	36	ARG	CD-NE-CZ	13.71	142.80	123.60
1	C	36	ARG	NH1-CZ-NH2	-13.71	104.32	119.40
1	M	401	HIS	O-C-N	12.36	142.48	122.70
1	A	383	ALA	N-CA-CB	11.87	126.72	110.10
1	C	383	ALA	N-CA-CB	11.85	126.69	110.10
1	F	383	ALA	N-CA-CB	11.85	126.69	110.10
1	E	383	ALA	N-CA-CB	11.84	126.68	110.10
1	G	383	ALA	N-CA-CB	11.81	126.64	110.10
1	D	383	ALA	N-CA-CB	11.79	126.60	110.10
1	B	383	ALA	N-CA-CB	11.78	126.60	110.10
1	B	114	MET	N-CA-CB	11.71	131.69	110.60
1	D	114	MET	N-CA-CB	11.70	131.66	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	114	MET	N-CA-CB	11.69	131.64	110.60
1	F	114	MET	N-CA-CB	11.68	131.62	110.60
1	C	114	MET	N-CA-CB	11.67	131.61	110.60
1	G	114	MET	N-CA-CB	11.67	131.61	110.60
1	E	114	MET	N-CA-CB	11.67	131.60	110.60
1	C	46	ALA	N-CA-CB	-11.17	94.46	110.10
1	A	46	ALA	N-CA-CB	-11.15	94.49	110.10
1	B	46	ALA	N-CA-CB	-11.15	94.49	110.10
1	G	46	ALA	N-CA-CB	-11.15	94.49	110.10
1	F	46	ALA	N-CA-CB	-11.14	94.51	110.10
1	E	46	ALA	N-CA-CB	-11.13	94.51	110.10
1	D	46	ALA	N-CA-CB	-11.12	94.53	110.10
1	L	401	HIS	O-C-N	-11.05	105.02	122.70
1	C	49	ILE	CB-CA-C	-10.33	90.94	111.60
1	D	49	ILE	CB-CA-C	-10.33	90.94	111.60
1	F	49	ILE	CB-CA-C	-10.32	90.95	111.60
1	B	49	ILE	CB-CA-C	-10.32	90.96	111.60
1	E	49	ILE	CB-CA-C	-10.32	90.96	111.60
1	A	49	ILE	CB-CA-C	-10.31	90.97	111.60
1	G	49	ILE	CB-CA-C	-10.31	90.98	111.60
1	C	36	ARG	NE-CZ-NH2	-10.05	115.27	120.30
1	D	36	ARG	NE-CZ-NH2	-9.95	115.32	120.30
1	F	36	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	A	36	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	G	36	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	B	36	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	E	36	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	M	401	HIS	CA-C-N	-9.26	96.83	117.20
1	D	36	ARG	CB-CA-C	9.17	128.73	110.40
1	C	36	ARG	CB-CA-C	9.15	128.70	110.40
1	A	36	ARG	CB-CA-C	9.14	128.68	110.40
1	F	36	ARG	CB-CA-C	9.14	128.68	110.40
1	G	36	ARG	CB-CA-C	9.13	128.67	110.40
1	E	36	ARG	CB-CA-C	9.13	128.66	110.40
1	B	36	ARG	CB-CA-C	9.12	128.64	110.40
1	C	231	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	G	231	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	F	231	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	B	231	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	D	231	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	E	112	ASN	N-CA-CB	-8.82	94.72	110.60
1	E	231	ARG	NE-CZ-NH1	8.81	124.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	112	ASN	N-CA-CB	-8.80	94.75	110.60
1	B	112	ASN	N-CA-CB	-8.79	94.77	110.60
1	A	112	ASN	N-CA-CB	-8.79	94.78	110.60
1	C	112	ASN	N-CA-CB	-8.79	94.78	110.60
1	F	112	ASN	N-CA-CB	-8.78	94.79	110.60
1	G	112	ASN	N-CA-CB	-8.77	94.82	110.60
1	A	231	ARG	NE-CZ-NH1	8.75	124.68	120.30
1	C	517	THR	CA-CB-OG1	8.71	127.30	109.00
1	K	452	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	B	517	THR	CA-CB-OG1	8.67	127.20	109.00
1	F	517	THR	CA-CB-OG1	8.66	127.19	109.00
1	D	517	THR	CA-CB-OG1	8.66	127.18	109.00
1	G	517	THR	CA-CB-OG1	8.66	127.18	109.00
1	A	517	THR	CA-CB-OG1	8.64	127.16	109.00
1	E	517	THR	CA-CB-OG1	8.64	127.15	109.00
1	A	41	ASP	N-CA-CB	8.60	126.07	110.60
1	E	41	ASP	N-CA-CB	8.59	126.06	110.60
1	B	41	ASP	N-CA-CB	8.59	126.05	110.60
1	F	41	ASP	N-CA-CB	8.57	126.03	110.60
1	C	41	ASP	N-CA-CB	8.57	126.02	110.60
1	N	452	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	G	41	ASP	N-CA-CB	8.55	126.00	110.60
1	M	452	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	J	452	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	D	41	ASP	N-CA-CB	8.53	125.96	110.60
1	B	152	ALA	CB-CA-C	8.53	122.89	110.10
1	F	152	ALA	CB-CA-C	8.52	122.88	110.10
1	H	452	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	I	452	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	D	152	ALA	CB-CA-C	8.50	122.85	110.10
1	L	231	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	K	58	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	C	152	ALA	CB-CA-C	8.48	122.82	110.10
1	G	152	ALA	CB-CA-C	8.48	122.81	110.10
1	E	152	ALA	CB-CA-C	8.46	122.79	110.10
1	D	461	GLU	CB-CA-C	8.46	127.31	110.40
1	A	461	GLU	CB-CA-C	8.45	127.30	110.40
1	A	152	ALA	CB-CA-C	8.45	122.77	110.10
1	F	461	GLU	CB-CA-C	8.45	127.30	110.40
1	L	452	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	C	461	GLU	CB-CA-C	8.44	127.28	110.40
1	B	461	GLU	CB-CA-C	8.43	127.27	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	58	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	E	461	GLU	CB-CA-C	8.43	127.25	110.40
1	G	461	GLU	CB-CA-C	8.42	127.23	110.40
1	H	58	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	M	231	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	M	58	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	I	58	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	H	231	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	K	231	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	L	58	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	J	36	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	I	231	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	N	58	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	J	231	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	N	231	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	M	36	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	473	ASP	N-CA-CB	8.15	125.28	110.60
1	G	473	ASP	N-CA-CB	8.15	125.27	110.60
1	D	473	ASP	N-CA-CB	8.14	125.25	110.60
1	E	473	ASP	N-CA-CB	8.14	125.25	110.60
1	H	36	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	F	473	ASP	N-CA-CB	8.13	125.24	110.60
1	B	153	ASN	CB-CA-C	8.13	126.67	110.40
1	C	153	ASN	CB-CA-C	8.13	126.66	110.40
1	I	36	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	C	473	ASP	N-CA-CB	8.12	125.22	110.60
1	A	231	ARG	CB-CA-C	-8.12	94.17	110.40
1	A	473	ASP	N-CA-CB	8.12	125.21	110.60
1	D	153	ASN	CB-CA-C	8.12	126.63	110.40
1	K	36	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	G	153	ASN	CB-CA-C	8.11	126.62	110.40
1	E	153	ASN	CB-CA-C	8.11	126.62	110.40
1	A	153	ASN	CB-CA-C	8.11	126.61	110.40
1	D	231	ARG	CB-CA-C	-8.11	94.19	110.40
1	E	231	ARG	CB-CA-C	-8.10	94.21	110.40
1	L	36	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	C	231	ARG	CB-CA-C	-8.09	94.23	110.40
1	F	153	ASN	CB-CA-C	8.09	126.58	110.40
1	F	231	ARG	CB-CA-C	-8.09	94.22	110.40
1	G	231	ARG	CB-CA-C	-8.08	94.24	110.40
1	N	36	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	B	231	ARG	CB-CA-C	-8.06	94.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	112	ASN	CB-CA-C	8.02	126.44	110.40
1	C	112	ASN	CB-CA-C	8.02	126.43	110.40
1	A	112	ASN	CB-CA-C	8.01	126.42	110.40
1	D	112	ASN	CB-CA-C	8.00	126.41	110.40
1	B	112	ASN	CB-CA-C	8.00	126.40	110.40
1	E	112	ASN	CB-CA-C	8.00	126.40	110.40
1	F	112	ASN	CB-CA-C	8.00	126.39	110.40
1	F	391	GLU	CB-CA-C	-7.94	94.51	110.40
1	A	391	GLU	CB-CA-C	-7.94	94.53	110.40
1	E	391	GLU	CB-CA-C	-7.91	94.57	110.40
1	C	391	GLU	CB-CA-C	-7.91	94.58	110.40
1	D	391	GLU	CB-CA-C	-7.91	94.58	110.40
1	B	391	GLU	CB-CA-C	-7.91	94.58	110.40
1	G	391	GLU	CB-CA-C	-7.90	94.59	110.40
1	G	73	MET	CB-CA-C	-7.89	94.62	110.40
1	J	401	HIS	O-C-N	7.88	135.32	122.70
1	E	73	MET	CB-CA-C	-7.86	94.67	110.40
1	D	73	MET	CB-CA-C	-7.86	94.69	110.40
1	F	73	MET	CB-CA-C	-7.85	94.70	110.40
1	B	73	MET	CB-CA-C	-7.84	94.71	110.40
1	C	73	MET	CB-CA-C	-7.84	94.72	110.40
1	B	39	VAL	CB-CA-C	7.83	126.28	111.40
1	A	73	MET	CB-CA-C	-7.83	94.75	110.40
1	E	39	VAL	CB-CA-C	7.81	126.24	111.40
1	F	39	VAL	CB-CA-C	7.79	126.20	111.40
1	A	39	VAL	CB-CA-C	7.77	126.16	111.40
1	C	39	VAL	CB-CA-C	7.77	126.16	111.40
1	G	39	VAL	CB-CA-C	7.75	126.12	111.40
1	D	39	VAL	CB-CA-C	7.74	126.10	111.40
1	J	401	HIS	CA-C-N	-7.63	100.42	117.20
1	G	404	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	404	ARG	NE-CZ-NH2	-7.49	116.55	120.30
1	M	400	LEU	O-C-N	-7.49	110.72	122.70
1	C	404	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	D	404	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	E	404	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	L	400	LEU	O-C-N	7.43	134.59	122.70
1	B	404	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	F	52	ASP	CB-CA-C	7.25	124.89	110.40
1	F	404	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	G	52	ASP	CB-CA-C	7.23	124.86	110.40
1	C	52	ASP	CB-CA-C	7.22	124.84	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	52	ASP	CB-CA-C	7.21	124.82	110.40
1	N	367	GLU	CB-CA-C	-7.20	96.00	110.40
1	J	367	GLU	CB-CA-C	-7.19	96.02	110.40
1	B	52	ASP	CB-CA-C	7.19	124.78	110.40
1	D	52	ASP	CB-CA-C	7.19	124.78	110.40
1	E	52	ASP	CB-CA-C	7.19	124.78	110.40
1	L	367	GLU	CB-CA-C	-7.18	96.04	110.40
1	H	367	GLU	CB-CA-C	-7.18	96.04	110.40
1	I	367	GLU	CB-CA-C	-7.17	96.05	110.40
1	M	367	GLU	CB-CA-C	-7.17	96.05	110.40
1	K	367	GLU	CB-CA-C	-7.17	96.06	110.40
1	M	401	HIS	C-N-CA	-7.12	103.89	121.70
1	L	362	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	M	362	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	J	362	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	K	362	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	H	362	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	F	118	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	N	362	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	I	362	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	D	118	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	115	ASP	N-CA-CB	6.96	123.12	110.60
1	A	115	ASP	N-CA-CB	6.95	123.12	110.60
1	A	118	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	C	118	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	G	115	ASP	N-CA-CB	6.95	123.10	110.60
1	D	115	ASP	N-CA-CB	6.93	123.08	110.60
1	E	115	ASP	N-CA-CB	6.93	123.08	110.60
1	L	401	HIS	CA-C-N	6.92	132.43	117.20
1	C	115	ASP	N-CA-CB	6.91	123.04	110.60
1	F	115	ASP	N-CA-CB	6.90	123.02	110.60
1	A	294	THR	CA-CB-CG2	-6.89	102.76	112.40
1	E	118	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	87	ASP	CB-CG-OD2	6.88	124.49	118.30
1	F	294	THR	CA-CB-CG2	-6.88	102.77	112.40
1	C	46	ALA	CB-CA-C	-6.87	99.80	110.10
1	D	87	ASP	CB-CG-OD2	6.86	124.48	118.30
1	B	294	THR	CA-CB-CG2	-6.86	102.80	112.40
1	G	118	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	G	294	THR	CA-CB-CG2	-6.86	102.80	112.40
1	G	46	ALA	CB-CA-C	-6.86	99.82	110.10
1	G	87	ASP	CB-CG-OD2	6.86	124.47	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	294	THR	CA-CB-CG2	-6.85	102.81	112.40
1	D	46	ALA	CB-CA-C	-6.85	99.82	110.10
1	E	294	THR	CA-CB-CG2	-6.85	102.81	112.40
1	D	294	THR	CA-CB-CG2	-6.85	102.81	112.40
1	E	87	ASP	CB-CG-OD2	6.84	124.46	118.30
1	B	46	ALA	CB-CA-C	-6.83	99.86	110.10
1	A	46	ALA	CB-CA-C	-6.83	99.86	110.10
1	F	46	ALA	CB-CA-C	-6.83	99.86	110.10
1	E	46	ALA	CB-CA-C	-6.82	99.87	110.10
1	A	87	ASP	CB-CG-OD2	6.82	124.44	118.30
1	C	231	ARG	CA-CB-CG	6.80	128.35	113.40
1	D	39	VAL	CA-CB-CG1	6.79	121.08	110.90
1	B	87	ASP	CB-CG-OD2	6.79	124.41	118.30
1	B	231	ARG	CA-CB-CG	6.79	128.33	113.40
1	G	231	ARG	CA-CB-CG	6.78	128.32	113.40
1	A	231	ARG	CA-CB-CG	6.78	128.32	113.40
1	C	39	VAL	CA-CB-CG1	6.78	121.07	110.90
1	G	39	VAL	CA-CB-CG1	6.78	121.07	110.90
1	F	87	ASP	CB-CG-OD2	6.77	124.40	118.30
1	D	231	ARG	CA-CB-CG	6.77	128.30	113.40
1	B	39	VAL	CA-CB-CG1	6.76	121.05	110.90
1	F	231	ARG	CA-CB-CG	6.76	128.28	113.40
1	A	39	VAL	CA-CB-CG1	6.76	121.05	110.90
1	E	39	VAL	CA-CB-CG1	6.76	121.03	110.90
1	E	231	ARG	CA-CB-CG	6.75	128.25	113.40
1	F	39	VAL	CA-CB-CG1	6.74	121.01	110.90
1	B	139	SER	CB-CA-C	6.72	122.86	110.10
1	E	139	SER	CB-CA-C	6.71	122.85	110.10
1	B	118	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	517	THR	N-CA-CB	6.71	123.04	110.30
1	L	401	HIS	C-N-CA	6.71	138.47	121.70
1	F	139	SER	CB-CA-C	6.69	122.81	110.10
1	G	139	SER	CB-CA-C	6.69	122.80	110.10
1	E	517	THR	N-CA-CB	6.68	123.00	110.30
1	A	139	SER	CB-CA-C	6.68	122.80	110.10
1	D	139	SER	CB-CA-C	6.67	122.78	110.10
1	F	517	THR	N-CA-CB	6.67	122.98	110.30
1	D	517	THR	N-CA-CB	6.67	122.98	110.30
1	B	517	THR	N-CA-CB	6.66	122.96	110.30
1	G	517	THR	N-CA-CB	6.66	122.95	110.30
1	C	517	THR	N-CA-CB	6.64	122.92	110.30
1	C	139	SER	CB-CA-C	6.64	122.71	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	285	ARG	CB-CA-C	-6.60	97.20	110.40
1	A	285	ARG	CB-CA-C	-6.59	97.22	110.40
1	G	285	ARG	CB-CA-C	-6.59	97.22	110.40
1	D	285	ARG	CB-CA-C	-6.58	97.25	110.40
1	F	285	ARG	CB-CA-C	-6.57	97.27	110.40
1	C	285	ARG	CB-CA-C	-6.56	97.28	110.40
1	B	285	ARG	CB-CA-C	-6.56	97.28	110.40
1	D	322	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	C	140	ASP	N-CA-CB	-6.54	98.82	110.60
1	D	140	ASP	N-CA-CB	-6.54	98.82	110.60
1	E	140	ASP	N-CA-CB	-6.54	98.83	110.60
1	A	140	ASP	N-CA-CB	-6.54	98.83	110.60
1	B	140	ASP	N-CA-CB	-6.54	98.83	110.60
1	J	473	ASP	N-CA-CB	6.53	122.35	110.60
1	N	473	ASP	N-CA-CB	6.52	122.34	110.60
1	F	140	ASP	N-CA-CB	-6.52	98.86	110.60
1	G	140	ASP	N-CA-CB	-6.52	98.87	110.60
1	C	425	LYS	CB-CA-C	6.51	123.42	110.40
1	E	371	LYS	CB-CA-C	6.51	123.41	110.40
1	I	473	ASP	N-CA-CB	6.51	122.31	110.60
1	F	425	LYS	CB-CA-C	6.50	123.41	110.40
1	G	425	LYS	CB-CA-C	6.50	123.41	110.40
1	N	404	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	K	473	ASP	N-CA-CB	6.50	122.30	110.60
1	A	425	LYS	CB-CA-C	6.50	123.39	110.40
1	B	425	LYS	CB-CA-C	6.50	123.39	110.40
1	L	118	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	B	371	LYS	CB-CA-C	6.50	123.39	110.40
1	M	118	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	N	118	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	E	425	LYS	CB-CA-C	6.49	123.38	110.40
1	H	501	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	C	371	LYS	CB-CA-C	6.49	123.38	110.40
1	J	501	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	M	473	ASP	N-CA-CB	6.48	122.27	110.60
1	H	473	ASP	N-CA-CB	6.48	122.27	110.60
1	G	322	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	425	LYS	CB-CA-C	6.47	123.34	110.40
1	L	473	ASP	N-CA-CB	6.47	122.24	110.60
1	C	322	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	371	LYS	CB-CA-C	6.46	123.31	110.40
1	F	322	ARG	NE-CZ-NH2	-6.45	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	118	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	K	118	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	M	501	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	K	350	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	D	371	LYS	CB-CA-C	6.43	123.26	110.40
1	G	371	LYS	CB-CA-C	6.42	123.25	110.40
1	H	118	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	F	371	LYS	CB-CA-C	6.42	123.24	110.40
1	K	501	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	322	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	52	ASP	N-CA-CB	6.39	122.11	110.60
1	C	52	ASP	N-CA-CB	6.39	122.11	110.60
1	J	118	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	E	52	ASP	N-CA-CB	6.39	122.10	110.60
1	A	52	ASP	N-CA-CB	6.39	122.10	110.60
1	N	501	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	F	52	ASP	N-CA-CB	6.37	122.06	110.60
1	D	52	ASP	N-CA-CB	6.37	122.06	110.60
1	G	52	ASP	N-CA-CB	6.37	122.06	110.60
1	H	350	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	I	350	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	322	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	L	395	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	L	350	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	L	501	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	E	322	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	I	501	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	I	395	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	482	THR	N-CA-CB	6.25	122.18	110.30
1	M	350	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	J	350	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	482	THR	N-CA-CB	6.24	122.15	110.30
1	K	395	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	N	350	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	F	362	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	E	510	VAL	CB-CA-C	-6.21	99.61	111.40
1	D	482	THR	N-CA-CB	6.20	122.09	110.30
1	C	510	VAL	CB-CA-C	-6.20	99.63	111.40
1	H	395	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	482	THR	N-CA-CB	6.19	122.07	110.30
1	G	482	THR	N-CA-CB	6.19	122.07	110.30
1	A	510	VAL	CB-CA-C	-6.19	99.64	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	482	THR	N-CA-CB	6.19	122.06	110.30
1	F	510	VAL	CB-CA-C	-6.19	99.64	111.40
1	M	395	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	D	510	VAL	CB-CA-C	-6.19	99.65	111.40
1	B	510	VAL	CB-CA-C	-6.18	99.65	111.40
1	F	482	THR	N-CA-CB	6.18	122.04	110.30
1	J	395	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	G	362	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	G	510	VAL	CB-CA-C	-6.16	99.70	111.40
1	J	404	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	362	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	L	404	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	D	362	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	N	395	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	362	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	362	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	F	85	ALA	N-CA-CB	-6.02	101.67	110.10
1	L	196	ASP	N-CA-CB	-6.02	99.76	110.60
1	C	435	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	M	5	ASP	N-CA-CB	6.01	121.42	110.60
1	H	284	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	I	5	ASP	N-CA-CB	6.01	121.41	110.60
1	E	435	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	M	196	ASP	N-CA-CB	-6.00	99.80	110.60
1	N	196	ASP	N-CA-CB	-6.00	99.80	110.60
1	J	196	ASP	N-CA-CB	-6.00	99.80	110.60
1	N	5	ASP	N-CA-CB	6.00	121.40	110.60
1	I	196	ASP	N-CA-CB	-6.00	99.81	110.60
1	K	196	ASP	N-CA-CB	-5.99	99.83	110.60
1	J	5	ASP	N-CA-CB	5.98	121.37	110.60
1	L	5	ASP	N-CA-CB	5.98	121.37	110.60
1	D	435	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	E	85	ALA	N-CA-CB	-5.98	101.73	110.10
1	G	435	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	H	196	ASP	N-CA-CB	-5.98	99.83	110.60
1	C	85	ALA	N-CA-CB	-5.97	101.74	110.10
1	D	40	LEU	N-CA-CB	-5.97	98.46	110.40
1	G	85	ALA	N-CA-CB	-5.97	101.74	110.10
1	B	85	ALA	N-CA-CB	-5.97	101.75	110.10
1	K	5	ASP	N-CA-CB	5.96	121.33	110.60
1	D	85	ALA	N-CA-CB	-5.96	101.75	110.10
1	N	284	ARG	NE-CZ-NH1	5.96	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	5	ASP	N-CA-CB	5.96	121.33	110.60
1	A	85	ALA	N-CA-CB	-5.96	101.76	110.10
1	G	40	LEU	N-CA-CB	-5.95	98.49	110.40
1	A	435	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	B	362	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	I	284	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	40	LEU	N-CA-CB	-5.93	98.53	110.40
1	B	435	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	F	40	LEU	N-CA-CB	-5.93	98.53	110.40
1	F	435	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	E	40	LEU	N-CA-CB	-5.93	98.55	110.40
1	C	40	LEU	N-CA-CB	-5.92	98.55	110.40
1	B	40	LEU	N-CA-CB	-5.92	98.56	110.40
1	M	284	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	391	GLU	CA-CB-CG	5.85	126.27	113.40
1	E	391	GLU	CA-CB-CG	5.85	126.27	113.40
1	B	391	GLU	CA-CB-CG	5.85	126.27	113.40
1	G	391	GLU	CA-CB-CG	5.84	126.26	113.40
1	N	285	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	K	284	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	M	285	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	E	367	GLU	CB-CA-C	-5.83	98.73	110.40
1	D	367	GLU	CB-CA-C	-5.83	98.73	110.40
1	F	391	GLU	CA-CB-CG	5.83	126.22	113.40
1	A	391	GLU	CA-CB-CG	5.83	126.21	113.40
1	L	284	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	417	VAL	CA-CB-CG2	-5.82	102.17	110.90
1	B	367	GLU	CB-CA-C	-5.82	98.76	110.40
1	C	391	GLU	CA-CB-CG	5.82	126.20	113.40
1	A	367	GLU	CB-CA-C	-5.82	98.77	110.40
1	C	367	GLU	CB-CA-C	-5.81	98.77	110.40
1	F	367	GLU	CB-CA-C	-5.80	98.79	110.40
1	G	367	GLU	CB-CA-C	-5.80	98.79	110.40
1	K	404	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	F	87	ASP	OD1-CG-OD2	-5.80	112.28	123.30
1	E	417	VAL	CA-CB-CG2	-5.80	102.20	110.90
1	G	417	VAL	CA-CB-CG2	-5.79	102.21	110.90
1	B	417	VAL	CA-CB-CG2	-5.79	102.21	110.90
1	C	417	VAL	CA-CB-CG2	-5.79	102.21	110.90
1	D	87	ASP	OD1-CG-OD2	-5.79	112.30	123.30
1	E	87	ASP	OD1-CG-OD2	-5.79	112.30	123.30
1	B	87	ASP	OD1-CG-OD2	-5.78	112.32	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	417	VAL	CA-CB-CG2	-5.78	102.23	110.90
1	A	87	ASP	OD1-CG-OD2	-5.78	112.32	123.30
1	C	87	ASP	OD1-CG-OD2	-5.77	112.33	123.30
1	F	417	VAL	CA-CB-CG2	-5.77	102.24	110.90
1	G	87	ASP	OD1-CG-OD2	-5.77	112.34	123.30
1	J	284	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	E	149	THR	N-CA-CB	5.76	121.25	110.30
1	D	149	THR	N-CA-CB	5.75	121.23	110.30
1	I	285	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	G	149	THR	N-CA-CB	5.75	121.22	110.30
1	K	115	ASP	CB-CA-C	5.75	121.90	110.40
1	K	285	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	F	149	THR	N-CA-CB	5.75	121.22	110.30
1	H	285	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	L	285	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	C	149	THR	N-CA-CB	5.71	121.16	110.30
1	J	285	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	149	THR	N-CA-CB	5.71	121.15	110.30
1	L	115	ASP	CB-CA-C	5.71	121.82	110.40
1	B	149	THR	N-CA-CB	5.71	121.14	110.30
1	C	39	VAL	CG1-CB-CG2	5.71	120.03	110.90
1	B	39	VAL	CG1-CB-CG2	5.70	120.02	110.90
1	L	400	LEU	CA-C-N	-5.70	104.66	117.20
1	I	115	ASP	CB-CA-C	5.70	121.80	110.40
1	N	115	ASP	CB-CA-C	5.70	121.79	110.40
1	E	452	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	E	39	VAL	CG1-CB-CG2	5.69	120.00	110.90
1	J	115	ASP	CB-CA-C	5.68	121.77	110.40
1	F	39	VAL	CG1-CB-CG2	5.68	119.99	110.90
1	D	452	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	M	115	ASP	CB-CA-C	5.68	121.76	110.40
1	D	353	ILE	CB-CA-C	-5.68	100.25	111.60
1	A	353	ILE	CB-CA-C	-5.67	100.25	111.60
1	E	412	VAL	CB-CA-C	-5.67	100.62	111.40
1	A	452	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	F	353	ILE	CB-CA-C	-5.67	100.26	111.60
1	H	115	ASP	CB-CA-C	5.67	121.74	110.40
1	C	353	ILE	CB-CA-C	-5.67	100.26	111.60
1	G	39	VAL	CG1-CB-CG2	5.67	119.97	110.90
1	C	412	VAL	CB-CA-C	-5.66	100.64	111.40
1	B	353	ILE	CB-CA-C	-5.66	100.28	111.60
1	D	412	VAL	CB-CA-C	-5.66	100.65	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	353	ILE	CB-CA-C	-5.66	100.28	111.60
1	F	412	VAL	CB-CA-C	-5.66	100.65	111.40
1	G	412	VAL	CB-CA-C	-5.66	100.65	111.40
1	E	353	ILE	CB-CA-C	-5.65	100.30	111.60
1	B	412	VAL	CB-CA-C	-5.65	100.66	111.40
1	C	452	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	39	VAL	CG1-CB-CG2	5.64	119.92	110.90
1	A	39	VAL	CG1-CB-CG2	5.64	119.92	110.90
1	I	404	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	412	VAL	CB-CA-C	-5.63	100.71	111.40
1	E	231	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	C	231	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	231	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	G	452	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	G	126	ALA	CB-CA-C	5.60	118.50	110.10
1	C	126	ALA	CB-CA-C	5.59	118.49	110.10
1	B	400	LEU	O-C-N	-5.59	113.76	122.70
1	A	126	ALA	CB-CA-C	5.58	118.48	110.10
1	H	463	SER	N-CA-CB	-5.58	102.12	110.50
1	F	126	ALA	CB-CA-C	5.58	118.47	110.10
1	B	126	ALA	CB-CA-C	5.57	118.46	110.10
1	J	463	SER	N-CA-CB	-5.57	102.14	110.50
1	G	231	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	F	452	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	M	463	SER	N-CA-CB	-5.57	102.15	110.50
1	E	126	ALA	CB-CA-C	5.57	118.45	110.10
1	K	463	SER	N-CA-CB	-5.57	102.15	110.50
1	I	463	SER	N-CA-CB	-5.56	102.15	110.50
1	B	452	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	126	ALA	CB-CA-C	5.56	118.44	110.10
1	L	463	SER	N-CA-CB	-5.55	102.17	110.50
1	A	400	LEU	O-C-N	-5.55	113.82	122.70
1	N	463	SER	N-CA-CB	-5.53	102.20	110.50
1	D	231	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	H	404	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	166	MET	CG-SD-CE	-5.47	91.44	100.20
1	F	166	MET	CG-SD-CE	-5.47	91.44	100.20
1	G	166	MET	CG-SD-CE	-5.47	91.44	100.20
1	M	404	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	166	MET	CG-SD-CE	-5.46	91.46	100.20
1	D	166	MET	CG-SD-CE	-5.46	91.47	100.20
1	F	231	ARG	NE-CZ-NH2	-5.46	117.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	113	PRO	CA-N-CD	-5.45	103.87	111.50
1	C	166	MET	CG-SD-CE	-5.45	91.48	100.20
1	E	166	MET	CG-SD-CE	-5.44	91.49	100.20
1	E	113	PRO	CA-N-CD	-5.43	103.89	111.50
1	C	409	GLU	N-CA-CB	5.42	120.36	110.60
1	F	517	THR	CB-CA-C	-5.42	96.96	111.60
1	G	400	LEU	O-C-N	-5.42	114.03	122.70
1	G	517	THR	CB-CA-C	-5.42	96.96	111.60
1	C	517	THR	CB-CA-C	-5.42	96.97	111.60
1	I	281	PHE	N-CA-CB	5.42	120.36	110.60
1	H	281	PHE	N-CA-CB	5.42	120.36	110.60
1	F	369	VAL	N-CA-CB	5.42	123.42	111.50
1	B	517	THR	CB-CA-C	-5.42	96.98	111.60
1	A	435	ASP	CB-CA-C	-5.41	99.57	110.40
1	C	435	ASP	CB-CA-C	-5.41	99.57	110.40
1	G	435	ASP	CB-CA-C	-5.41	99.58	110.40
1	A	409	GLU	N-CA-CB	5.41	120.34	110.60
1	E	435	ASP	CB-CA-C	-5.41	99.58	110.40
1	J	294	THR	CA-CB-CG2	-5.41	104.83	112.40
1	L	281	PHE	N-CA-CB	5.41	120.33	110.60
1	M	281	PHE	N-CA-CB	5.41	120.33	110.60
1	A	117	LYS	N-CA-CB	5.40	120.33	110.60
1	A	369	VAL	N-CA-CB	5.40	123.39	111.50
1	E	369	VAL	N-CA-CB	5.40	123.39	111.50
1	A	517	THR	CB-CA-C	-5.40	97.02	111.60
1	F	435	ASP	CB-CA-C	-5.40	99.60	110.40
1	F	113	PRO	CA-N-CD	-5.40	103.94	111.50
1	J	281	PHE	N-CA-CB	5.40	120.32	110.60
1	B	113	PRO	CA-N-CD	-5.40	103.94	111.50
1	G	369	VAL	N-CA-CB	5.40	123.38	111.50
1	B	369	VAL	N-CA-CB	5.40	123.37	111.50
1	D	409	GLU	N-CA-CB	5.39	120.31	110.60
1	A	113	PRO	CA-N-CD	-5.39	103.95	111.50
1	B	59	GLU	CB-CA-C	5.39	121.18	110.40
1	D	517	THR	CB-CA-C	-5.39	97.04	111.60
1	D	435	ASP	CB-CA-C	-5.39	99.62	110.40
1	B	435	ASP	CB-CA-C	-5.39	99.62	110.40
1	D	369	VAL	N-CA-CB	5.39	123.36	111.50
1	E	117	LYS	N-CA-CB	5.39	120.30	110.60
1	K	281	PHE	N-CA-CB	5.39	120.30	110.60
1	E	409	GLU	N-CA-CB	5.39	120.30	110.60
1	E	517	THR	CB-CA-C	-5.39	97.06	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	294	THR	CA-CB-CG2	-5.39	104.86	112.40
1	K	294	THR	CA-CB-CG2	-5.39	104.86	112.40
1	N	294	THR	CA-CB-CG2	-5.39	104.86	112.40
1	C	117	LYS	N-CA-CB	5.38	120.29	110.60
1	A	231	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	59	GLU	CB-CA-C	5.38	121.16	110.40
1	L	294	THR	CA-CB-CG2	-5.38	104.87	112.40
1	C	369	VAL	N-CA-CB	5.37	123.32	111.50
1	G	117	LYS	N-CA-CB	5.37	120.27	110.60
1	B	117	LYS	N-CA-CB	5.37	120.27	110.60
1	D	285	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	409	GLU	N-CA-CB	5.37	120.27	110.60
1	D	117	LYS	N-CA-CB	5.37	120.26	110.60
1	F	117	LYS	N-CA-CB	5.37	120.26	110.60
1	G	59	GLU	CB-CA-C	5.36	121.12	110.40
1	N	281	PHE	N-CA-CB	5.36	120.26	110.60
1	F	409	GLU	N-CA-CB	5.36	120.25	110.60
1	M	294	THR	CA-CB-CG2	-5.36	104.90	112.40
1	D	113	PRO	CA-N-CD	-5.35	104.01	111.50
1	F	59	GLU	CB-CA-C	5.35	121.09	110.40
1	E	59	GLU	CB-CA-C	5.35	121.09	110.40
1	G	113	PRO	CA-N-CD	-5.35	104.02	111.50
1	G	285	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	H	294	THR	CA-CB-CG2	-5.34	104.92	112.40
1	A	285	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	G	409	GLU	N-CA-CB	5.34	120.22	110.60
1	C	59	GLU	CB-CA-C	5.34	121.07	110.40
1	A	59	GLU	CB-CA-C	5.33	121.06	110.40
1	B	58	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	257	GLU	N-CA-CB	5.32	120.18	110.60
1	C	400	LEU	O-C-N	-5.31	114.20	122.70
1	F	257	GLU	N-CA-CB	5.31	120.16	110.60
1	A	368	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	L	400	LEU	C-N-CA	-5.30	108.44	121.70
1	C	257	GLU	N-CA-CB	5.30	120.15	110.60
1	F	196	ASP	N-CA-CB	-5.30	101.05	110.60
1	E	113	PRO	N-CA-CB	5.30	109.66	103.30
1	E	257	GLU	N-CA-CB	5.29	120.13	110.60
1	A	196	ASP	N-CA-CB	-5.29	101.08	110.60
1	D	196	ASP	N-CA-CB	-5.29	101.08	110.60
1	C	196	ASP	N-CA-CB	-5.29	101.08	110.60
1	B	473	ASP	CB-CA-C	5.29	120.97	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	140	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	473	ASP	CB-CA-C	5.28	120.97	110.40
1	G	58	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	257	GLU	N-CA-CB	5.28	120.11	110.60
1	G	473	ASP	CB-CA-C	5.28	120.96	110.40
1	C	58	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	140	ASP	CB-CG-OD1	5.28	123.05	118.30
1	E	196	ASP	N-CA-CB	-5.28	101.10	110.60
1	B	196	ASP	N-CA-CB	-5.28	101.10	110.60
1	F	58	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	322	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	J	258	ALA	CB-CA-C	5.27	118.01	110.10
1	C	113	PRO	N-CA-CB	5.27	109.62	103.30
1	I	258	ALA	CB-CA-C	5.27	118.01	110.10
1	E	473	ASP	CB-CA-C	5.27	120.94	110.40
1	C	368	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	473	ASP	CB-CA-C	5.26	120.92	110.40
1	F	473	ASP	CB-CA-C	5.26	120.92	110.40
1	G	140	ASP	CB-CG-OD1	5.26	123.04	118.30
1	J	401	HIS	C-N-CA	-5.26	108.55	121.70
1	A	106	ALA	CB-CA-C	5.26	117.99	110.10
1	G	196	ASP	N-CA-CB	-5.26	101.13	110.60
1	N	258	ALA	CB-CA-C	5.26	117.99	110.10
1	C	473	ASP	CB-CA-C	5.26	120.92	110.40
1	B	140	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	257	GLU	N-CA-CB	5.25	120.06	110.60
1	E	106	ALA	CB-CA-C	5.25	117.98	110.10
1	F	322	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	H	258	ALA	CB-CA-C	5.25	117.98	110.10
1	M	258	ALA	CB-CA-C	5.25	117.97	110.10
1	F	113	PRO	N-CA-CB	5.25	109.60	103.30
1	K	258	ALA	CB-CA-C	5.25	117.97	110.10
1	L	258	ALA	CB-CA-C	5.24	117.97	110.10
1	F	106	ALA	CB-CA-C	5.24	117.96	110.10
1	B	285	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	F	368	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	G	322	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	106	ALA	CB-CA-C	5.23	117.94	110.10
1	G	257	GLU	N-CA-CB	5.23	120.02	110.60
1	E	58	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	106	ALA	CB-CA-C	5.23	117.94	110.10
1	E	285	ARG	NE-CZ-NH1	5.23	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	320	ALA	N-CA-CB	5.22	117.41	110.10
1	G	368	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	58	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	106	ALA	CB-CA-C	5.22	117.93	110.10
1	B	106	ALA	CB-CA-C	5.22	117.92	110.10
1	D	113	PRO	N-CA-CB	5.22	109.56	103.30
1	G	113	PRO	N-CA-CB	5.22	109.56	103.30
1	G	268	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	368	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	F	320	ALA	N-CA-CB	5.21	117.40	110.10
1	A	113	PRO	N-CA-CB	5.21	109.55	103.30
1	C	322	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	320	ALA	N-CA-CB	5.21	117.39	110.10
1	B	113	PRO	N-CA-CB	5.21	109.55	103.30
1	C	140	ASP	CB-CG-OD1	5.20	122.98	118.30
1	E	140	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	320	ALA	N-CA-CB	5.20	117.38	110.10
1	E	320	ALA	N-CA-CB	5.20	117.38	110.10
1	F	285	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	320	ALA	N-CA-CB	5.20	117.38	110.10
1	D	320	ALA	N-CA-CB	5.20	117.38	110.10
1	B	268	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	140	ASP	CB-CG-OD1	5.19	122.97	118.30
1	E	368	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	203	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	D	322	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	F	400	LEU	O-C-N	-5.18	114.41	122.70
1	D	268	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	F	87	ASP	CB-CG-OD1	5.17	122.95	118.30
1	F	268	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	F	284	ARG	CB-CA-C	-5.15	100.10	110.40
1	A	58	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	284	ARG	CB-CA-C	-5.15	100.10	110.40
1	C	203	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	B	203	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	C	285	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	140	ASP	CA-CB-CG	5.13	124.70	113.40
1	F	140	ASP	CA-CB-CG	5.13	124.68	113.40
1	G	284	ARG	CB-CA-C	-5.13	100.14	110.40
1	C	284	ARG	CB-CA-C	-5.13	100.15	110.40
1	B	284	ARG	CB-CA-C	-5.12	100.15	110.40
1	D	284	ARG	CB-CA-C	-5.12	100.15	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	322	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	368	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	E	140	ASP	CA-CB-CG	5.12	124.66	113.40
1	B	87	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	140	ASP	CA-CB-CG	5.12	124.65	113.40
1	M	285	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	E	284	ARG	CB-CA-C	-5.11	100.18	110.40
1	A	204	PHE	CB-CG-CD2	-5.10	117.23	120.80
1	B	140	ASP	CA-CB-CG	5.10	124.62	113.40
1	E	322	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	G	140	ASP	CA-CB-CG	5.10	124.62	113.40
1	A	87	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	140	ASP	CA-CB-CG	5.10	124.61	113.40
1	E	268	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	203	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	E	87	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	73	MET	CA-CB-CG	5.08	121.93	113.30
1	C	268	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	73	MET	CA-CB-CG	5.07	121.92	113.30
1	D	203	TYR	CB-CG-CD1	5.07	124.04	121.00
1	E	73	MET	CA-CB-CG	5.07	121.92	113.30
1	B	73	MET	CA-CB-CG	5.07	121.92	113.30
1	D	369	VAL	CB-CA-C	-5.07	101.77	111.40
1	E	203	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	B	204	PHE	CB-CG-CD2	-5.06	117.25	120.80
1	D	104	LEU	CB-CA-C	5.06	119.82	110.20
1	F	203	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	M	59	GLU	CB-CA-C	5.06	120.52	110.40
1	C	361	ASP	CB-CA-C	5.06	120.52	110.40
1	C	436	GLN	N-CA-CB	5.06	119.70	110.60
1	E	369	VAL	CB-CA-C	-5.06	101.79	111.40
1	F	104	LEU	CB-CA-C	5.05	119.80	110.20
1	K	285	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	436	GLN	N-CA-CB	5.05	119.69	110.60
1	C	369	VAL	CB-CA-C	-5.05	101.80	111.40
1	F	73	MET	CA-CB-CG	5.05	121.89	113.30
1	I	59	GLU	CB-CA-C	5.05	120.50	110.40
1	B	361	ASP	CB-CA-C	5.05	120.50	110.40
1	C	73	MET	CA-CB-CG	5.05	121.88	113.30
1	G	73	MET	CA-CB-CG	5.05	121.88	113.30
1	D	87	ASP	CB-CG-OD1	5.05	122.84	118.30
1	G	361	ASP	CB-CA-C	5.05	120.49	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	369	VAL	CB-CA-C	-5.04	101.81	111.40
1	G	436	GLN	N-CA-CB	5.04	119.68	110.60
1	A	436	GLN	N-CA-CB	5.04	119.67	110.60
1	E	501	ARG	N-CA-CB	-5.04	101.52	110.60
1	A	361	ASP	CB-CA-C	5.04	120.48	110.40
1	F	501	ARG	N-CA-CB	-5.04	101.53	110.60
1	C	501	ARG	N-CA-CB	-5.04	101.53	110.60
1	F	203	TYR	CB-CG-CD1	5.04	124.02	121.00
1	B	369	VAL	CB-CA-C	-5.04	101.83	111.40
1	D	400	LEU	O-C-N	-5.04	114.64	122.70
1	E	436	GLN	N-CA-CB	5.04	119.67	110.60
1	F	436	GLN	N-CA-CB	5.04	119.67	110.60
1	G	203	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	H	59	GLU	CB-CA-C	5.04	120.47	110.40
1	F	361	ASP	CB-CA-C	5.03	120.47	110.40
1	L	59	GLU	CB-CA-C	5.03	120.47	110.40
1	D	361	ASP	CB-CA-C	5.03	120.47	110.40
1	D	436	GLN	N-CA-CB	5.03	119.66	110.60
1	E	203	TYR	CB-CG-CD1	5.03	124.02	121.00
1	E	321	LYS	N-CA-CB	5.03	119.66	110.60
1	A	104	LEU	CB-CA-C	5.03	119.76	110.20
1	B	104	LEU	CB-CA-C	5.03	119.76	110.20
1	G	204	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	K	59	GLU	CB-CA-C	5.03	120.46	110.40
1	B	501	ARG	N-CA-CB	-5.03	101.55	110.60
1	E	104	LEU	CB-CA-C	5.03	119.75	110.20
1	G	87	ASP	CB-CG-OD1	5.03	122.83	118.30
1	F	321	LYS	N-CA-CB	5.03	119.65	110.60
1	N	59	GLU	CB-CA-C	5.02	120.45	110.40
1	N	285	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	G	321	LYS	N-CA-CB	5.02	119.64	110.60
1	A	321	LYS	N-CA-CB	5.02	119.64	110.60
1	G	369	VAL	CB-CA-C	-5.02	101.86	111.40
1	B	203	TYR	CB-CG-CD1	5.01	124.01	121.00
1	D	321	LYS	N-CA-CB	5.01	119.62	110.60
1	E	361	ASP	CB-CA-C	5.01	120.43	110.40
1	C	87	ASP	CB-CG-OD1	5.01	122.81	118.30
1	G	104	LEU	CB-CA-C	5.01	119.72	110.20
1	E	204	PHE	CB-CG-CD2	-5.01	117.29	120.80
1	A	369	VAL	CB-CA-C	-5.01	101.89	111.40
1	D	501	ARG	N-CA-CB	-5.01	101.59	110.60
1	G	501	ARG	N-CA-CB	-5.01	101.59	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	203	TYR	CB-CG-CD1	5.00	124.00	121.00
1	A	268	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	B	321	LYS	N-CA-CB	5.00	119.60	110.60
1	C	104	LEU	CB-CA-C	5.00	119.70	110.20

