



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:07 PM BST

PDB ID : 4AAR  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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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

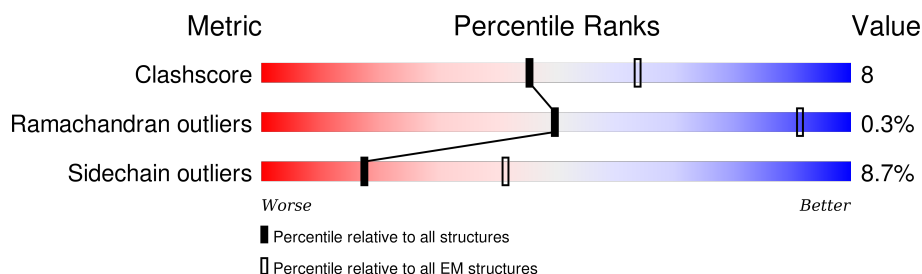
# 1 Overall quality at a glance

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	548	60% 27% 8% . .
1	B	548	61% 27% 8% . .
1	C	548	60% 27% 8% . .
1	D	548	61% 26% 8% . .
1	E	548	61% 27% 7% . .
1	F	548	60% 28% 7% . .
1	G	548	60% 28% 7% . .
1	H	548	79% 14% . . .
1	I	548	78% 14% . .

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Mol	Chain	Length	Quality of chain
1	J	548	 78%15% . .
1	K	548	 78%14% . . .
1	L	548	 78%15% . .
1	M	548	 78%14% . . .
1	N	548	 77%15% . .

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 [i](#)

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:

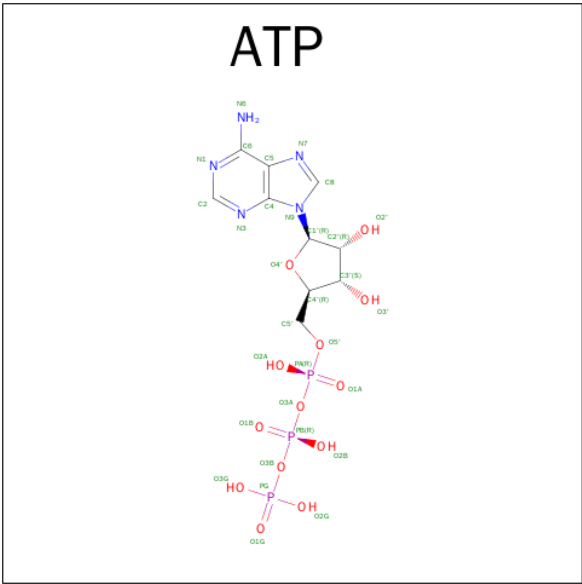
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5
B	398	ALA	ASP	ENGINEERED MUTATION	UNP P0A6F5

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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

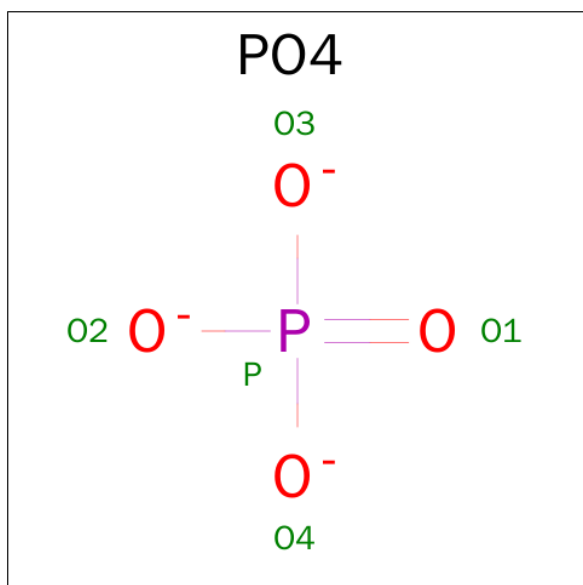
- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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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<sub>4</sub>P).