There are no chirality outliers.

All (138) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	268	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	36	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	395	ARG	Sidechain
1	A	404	ARG	Sidechain
1	B	13	ARG	Sidechain
1	B	197	ARG	Sidechain
1	B	231	ARG	Sidechain
1	B	268	ARG	Sidechain
1	B	350	ARG	Sidechain
1	B	36	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	395	ARG	Sidechain
1	B	404	ARG	Sidechain
1	C	13	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	219	PHE	Sidechain
1	C	231	ARG	Sidechain
1	C	268	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	36	ARG	Sidechain
1	C	362	ARG	Sidechain
1	C	395	ARG	Sidechain
1	C	404	ARG	Sidechain
1	D	13	ARG	Sidechain
1	D	197	ARG	Sidechain
1	D	219	PHE	Sidechain
1	D	231	ARG	Sidechain
1	D	268	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	350	ARG	Sidechain
1	D	36	ARG	Sidechain
1	D	362	ARG	Sidechain
1	D	395	ARG	Sidechain
1	D	404	ARG	Sidechain
1	E	13	ARG	Sidechain
1	E	197	ARG	Sidechain
1	E	231	ARG	Sidechain
1	E	268	ARG	Sidechain
1	E	350	ARG	Sidechain
1	E	36	ARG	Sidechain
1	E	362	ARG	Sidechain
1	E	395	ARG	Sidechain
1	E	404	ARG	Sidechain
1	F	13	ARG	Sidechain
1	F	197	ARG	Sidechain
1	F	219	PHE	Sidechain
1	F	231	ARG	Sidechain
1	F	268	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	36	ARG	Sidechain
1	F	362	ARG	Sidechain
1	F	395	ARG	Sidechain
1	F	404	ARG	Sidechain
1	G	13	ARG	Sidechain
1	G	197	ARG	Sidechain
1	G	231	ARG	Sidechain
1	G	268	ARG	Sidechain
1	G	350	ARG	Sidechain
1	G	36	ARG	Sidechain
1	G	362	ARG	Sidechain
1	G	395	ARG	Sidechain
1	G	404	ARG	Sidechain
1	H	118	ARG	Sidechain
1	H	197	ARG	Sidechain
1	H	231	ARG	Sidechain
1	H	284	ARG	Sidechain
1	H	285	ARG	Sidechain
1	H	350	ARG	Sidechain
1	H	362	ARG	Sidechain
1	H	421	ARG	Sidechain
1	H	445	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	H	478	TYR	Sidechain
1	I	118	ARG	Sidechain
1	I	197	ARG	Sidechain
1	I	231	ARG	Sidechain
1	I	284	ARG	Sidechain
1	I	285	ARG	Sidechain
1	I	350	ARG	Sidechain
1	I	362	ARG	Sidechain
1	I	421	ARG	Sidechain
1	I	445	ARG	Sidechain
1	I	478	TYR	Sidechain
1	J	118	ARG	Sidechain
1	J	197	ARG	Sidechain
1	J	231	ARG	Sidechain
1	J	284	ARG	Sidechain
1	J	285	ARG	Sidechain
1	J	350	ARG	Sidechain
1	J	362	ARG	Sidechain
1	J	421	ARG	Sidechain
1	J	445	ARG	Sidechain
1	J	478	TYR	Sidechain
1	K	118	ARG	Sidechain
1	K	197	ARG	Sidechain
1	K	231	ARG	Sidechain
1	K	284	ARG	Sidechain
1	K	285	ARG	Sidechain
1	K	350	ARG	Sidechain
1	K	362	ARG	Sidechain
1	K	421	ARG	Sidechain
1	K	445	ARG	Sidechain
1	K	478	TYR	Sidechain
1	L	118	ARG	Sidechain
1	L	197	ARG	Sidechain
1	L	231	ARG	Sidechain
1	L	284	ARG	Sidechain
1	L	285	ARG	Sidechain
1	L	350	ARG	Sidechain
1	L	362	ARG	Sidechain
1	L	401	HIS	Mainchain
1	L	421	ARG	Sidechain
1	L	445	ARG	Sidechain
1	L	478	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	M	118	ARG	Sidechain
1	M	197	ARG	Sidechain
1	M	231	ARG	Sidechain
1	M	284	ARG	Sidechain
1	M	285	ARG	Sidechain
1	M	350	ARG	Sidechain
1	M	362	ARG	Sidechain
1	M	421	ARG	Sidechain
1	M	445	ARG	Sidechain
1	M	478	TYR	Sidechain
1	N	118	ARG	Sidechain
1	N	197	ARG	Sidechain
1	N	231	ARG	Sidechain
1	N	284	ARG	Sidechain
1	N	285	ARG	Sidechain
1	N	350	ARG	Sidechain
1	N	362	ARG	Sidechain
1	N	401	HIS	Mainchain
1	N	421	ARG	Sidechain
1	N	445	ARG	Sidechain
1	N	478	TYR	Sidechain

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	3846	0	3970	203	0
1	B	3846	0	3970	205	0
1	C	3846	0	3970	205	0
1	D	3846	0	3970	210	0
1	E	3846	0	3970	209	0
1	F	3846	0	3970	208	0
1	G	3846	0	3970	207	0
1	H	3846	0	3970	28	0
1	I	3846	0	3970	28	0
1	J	3846	0	3968	29	0
1	K	3846	0	3969	27	0
1	L	3846	0	3969	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3846	0	3970	27	0
1	N	3846	0	3968	32	0
2	A	31	12	12	4	0
2	B	31	12	12	3	0
2	C	31	12	12	3	0
2	D	31	12	12	3	0
2	E	31	12	12	3	0
2	F	31	12	12	4	0
2	G	31	12	12	4	0
3	A	1	0	0	5	0
3	B	1	0	0	4	0
3	C	1	0	0	4	0
3	D	1	0	0	4	0
3	E	1	0	0	4	0
3	F	1	0	0	5	0
3	G	1	0	0	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
All	All	54075	84	55658	1291	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 12.

All (1291) 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:J:400:LEU:C	1:J:401:HIS:N	1.72	1.43
1:A:115:ASP:H	1:B:36:ARG:CZ	1.37	1.37
1:C:115:ASP:H	1:D:36:ARG:CZ	1.37	1.37
1:D:115:ASP:H	1:E:36:ARG:CZ	1.37	1.36
1:A:116:LEU:H	1:B:36:ARG:NH1	1.24	1.36
1:C:116:LEU:H	1:D:36:ARG:NH1	1.24	1.36
1:B:115:ASP:H	1:C:36:ARG:CZ	1.37	1.36
1:F:115:ASP:H	1:G:36:ARG:CZ	1.37	1.35
1:L:400:LEU:C	1:L:401:HIS:N	1.78	1.35
1:A:36:ARG:CZ	1:G:115:ASP:H	1.37	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:ASP:H	1:F:36:ARG:CZ	1.37	1.34
1:F:116:LEU:H	1:G:36:ARG:NH1	1.24	1.33
1:E:116:LEU:H	1:F:36:ARG:NH1	1.24	1.33
1:D:116:LEU:H	1:E:36:ARG:NH1	1.24	1.33
1:B:116:LEU:H	1:C:36:ARG:NH1	1.24	1.32
1:A:36:ARG:NH1	1:G:116:LEU:H	1.24	1.32
1:N:400:LEU:C	1:N:401:HIS:N	1.83	1.32
1:B:116:LEU:N	1:C:36:ARG:HH12	1.29	1.30
1:C:116:LEU:N	1:D:36:ARG:HH12	1.30	1.29
1:D:116:LEU:N	1:E:36:ARG:HH12	1.29	1.29
1:A:36:ARG:HH12	1:G:116:LEU:N	1.30	1.29
1:E:116:LEU:N	1:F:36:ARG:HH12	1.30	1.28
1:A:116:LEU:N	1:B:36:ARG:HH12	1.30	1.27
1:F:116:LEU:N	1:G:36:ARG:HH12	1.30	1.26
1:A:112:ASN:O	1:B:36:ARG:NH1	1.85	1.10
1:F:112:ASN:O	1:G:36:ARG:NH1	1.85	1.10
1:C:112:ASN:O	1:D:36:ARG:NH1	1.85	1.10
1:E:112:ASN:O	1:F:36:ARG:NH1	1.85	1.09
1:B:112:ASN:O	1:C:36:ARG:NH1	1.85	1.09
1:A:36:ARG:NH1	1:G:112:ASN:O	1.84	1.08
1:D:112:ASN:O	1:E:36:ARG:NH1	1.85	1.08
1:B:115:ASP:N	1:C:36:ARG:CZ	2.18	1.07
1:C:113:PRO:C	1:D:36:ARG:HH11	1.59	1.07
1:C:115:ASP:N	1:D:36:ARG:CZ	2.18	1.07
1:D:113:PRO:C	1:E:36:ARG:HH11	1.59	1.06
1:A:36:ARG:HH11	1:G:113:PRO:C	1.59	1.06
1:A:113:PRO:C	1:B:36:ARG:HH11	1.59	1.06
1:B:113:PRO:C	1:C:36:ARG:HH11	1.59	1.06
1:F:113:PRO:C	1:G:36:ARG:HH11	1.59	1.06
1:E:113:PRO:C	1:F:36:ARG:HH11	1.59	1.06
1:A:115:ASP:N	1:B:36:ARG:CZ	2.18	1.06
1:A:113:PRO:C	1:B:36:ARG:NH1	2.09	1.06
1:B:113:PRO:C	1:C:36:ARG:NH1	2.10	1.06
1:A:36:ARG:CZ	1:G:115:ASP:N	2.18	1.06
1:F:115:ASP:N	1:G:36:ARG:CZ	2.18	1.05
1:A:36:ARG:NH1	1:G:113:PRO:C	2.10	1.05
1:D:115:ASP:N	1:E:36:ARG:CZ	2.18	1.05
1:F:113:PRO:C	1:G:36:ARG:NH1	2.10	1.05
1:C:113:PRO:C	1:D:36:ARG:NH1	2.10	1.05
1:E:115:ASP:N	1:F:36:ARG:CZ	2.18	1.05
1:E:113:PRO:C	1:F:36:ARG:NH1	2.10	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ASP:N	1:D:36:ARG:NH1	2.05	1.05
1:D:115:ASP:N	1:E:36:ARG:NH1	2.05	1.05
1:D:113:PRO:C	1:E:36:ARG:NH1	2.10	1.04
1:B:115:ASP:N	1:C:36:ARG:NH1	2.05	1.04
1:E:115:ASP:N	1:F:36:ARG:NH1	2.05	1.04
1:F:115:ASP:N	1:G:36:ARG:NH1	2.05	1.03
1:A:36:ARG:NH1	1:G:115:ASP:N	2.05	1.03
1:A:115:ASP:N	1:B:36:ARG:NH1	2.05	1.02
1:B:112:ASN:O	1:C:36:ARG:CZ	2.08	1.02
1:D:112:ASN:O	1:E:36:ARG:CZ	2.08	1.01
1:A:36:ARG:CZ	1:G:112:ASN:O	2.08	1.01
1:F:112:ASN:O	1:G:36:ARG:CZ	2.08	1.01
1:C:112:ASN:O	1:D:36:ARG:CZ	2.08	1.01
1:E:112:ASN:O	1:F:36:ARG:CZ	2.08	1.01
1:A:112:ASN:O	1:B:36:ARG:CZ	2.08	1.00
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.51	0.93
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.50	0.92
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.51	0.92
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.50	0.91
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.51	0.91
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.51	0.91
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.50	0.90
1:E:114:MET:N	1:F:36:ARG:CZ	2.38	0.87
1:D:114:MET:N	1:E:36:ARG:CZ	2.38	0.87
1:A:36:ARG:CZ	1:G:114:MET:N	2.38	0.87
1:F:114:MET:N	1:G:36:ARG:CZ	2.38	0.87
1:C:114:MET:N	1:D:36:ARG:CZ	2.38	0.86
1:B:114:MET:N	1:C:36:ARG:CZ	2.38	0.86
1:A:114:MET:N	1:B:36:ARG:CZ	2.38	0.86
1:A:49:ILE:HD11	1:G:513:LEU:HA	1.61	0.83
1:F:513:LEU:HA	1:G:49:ILE:HD11	1.61	0.83
1:E:513:LEU:HA	1:F:49:ILE:HD11	1.61	0.83
1:A:513:LEU:HA	1:B:49:ILE:HD11	1.61	0.82
1:D:513:LEU:HA	1:E:49:ILE:HD11	1.61	0.82
1:C:513:LEU:HA	1:D:49:ILE:HD11	1.61	0.82
1:B:513:LEU:HA	1:C:49:ILE:HD11	1.61	0.82
1:C:112:ASN:C	1:D:36:ARG:CZ	2.49	0.81
1:E:112:ASN:C	1:F:36:ARG:CZ	2.49	0.81
1:A:112:ASN:C	1:B:36:ARG:CZ	2.49	0.81
1:F:112:ASN:C	1:G:36:ARG:CZ	2.49	0.81
1:A:36:ARG:CZ	1:G:112:ASN:C	2.49	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ASN:C	1:E:36:ARG:CZ	2.49	0.80
1:A:183:LEU:O	1:A:382:GLY:HA3	1.82	0.80
1:B:183:LEU:O	1:B:382:GLY:HA3	1.82	0.80
1:F:183:LEU:O	1:F:382:GLY:HA3	1.82	0.80
1:C:183:LEU:O	1:C:382:GLY:HA3	1.82	0.80
1:D:183:LEU:O	1:D:382:GLY:HA3	1.82	0.80
1:B:112:ASN:C	1:C:36:ARG:CZ	2.49	0.79
1:B:114:MET:H	1:C:36:ARG:NE	1.80	0.79
1:G:183:LEU:O	1:G:382:GLY:HA3	1.82	0.79
1:D:114:MET:H	1:E:36:ARG:NE	1.80	0.79
1:E:114:MET:H	1:F:36:ARG:NE	1.81	0.79
1:E:116:LEU:N	1:F:36:ARG:NH1	2.05	0.79
1:E:183:LEU:O	1:E:382:GLY:HA3	1.82	0.79
1:A:36:ARG:NE	1:G:114:MET:H	1.80	0.79
1:A:113:PRO:CA	1:B:36:ARG:HH11	1.96	0.79
1:C:114:MET:H	1:D:36:ARG:NE	1.80	0.78
1:A:114:MET:H	1:B:36:ARG:NE	1.80	0.78
1:F:114:MET:H	1:G:36:ARG:NE	1.80	0.78
1:E:199:TYR:CD2	1:E:205:ILE:HD11	2.19	0.78
1:F:199:TYR:CD2	1:F:205:ILE:HD11	2.19	0.78
1:A:199:TYR:CD2	1:A:205:ILE:HD11	2.19	0.78
1:C:113:PRO:CA	1:D:36:ARG:HH11	1.96	0.78
1:E:115:ASP:HB2	1:F:36:ARG:HH22	1.49	0.78
1:A:135:SER:HA	1:A:412:VAL:HG12	1.66	0.78
1:G:199:TYR:CD2	1:G:205:ILE:HD11	2.19	0.78
1:B:199:TYR:CD2	1:B:205:ILE:HD11	2.19	0.78
1:D:115:ASP:HB2	1:E:36:ARG:HH22	1.49	0.78
1:D:113:PRO:CA	1:E:36:ARG:HH11	1.96	0.78
1:F:113:PRO:CA	1:G:36:ARG:HH11	1.96	0.78
1:F:115:ASP:HB2	1:G:36:ARG:HH22	1.49	0.78
1:B:135:SER:HA	1:B:412:VAL:HG12	1.66	0.78
1:D:199:TYR:CD2	1:D:205:ILE:HD11	2.19	0.77
1:G:135:SER:HA	1:G:412:VAL:HG12	1.66	0.77
1:B:113:PRO:CA	1:C:36:ARG:HH11	1.96	0.77
1:A:36:ARG:HH22	1:G:115:ASP:HB2	1.49	0.77
1:A:36:ARG:HH11	1:G:113:PRO:CA	1.96	0.77
1:E:113:PRO:CA	1:F:36:ARG:HH11	1.96	0.77
1:C:199:TYR:CD2	1:C:205:ILE:HD11	2.19	0.77
1:C:135:SER:HA	1:C:412:VAL:HG12	1.66	0.77
1:F:198:GLY:HA2	1:F:327:LYS:O	1.86	0.76
1:D:198:GLY:HA2	1:D:327:LYS:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ASP:HB2	1:C:36:ARG:HH22	1.49	0.76
1:G:198:GLY:HA2	1:G:327:LYS:O	1.86	0.76
1:F:135:SER:HA	1:F:412:VAL:HG12	1.66	0.76
1:C:115:ASP:HB2	1:D:36:ARG:HH22	1.49	0.76
1:D:135:SER:HA	1:D:412:VAL:HG12	1.66	0.76
1:D:115:ASP:H	1:E:36:ARG:NH1	1.84	0.75
1:C:198:GLY:HA2	1:C:327:LYS:O	1.86	0.75
1:D:116:LEU:N	1:E:36:ARG:NH1	2.05	0.75
1:E:135:SER:HA	1:E:412:VAL:HG12	1.66	0.75
1:A:115:ASP:HB2	1:B:36:ARG:HH22	1.49	0.75
1:A:198:GLY:HA2	1:A:327:LYS:O	1.86	0.75
1:C:115:ASP:H	1:D:36:ARG:NH1	1.84	0.75
1:B:115:ASP:H	1:C:36:ARG:NH1	1.84	0.75
1:B:198:GLY:HA2	1:B:327:LYS:O	1.86	0.74
1:E:198:GLY:HA2	1:E:327:LYS:O	1.86	0.74
1:A:36:ARG:CZ	1:A:36:ARG:NH1	2.51	0.74
1:B:521:VAL:HG21	1:C:59:GLU:HB3	1.70	0.74
1:A:30:THR:HG22	1:A:38:VAL:HG21	1.69	0.74
1:G:36:ARG:CZ	1:G:36:ARG:NH1	2.51	0.74
1:D:30:THR:HG22	1:D:38:VAL:HG21	1.69	0.74
1:A:36:ARG:NH1	1:G:115:ASP:H	1.84	0.73
1:F:521:VAL:HG21	1:G:59:GLU:HB3	1.70	0.73
1:G:30:THR:HG22	1:G:38:VAL:HG21	1.69	0.73
1:A:115:ASP:H	1:B:36:ARG:NH1	1.84	0.73
1:D:36:ARG:NH1	1:D:36:ARG:CZ	2.51	0.73
1:C:521:VAL:HG21	1:D:59:GLU:HB3	1.70	0.73
1:F:36:ARG:CZ	1:F:36:ARG:NH1	2.51	0.73
1:E:30:THR:HG22	1:E:38:VAL:HG21	1.69	0.73
1:B:36:ARG:NH1	1:B:36:ARG:CZ	2.51	0.73
1:A:36:ARG:NH1	1:G:116:LEU:N	2.05	0.73
1:B:30:THR:HG22	1:B:38:VAL:HG21	1.69	0.73
1:E:521:VAL:HG21	1:F:59:GLU:HB3	1.70	0.73
1:C:30:THR:HG22	1:C:38:VAL:HG21	1.69	0.73
1:A:521:VAL:HG21	1:B:59:GLU:HB3	1.70	0.73
1:C:36:ARG:CZ	1:C:36:ARG:NH1	2.51	0.73
1:F:30:THR:HG22	1:F:38:VAL:HG21	1.69	0.72
1:D:521:VAL:HG21	1:E:59:GLU:HB3	1.70	0.72
3:E:1526:PO4:P	2:E:1527:ATP:O1G	2.48	0.72
3:G:1525:PO4:P	2:G:1527:ATP:O1G	2.48	0.72
1:E:36:ARG:NH1	1:E:36:ARG:CZ	2.51	0.72
1:F:115:ASP:H	1:G:36:ARG:NH1	1.84	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1525:PO4:P	2:F:1527:ATP:O1G	2.48	0.72
1:A:59:GLU:HB3	1:G:521:VAL:HG21	1.70	0.72
2:D:1525:ATP:O1G	3:D:1526:PO4:P	2.48	0.72
2:C:1526:ATP:O1G	3:C:1527:PO4:P	2.48	0.71
2:A:1525:ATP:O1G	3:A:1526:PO4:P	2.48	0.71
1:L:181:THR:O	1:M:283:ASP:N	2.24	0.71
1:M:181:THR:O	1:N:283:ASP:N	2.24	0.71
1:E:115:ASP:H	1:F:36:ARG:NH2	1.86	0.71
1:E:115:ASP:H	1:F:36:ARG:NH1	1.84	0.71
2:B:1525:ATP:O1G	3:B:1526:PO4:P	2.48	0.71
2:B:1525:ATP:O1A	3:B:1526:PO4:P	2.49	0.71
1:D:115:ASP:H	1:E:36:ARG:NH2	1.86	0.71
2:D:1525:ATP:O1A	3:D:1526:PO4:P	2.49	0.71
1:I:181:THR:O	1:J:283:ASP:N	2.23	0.70
1:F:115:ASP:H	1:G:36:ARG:NH2	1.86	0.70
3:E:1526:PO4:P	2:E:1527:ATP:O1A	2.49	0.70
1:J:181:THR:O	1:K:283:ASP:N	2.24	0.70
3:G:1525:PO4:P	2:G:1527:ATP:O1A	2.49	0.70
2:C:1526:ATP:O1A	3:C:1527:PO4:P	2.49	0.70
3:F:1525:PO4:P	2:F:1527:ATP:O1A	2.49	0.70
1:K:181:THR:O	1:L:283:ASP:N	2.23	0.70
2:A:1525:ATP:O1A	3:A:1526:PO4:P	2.49	0.70
1:D:191:GLU:O	1:D:334:ASP:HA	1.92	0.70
1:C:115:ASP:H	1:D:36:ARG:NH2	1.86	0.70
1:C:191:GLU:O	1:C:334:ASP:HA	1.92	0.70
1:H:283:ASP:N	1:N:181:THR:O	2.24	0.70
1:B:116:LEU:N	1:C:36:ARG:NH1	2.05	0.69
1:A:36:ARG:NH2	1:G:115:ASP:H	1.86	0.69
1:E:191:GLU:O	1:E:334:ASP:HA	1.92	0.69
1:H:181:THR:O	1:I:283:ASP:N	2.24	0.69
1:C:116:LEU:N	1:D:36:ARG:NH1	2.05	0.69
1:B:115:ASP:H	1:C:36:ARG:NH2	1.86	0.69
1:A:115:ASP:H	1:B:36:ARG:NH2	1.86	0.69
1:F:191:GLU:O	1:F:334:ASP:HA	1.92	0.69
1:G:191:GLU:O	1:G:334:ASP:HA	1.92	0.69
1:B:191:GLU:O	1:B:334:ASP:HA	1.92	0.69
1:E:517:THR:HB	1:F:39:VAL:HB	1.76	0.68
1:A:191:GLU:O	1:A:334:ASP:HA	1.92	0.68
1:B:114:MET:H	1:C:36:ARG:CZ	2.05	0.68
1:F:517:THR:HB	1:G:39:VAL:HB	1.76	0.68
1:F:114:MET:H	1:G:36:ARG:CZ	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:THR:HB	1:E:39:VAL:HB	1.76	0.68
1:A:6:VAL:HG22	1:A:521:VAL:HG22	1.76	0.68
1:F:116:LEU:N	1:G:36:ARG:NH1	2.05	0.68
1:B:6:VAL:HG22	1:B:521:VAL:HG22	1.76	0.68
1:E:114:MET:H	1:F:36:ARG:CZ	2.05	0.67
1:C:6:VAL:HG22	1:C:521:VAL:HG22	1.76	0.67
1:A:36:ARG:CZ	1:G:114:MET:H	2.05	0.67
1:L:400:LEU:C	1:L:401:HIS:CA	2.63	0.67
1:B:517:THR:HB	1:C:39:VAL:HB	1.76	0.67
1:G:6:VAL:HG22	1:G:521:VAL:HG22	1.76	0.67
1:A:517:THR:HB	1:B:39:VAL:HB	1.76	0.66
1:A:116:LEU:N	1:B:36:ARG:NH1	2.05	0.66
1:C:517:THR:HB	1:D:39:VAL:HB	1.76	0.66
1:F:6:VAL:HG22	1:F:521:VAL:HG22	1.76	0.66
1:D:6:VAL:HG22	1:D:521:VAL:HG22	1.76	0.66
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.78	0.66
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.78	0.66
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.78	0.66
1:K:223:ALA:O	1:K:251:ALA:HA	1.96	0.66
1:A:39:VAL:HB	1:G:517:THR:HB	1.76	0.66
1:G:40:LEU:HD21	1:G:55:SER:HB3	1.78	0.66
1:I:223:ALA:O	1:I:251:ALA:HA	1.96	0.66
1:C:114:MET:H	1:D:36:ARG:CZ	2.05	0.66
1:E:6:VAL:HG22	1:E:521:VAL:HG22	1.76	0.66
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.78	0.66
1:A:40:LEU:HD21	1:A:55:SER:HB3	1.78	0.65
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.78	0.65
1:F:73:MET:HA	1:G:46:ALA:CB	2.26	0.65
1:D:114:MET:H	1:E:36:ARG:CZ	2.05	0.65
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.78	0.65
1:C:39:VAL:HG13	1:C:48:THR:O	1.97	0.65
1:B:73:MET:HA	1:C:46:ALA:HB2	1.78	0.65
1:M:223:ALA:O	1:M:251:ALA:HA	1.96	0.65
1:F:40:LEU:HD21	1:F:55:SER:HB3	1.78	0.65
1:B:73:MET:HA	1:C:46:ALA:CB	2.26	0.65
1:L:223:ALA:O	1:L:251:ALA:HA	1.96	0.65
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.78	0.65
1:J:223:ALA:O	1:J:251:ALA:HA	1.96	0.65
1:G:39:VAL:HG13	1:G:48:THR:O	1.97	0.65
1:F:39:VAL:HG13	1:F:48:THR:O	1.97	0.65
1:C:73:MET:HA	1:D:46:ALA:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG12	1:A:90:THR:CG2	2.27	0.65
1:B:40:LEU:HD21	1:B:55:SER:HB3	1.78	0.65
1:N:223:ALA:O	1:N:251:ALA:HA	1.96	0.65
1:D:73:MET:HA	1:E:46:ALA:CB	2.26	0.65
1:E:73:MET:HA	1:F:46:ALA:CB	2.26	0.65
1:A:46:ALA:CB	1:G:73:MET:HA	2.26	0.65
1:A:73:MET:HA	1:B:46:ALA:CB	2.26	0.65
1:A:73:MET:HA	1:B:46:ALA:HB2	1.79	0.65
1:H:223:ALA:O	1:H:251:ALA:HA	1.96	0.65
1:F:114:MET:HB2	1:G:36:ARG:HD2	1.79	0.64
1:E:39:VAL:HG13	1:E:48:THR:O	1.97	0.64
1:A:39:VAL:HG13	1:A:48:THR:O	1.97	0.64
1:C:73:MET:HA	1:D:46:ALA:CB	2.26	0.64
1:E:114:MET:HB2	1:F:36:ARG:HD2	1.79	0.64
1:B:27:VAL:HG12	1:B:90:THR:CG2	2.27	0.64
1:A:46:ALA:HB2	1:G:73:MET:HA	1.78	0.64
1:A:36:ARG:HD2	1:G:114:MET:HB2	1.79	0.64
1:D:40:LEU:HD21	1:D:55:SER:HB3	1.78	0.64
1:E:40:LEU:HD21	1:E:55:SER:HB3	1.78	0.64
1:D:73:MET:HA	1:E:46:ALA:HB2	1.79	0.64
1:A:39:VAL:HB	1:G:517:THR:CB	2.28	0.64
1:A:517:THR:CB	1:B:39:VAL:HB	2.28	0.64
1:C:40:LEU:HD21	1:C:55:SER:HB3	1.78	0.64
1:D:114:MET:HB2	1:E:36:ARG:HD2	1.79	0.64
1:D:39:VAL:HG13	1:D:48:THR:O	1.97	0.64
1:E:517:THR:CB	1:F:39:VAL:HB	2.28	0.63
1:F:73:MET:HA	1:G:46:ALA:HB2	1.79	0.63
1:E:73:MET:HA	1:F:46:ALA:HB2	1.79	0.63
1:A:114:MET:HB2	1:B:36:ARG:HD2	1.79	0.63
1:B:114:MET:HB2	1:C:36:ARG:HD2	1.79	0.63
1:F:517:THR:CB	1:G:39:VAL:HB	2.28	0.63
1:C:27:VAL:HG12	1:C:90:THR:CG2	2.27	0.63
1:B:39:VAL:HG13	1:B:48:THR:O	1.97	0.63
1:C:517:THR:HA	1:D:39:VAL:HG23	1.81	0.63
1:C:114:MET:HB2	1:D:36:ARG:HD2	1.79	0.63
1:A:114:MET:H	1:B:36:ARG:CD	2.12	0.63
1:D:114:MET:H	1:E:36:ARG:CD	2.12	0.63
1:A:39:VAL:HG23	1:G:517:THR:HA	1.81	0.63
1:E:114:MET:H	1:F:36:ARG:CD	2.12	0.63
1:B:517:THR:HA	1:C:39:VAL:HG23	1.81	0.63
1:F:114:MET:H	1:G:36:ARG:CD	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:THR:CB	1:C:39:VAL:HB	2.29	0.62
1:F:517:THR:HA	1:G:39:VAL:HG23	1.81	0.62
1:E:517:THR:HA	1:F:39:VAL:HG23	1.81	0.62
1:A:517:THR:HA	1:B:39:VAL:HG23	1.81	0.62
1:D:517:THR:CB	1:E:39:VAL:HB	2.28	0.62
1:B:114:MET:H	1:C:36:ARG:CD	2.12	0.62
1:B:31:LEU:HB3	1:B:90:THR:HG21	1.82	0.62
1:C:114:MET:H	1:D:36:ARG:CD	2.12	0.62
1:D:517:THR:HA	1:E:39:VAL:HG23	1.81	0.62
1:A:114:MET:H	1:B:36:ARG:CZ	2.05	0.62
1:D:30:THR:HG21	1:D:56:VAL:HG21	1.82	0.62
1:E:30:THR:HG21	1:E:56:VAL:HG21	1.82	0.62
1:A:521:VAL:H	1:B:41:ASP:HB3	1.65	0.62
1:C:31:LEU:HB3	1:C:90:THR:HG21	1.82	0.62
1:F:30:THR:HG21	1:F:56:VAL:HG21	1.82	0.62
1:C:517:THR:CB	1:D:39:VAL:HB	2.28	0.62
1:B:520:MET:HA	1:C:41:ASP:HB2	1.82	0.62
1:D:521:VAL:H	1:E:41:ASP:HB3	1.65	0.62
1:D:27:VAL:HG12	1:D:90:THR:CG2	2.27	0.62
1:B:521:VAL:H	1:C:41:ASP:HB3	1.65	0.62
1:A:41:ASP:HB3	1:G:521:VAL:H	1.65	0.62
1:A:31:LEU:HB3	1:A:90:THR:HG21	1.82	0.61
1:G:30:THR:HG21	1:G:56:VAL:HG21	1.82	0.61
1:A:520:MET:HA	1:B:41:ASP:HB2	1.82	0.61
1:F:27:VAL:HG12	1:F:90:THR:CG2	2.27	0.61
1:D:520:MET:HA	1:E:41:ASP:HB2	1.82	0.61
1:A:36:ARG:CD	1:G:114:MET:H	2.12	0.61
1:C:520:MET:HA	1:D:41:ASP:HB2	1.82	0.61
1:E:520:MET:HA	1:F:41:ASP:HB2	1.82	0.61
1:C:30:THR:HG21	1:C:56:VAL:HG21	1.82	0.61
1:D:31:LEU:HB3	1:D:90:THR:HG21	1.82	0.61
1:E:214:GLU:HA	1:E:323:VAL:O	2.01	0.61
1:A:30:THR:HG21	1:A:56:VAL:HG21	1.82	0.61
1:F:521:VAL:H	1:G:41:ASP:HB3	1.65	0.61