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	

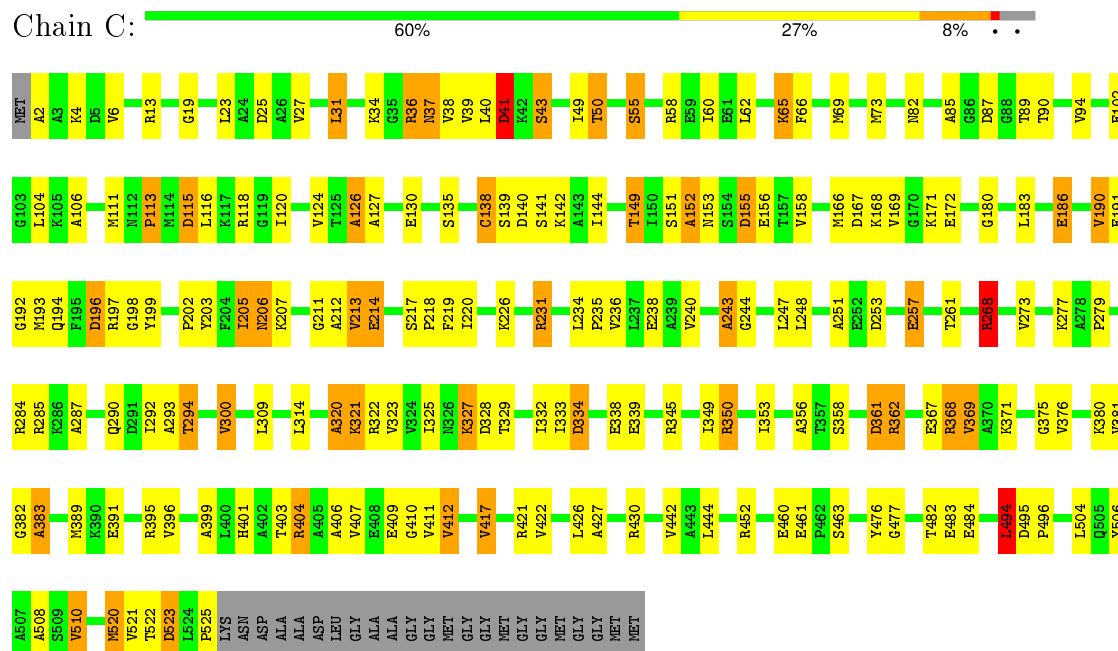
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