1:D:214:GLU:HA	1:D:323:VAL:O	2.01	0.61
1:F:520:MET:HA	1:G:41:ASP:HB2	1.82	0.61
1:A:41:ASP:HB2	1:G:520:MET:HA	1.82	0.61
1:G:214:GLU:HA	1:G:323:VAL:O	2.01	0.61
1:G:31:LEU:HB3	1:G:90:THR:HG21	1.82	0.61
1:E:521:VAL:H	1:F:41:ASP:HB3	1.65	0.61
1:C:214:GLU:HA	1:C:323:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:NH1	1:G:114:MET:N	2.49	0.61
1:F:31:LEU:HB3	1:F:90:THR:HG21	1.82	0.61
1:A:214:GLU:HA	1:A:323:VAL:O	2.00	0.61
1:F:214:GLU:HA	1:F:323:VAL:O	2.01	0.61
1:E:31:LEU:HB3	1:E:90:THR:HG21	1.82	0.60
1:C:521:VAL:H	1:D:41:ASP:HB3	1.65	0.60
1:B:214:GLU:HA	1:B:323:VAL:O	2.01	0.60
1:E:27:VAL:HG12	1:E:90:THR:CG2	2.27	0.60
1:B:114:MET:N	1:C:36:ARG:NH1	2.49	0.60
1:B:30:THR:HG21	1:B:56:VAL:HG21	1.82	0.60
1:D:114:MET:N	1:E:36:ARG:NH1	2.50	0.60
1:A:114:MET:N	1:B:36:ARG:NH1	2.49	0.60
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.84	0.60
1:E:114:MET:N	1:F:36:ARG:NH1	2.50	0.60
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.84	0.60
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.84	0.60
1:C:114:MET:N	1:D:36:ARG:NH1	2.49	0.60
1:G:40:LEU:HB3	1:G:59:GLU:HG3	1.84	0.60
1:G:27:VAL:HG12	1:G:90:THR:CG2	2.27	0.59
1:E:40:LEU:HB3	1:E:59:GLU:HG3	1.84	0.59
1:F:40:LEU:HB3	1:F:59:GLU:HG3	1.84	0.59
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.84	0.59
1:A:40:LEU:HB3	1:A:59:GLU:HG3	1.84	0.59
1:C:417:VAL:HG21	1:C:477:GLY:HA3	1.84	0.59
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.84	0.59
1:G:151:SER:HB3	1:G:399:ALA:HA	1.85	0.59
1:F:114:MET:N	1:G:36:ARG:NH1	2.49	0.59
1:B:417:VAL:HG21	1:B:477:GLY:HA3	1.84	0.59
1:D:40:LEU:HB3	1:D:59:GLU:HG3	1.84	0.59
1:B:40:LEU:HB3	1:B:59:GLU:HG3	1.84	0.59
1:L:400:LEU:CA	1:L:401:HIS:N	2.62	0.58
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.85	0.58
1:A:36:ARG:HH12	1:G:116:LEU:H	0.62	0.58
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.85	0.58
1:F:151:SER:HB3	1:F:399:ALA:HA	1.85	0.58
1:B:116:LEU:H	1:C:36:ARG:HH12	0.61	0.58
1:A:217:SER:HA	1:A:320:ALA:O	2.04	0.58
1:A:151:SER:HB3	1:A:399:ALA:HA	1.85	0.58
1:A:115:ASP:CB	1:B:36:ARG:HH22	2.15	0.58
1:C:40:LEU:HB3	1:C:59:GLU:HG3	1.84	0.58
1:B:217:SER:HA	1:B:320:ALA:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:SER:HA	1:C:320:ALA:O	2.04	0.58
1:G:217:SER:HA	1:G:320:ALA:O	2.04	0.58
1:D:116:LEU:H	1:E:36:ARG:HH12	0.61	0.58
1:G:151:SER:CB	1:G:399:ALA:HA	2.34	0.58
1:F:192:GLY:O	1:F:375:GLY:HA2	2.04	0.58
1:E:151:SER:CB	1:E:399:ALA:HA	2.34	0.58
1:E:151:SER:HB3	1:E:399:ALA:HA	1.85	0.58
1:B:240:VAL:HG11	1:B:247:LEU:HB2	1.85	0.58
1:D:151:SER:CB	1:D:399:ALA:HA	2.34	0.58
1:F:217:SER:HA	1:F:320:ALA:O	2.04	0.58
1:E:116:LEU:H	1:F:36:ARG:HH12	0.62	0.58
1:A:151:SER:CB	1:A:399:ALA:HA	2.34	0.58
1:G:192:GLY:O	1:G:375:GLY:HA2	2.04	0.58
1:E:240:VAL:HG11	1:E:247:LEU:HB2	1.85	0.58
1:G:240:VAL:HG11	1:G:247:LEU:HB2	1.85	0.57
1:F:240:VAL:HG11	1:F:247:LEU:HB2	1.85	0.57
1:E:217:SER:HA	1:E:320:ALA:O	2.04	0.57
1:D:217:SER:HA	1:D:320:ALA:O	2.04	0.57
1:F:115:ASP:CB	1:G:36:ARG:HH22	2.15	0.57
1:C:192:GLY:O	1:C:375:GLY:HA2	2.04	0.57
1:D:192:GLY:O	1:D:375:GLY:HA2	2.04	0.57
1:G:127:ALA:HB2	1:G:426:LEU:HD11	1.86	0.57
1:B:151:SER:HB3	1:B:399:ALA:HA	1.85	0.57
1:C:151:SER:CB	1:C:399:ALA:HA	2.34	0.57
1:B:192:GLY:O	1:B:375:GLY:HA2	2.04	0.57
1:E:115:ASP:CB	1:F:36:ARG:HH22	2.15	0.57
1:D:151:SER:HB3	1:D:399:ALA:HA	1.85	0.57
1:B:151:SER:CB	1:B:399:ALA:HA	2.34	0.57
1:E:192:GLY:O	1:E:375:GLY:HA2	2.04	0.57
1:A:192:GLY:O	1:A:375:GLY:HA2	2.04	0.57
1:F:127:ALA:HB2	1:F:426:LEU:HD11	1.87	0.57
1:D:115:ASP:CB	1:E:36:ARG:HH22	2.15	0.57
1:A:36:ARG:NH2	1:G:112:ASN:O	2.38	0.57
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.86	0.57
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.86	0.57
1:D:127:ALA:HB2	1:D:426:LEU:HD11	1.86	0.57
1:F:151:SER:CB	1:F:399:ALA:HA	2.34	0.57
1:C:151:SER:HB3	1:C:399:ALA:HA	1.85	0.57
1:A:240:VAL:HG11	1:A:247:LEU:HB2	1.85	0.57
1:E:127:ALA:HB2	1:E:426:LEU:HD11	1.87	0.57
1:A:36:ARG:HH22	1:G:115:ASP:CB	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ASN:O	1:B:36:ARG:NH2	2.38	0.57
1:F:39:VAL:HG21	1:F:49:ILE:CD1	2.35	0.57
1:E:112:ASN:O	1:F:36:ARG:NH2	2.38	0.56
1:E:39:VAL:HG21	1:E:49:ILE:CD1	2.35	0.56
1:A:127:ALA:HB2	1:A:426:LEU:HD11	1.87	0.56
1:D:212:ALA:HA	1:D:325:ILE:O	2.06	0.56
1:K:229:ASN:HA	1:K:258:ALA:HB3	1.87	0.56
1:E:212:ALA:HA	1:E:325:ILE:O	2.06	0.56
1:M:229:ASN:HA	1:M:258:ALA:HB3	1.88	0.56
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.86	0.56
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.86	0.56
1:N:229:ASN:HA	1:N:258:ALA:HB3	1.88	0.56
1:C:127:ALA:HB2	1:C:426:LEU:HD11	1.87	0.56
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.56
1:F:212:ALA:HA	1:F:325:ILE:O	2.06	0.56
1:L:229:ASN:HA	1:L:258:ALA:HB3	1.88	0.56
1:F:113:PRO:O	1:G:36:ARG:NH1	2.39	0.56
1:F:112:ASN:O	1:G:36:ARG:NH2	2.38	0.56
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.86	0.56
1:E:152:ALA:HB1	1:E:155:ASP:HB2	1.87	0.56
1:C:112:ASN:O	1:D:36:ARG:NH2	2.38	0.56
1:B:112:ASN:O	1:C:36:ARG:NH2	2.38	0.56
1:B:39:VAL:HG21	1:B:49:ILE:CD1	2.35	0.56
1:G:152:ALA:HB1	1:G:155:ASP:HB2	1.87	0.56
1:J:229:ASN:HA	1:J:258:ALA:HB3	1.87	0.56
1:D:152:ALA:HB1	1:D:155:ASP:HB2	1.87	0.56
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.86	0.56
1:A:113:PRO:O	1:B:36:ARG:NH1	2.39	0.56
1:C:115:ASP:CB	1:D:36:ARG:HH22	2.15	0.56
1:B:115:ASP:CB	1:C:36:ARG:HH22	2.15	0.56
1:D:39:VAL:HG21	1:D:49:ILE:CD1	2.35	0.56
1:A:152:ALA:HB1	1:A:155:ASP:HB2	1.87	0.56
1:B:127:ALA:HB2	1:B:426:LEU:HD11	1.86	0.56
1:C:113:PRO:O	1:D:36:ARG:NH1	2.39	0.56
1:D:112:ASN:C	1:E:36:ARG:NE	2.59	0.56
1:B:115:ASP:C	1:C:36:ARG:HH12	2.07	0.56
1:B:212:ALA:HA	1:B:325:ILE:O	2.05	0.56
1:A:212:ALA:HA	1:A:325:ILE:O	2.06	0.56
1:C:112:ASN:C	1:D:36:ARG:NE	2.59	0.56
1:B:113:PRO:O	1:C:36:ARG:NH1	2.39	0.56
1:A:39:VAL:HG21	1:A:49:ILE:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:39:VAL:HG21	1:G:49:ILE:CD1	2.35	0.56
1:B:152:ALA:HB1	1:B:155:ASP:HB2	1.87	0.56
1:B:112:ASN:C	1:C:36:ARG:NE	2.59	0.56
1:F:112:ASN:C	1:G:36:ARG:NE	2.59	0.56
1:C:212:ALA:HA	1:C:325:ILE:O	2.05	0.56
1:C:152:ALA:HB1	1:C:155:ASP:HB2	1.87	0.56
1:A:36:ARG:NE	1:G:112:ASN:C	2.59	0.55
1:A:36:ARG:NH1	1:G:113:PRO:O	2.39	0.55
1:E:113:PRO:O	1:F:36:ARG:NH1	2.39	0.55
1:H:229:ASN:HA	1:H:258:ALA:HB3	1.88	0.55
1:D:112:ASN:O	1:E:36:ARG:NH2	2.38	0.55
1:C:39:VAL:HG21	1:C:49:ILE:CD1	2.35	0.55
1:C:186:GLU:H	1:C:380:LYS:HB2	1.72	0.55
1:F:152:ALA:HB1	1:F:155:ASP:HB2	1.87	0.55
1:G:212:ALA:HA	1:G:325:ILE:O	2.06	0.55
1:A:112:ASN:C	1:B:36:ARG:NE	2.59	0.55
1:C:116:LEU:H	1:D:36:ARG:HH12	0.62	0.55
1:C:115:ASP:C	1:D:36:ARG:HH12	2.07	0.55
1:B:114:MET:CB	1:C:36:ARG:HD2	2.36	0.55
1:A:26:ALA:O	1:A:30:THR:HG23	2.07	0.55
1:C:114:MET:CB	1:D:36:ARG:HD2	2.37	0.55
1:D:114:MET:CB	1:E:36:ARG:HD2	2.36	0.55
1:E:112:ASN:C	1:F:36:ARG:NE	2.59	0.55
1:D:246:PRO:HB3	1:D:272:LYS:HB2	1.89	0.55
1:E:246:PRO:HB3	1:E:272:LYS:HB2	1.89	0.55
1:A:114:MET:CB	1:B:36:ARG:HD2	2.36	0.55
1:I:229:ASN:HA	1:I:258:ALA:HB3	1.88	0.55
1:G:26:ALA:O	1:G:30:THR:HG23	2.07	0.55
1:G:246:PRO:HB3	1:G:272:LYS:HB2	1.89	0.55
1:F:246:PRO:HB3	1:F:272:LYS:HB2	1.89	0.55
1:A:186:GLU:H	1:A:380:LYS:HB2	1.72	0.54
1:E:186:GLU:H	1:E:380:LYS:HB2	1.72	0.54
1:E:114:MET:CB	1:F:36:ARG:HD2	2.37	0.54
1:H:25:ASP:CG	1:H:28:LYS:HZ3	2.11	0.54
1:N:398:ALA:O	1:N:401:HIS:N	2.41	0.54
1:D:39:VAL:HG21	1:D:49:ILE:HG12	1.89	0.54
1:D:26:ALA:O	1:D:30:THR:HG23	2.07	0.54
1:B:26:ALA:O	1:B:30:THR:HG23	2.07	0.54
1:C:26:ALA:O	1:C:30:THR:HG23	2.07	0.54
1:G:186:GLU:H	1:G:380:LYS:HB2	1.72	0.54
1:A:246:PRO:HB3	1:A:272:LYS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:MET:CB	1:G:36:ARG:HD2	2.36	0.54
1:C:39:VAL:HG21	1:C:49:ILE:HG12	1.89	0.54
1:G:39:VAL:HG21	1:G:49:ILE:HG12	1.89	0.54
1:D:40:LEU:HD11	1:D:55:SER:HB3	1.90	0.54
1:B:186:GLU:H	1:B:380:LYS:HB2	1.72	0.54
1:C:218:PRO:HG2	1:C:320:ALA:HB3	1.90	0.54
1:A:36:ARG:HD2	1:G:114:MET:CB	2.36	0.54
1:F:39:VAL:HG21	1:F:49:ILE:HG12	1.89	0.54
1:E:26:ALA:O	1:E:30:THR:HG23	2.07	0.54
1:F:26:ALA:O	1:F:30:THR:HG23	2.07	0.54
1:J:25:ASP:CG	1:J:28:LYS:HZ3	2.11	0.54
1:N:25:ASP:CG	1:N:28:LYS:HZ3	2.11	0.54
1:C:246:PRO:HB3	1:C:272:LYS:HB2	1.89	0.54
1:A:218:PRO:HG2	1:A:320:ALA:HB3	1.90	0.54
1:G:218:PRO:HG2	1:G:320:ALA:HB3	1.90	0.54
1:B:39:VAL:HG21	1:B:49:ILE:HG12	1.89	0.54
1:E:39:VAL:HG21	1:E:49:ILE:HG12	1.89	0.54
1:F:186:GLU:H	1:F:380:LYS:HB2	1.72	0.54
1:B:218:PRO:HG2	1:B:320:ALA:HB3	1.90	0.54
1:E:115:ASP:C	1:F:36:ARG:HH12	2.07	0.54
1:C:40:LEU:HD11	1:C:55:SER:HB3	1.90	0.54
1:F:40:LEU:HD11	1:F:55:SER:HB3	1.90	0.54
1:E:40:LEU:HD11	1:E:55:SER:HB3	1.90	0.54
1:B:246:PRO:HB3	1:B:272:LYS:HB2	1.89	0.54
1:B:205:ILE:HD12	1:B:211:GLY:O	2.09	0.53
1:C:205:ILE:HD12	1:C:211:GLY:O	2.09	0.53
1:B:40:LEU:HD11	1:B:55:SER:HB3	1.90	0.53
1:D:218:PRO:HG2	1:D:320:ALA:HB3	1.90	0.53
1:D:113:PRO:O	1:E:36:ARG:NH1	2.39	0.53
1:E:31:LEU:CB	1:E:90:THR:HG21	2.39	0.53
1:D:186:GLU:H	1:D:380:LYS:HB2	1.72	0.53
1:L:25:ASP:CG	1:L:28:LYS:HZ3	2.11	0.53
1:D:31:LEU:CB	1:D:90:THR:HG21	2.39	0.53
1:G:39:VAL:HG13	1:G:48:THR:C	2.29	0.53
1:F:218:PRO:HG2	1:F:320:ALA:HB3	1.90	0.53
1:I:25:ASP:CG	1:I:28:LYS:HZ3	2.12	0.53
1:C:31:LEU:CB	1:C:90:THR:HG21	2.39	0.53
1:A:205:ILE:HD12	1:A:211:GLY:O	2.08	0.53
1:D:205:ILE:HD12	1:D:211:GLY:O	2.09	0.53
1:D:39:VAL:HG13	1:D:48:THR:C	2.29	0.53
1:F:31:LEU:CB	1:F:90:THR:HG21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:VAL:HG21	1:A:49:ILE:HG12	1.89	0.53
1:F:205:ILE:HD12	1:F:211:GLY:O	2.09	0.53
1:G:40:LEU:HD11	1:G:55:SER:HB3	1.90	0.53
1:K:25:ASP:CG	1:K:28:LYS:HZ3	2.12	0.53
1:C:113:PRO:CA	1:D:36:ARG:NH1	2.66	0.53
1:F:113:PRO:HA	1:G:36:ARG:HH11	1.73	0.53
1:E:39:VAL:HG13	1:E:48:THR:C	2.29	0.53
1:F:112:ASN:CB	1:G:36:ARG:HE	2.22	0.53
1:B:31:LEU:CB	1:B:90:THR:HG21	2.39	0.53
1:A:39:VAL:HG13	1:A:48:THR:C	2.29	0.53
1:B:239:ALA:HB1	1:B:314:LEU:HG	1.91	0.53
1:A:36:ARG:HE	1:G:112:ASN:CB	2.22	0.52
1:G:31:LEU:CB	1:G:90:THR:HG21	2.39	0.52
1:E:218:PRO:HG2	1:E:320:ALA:HB3	1.90	0.52
1:B:411:VAL:HB	1:B:494:LEU:HB3	1.92	0.52
1:C:239:ALA:HB1	1:C:314:LEU:HG	1.91	0.52
1:B:144:ILE:HG23	1:B:403:THR:CG2	2.40	0.52
1:C:144:ILE:HG23	1:C:403:THR:CG2	2.40	0.52
1:G:411:VAL:HB	1:G:494:LEU:HB3	1.92	0.52
1:A:239:ALA:HB1	1:A:314:LEU:HG	1.91	0.52
1:A:112:ASN:CB	1:B:36:ARG:HE	2.23	0.52
1:A:36:ARG:HH11	1:G:113:PRO:HA	1.73	0.52
1:E:113:PRO:HA	1:F:36:ARG:HH11	1.73	0.52
1:A:40:LEU:HD11	1:A:55:SER:HB3	1.90	0.52
1:D:247:LEU:O	1:D:273:VAL:HA	2.10	0.52
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.40	0.52
1:F:411:VAL:HB	1:F:494:LEU:HB3	1.92	0.52
1:C:142:LYS:H	1:C:142:LYS:HD2	1.75	0.52
1:F:39:VAL:HG13	1:F:48:THR:C	2.29	0.52
1:C:39:VAL:HG13	1:C:48:THR:C	2.29	0.52
1:A:247:LEU:O	1:A:273:VAL:HA	2.10	0.52
1:G:142:LYS:H	1:G:142:LYS:HD2	1.75	0.52
1:E:205:ILE:HD12	1:E:211:GLY:O	2.09	0.52
1:A:31:LEU:CB	1:A:90:THR:HG21	2.39	0.52
1:C:247:LEU:O	1:C:273:VAL:HA	2.10	0.52
1:G:247:LEU:O	1:G:273:VAL:HA	2.10	0.52
1:B:142:LYS:H	1:B:142:LYS:HD2	1.75	0.52
1:E:142:LYS:HD2	1:E:142:LYS:H	1.75	0.52
1:G:239:ALA:HB1	1:G:314:LEU:HG	1.92	0.52
1:B:39:VAL:HG13	1:B:48:THR:C	2.29	0.52
1:G:205:ILE:HD12	1:G:211:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:LEU:O	1:B:273:VAL:HA	2.10	0.52
1:F:247:LEU:O	1:F:273:VAL:HA	2.10	0.52
1:D:142:LYS:HD2	1:D:142:LYS:H	1.75	0.52
2:C:1526:ATP:O3B	3:C:1527:PO4:P	2.68	0.52
2:A:1525:ATP:O3B	3:A:1526:PO4:P	2.68	0.52
1:E:247:LEU:O	1:E:273:VAL:HA	2.10	0.52
1:C:411:VAL:HB	1:C:494:LEU:HB3	1.92	0.52
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.40	0.52
1:E:13:ARG:HG2	1:E:13:ARG:HH11	1.75	0.52
1:A:142:LYS:H	1:A:142:LYS:HD2	1.75	0.52
1:A:113:PRO:HA	1:B:36:ARG:HH11	1.73	0.52
1:E:112:ASN:CB	1:F:36:ARG:HE	2.22	0.52
3:E:1526:PO4:P	2:E:1527:ATP:O3B	2.68	0.52
1:D:113:PRO:HA	1:E:36:ARG:HH11	1.73	0.51
1:D:13:ARG:HH11	1:D:13:ARG:HG2	1.75	0.51
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.40	0.51
1:F:239:ALA:HB1	1:F:314:LEU:HG	1.91	0.51
1:D:106:ALA:HB3	1:D:116:LEU:HD21	1.92	0.51
1:B:113:PRO:HA	1:C:36:ARG:HH11	1.73	0.51
1:F:113:PRO:CA	1:G:36:ARG:NH1	2.66	0.51
1:F:251:ALA:HB3	1:F:254:VAL:HG23	1.93	0.51
1:A:13:ARG:HH11	1:A:13:ARG:HG2	1.75	0.51
1:D:239:ALA:HB1	1:D:314:LEU:HG	1.91	0.51
1:A:411:VAL:HB	1:A:494:LEU:HB3	1.91	0.51
1:E:106:ALA:HB3	1:E:116:LEU:HD21	1.93	0.51
3:F:1525:PO4:P	2:F:1527:ATP:O3B	2.68	0.51
1:A:149:THR:HA	1:A:152:ALA:HB3	1.92	0.51
1:B:251:ALA:HB3	1:B:254:VAL:HG23	1.92	0.51
1:D:251:ALA:HB3	1:D:254:VAL:HG23	1.92	0.51
1:F:13:ARG:HG2	1:F:13:ARG:HH11	1.75	0.51
1:C:112:ASN:CB	1:D:36:ARG:HE	2.22	0.51
1:B:112:ASN:CB	1:C:36:ARG:HE	2.22	0.51
1:C:13:ARG:HH11	1:C:13:ARG:HG2	1.75	0.51
1:C:113:PRO:HA	1:D:36:ARG:HH11	1.74	0.51
1:D:112:ASN:CB	1:E:36:ARG:HE	2.22	0.51
1:F:106:ALA:HB3	1:F:116:LEU:HD21	1.93	0.51
2:B:1525:ATP:O3B	3:B:1526:PO4:P	2.68	0.51
1:E:251:ALA:HB3	1:E:254:VAL:HG23	1.93	0.51
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.40	0.51
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.93	0.51
1:A:36:ARG:HH12	1:G:115:ASP:C	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:ALA:HB3	1:G:116:LEU:HD21	1.93	0.51
3:G:1525:PO4:P	2:G:1527:ATP:O3B	2.68	0.51
1:B:149:THR:HA	1:B:152:ALA:HB3	1.93	0.51
1:G:251:ALA:HB3	1:G:254:VAL:HG23	1.92	0.51
1:M:25:ASP:CG	1:M:28:LYS:HZ3	2.13	0.51
1:E:239:ALA:HB1	1:E:314:LEU:HG	1.91	0.51
1:E:213:VAL:HG13	1:E:325:ILE:HB	1.93	0.51
1:E:411:VAL:HB	1:E:494:LEU:HB3	1.92	0.51
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.40	0.51
1:B:106:ALA:HB3	1:B:116:LEU:HD21	1.93	0.51
2:D:1525:ATP:O3B	3:D:1526:PO4:P	2.68	0.51
1:D:411:VAL:HB	1:D:494:LEU:HB3	1.92	0.51
1:E:39:VAL:CG2	1:E:49:ILE:HD13	2.41	0.51
1:F:142:LYS:H	1:F:142:LYS:HD2	1.75	0.51
1:A:39:VAL:CG2	1:A:49:ILE:HD13	2.41	0.50
1:G:39:VAL:CG2	1:G:49:ILE:HD13	2.42	0.50
1:F:39:VAL:CG2	1:F:49:ILE:HD13	2.41	0.50
1:D:39:VAL:CG2	1:D:49:ILE:HD13	2.41	0.50
1:C:213:VAL:HG13	1:C:325:ILE:HB	1.94	0.50
1:F:213:VAL:HG13	1:F:325:ILE:HB	1.93	0.50
1:B:213:VAL:HG13	1:B:325:ILE:HB	1.93	0.50
1:E:34:LYS:HE2	1:E:458:CYS:HA	1.93	0.50
1:F:34:LYS:HE2	1:F:458:CYS:HA	1.94	0.50
1:G:149:THR:HA	1:G:152:ALA:HB3	1.93	0.50
1:C:106:ALA:HB3	1:C:116:LEU:HD21	1.92	0.50
1:B:39:VAL:CG2	1:B:49:ILE:HD13	2.41	0.50
1:C:39:VAL:CG2	1:C:49:ILE:HD13	2.42	0.50
1:D:213:VAL:HG13	1:D:325:ILE:HB	1.94	0.50
1:G:34:LYS:HE2	1:G:458:CYS:HA	1.94	0.50
1:D:113:PRO:CA	1:E:36:ARG:NH1	2.66	0.50