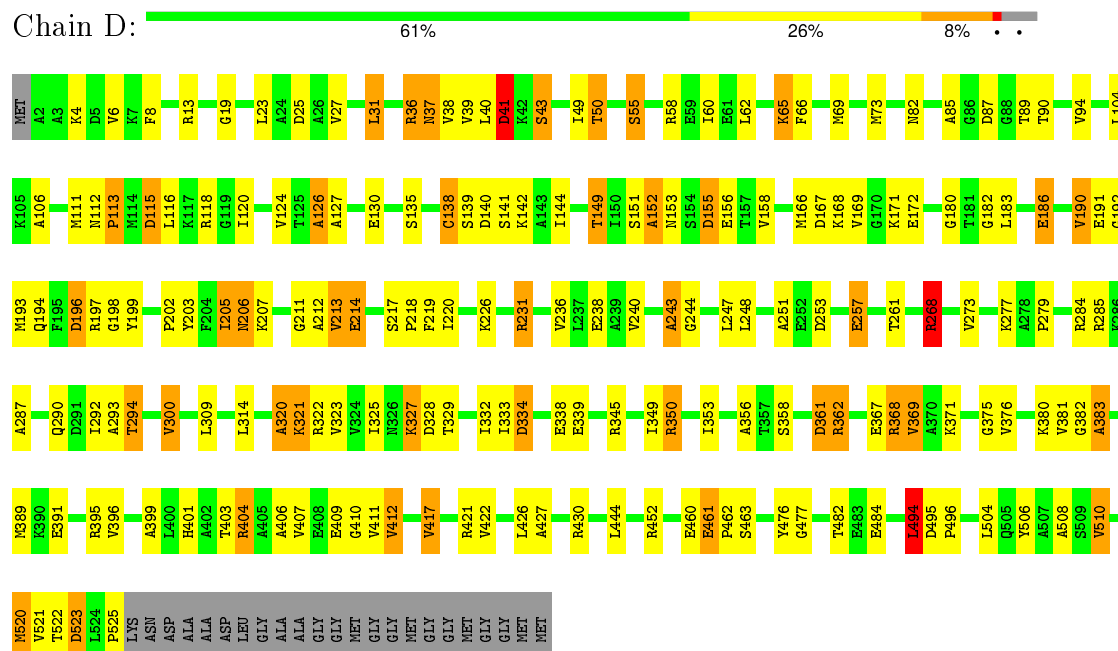




- Molecule 1: 60 KDA CHAPERONIN



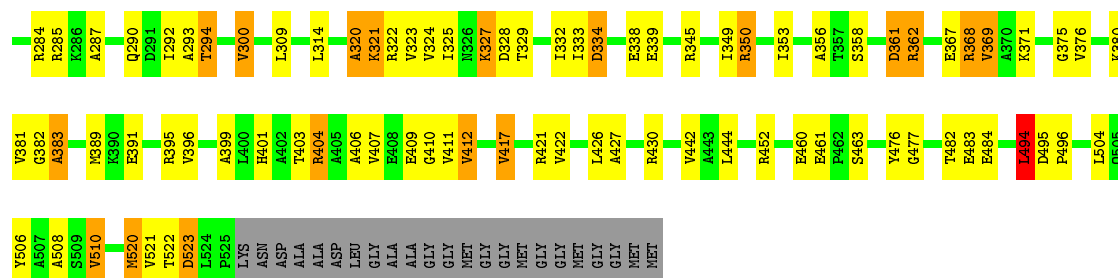
- Molecule 1: 60 KDA CHAPERONIN



- Molecule 1: 60 KDA CHAPERONIN

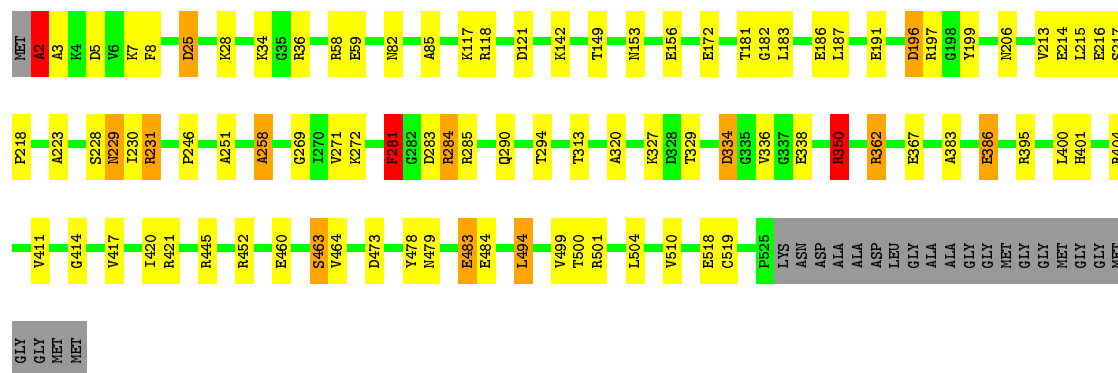






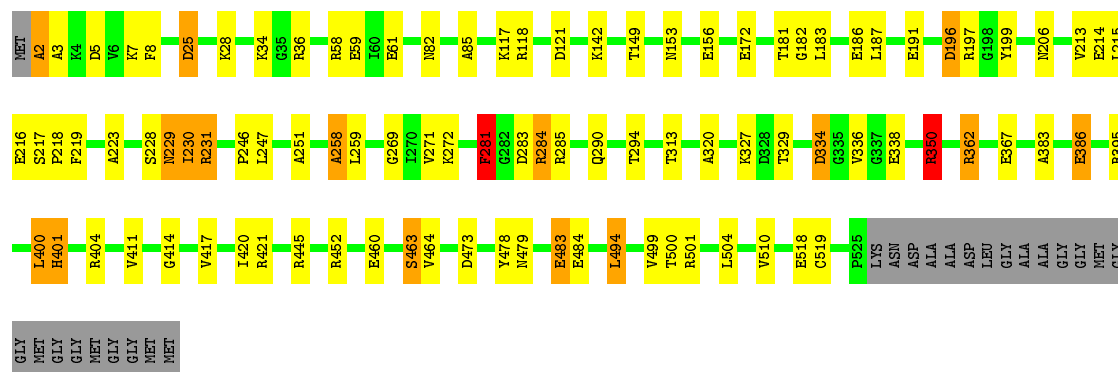
• Molecule 1: 60 KDA CHAPERONIN

Chain H: 79% 14% . . .



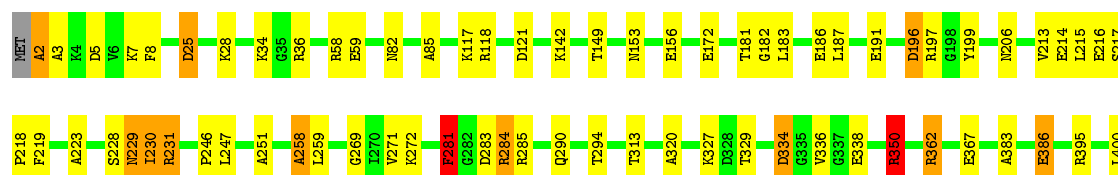
• Molecule 1: 60 KDA CHAPERONIN

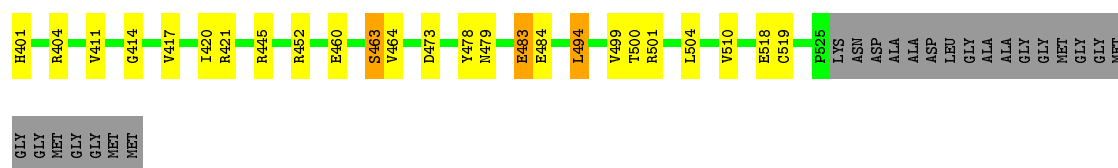
Chain I: 78% 14% . .



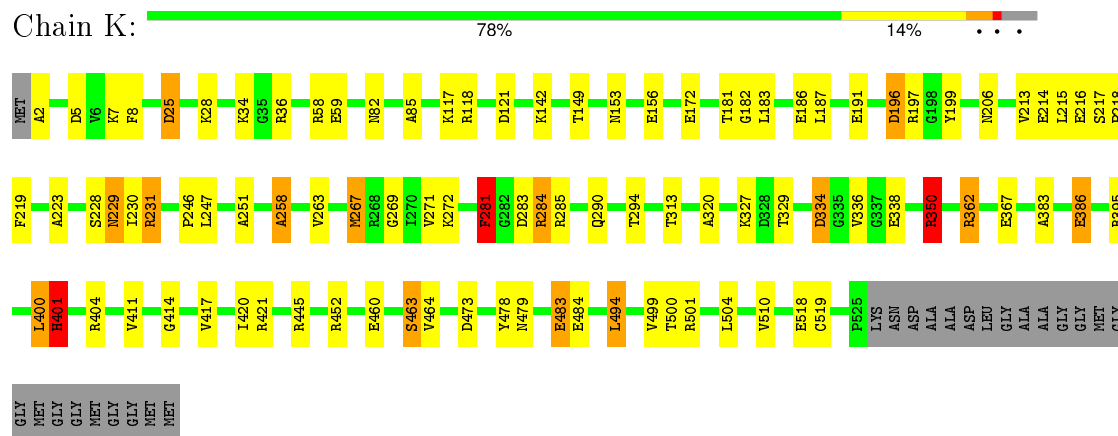
• Molecule 1: 60 KDA CHAPERONIN

Chain J: 78% 15% . .