1:N:400:LEU:C	1:N:401:HIS:CA	2.77	0.50
1:E:149:THR:HA	1:E:152:ALA:HB3	1.93	0.50
1:C:149:THR:HA	1:C:152:ALA:HB3	1.93	0.50
1:E:113:PRO:CA	1:F:36:ARG:NH1	2.66	0.49
1:A:213:VAL:HG13	1:A:325:ILE:HB	1.94	0.49
1:G:213:VAL:HG13	1:G:325:ILE:HB	1.93	0.49
1:F:149:THR:HA	1:F:152:ALA:HB3	1.93	0.49
1:A:34:LYS:HE2	1:A:458:CYS:HA	1.94	0.49
1:D:149:THR:HA	1:D:152:ALA:HB3	1.93	0.49
1:G:13:ARG:HH11	1:G:13:ARG:HG2	1.75	0.49
1:D:34:LYS:HE2	1:D:458:CYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:HH11	1:B:13:ARG:HG2	1.75	0.49
1:C:251:ALA:HB3	1:C:254:VAL:HG23	1.93	0.49
1:E:172:GLU:H	1:E:172:GLU:CD	2.16	0.49
1:E:138:CYS:HA	1:E:411:VAL:HG22	1.94	0.49
1:G:6:VAL:HG13	1:G:521:VAL:HG22	1.95	0.49
1:F:6:VAL:HG13	1:F:521:VAL:HG22	1.95	0.49
1:F:138:CYS:HA	1:F:411:VAL:HG22	1.95	0.49
1:F:114:MET:CA	1:G:36:ARG:CZ	2.91	0.49
1:A:36:ARG:NH1	1:G:113:PRO:CA	2.66	0.49
1:A:251:ALA:HB3	1:A:254:VAL:HG23	1.93	0.49
1:B:114:MET:CA	1:C:36:ARG:CZ	2.91	0.49
1:A:6:VAL:HG13	1:A:521:VAL:HG22	1.95	0.49
1:A:36:ARG:CZ	1:G:114:MET:CA	2.91	0.49
1:G:39:VAL:HG21	1:G:49:ILE:HD13	1.95	0.49
1:F:39:VAL:HG21	1:F:49:ILE:HD13	1.95	0.49
1:C:106:ALA:CB	1:C:116:LEU:HD21	2.43	0.48
1:E:517:THR:HA	1:F:39:VAL:CG2	2.43	0.48
1:G:138:CYS:HA	1:G:411:VAL:HG22	1.94	0.48
1:A:114:MET:CA	1:B:36:ARG:CZ	2.91	0.48
1:A:39:VAL:HG21	1:A:49:ILE:HD13	1.95	0.48
1:B:39:VAL:HG21	1:B:49:ILE:HD13	1.95	0.48
1:D:517:THR:HA	1:E:39:VAL:CG2	2.43	0.48
1:B:6:VAL:HG13	1:B:521:VAL:HG22	1.95	0.48
1:C:34:LYS:HE2	1:C:458:CYS:HA	1.94	0.48
1:E:39:VAL:HG21	1:E:49:ILE:HD13	1.95	0.48
1:E:6:VAL:HG13	1:E:521:VAL:HG22	1.95	0.48
1:B:34:LYS:HE2	1:B:458:CYS:HA	1.94	0.48
1:B:106:ALA:CB	1:B:116:LEU:HD21	2.43	0.48
1:D:106:ALA:CB	1:D:116:LEU:HD21	2.43	0.48
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.35	0.48
1:B:517:THR:HA	1:C:39:VAL:CG2	2.43	0.48
1:C:39:VAL:HG21	1:C:49:ILE:HD13	1.95	0.48
1:C:517:THR:HA	1:D:39:VAL:CG2	2.43	0.48
1:D:39:VAL:HG21	1:D:49:ILE:HD13	1.95	0.48
1:B:30:THR:CG2	1:B:38:VAL:HG21	2.42	0.48
1:B:138:CYS:HA	1:B:411:VAL:HG22	1.95	0.48
1:D:172:GLU:H	1:D:172:GLU:CD	2.16	0.48
1:F:106:ALA:CB	1:F:116:LEU:HD21	2.43	0.48
1:F:116:LEU:H	1:G:36:ARG:HH12	0.62	0.48
1:A:39:VAL:CG2	1:G:517:THR:HA	2.43	0.48
1:C:138:CYS:HA	1:C:411:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:ALA:CB	1:G:116:LEU:HD21	2.43	0.48
1:C:112:ASN:CG	1:D:36:ARG:HE	2.18	0.48
1:D:114:MET:CA	1:E:36:ARG:CZ	2.91	0.48
1:F:517:THR:HA	1:G:39:VAL:CG2	2.43	0.48
1:D:112:ASN:CG	1:E:36:ARG:HE	2.18	0.48
1:B:39:VAL:HG21	1:B:49:ILE:CG1	2.44	0.48
1:C:6:VAL:HG13	1:C:521:VAL:HG22	1.95	0.48
1:D:115:ASP:CA	1:E:36:ARG:NH1	2.77	0.47
1:B:112:ASN:CG	1:C:36:ARG:HE	2.18	0.47
1:B:172:GLU:CD	1:B:172:GLU:H	2.16	0.47
1:C:114:MET:CA	1:D:36:ARG:CZ	2.91	0.47
1:F:115:ASP:CA	1:G:36:ARG:NH1	2.77	0.47
1:E:112:ASN:CG	1:F:36:ARG:HE	2.17	0.47
1:C:39:VAL:HG21	1:C:49:ILE:CG1	2.44	0.47
1:A:138:CYS:HA	1:A:411:VAL:HG22	1.94	0.47
1:A:172:GLU:CD	1:A:172:GLU:H	2.16	0.47
1:A:112:ASN:CG	1:B:36:ARG:HE	2.18	0.47
1:L:326:ASN:HD22	1:L:327:LYS:HD2	1.80	0.47
1:E:106:ALA:CB	1:E:116:LEU:HD21	2.43	0.47
1:E:114:MET:CA	1:F:36:ARG:CZ	2.91	0.47
1:D:6:VAL:HG13	1:D:521:VAL:HG22	1.95	0.47
1:A:240:VAL:HG21	1:A:247:LEU:HD13	1.97	0.47
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.97	0.47
1:A:113:PRO:CA	1:B:36:ARG:NH1	2.66	0.47
1:E:144:ILE:HG23	1:E:403:THR:HG21	1.97	0.47
1:D:138:CYS:HA	1:D:411:VAL:HG22	1.95	0.47
1:H:326:ASN:HD22	1:H:327:LYS:HD2	1.80	0.47
1:A:106:ALA:CB	1:A:116:LEU:HD21	2.43	0.47
1:A:36:ARG:HE	1:G:112:ASN:CG	2.17	0.47
1:J:326:ASN:HD22	1:J:327:LYS:HD2	1.80	0.47
1:D:115:ASP:C	1:E:36:ARG:HH12	2.06	0.47
1:B:114:MET:C	1:C:36:ARG:NH1	2.67	0.47
1:F:112:ASN:CG	1:G:36:ARG:HE	2.18	0.47
1:F:115:ASP:C	1:G:36:ARG:HH12	2.07	0.47
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.35	0.47
1:B:240:VAL:HG21	1:B:247:LEU:HD13	1.97	0.47
1:G:196:ASP:HA	1:G:329:THR:HA	1.97	0.47
1:A:196:ASP:HA	1:A:329:THR:HA	1.97	0.47
1:N:326:ASN:HD22	1:N:327:LYS:HD2	1.79	0.47
1:J:320:ALA:HA	1:J:334:ASP:O	2.15	0.47
1:M:320:ALA:HA	1:M:334:ASP:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:326:ASN:HD22	1:I:327:LYS:HD2	1.80	0.47
1:C:196:ASP:HA	1:C:329:THR:HA	1.97	0.47
1:K:320:ALA:HA	1:K:334:ASP:O	2.15	0.47
1:G:172:GLU:H	1:G:172:GLU:CD	2.16	0.47
1:C:144:ILE:HG23	1:C:403:THR:HG21	1.97	0.47
1:E:427:ALA:HA	1:E:444:LEU:CD1	2.45	0.47
1:M:326:ASN:HD22	1:M:327:LYS:HD2	1.80	0.47
1:A:30:THR:CG2	1:A:38:VAL:HG21	2.42	0.47
1:F:144:ILE:HG23	1:F:403:THR:HG21	1.97	0.47
1:I:320:ALA:HA	1:I:334:ASP:O	2.15	0.47
1:B:196:ASP:HA	1:B:329:THR:HA	1.97	0.47
1:N:320:ALA:HA	1:N:334:ASP:O	2.15	0.47
1:L:320:ALA:HA	1:L:334:ASP:O	2.15	0.47
1:G:39:VAL:HG21	1:G:49:ILE:CG1	2.44	0.47
1:G:240:VAL:HG21	1:G:247:LEU:HD13	1.97	0.47
1:F:196:ASP:HA	1:F:329:THR:HA	1.97	0.47
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.45	0.47
1:F:172:GLU:CD	1:F:172:GLU:H	2.16	0.47
1:H:320:ALA:HA	1:H:334:ASP:O	2.15	0.47
1:E:39:VAL:HG21	1:E:49:ILE:CG1	2.44	0.46
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.97	0.46
1:E:356:ALA:HB1	1:E:361:ASP:HB2	1.97	0.46
1:N:479:ASN:O	1:N:483:GLU:N	2.49	0.46
1:D:427:ALA:HA	1:D:444:LEU:CD1	2.45	0.46
1:D:356:ALA:HB1	1:D:361:ASP:HB2	1.97	0.46
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.46	0.46
1:L:183:LEU:HA	1:L:383:ALA:O	2.15	0.46
1:K:183:LEU:HA	1:K:383:ALA:O	2.15	0.46
1:G:356:ALA:HB1	1:G:361:ASP:HB2	1.97	0.46
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.46	0.46
1:A:152:ALA:HB1	1:A:155:ASP:CB	2.45	0.46
1:A:144:ILE:HG23	1:A:403:THR:HG21	1.97	0.46
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.46	0.46
1:F:356:ALA:HB1	1:F:361:ASP:HB2	1.97	0.46
1:A:356:ALA:HB1	1:A:361:ASP:HB2	1.97	0.46
1:H:183:LEU:HA	1:H:383:ALA:O	2.15	0.46
1:F:114:MET:C	1:G:36:ARG:NH1	2.67	0.46
1:A:39:VAL:HG21	1:A:49:ILE:CG1	2.44	0.46
1:D:39:VAL:HG21	1:D:49:ILE:CG1	2.44	0.46
1:G:152:ALA:HB1	1:G:155:ASP:CB	2.46	0.46
1:A:120:ILE:O	1:A:124:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ILE:O	1:B:124:VAL:HG23	2.16	0.46
1:J:183:LEU:HA	1:J:383:ALA:O	2.15	0.46
1:M:183:LEU:HA	1:M:383:ALA:O	2.16	0.46
1:B:427:ALA:HA	1:B:444:LEU:CD1	2.45	0.46
1:E:120:ILE:O	1:E:124:VAL:HG23	2.16	0.46
1:D:517:THR:HA	1:E:39:VAL:CB	2.46	0.46
1:G:120:ILE:O	1:G:124:VAL:HG23	2.16	0.46
1:D:124:VAL:HG21	1:D:508:ALA:CB	2.45	0.46
1:D:196:ASP:HA	1:D:329:THR:HA	1.97	0.46
1:B:356:ALA:HB1	1:B:361:ASP:HB2	1.98	0.46
1:K:326:ASN:HD22	1:K:327:LYS:HD2	1.80	0.46
1:C:356:ALA:HB1	1:C:361:ASP:HB2	1.97	0.46
1:B:113:PRO:CA	1:C:36:ARG:NH1	2.66	0.46
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.98	0.46
1:D:139:SER:HB3	1:D:143:ALA:HB2	1.98	0.46
1:F:120:ILE:O	1:F:124:VAL:HG23	2.16	0.46
1:C:172:GLU:H	1:C:172:GLU:CD	2.16	0.46
1:E:517:THR:HA	1:F:39:VAL:CB	2.46	0.46
1:F:39:VAL:HG21	1:F:49:ILE:CG1	2.44	0.46
1:C:240:VAL:HG21	1:C:247:LEU:HD13	1.97	0.46
1:B:152:ALA:HB1	1:B:155:ASP:CB	2.45	0.46
1:J:246:PRO:HB3	1:J:272:LYS:HB2	1.98	0.46
1:M:479:ASN:O	1:M:483:GLU:N	2.48	0.46
1:K:414:GLY:N	1:K:494:LEU:HA	2.31	0.46
1:N:183:LEU:HA	1:N:383:ALA:O	2.16	0.46
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.98	0.46
1:B:144:ILE:HG23	1:B:403:THR:HG21	1.97	0.46
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.45	0.46
1:H:246:PRO:HB3	1:H:272:LYS:HB2	1.98	0.46
1:I:246:PRO:HB3	1:I:272:LYS:HB2	1.98	0.46
1:C:427:ALA:HA	1:C:444:LEU:CD1	2.45	0.46
1:E:139:SER:HB3	1:E:143:ALA:HB2	1.98	0.46
1:C:111:MET:O	1:C:113:PRO:HD3	2.16	0.46
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.35	0.46
1:F:517:THR:HA	1:G:39:VAL:CB	2.46	0.46
1:A:517:THR:HA	1:B:39:VAL:CB	2.46	0.46
1:F:240:VAL:HG21	1:F:247:LEU:HD13	1.97	0.46
1:F:152:ALA:HB1	1:F:155:ASP:CB	2.45	0.46
1:G:427:ALA:HA	1:G:444:LEU:CD1	2.45	0.46
1:E:196:ASP:HA	1:E:329:THR:HA	1.97	0.46
1:K:246:PRO:HB3	1:K:272:LYS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.98	0.46
1:A:115:ASP:CA	1:B:36:ARG:NH1	2.77	0.46
1:C:114:MET:C	1:D:36:ARG:NH1	2.67	0.46
1:C:115:ASP:CA	1:D:36:ARG:NH1	2.77	0.46
1:A:36:ARG:NH1	1:G:114:MET:C	2.67	0.46
1:A:36:ARG:NH1	1:G:115:ASP:CA	2.77	0.46
1:A:39:VAL:CB	1:G:517:THR:HA	2.46	0.46
1:A:517:THR:HA	1:B:39:VAL:CG2	2.43	0.46
1:C:517:THR:HA	1:D:39:VAL:CB	2.46	0.46
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.46	0.46
1:M:246:PRO:HB3	1:M:272:LYS:HB2	1.98	0.46
1:G:287:ALA:HB1	1:G:368:ARG:CZ	2.46	0.46
1:N:246:PRO:HB3	1:N:272:LYS:HB2	1.98	0.46
1:F:111:MET:O	1:F:113:PRO:HD3	2.17	0.45
1:F:13:ARG:HH21	1:F:518:GLU:CD	2.20	0.45
1:D:120:ILE:O	1:D:124:VAL:HG23	2.16	0.45
1:C:427:ALA:HA	1:C:444:LEU:HD11	1.98	0.45
1:L:246:PRO:HB3	1:L:272:LYS:HB2	1.98	0.45
1:C:139:SER:HB3	1:C:143:ALA:HB2	1.98	0.45
1:D:114:MET:C	1:E:36:ARG:NH1	2.67	0.45
1:G:111:MET:O	1:G:113:PRO:HD3	2.16	0.45
1:C:31:LEU:HA	3:C:1527:PO4:P	2.56	0.45
1:G:30:THR:CG2	1:G:38:VAL:HG21	2.42	0.45
1:B:427:ALA:HA	1:B:444:LEU:HD11	1.99	0.45
1:I:414:GLY:N	1:I:494:LEU:HA	2.32	0.45
1:N:414:GLY:N	1:N:494:LEU:HA	2.31	0.45
1:F:287:ALA:HB1	1:F:368:ARG:CZ	2.47	0.45
1:A:427:ALA:HA	1:A:444:LEU:CD1	2.45	0.45
1:C:287:ALA:HB1	1:C:368:ARG:CZ	2.46	0.45
1:F:427:ALA:HA	1:F:444:LEU:CD1	2.45	0.45
1:F:427:ALA:HA	1:F:444:LEU:HD11	1.99	0.45
1:B:139:SER:HB3	1:B:143:ALA:HB2	1.98	0.45
1:H:414:GLY:N	1:H:494:LEU:HA	2.31	0.45
1:A:287:ALA:HB1	1:A:368:ARG:CZ	2.46	0.45
1:B:287:ALA:HB1	1:B:368:ARG:CZ	2.47	0.45
1:M:414:GLY:N	1:M:494:LEU:HA	2.31	0.45
1:D:111:MET:O	1:D:113:PRO:HD3	2.16	0.45
1:A:31:LEU:HA	3:A:1526:PO4:P	2.57	0.45
1:G:31:LEU:HA	3:G:1525:PO4:P	2.57	0.45
1:D:13:ARG:HH21	1:D:518:GLU:CD	2.20	0.45
1:A:13:ARG:HH21	1:A:518:GLU:CD	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:ALA:HA	1:E:444:LEU:HD11	1.99	0.45
1:D:427:ALA:HA	1:D:444:LEU:HD11	1.99	0.45
1:C:120:ILE:O	1:C:124:VAL:HG23	2.16	0.45
1:J:479:ASN:O	1:J:483:GLU:N	2.48	0.45
1:E:287:ALA:HB1	1:E:368:ARG:CZ	2.46	0.45
1:J:149:THR:CG2	1:J:156:GLU:HA	2.47	0.45
1:D:287:ALA:HB1	1:D:368:ARG:CZ	2.47	0.45
1:L:149:THR:CG2	1:L:156:GLU:HA	2.47	0.45
1:A:112:ASN:HA	1:A:113:PRO:HD2	1.74	0.45
1:A:111:MET:O	1:A:113:PRO:HD3	2.16	0.45
1:B:115:ASP:CA	1:C:36:ARG:NH1	2.77	0.45
1:A:127:ALA:CB	1:A:426:LEU:HD11	2.47	0.45
1:M:217:SER:HA	1:M:320:ALA:O	2.17	0.45
1:A:427:ALA:HA	1:A:444:LEU:HD11	1.99	0.45
1:F:383:ALA:HB3	1:F:389:MET:HB2	1.98	0.45
1:C:349:ILE:HG22	1:C:369:VAL:HG13	1.98	0.45
1:K:149:THR:CG2	1:K:156:GLU:HA	2.47	0.45
1:M:284:ARG:HG3	1:M:284:ARG:HH11	1.81	0.45
1:E:115:ASP:CA	1:F:36:ARG:NH1	2.77	0.45
1:G:127:ALA:CB	1:G:426:LEU:HD11	2.46	0.45
1:G:427:ALA:HA	1:G:444:LEU:HD11	1.99	0.45
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.98	0.45
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.98	0.45
1:F:139:SER:HB3	1:F:143:ALA:HB2	1.98	0.45
1:I:284:ARG:HH11	1:I:284:ARG:HG3	1.81	0.45
1:I:479:ASN:O	1:I:483:GLU:N	2.48	0.45
1:D:31:LEU:HA	3:D:1526:PO4:P	2.56	0.45
1:B:31:LEU:HA	3:B:1526:PO4:P	2.56	0.45
1:D:152:ALA:HB1	1:D:155:ASP:CB	2.46	0.45
1:C:13:ARG:HH21	1:C:518:GLU:CD	2.20	0.45
1:N:217:SER:HA	1:N:320:ALA:O	2.17	0.45
1:K:479:ASN:O	1:K:483:GLU:N	2.49	0.45
1:I:149:THR:CG2	1:I:156:GLU:HA	2.46	0.45
1:I:183:LEU:HA	1:I:383:ALA:O	2.15	0.45
1:J:284:ARG:HH11	1:J:284:ARG:HG3	1.81	0.45
1:N:284:ARG:HH11	1:N:284:ARG:HG3	1.81	0.45
1:A:114:MET:C	1:B:36:ARG:NH1	2.67	0.45
1:F:30:THR:CG2	1:F:38:VAL:HG21	2.42	0.45
1:E:127:ALA:CB	1:E:426:LEU:HD11	2.47	0.45
1:E:152:ALA:HB1	1:E:155:ASP:CB	2.45	0.45
1:E:13:ARG:HH21	1:E:518:GLU:CD	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:217:SER:HA	1:I:320:ALA:O	2.17	0.45
1:H:149:THR:CG2	1:H:156:GLU:HA	2.46	0.45
1:F:406:ALA:HB2	1:F:496:PRO:HG3	1.99	0.45
1:D:240:VAL:HG21	1:D:247:LEU:HD13	1.97	0.45
1:C:152:ALA:HB1	1:C:155:ASP:CB	2.45	0.45
1:J:217:SER:HA	1:J:320:ALA:O	2.17	0.45
1:B:349:ILE:HG22	1:B:369:VAL:HG13	1.99	0.45
1:D:349:ILE:HG22	1:D:369:VAL:HG13	1.99	0.45
1:B:127:ALA:CB	1:B:426:LEU:HD11	2.46	0.45
1:G:406:ALA:HB2	1:G:496:PRO:HG3	1.99	0.45
1:K:284:ARG:HG3	1:K:284:ARG:HH11	1.81	0.45
1:B:111:MET:O	1:B:113:PRO:HD3	2.17	0.44
1:B:517:THR:HA	1:C:39:VAL:CB	2.46	0.44
1:E:240:VAL:HG21	1:E:247:LEU:HD13	1.97	0.44
1:A:139:SER:HB3	1:A:143:ALA:HB2	1.98	0.44
1:H:217:SER:HA	1:H:320:ALA:O	2.17	0.44
1:F:256:GLY:O	1:F:260:ALA:HB3	2.18	0.44
1:A:349:ILE:HG22	1:A:369:VAL:HG13	1.99	0.44
1:J:414:GLY:N	1:J:494:LEU:HA	2.31	0.44
1:L:414:GLY:N	1:L:494:LEU:HA	2.31	0.44
1:M:149:THR:CG2	1:M:156:GLU:HA	2.46	0.44
1:E:417:VAL:HG13	1:E:476:TYR:O	2.18	0.44
1:J:191:GLU:O	1:J:334:ASP:HA	2.18	0.44
1:E:349:ILE:HG22	1:E:369:VAL:HG13	1.98	0.44
1:A:256:GLY:O	1:A:260:ALA:HB3	2.18	0.44
1:N:149:THR:CG2	1:N:156:GLU:HA	2.47	0.44
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.35	0.44
1:D:521:VAL:HG21	1:E:59:GLU:CB	2.46	0.44
1:B:440:ILE:O	1:B:444:LEU:HG	2.18	0.44
1:M:417:VAL:HA	1:M:420:ILE:HG22	2.00	0.44
1:N:417:VAL:HA	1:N:420:ILE:HG22	2.00	0.44
1:H:8:PHE:HA	1:H:518:GLU:O	2.18	0.44
1:K:230:ILE:HG23	1:K:259:LEU:HD12	2.00	0.44
1:L:8:PHE:HA	1:L:518:GLU:O	2.18	0.44
1:B:115:ASP:CA	1:C:36:ARG:HH12	2.30	0.44
1:E:111:MET:O	1:E:113:PRO:HD3	2.17	0.44
1:F:521:VAL:N	1:G:41:ASP:HB3	2.32	0.44
1:F:417:VAL:HG13	1:F:476:TYR:O	2.18	0.44
1:G:417:VAL:HG13	1:G:476:TYR:O	2.18	0.44
1:F:127:ALA:CB	1:F:426:LEU:HD11	2.46	0.44
1:G:13:ARG:HH21	1:G:518:GLU:CD	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:ILE:O	1:C:444:LEU:HG	2.18	0.44
1:L:230:ILE:HG23	1:L:259:LEU:HD12	2.00	0.44
1:H:479:ASN:O	1:H:483:GLU:N	2.48	0.44
1:F:349:ILE:HG22	1:F:369:VAL:HG13	1.98	0.44
1:N:230:ILE:HG23	1:N:259:LEU:HD12	2.00	0.44
1:M:8:PHE:HA	1:M:518:GLU:O	2.18	0.44
1:D:256:GLY:O	1:D:260:ALA:HB3	2.18	0.44
1:N:8:PHE:HA	1:N:518:GLU:O	2.18	0.44
1:L:284:ARG:HG3	1:L:284:ARG:HH11	1.81	0.44
1:H:284:ARG:HG3	1:H:284:ARG:HH11	1.81	0.44
1:G:139:SER:HB3	1:G:143:ALA:HB2	1.98	0.44
1:E:90:THR:HG22	1:E:94:VAL:HG23	2.00	0.44
1:F:31:LEU:HA	3:F:1525:PO4:P	2.56	0.44
1:B:412:VAL:HG22	1:B:495:ASP:O	2.18	0.44
1:D:417:VAL:HG13	1:D:476:TYR:O	2.18	0.44
1:I:191:GLU:O	1:I:334:ASP:HA	2.18	0.44
1:A:440:ILE:O	1:A:444:LEU:HG	2.18	0.44
1:G:349:ILE:HG22	1:G:369:VAL:HG13	1.99	0.44
1:E:406:ALA:HB2	1:E:496:PRO:HG3	1.99	0.44
1:K:8:PHE:HA	1:K:518:GLU:O	2.18	0.44
1:A:115:ASP:CA	1:B:36:ARG:HH12	2.31	0.44
1:E:31:LEU:HA	3:E:1526:PO4:P	2.57	0.44
1:A:90:THR:HG22	1:A:94:VAL:HG23	2.00	0.44
1:B:90:THR:HG22	1:B:94:VAL:HG23	2.00	0.44
1:A:412:VAL:HG22	1:A:495:ASP:O	2.18	0.44
1:E:30:THR:CG2	1:E:38:VAL:HG21	2.42	0.44
1:D:127:ALA:CB	1:D:426:LEU:HD11	2.47	0.44
1:B:13:ARG:HH21	1:B:518:GLU:CD	2.20	0.44
1:F:440:ILE:O	1:F:444:LEU:HG	2.18	0.44
1:D:279:PRO:HG3	1:D:292:ILE:HD11	2.00	0.44
1:J:8:PHE:HA	1:J:518:GLU:O	2.18	0.44
1:L:479:ASN:O	1:L:483:GLU:N	2.48	0.44
1:I:386:GLU:HA	1:J:281:PHE:CG	2.53	0.44
1:I:8:PHE:HA	1:I:518:GLU:O	2.18	0.44
1:A:36:ARG:HH12	1:G:115:ASP:CA	2.30	0.44
1:D:90:THR:HG22	1:D:94:VAL:HG23	2.00	0.44
1:E:412:VAL:HG22	1:E:495:ASP:O	2.18	0.44
1:K:217:SER:HA	1:K:320:ALA:O	2.17	0.44
1:L:217:SER:HA	1:L:320:ALA:O	2.17	0.44
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.98	0.44
1:H:230:ILE:HG23	1:H:259:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:230:ILE:HG23	1:J:259:LEU:HD12	2.00	0.44
1:H:386:GLU:HA	1:I:281:PHE:CG	2.53	0.44
1:C:279:PRO:HG3	1:C:292:ILE:HD11	2.00	0.44
1:A:115:ASP:C	1:B:36:ARG:HH12	2.07	0.44
1:C:412:VAL:HG22	1:C:495:ASP:O	2.18	0.44
1:F:412:VAL:HG22	1:F:495:ASP:O	2.18	0.44
1:C:521:VAL:HG21	1:D:59:GLU:CB	2.45	0.44
1:B:417:VAL:HG13	1:B:476:TYR:O	2.18	0.44
1:E:440:ILE:O	1:E:444:LEU:HG	2.18	0.44
1:M:230:ILE:HG23	1:M:259:LEU:HD12	2.00	0.44
1:G:412:VAL:HG22	1:G:495:ASP:O	2.18	0.43
1:D:412:VAL:HG22	1:D:495:ASP:O	2.18	0.43
1:C:417:VAL:HG13	1:C:476:TYR:O	2.18	0.43
1:J:386:GLU:HA	1:K:281:PHE:CG	2.53	0.43
1:L:386:GLU:HA	1:M:281:PHE:CG	2.53	0.43
1:C:115:ASP:CA	1:D:36:ARG:HH12	2.31	0.43
1:F:90:THR:HG22	1:F:94:VAL:HG23	2.00	0.43
1:A:417:VAL:HG13	1:A:476:TYR:O	2.18	0.43
1:K:191:GLU:O	1:K:334:ASP:HA	2.18	0.43
1:E:279:PRO:HG3	1:E:292:ILE:HD11	2.00	0.43
1:E:256:GLY:O	1:E:260:ALA:HB3	2.18	0.43
1:L:215:LEU:O	1:L:218:PRO:HD3	2.18	0.43
1:H:281:PHE:CG	1:N:386:GLU:HA	2.53	0.43
1:L:417:VAL:HA	1:L:420:ILE:HG22	2.00	0.43
1:B:521:VAL:N	1:C:41:ASP:HB3	2.31	0.43
1:D:520:MET:CA	1:E:41:ASP:HB2	2.48	0.43
1:E:293:ALA:HB2	1:E:300:VAL:CG2	2.49	0.43
1:C:256:GLY:O	1:C:260:ALA:HB3	2.18	0.43
1:H:117:LYS:HZ2	1:H:121:ASP:CG	2.21	0.43
1:F:115:ASP:CA	1:G:36:ARG:HH12	2.30	0.43
1:C:90:THR:HG22	1:C:94:VAL:HG23	2.00	0.43
1:B:520:MET:CA	1:C:41:ASP:HB2	2.48	0.43
1:C:406:ALA:HB2	1:C:496:PRO:HG3	1.99	0.43
1:G:256:GLY:O	1:G:260:ALA:HB3	2.18	0.43
1:I:230:ILE:HG23	1:I:259:LEU:HD12	2.00	0.43
1:F:293:ALA:HB2	1:F:300:VAL:CG2	2.49	0.43
1:M:7:LYS:O	1:M:519:CYS:HA	2.18	0.43
1:B:279:PRO:HG3	1:B:292:ILE:HD11	2.00	0.43
1:C:520:MET:CA	1:D:41:ASP:HB2	2.48	0.43
1:D:40:LEU:HD11	1:D:55:SER:CB	2.48	0.43
1:H:191:GLU:O	1:H:334:ASP:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:7:LYS:O	1:J:519:CYS:HA	2.18	0.43
1:M:215:LEU:O	1:M:218:PRO:HD3	2.18	0.43
1:A:406:ALA:HB2	1:A:496:PRO:HG3	1.99	0.43
1:B:513:LEU:CA	1:C:49:ILE:HD11	2.43	0.43
1:B:202:PRO:O	1:B:205:ILE:HB	2.19	0.43
1:G:40:LEU:HD11	1:G:55:SER:CB	2.48	0.43
1:A:41:ASP:HB3	1:G:521:VAL:N	2.32	0.43
1:C:180:GLY:HA3	1:C:381:VAL:O	2.19	0.43
1:A:10:ASN:HA	1:A:13:ARG:HD2	2.01	0.43
1:F:10:ASN:HA	1:F:13:ARG:HD2	2.01	0.43
1:F:13:ARG:NH1	1:F:515:ILE:O	2.49	0.43
1:C:10:ASN:HA	1:C:13:ARG:HD2	2.01	0.43
1:G:440:ILE:O	1:G:444:LEU:HG	2.18	0.43
1:B:406:ALA:HB2	1:B:496:PRO:HG3	1.99	0.43
1:H:417:VAL:HA	1:H:420:ILE:HG22	2.00	0.43
1:B:256:GLY:O	1:B:260:ALA:HB3	2.18	0.43
1:F:279:PRO:HG3	1:F:292:ILE:HD11	2.00	0.43
1:K:215:LEU:O	1:K:218:PRO:HD3	2.18	0.43
1:G:293:ALA:HB2	1:G:300:VAL:CG2	2.49	0.43
1:D:115:ASP:CA	1:E:36:ARG:HH12	2.30	0.43
1:C:182:GLY:O	1:C:382:GLY:HA2	2.19	0.43
1:E:40:LEU:HD11	1:E:55:SER:CB	2.48	0.43
1:F:180:GLY:HA3	1:F:381:VAL:O	2.19	0.43
1:B:10:ASN:HA	1:B:13:ARG:HD2	2.01	0.43
1:M:191:GLU:O	1:M:334:ASP:HA	2.18	0.43
1:I:215:LEU:O	1:I:218:PRO:HD3	2.18	0.43
1:J:117:LYS:HZ2	1:J:121:ASP:CG	2.22	0.43
1:A:293:ALA:HB2	1:A:300:VAL:CG2	2.49	0.43
1:I:417:VAL:HA	1:I:420:ILE:HG22	2.00	0.43
1:M:386:GLU:HA	1:N:281:PHE:CG	2.53	0.43
1:M:117:LYS:HZ2	1:M:121:ASP:CG	2.21	0.43
1:E:114:MET:C	1:F:36:ARG:NH1	2.67	0.43
1:G:90:THR:HG22	1:G:94:VAL:HG23	2.00	0.43
1:D:182:GLY:O	1:D:382:GLY:HA2	2.18	0.43
1:F:40:LEU:HD11	1:F:55:SER:CB	2.48	0.43
1:A:40:LEU:HD11	1:A:55:SER:CB	2.48	0.43
1:E:10:ASN:HA	1:E:13:ARG:HD2	2.01	0.43
1:M:219:PHE:O	1:M:247:LEU:HD12	2.19	0.43
1:D:293:ALA:HB2	1:D:300:VAL:CG2	2.49	0.43
1:N:7:LYS:O	1:N:519:CYS:HA	2.18	0.43
1:H:7:LYS:O	1:H:519:CYS:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:215:LEU:O	1:N:218:PRO:HD3	2.18	0.43
1:H:215:LEU:O	1:H:218:PRO:HD3	2.18	0.43
1:E:115:ASP:CA	1:F:36:ARG:HH12	2.31	0.43
1:F:39:VAL:HG13	1:F:49:ILE:HA	2.01	0.43
1:C:202:PRO:O	1:C:205:ILE:HB	2.19	0.43
1:D:30:THR:CG2	1:D:38:VAL:HG21	2.42	0.43
1:C:521:VAL:N	1:D:41:ASP:HB3	2.32	0.43
1:B:30:THR:HG22	1:B:38:VAL:CG2	2.45	0.43
1:A:520:MET:CA	1:B:41:ASP:HB2	2.48	0.43
1:B:180:GLY:HA3	1:B:381:VAL:O	2.19	0.43
1:D:440:ILE:O	1:D:444:LEU:HG	2.18	0.43
1:L:7:LYS:O	1:L:519:CYS:HA	2.18	0.43
1:I:219:PHE:O	1:I:247:LEU:HD12	2.19	0.43
1:A:279:PRO:HG3	1:A:292:ILE:HD11	2.00	0.43
1:L:219:PHE:O	1:L:247:LEU:HD12	2.19	0.43
1:A:513:LEU:CA	1:B:49:ILE:HD11	2.43	0.43
1:E:39:VAL:HG13	1:E:49:ILE:HA	2.01	0.43
1:C:513:LEU:CA	1:D:49:ILE:HD11	2.43	0.43
1:F:182:GLY:O	1:F:382:GLY:HA2	2.19	0.43
1:G:182:GLY:O	1:G:382:GLY:HA2	2.19	0.43
1:C:40:LEU:HD11	1:C:55:SER:CB	2.48	0.43
1:A:30:THR:HG22	1:A:38:VAL:CG2	2.45	0.43
1:A:41:ASP:HB2	1:G:520:MET:CA	2.48	0.43
1:E:180:GLY:HA3	1:E:381:VAL:O	2.19	0.43
1:D:10:ASN:HA	1:D:13:ARG:HD2	2.01	0.43
1:G:10:ASN:HA	1:G:13:ARG:HD2	2.01	0.43
1:G:13:ARG:NH1	1:G:515:ILE:O	2.49	0.43
1:J:417:VAL:HA	1:J:420:ILE:HG22	2.00	0.43
1:K:417:VAL:HA	1:K:420:ILE:HG22	2.00	0.43
1:C:112:ASN:HA	1:C:113:PRO:HD2	1.74	0.42
1:F:112:ASN:HA	1:F:113:PRO:HD2	1.74	0.42
1:D:23:LEU:O	1:D:27:VAL:HG23	2.19	0.42
1:B:182:GLY:O	1:B:382:GLY:HA2	2.19	0.42
1:A:202:PRO:O	1:A:205:ILE:HB	2.19	0.42
1:D:521:VAL:N	1:E:41:ASP:HB3	2.32	0.42
1:C:127:ALA:CB	1:C:426:LEU:HD11	2.47	0.42
1:L:191:GLU:O	1:L:334:ASP:HA	2.18	0.42
1:K:386:GLU:HA	1:L:281:PHE:CG	2.54	0.42
1:D:406:ALA:HB2	1:D:496:PRO:HG3	1.99	0.42
1:G:279:PRO:HG3	1:G:292:ILE:HD11	2.00	0.42
1:N:219:PHE:O	1:N:247:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ALA:HB2	1:B:300:VAL:CG2	2.49	0.42
1:D:39:VAL:HG13	1:D:49:ILE:HA	2.01	0.42
1:G:180:GLY:HA3	1:G:381:VAL:O	2.19	0.42
1:A:73:MET:HA	1:B:46:ALA:HB1	2.01	0.42
1:H:219:PHE:O	1:H:247:LEU:HD12	2.19	0.42
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.35	0.42
1:G:23:LEU:O	1:G:27:VAL:HG23	2.19	0.42
1:E:182:GLY:O	1:E:382:GLY:HA2	2.19	0.42
1:F:73:MET:HA	1:G:46:ALA:HB1	2.01	0.42
1:N:271:VAL:HG12	1:N:272:LYS:H	1.85	0.42
1:K:219:PHE:O	1:K:247:LEU:HD12	2.19	0.42
1:J:219:PHE:O	1:J:247:LEU:HD12	2.19	0.42
1:N:400:LEU:CA	1:N:401:HIS:N	2.76	0.42
1:E:23:LEU:O	1:E:27:VAL:HG23	2.19	0.42
1:A:517:THR:HA	1:B:39:VAL:HB	2.02	0.42
1:A:182:GLY:O	1:A:382:GLY:HA2	2.19	0.42
1:E:521:VAL:N	1:F:41:ASP:HB3	2.32	0.42
1:C:30:THR:HG22	1:C:38:VAL:CG2	2.45	0.42
1:H:271:VAL:HG12	1:H:272:LYS:H	1.85	0.42
1:I:271:VAL:HG12	1:I:272:LYS:H	1.85	0.42
1:I:117:LYS:HZ2	1:I:121:ASP:CG	2.22	0.42
1:J:215:LEU:O	1:J:218:PRO:HD3	2.18	0.42
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.50	0.42
1:E:520:MET:CA	1:F:41:ASP:HB2	2.48	0.42
1:D:180:GLY:HA3	1:D:381:VAL:O	2.19	0.42
1:A:46:ALA:HB1	1:G:73:MET:HA	2.01	0.42
1:M:271:VAL:HG12	1:M:272:LYS:H	1.85	0.42
1:F:294:THR:HG21	1:F:345:ARG:HG3	2.01	0.42
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.50	0.42
1:E:112:ASN:HA	1:E:113:PRO:HD2	1.74	0.42
1:A:23:LEU:O	1:A:27:VAL:HG23	2.19	0.42
1:A:39:VAL:HB	1:G:517:THR:HA	2.02	0.42
1:G:39:VAL:HG13	1:G:49:ILE:HA	2.01	0.42
1:C:39:VAL:HG13	1:C:49:ILE:HA	2.01	0.42
1:A:13:ARG:NH1	1:A:515:ILE:O	2.49	0.42
1:J:271:VAL:HG12	1:J:272:LYS:H	1.85	0.42
1:K:117:LYS:HZ2	1:K:121:ASP:CG	2.21	0.42
1:N:117:LYS:HZ2	1:N:121:ASP:CG	2.23	0.42
1:I:7:LYS:O	1:I:519:CYS:HA	2.18	0.42
1:C:23:LEU:O	1:C:27:VAL:HG23	2.19	0.42
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:LEU:CA	1:E:49:ILE:HD11	2.43	0.42
1:B:73:MET:HA	1:C:46:ALA:HB1	2.01	0.42
1:E:73:MET:HA	1:F:46:ALA:HB1	2.01	0.42
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.49	0.42
1:G:294:THR:HG21	1:G:345:ARG:HG3	2.01	0.42
1:B:23:LEU:O	1:B:27:VAL:HG23	2.19	0.42
1:D:30:THR:HG22	1:D:38:VAL:CG2	2.45	0.42
1:F:520:MET:CA	1:G:41:ASP:HB2	2.48	0.42
1:C:30:THR:CG2	1:C:38:VAL:HG21	2.42	0.42
1:B:40:LEU:HD11	1:B:55:SER:CB	2.48	0.42
1:D:46:ALA:HA	1:D:47:PRO:HD2	1.85	0.42
1:N:191:GLU:O	1:N:334:ASP:HA	2.18	0.42
1:L:271:VAL:HG12	1:L:272:LYS:H	1.85	0.42
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.50	0.42
1:E:294:THR:HG21	1:E:345:ARG:HG3	2.02	0.42
1:F:202:PRO:O	1:F:205:ILE:HB	2.19	0.42
1:A:521:VAL:N	1:B:41:ASP:HB3	2.32	0.42
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.50	0.42
1:K:7:LYS:O	1:K:519:CYS:HA	2.18	0.42
1:F:517:THR:HA	1:G:39:VAL:HB	2.02	0.42
1:B:39:VAL:HG13	1:B:49:ILE:HA	2.01	0.42
1:G:30:THR:HG22	1:G:38:VAL:CG2	2.45	0.42
1:E:30:THR:HG22	1:E:38:VAL:CG2	2.45	0.42
1:F:30:THR:HG22	1:F:38:VAL:CG2	2.45	0.42
1:A:180:GLY:HA3	1:A:381:VAL:O	2.19	0.42
1:A:383:ALA:HB3	1:A:389:MET:N	2.35	0.42
1:L:117:LYS:HZ2	1:L:121:ASP:CG	2.22	0.42
1:A:39:VAL:HG13	1:A:49:ILE:HA	2.01	0.41
1:E:202:PRO:O	1:E:205:ILE:HB	2.19	0.41
1:D:73:MET:HA	1:E:46:ALA:HB1	2.01	0.41
1:C:34:LYS:HZ1	1:C:483:GLU:CD	2.23	0.41
1:K:254:VAL:CG1	1:K:259:LEU:HD23	2.50	0.41
1:C:293:ALA:HB2	1:C:300:VAL:CG2	2.49	0.41
1:G:112:ASN:HA	1:G:113:PRO:HD2	1.74	0.41
1:B:517:THR:HA	1:C:39:VAL:HB	2.02	0.41
1:G:383:ALA:HB3	1:G:389:MET:N	2.35	0.41
1:J:254:VAL:CG1	1:J:259:LEU:HD23	2.50	0.41
1:D:294:THR:HG21	1:D:345:ARG:HG3	2.02	0.41
1:E:102:GLU:HB2	1:E:442:VAL:HG13	2.02	0.41
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.50	0.41
1:F:23:LEU:O	1:F:27:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HD11	1:G:513:LEU:CA	2.43	0.41
1:C:73:MET:HA	1:D:46:ALA:HB1	2.01	0.41
1:B:323:VAL:HG22	1:B:332:ILE:HA	2.03	0.41
1:F:126:ALA:HB3	1:F:426:LEU:HD22	2.03	0.41
1:N:254:VAL:CG1	1:N:259:LEU:HD23	2.50	0.41
1:C:294:THR:HG21	1:C:345:ARG:HG3	2.01	0.41
1:A:323:VAL:HG22	1:A:332:ILE:HA	2.03	0.41
1:G:126:ALA:HB3	1:G:426:LEU:HD22	2.03	0.41
1:C:383:ALA:HB3	1:C:389:MET:N	2.35	0.41
1:L:2:ALA:O	1:L:3:ALA:C	2.59	0.41
1:B:19:GLY:HA2	1:B:62:LEU:CD1	2.50	0.41
1:D:202:PRO:O	1:D:205:ILE:HB	2.19	0.41
1:D:13:ARG:NH1	1:D:515:ILE:O	2.49	0.41
1:I:254:VAL:CG1	1:I:259:LEU:HD23	2.50	0.41
1:A:294:THR:HG21	1:A:345:ARG:HG3	2.01	0.41
1:N:2:ALA:O	1:N:3:ALA:C	2.59	0.41
1:E:517:THR:HA	1:F:39:VAL:HB	2.02	0.41
1:E:513:LEU:CA	1:F:49:ILE:HD11	2.43	0.41
1:E:205:ILE:HG23	1:E:211:GLY:HA2	2.03	0.41
1:E:126:ALA:HB3	1:E:426:LEU:HD22	2.03	0.41
1:M:254:VAL:CG1	1:M:259:LEU:HD23	2.50	0.41
1:H:2:ALA:O	1:H:3:ALA:C	2.59	0.41
1:A:268:ARG:CZ	1:A:268:ARG:HA	2.51	0.41
1:D:517:THR:HA	1:E:39:VAL:HB	2.02	0.41
1:G:202:PRO:O	1:G:205:ILE:HB	2.19	0.41
1:C:135:SER:CA	1:C:412:VAL:HG12	2.45	0.41
1:G:323:VAL:HG22	1:G:332:ILE:HA	2.03	0.41
1:A:126:ALA:HB3	1:A:426:LEU:HD22	2.03	0.41
1:A:102:GLU:HB2	1:A:442:VAL:HG13	2.02	0.41
1:C:323:VAL:HG22	1:C:332:ILE:HA	2.03	0.41
1:D:383:ALA:HB3	1:D:389:MET:N	2.35	0.41
1:B:383:ALA:HB3	1:B:389:MET:N	2.35	0.41
1:F:102:GLU:HB2	1:F:442:VAL:HG13	2.02	0.41
1:B:294:THR:HG21	1:B:345:ARG:HG3	2.01	0.41
1:F:513:LEU:CA	1:G:49:ILE:HD11	2.43	0.41
1:E:46:ALA:HA	1:E:47:PRO:HD2	1.84	0.41
1:B:13:ARG:NH1	1:B:515:ILE:O	2.49	0.41
1:K:271:VAL:HG12	1:K:272:LYS:H	1.85	0.41
1:F:383:ALA:HB3	1:F:389:MET:N	2.35	0.41
1:F:85:ALA:HB1	1:F:499:VAL:HA	2.03	0.41
1:B:268:ARG:CZ	1:B:268:ARG:HA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:2:ALA:O	1:J:3:ALA:C	2.59	0.41
1:D:102:GLU:HB2	1:D:442:VAL:HG13	2.02	0.41
1:D:112:ASN:HA	1:D:113:PRO:HD2	1.74	0.41
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.35	0.41
1:F:205:ILE:HG23	1:F:211:GLY:HA2	2.03	0.41
1:C:152:ALA:HB1	1:C:155:ASP:CA	2.51	0.41
1:F:51:LYS:HB2	1:F:395:ARG:HD3	2.03	0.41
1:G:268:ARG:HA	1:G:268:ARG:CZ	2.51	0.41
1:B:126:ALA:HB3	1:B:426:LEU:HD22	2.03	0.40
1:B:152:ALA:HB1	1:B:155:ASP:CA	2.51	0.40
1:B:102:GLU:HB2	1:B:442:VAL:HG13	2.02	0.40
1:G:102:GLU:HB2	1:G:442:VAL:HG13	2.02	0.40
3:G:1525:PO4:P	2:G:1527:ATP:PG	3.20	0.40
1:D:152:ALA:HB1	1:D:155:ASP:CA	2.51	0.40
1:E:13:ARG:NH1	1:E:515:ILE:O	2.49	0.40
1:E:383:ALA:HB3	1:E:389:MET:N	2.35	0.40
1:I:2:ALA:O	1:I:3:ALA:C	2.59	0.40
1:D:461:GLU:HA	1:D:462:PRO:HD2	1.83	0.40
3:F:1525:PO4:P	2:F:1527:ATP:PG	3.20	0.40
1:G:205:ILE:HG23	1:G:211:GLY:HA2	2.03	0.40
1:D:205:ILE:HG23	1:D:211:GLY:HA2	2.03	0.40
1:D:323:VAL:HG22	1:D:332:ILE:HA	2.03	0.40
1:D:126:ALA:HB3	1:D:426:LEU:HD22	2.03	0.40
1:D:206:ASN:HB2	1:D:213:VAL:CB	2.52	0.40
1:E:206:ASN:HB2	1:E:213:VAL:CB	2.51	0.40
1:A:152:ALA:HB1	1:A:155:ASP:CA	2.51	0.40
1:B:34:LYS:HZ1	1:B:483:GLU:CD	2.24	0.40
1:H:254:VAL:CG1	1:H:259:LEU:HD23	2.50	0.40
1:F:231:ARG:O	1:F:235:PRO:HD2	2.22	0.40
1:E:85:ALA:HB1	1:E:499:VAL:HA	2.04	0.40
2:A:1525:ATP:PG	3:A:1526:PO4:P	3.20	0.40
1:D:517:THR:CA	1:E:39:VAL:HB	2.52	0.40
1:C:517:THR:HA	1:D:39:VAL:HB	2.02	0.40
1:F:323:VAL:HG22	1:F:332:ILE:HA	2.03	0.40
1:F:152:ALA:HB1	1:F:155:ASP:CA	2.51	0.40
1:B:13:ARG:CG	1:B:13:ARG:HH11	2.34	0.40
1:G:62:LEU:HB2	1:G:68:ASN:HA	2.04	0.40
1:G:166:MET:HA	1:G:175:ILE:HD11	2.04	0.40
1:D:85:ALA:HB1	1:D:499:VAL:HA	2.03	0.40
1:C:166:MET:HA	1:C:175:ILE:HD11	2.04	0.40
1:C:268:ARG:CZ	1:C:268:ARG:HA	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ALA:HB1	1:B:499:VAL:HA	2.04	0.40
1:E:517:THR:CA	1:F:39:VAL:HB	2.52	0.40
1:A:62:LEU:HB2	1:A:68:ASN:HA	2.04	0.40
1:B:62:LEU:HB2	1:B:68:ASN:HA	2.04	0.40
1:C:85:ALA:HB1	1:C:499:VAL:HA	2.04	0.40
1:G:51:LYS:HB2	1:G:395:ARG:HD3	2.03	0.40
1:G:85:ALA:HB1	1:G:499:VAL:HA	2.04	0.40
1:E:231:ARG:O	1:E:235:PRO:HD2	2.22	0.40
1:E:268:ARG:CZ	1:E:268:ARG:HA	2.51	0.40
1:F:268:ARG:HA	1:F:268:ARG:NE	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	B	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	C	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	D	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	E	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	F	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	G	522/548 (95%)	517 (99%)	5 (1%)	0	100	100
1	H	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	I	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	J	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	K	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80
1	L	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39 80
1	N	522/548 (95%)	498 (95%)	22 (4%)	2 (0%)	39 80
All	All	7308/7672 (95%)	7105 (97%)	189 (3%)	14 (0%)	56 86

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	269	GLY
1	I	269	GLY
1	J	269	GLY
1	K	269	GLY
1	L	269	GLY
1	M	269	GLY
1	N	269	GLY
1	H	336	VAL
1	I	336	VAL
1	J	336	VAL
1	K	336	VAL
1	L	336	VAL
1	M	336	VAL
1	N	336	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	402/414 (97%)	364 (90%)	38 (10%)	11 41
1	B	402/414 (97%)	364 (90%)	38 (10%)	11 41
1	C	402/414 (97%)	364 (90%)	38 (10%)	11 41
1	D	402/414 (97%)	364 (90%)	38 (10%)	11 41
1	E	402/414 (97%)	364 (90%)	38 (10%)	11 41
1	F	402/414 (97%)	364 (90%)	38 (10%)	11 41
1	G	402/414 (97%)	364 (90%)	38 (10%)	11 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	I	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	J	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	K	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	L	402/414 (97%)	366 (91%)	36 (9%)	12	44
1	M	402/414 (97%)	367 (91%)	35 (9%)	13	45
1	N	402/414 (97%)	367 (91%)	35 (9%)	13	45
All	All	5628/5796 (97%)	5116 (91%)	512 (9%)	16	43

All (512) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	25	ASP
1	A	31	LEU
1	A	37	ASN
1	A	49	ILE
1	A	55	SER
1	A	130	GLU
1	A	142	LYS
1	A	155	ASP
1	A	156	GLU
1	A	164	GLU
1	A	169	VAL
1	A	171	LYS
1	A	190	VAL
1	A	207	LYS
1	A	213	VAL
1	A	214	GLU
1	A	219	PHE
1	A	228	SER
1	A	253	ASP
1	A	257	GLU
1	A	290	GLN
1	A	295	LEU
1	A	327	LYS
1	A	328	ASP
1	A	334	ASP
1	A	350	ARG
1	A	358	SER

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Mol	Chain	Res	Type
1	A	363	GLU
1	A	421	ARG
1	A	453	GLN
1	A	460	GLU
1	A	473	ASP
1	A	484	GLU
1	A	504	LEU
1	A	516	THR
1	A	517	THR
1	A	523	ASP
1	B	8	PHE
1	B	25	ASP
1	B	31	LEU
1	B	37	ASN
1	B	49	ILE
1	B	55	SER
1	B	130	GLU
1	B	142	LYS
1	B	155	ASP
1	B	156	GLU
1	B	164	GLU
1	B	169	VAL
1	B	171	LYS
1	B	190	VAL
1	B	207	LYS
1	B	213	VAL
1	B	214	GLU
1	B	219	PHE
1	B	228	SER
1	B	253	ASP
1	B	257	GLU
1	B	290	GLN
1	B	295	LEU
1	B	327	LYS
1	B	328	ASP
1	B	334	ASP
1	B	350	ARG
1	B	358	SER
1	B	363	GLU
1	B	421	ARG
1	B	453	GLN
1	B	460	GLU

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Mol	Chain	Res	Type
1	B	473	ASP
1	B	484	GLU
1	B	504	LEU
1	B	516	THR
1	B	517	THR
1	B	523	ASP
1	C	8	PHE
1	C	25	ASP
1	C	31	LEU
1	C	37	ASN
1	C	49	ILE
1	C	55	SER
1	C	130	GLU
1	C	142	LYS
1	C	155	ASP
1	C	156	GLU
1	C	164	GLU
1	C	169	VAL
1	C	171	LYS
1	C	190	VAL
1	C	207	LYS
1	C	213	VAL
1	C	214	GLU
1	C	219	PHE
1	C	228	SER
1	C	253	ASP
1	C	257	GLU
1	C	290	GLN
1	C	295	LEU
1	C	327	LYS
1	C	328	ASP
1	C	334	ASP
1	C	350	ARG
1	C	358	SER
1	C	363	GLU
1	C	421	ARG
1	C	453	GLN
1	C	460	GLU
1	C	473	ASP
1	C	484	GLU
1	C	504	LEU
1	C	516	THR

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Mol	Chain	Res	Type
1	C	517	THR
1	C	523	ASP
1	D	8	PHE
1	D	25	ASP
1	D	31	LEU
1	D	37	ASN
1	D	49	ILE
1	D	55	SER
1	D	130	GLU
1	D	142	LYS
1	D	155	ASP
1	D	156	GLU
1	D	164	GLU
1	D	169	VAL
1	D	171	LYS
1	D	190	VAL
1	D	207	LYS
1	D	213	VAL
1	D	214	GLU
1	D	219	PHE
1	D	228	SER
1	D	253	ASP
1	D	257	GLU
1	D	290	GLN
1	D	295	LEU
1	D	327	LYS
1	D	328	ASP
1	D	334	ASP
1	D	350	ARG
1	D	358	SER
1	D	363	GLU
1	D	421	ARG
1	D	453	GLN
1	D	460	GLU
1	D	473	ASP
1	D	484	GLU
1	D	504	LEU
1	D	516	THR
1	D	517	THR
1	D	523	ASP
1	E	8	PHE
1	E	25	ASP

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Mol	Chain	Res	Type
1	E	31	LEU
1	E	37	ASN
1	E	49	ILE
1	E	55	SER
1	E	130	GLU
1	E	142	LYS
1	E	155	ASP
1	E	156	GLU
1	E	164	GLU
1	E	169	VAL
1	E	171	LYS
1	E	190	VAL
1	E	207	LYS
1	E	213	VAL
1	E	214	GLU
1	E	219	PHE
1	E	228	SER
1	E	253	ASP
1	E	257	GLU
1	E	290	GLN
1	E	295	LEU
1	E	327	LYS
1	E	328	ASP
1	E	334	ASP
1	E	350	ARG
1	E	358	SER
1	E	363	GLU
1	E	421	ARG
1	E	453	GLN
1	E	460	GLU
1	E	473	ASP
1	E	484	GLU
1	E	504	LEU
1	E	516	THR
1	E	517	THR
1	E	523	ASP
1	F	8	PHE
1	F	25	ASP
1	F	31	LEU
1	F	37	ASN
1	F	49	ILE
1	F	55	SER

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Mol	Chain	Res	Type
1	F	130	GLU
1	F	142	LYS
1	F	155	ASP
1	F	156	GLU
1	F	164	GLU
1	F	169	VAL
1	F	171	LYS
1	F	190	VAL
1	F	207	LYS
1	F	213	VAL
1	F	214	GLU
1	F	219	PHE
1	F	228	SER
1	F	253	ASP
1	F	257	GLU
1	F	290	GLN
1	F	295	LEU
1	F	327	LYS
1	F	328	ASP
1	F	334	ASP
1	F	350	ARG
1	F	358	SER
1	F	363	GLU
1	F	421	ARG
1	F	453	GLN
1	F	460	GLU
1	F	473	ASP
1	F	484	GLU
1	F	504	LEU
1	F	516	THR
1	F	517	THR
1	F	523	ASP
1	G	8	PHE
1	G	25	ASP
1	G	31	LEU
1	G	37	ASN
1	G	49	ILE
1	G	55	SER
1	G	130	GLU
1	G	142	LYS
1	G	155	ASP
1	G	156	GLU

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Mol	Chain	Res	Type
1	G	164	GLU
1	G	169	VAL
1	G	171	LYS
1	G	190	VAL
1	G	207	LYS
1	G	213	VAL
1	G	214	GLU
1	G	219	PHE
1	G	228	SER
1	G	253	ASP
1	G	257	GLU
1	G	290	GLN
1	G	295	LEU
1	G	327	LYS
1	G	328	ASP
1	G	334	ASP
1	G	350	ARG
1	G	358	SER
1	G	363	GLU
1	G	421	ARG
1	G	453	GLN
1	G	460	GLU
1	G	473	ASP
1	G	484	GLU
1	G	504	LEU
1	G	516	THR
1	G	517	THR
1	G	523	ASP
1	H	25	ASP
1	H	34	LYS
1	H	82	ASN
1	H	115	ASP
1	H	140	ASP
1	H	142	LYS
1	H	153	ASN
1	H	172	GLU
1	H	174	VAL
1	H	186	GLU
1	H	196	ASP
1	H	199	TYR
1	H	213	VAL
1	H	214	GLU

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Mol	Chain	Res	Type
1	H	216	GLU
1	H	228	SER
1	H	229	ASN
1	H	230	ILE
1	H	281	PHE
1	H	290	GLN
1	H	327	LYS
1	H	329	THR
1	H	334	ASP
1	H	338	GLU
1	H	350	ARG
1	H	404	ARG
1	H	411	VAL
1	H	460	GLU
1	H	463	SER
1	H	483	GLU
1	H	484	GLU
1	H	494	LEU
1	H	500	THR
1	H	504	LEU
1	H	510	VAL
1	I	25	ASP
1	I	34	LYS
1	I	82	ASN
1	I	115	ASP
1	I	140	ASP
1	I	142	LYS
1	I	153	ASN
1	I	172	GLU
1	I	174	VAL
1	I	186	GLU
1	I	196	ASP
1	I	199	TYR
1	I	213	VAL
1	I	214	GLU
1	I	216	GLU
1	I	228	SER
1	I	229	ASN
1	I	230	ILE
1	I	281	PHE
1	I	290	GLN
1	I	327	LYS

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Mol	Chain	Res	Type
1	I	329	THR
1	I	334	ASP
1	I	338	GLU
1	I	350	ARG
1	I	404	ARG
1	I	411	VAL
1	I	460	GLU
1	I	463	SER
1	I	483	GLU
1	I	484	GLU
1	I	494	LEU
1	I	500	THR
1	I	504	LEU
1	I	510	VAL
1	J	25	ASP
1	J	34	LYS
1	J	82	ASN
1	J	115	ASP
1	J	140	ASP
1	J	142	LYS
1	J	153	ASN
1	J	172	GLU
1	J	174	VAL
1	J	186	GLU
1	J	196	ASP
1	J	199	TYR
1	J	213	VAL
1	J	214	GLU
1	J	216	GLU
1	J	228	SER
1	J	229	ASN
1	J	230	ILE
1	J	281	PHE
1	J	290	GLN
1	J	327	LYS
1	J	329	THR
1	J	334	ASP
1	J	338	GLU
1	J	350	ARG
1	J	404	ARG
1	J	411	VAL
1	J	460	GLU

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Mol	Chain	Res	Type
1	J	463	SER
1	J	483	GLU
1	J	484	GLU
1	J	494	LEU
1	J	500	THR
1	J	504	LEU
1	J	510	VAL
1	K	25	ASP
1	K	34	LYS
1	K	82	ASN
1	K	115	ASP
1	K	140	ASP
1	K	142	LYS
1	K	153	ASN
1	K	172	GLU
1	K	174	VAL
1	K	186	GLU
1	K	196	ASP
1	K	199	TYR
1	K	213	VAL
1	K	214	GLU
1	K	216	GLU
1	K	228	SER
1	K	229	ASN
1	K	230	ILE
1	K	281	PHE
1	K	290	GLN
1	K	327	LYS
1	K	329	THR
1	K	334	ASP
1	K	338	GLU
1	K	350	ARG
1	K	404	ARG
1	K	411	VAL
1	K	460	GLU
1	K	463	SER
1	K	483	GLU
1	K	484	GLU
1	K	494	LEU
1	K	500	THR
1	K	504	LEU
1	K	510	VAL

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Mol	Chain	Res	Type
1	L	25	ASP
1	L	34	LYS
1	L	82	ASN
1	L	115	ASP
1	L	140	ASP
1	L	142	LYS
1	L	153	ASN
1	L	172	GLU
1	L	174	VAL
1	L	186	GLU
1	L	187	LEU
1	L	196	ASP
1	L	199	TYR
1	L	213	VAL
1	L	214	GLU
1	L	216	GLU
1	L	228	SER
1	L	229	ASN
1	L	230	ILE
1	L	281	PHE
1	L	290	GLN
1	L	327	LYS
1	L	329	THR
1	L	334	ASP
1	L	338	GLU
1	L	350	ARG
1	L	404	ARG
1	L	411	VAL
1	L	460	GLU
1	L	463	SER
1	L	483	GLU
1	L	484	GLU
1	L	494	LEU
1	L	500	THR
1	L	504	LEU
1	L	510	VAL
1	M	25	ASP
1	M	34	LYS
1	M	82	ASN
1	M	115	ASP
1	M	140	ASP
1	M	142	LYS

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Mol	Chain	Res	Type
1	M	153	ASN
1	M	172	GLU
1	M	174	VAL
1	M	186	GLU
1	M	196	ASP
1	M	199	TYR
1	M	213	VAL
1	M	214	GLU
1	M	216	GLU
1	M	228	SER
1	M	229	ASN
1	M	230	ILE
1	M	281	PHE
1	M	290	GLN
1	M	327	LYS
1	M	329	THR
1	M	334	ASP
1	M	338	GLU
1	M	350	ARG
1	M	404	ARG
1	M	411	VAL
1	M	460	GLU
1	M	463	SER
1	M	483	GLU
1	M	484	GLU
1	M	494	LEU
1	M	500	THR
1	M	504	LEU
1	M	510	VAL
1	N	25	ASP
1	N	34	LYS
1	N	82	ASN
1	N	115	ASP
1	N	140	ASP
1	N	142	LYS
1	N	153	ASN
1	N	172	GLU
1	N	174	VAL
1	N	186	GLU
1	N	196	ASP
1	N	199	TYR
1	N	213	VAL

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Mol	Chain	Res	Type
1	N	214	GLU
1	N	216	GLU
1	N	228	SER
1	N	229	ASN
1	N	230	ILE
1	N	281	PHE
1	N	290	GLN
1	N	327	LYS
1	N	329	THR
1	N	334	ASP
1	N	338	GLU
1	N	350	ARG
1	N	404	ARG
1	N	411	VAL
1	N	460	GLU
1	N	463	SER
1	N	483	GLU
1	N	484	GLU
1	N	494	LEU
1	N	500	THR
1	N	504	LEU
1	N	510	VAL

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

Mol	Chain	Res	Type
1	A	366	GLN
1	B	366	GLN
1	C	366	GLN
1	D	366	GLN
1	E	366	GLN
1	F	366	GLN
1	G	366	GLN
1	H	68	ASN
1	H	326	ASN
1	I	68	ASN
1	I	326	ASN
1	J	68	ASN
1	J	326	ASN
1	K	68	ASN
1	K	326	ASN
1	L	68	ASN

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Mol	Chain	Res	Type
1	L	326	ASN
1	M	68	ASN
1	M	326	ASN
1	N	68	ASN
1	N	326	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 7 are modelled with single atom and 7 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ATP	A	1525	4	26,33,33	0.96	1 (3%)	26,52,52	1.34	5 (19%)
2	ATP	B	1525	4	26,33,33	0.97	1 (3%)	26,52,52	1.35	5 (19%)
2	ATP	C	1526	4	26,33,33	0.98	1 (3%)	26,52,52	1.34	5 (19%)
2	ATP	D	1525	4	26,33,33	0.98	1 (3%)	26,52,52	1.35	5 (19%)
2	ATP	E	1527	4	26,33,33	0.99	1 (3%)	26,52,52	1.35	5 (19%)
2	ATP	F	1527	4	26,33,33	0.98	1 (3%)	26,52,52	1.35	5 (19%)
2	ATP	G	1527	4	26,33,33	0.97	1 (3%)	26,52,52	1.35	5 (19%)

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	ATP	A	1525	4	-	0/18/38/38	0/3/3/3
2	ATP	B	1525	4	-	0/18/38/38	0/3/3/3
2	ATP	C	1526	4	-	0/18/38/38	0/3/3/3
2	ATP	D	1525	4	-	0/18/38/38	0/3/3/3
2	ATP	E	1527	4	-	0/18/38/38	0/3/3/3
2	ATP	F	1527	4	-	0/18/38/38	0/3/3/3
2	ATP	G	1527	4	-	0/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1527	ATP	C2'-C1'	-3.34	1.48	1.53
2	C	1526	ATP	C2'-C1'	-3.33	1.48	1.53
2	D	1525	ATP	C2'-C1'	-3.32	1.48	1.53
2	G	1527	ATP	C2'-C1'	-3.29	1.48	1.53
2	B	1525	ATP	C2'-C1'	-3.29	1.48	1.53
2	F	1527	ATP	C2'-C1'	-3.29	1.48	1.53
2	A	1525	ATP	C2'-C1'	-3.24	1.48	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1527	ATP	C4'-O4'-C1'	-2.51	106.98	109.64
2	D	1525	ATP	C4'-O4'-C1'	-2.50	106.99	109.64
2	B	1525	ATP	C4'-O4'-C1'	-2.48	107.02	109.64
2	C	1526	ATP	C4'-O4'-C1'	-2.48	107.02	109.64
2	F	1527	ATP	C4'-O4'-C1'	-2.48	107.02	109.64
2	A	1525	ATP	C4'-O4'-C1'	-2.47	107.03	109.64
2	G	1527	ATP	C4'-O4'-C1'	-2.45	107.05	109.64
2	G	1527	ATP	C1'-N9-C4	-2.33	124.21	126.81
2	D	1525	ATP	C1'-N9-C4	-2.29	124.24	126.81
2	A	1525	ATP	C1'-N9-C4	-2.28	124.27	126.81
2	E	1527	ATP	C1'-N9-C4	-2.27	124.28	126.81
2	F	1527	ATP	C1'-N9-C4	-2.25	124.29	126.81
2	C	1526	ATP	C1'-N9-C4	-2.24	124.30	126.81
2	B	1525	ATP	C1'-N9-C4	-2.24	124.31	126.81
2	F	1527	ATP	O2A-PA-O3A	2.23	114.83	105.27
2	B	1525	ATP	O2A-PA-O3A	2.24	114.85	105.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1525	ATP	O2A-PA-O3A	2.24	114.86	105.27
2	G	1527	ATP	O2A-PA-O3A	2.24	114.86	105.27
2	E	1527	ATP	O2A-PA-O3A	2.24	114.87	105.27
2	D	1525	ATP	O2A-PA-O3A	2.24	114.88	105.27
2	C	1526	ATP	O2A-PA-O3A	2.25	114.90	105.27
2	D	1525	ATP	O4'-C1'-N9	2.37	112.59	108.11
2	E	1527	ATP	O4'-C1'-N9	2.38	112.61	108.11
2	C	1526	ATP	O4'-C1'-N9	2.39	112.62	108.11
2	G	1527	ATP	O4'-C1'-N9	2.40	112.64	108.11
2	G	1527	ATP	O3G-PG-O2G	2.41	116.30	107.44
2	A	1525	ATP	O4'-C1'-N9	2.42	112.67	108.11
2	B	1525	ATP	O4'-C1'-N9	2.42	112.67	108.11
2	F	1527	ATP	O4'-C1'-N9	2.42	112.67	108.11
2	A	1525	ATP	O3G-PG-O2G	2.42	116.33	107.44
2	D	1525	ATP	O3G-PG-O2G	2.43	116.36	107.44
2	E	1527	ATP	O3G-PG-O2G	2.43	116.36	107.44
2	C	1526	ATP	O3G-PG-O2G	2.43	116.37	107.44
2	B	1525	ATP	O3G-PG-O2G	2.44	116.40	107.44
2	F	1527	ATP	O3G-PG-O2G	2.45	116.43	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1525	ATP	4	0
2	B	1525	ATP	3	0
2	C	1526	ATP	3	0
2	D	1525	ATP	3	0
2	E	1527	ATP	3	0
2	F	1527	ATP	4	0
2	G	1527	ATP	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.