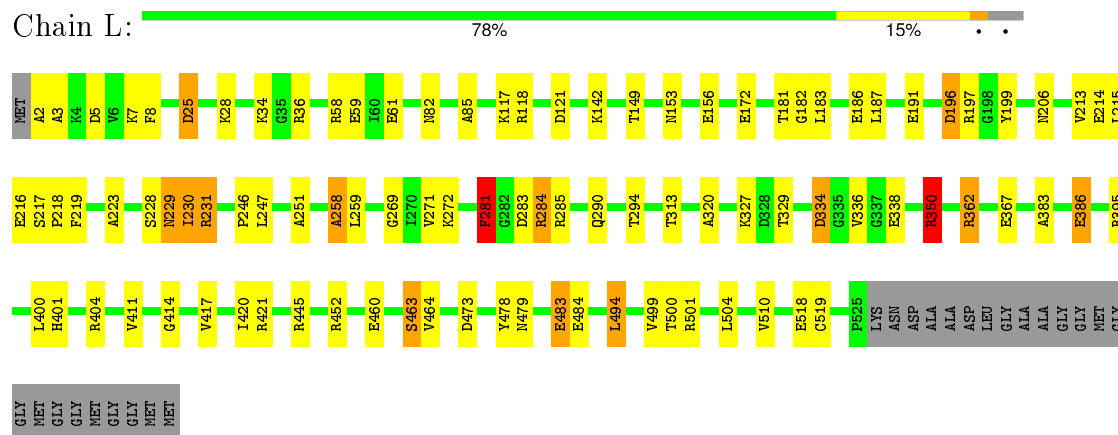




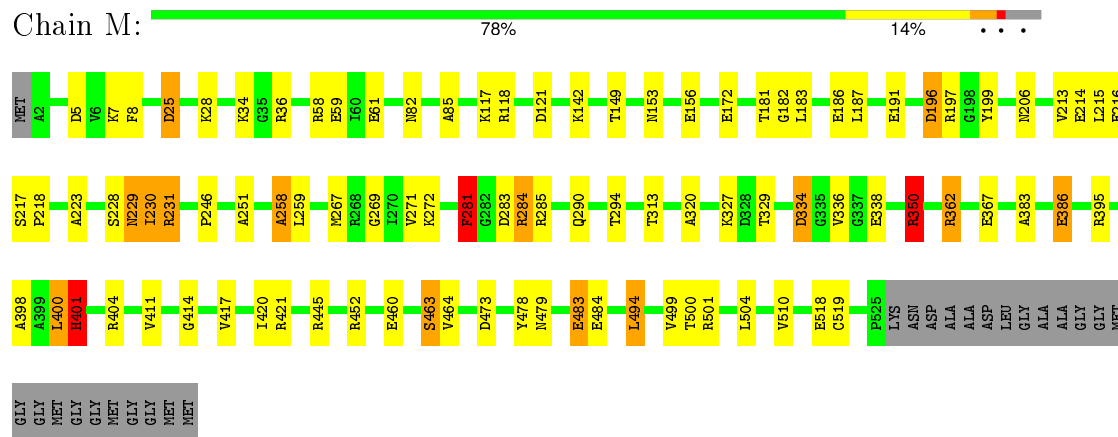
• Molecule 1: 60 KDA CHAPERONIN



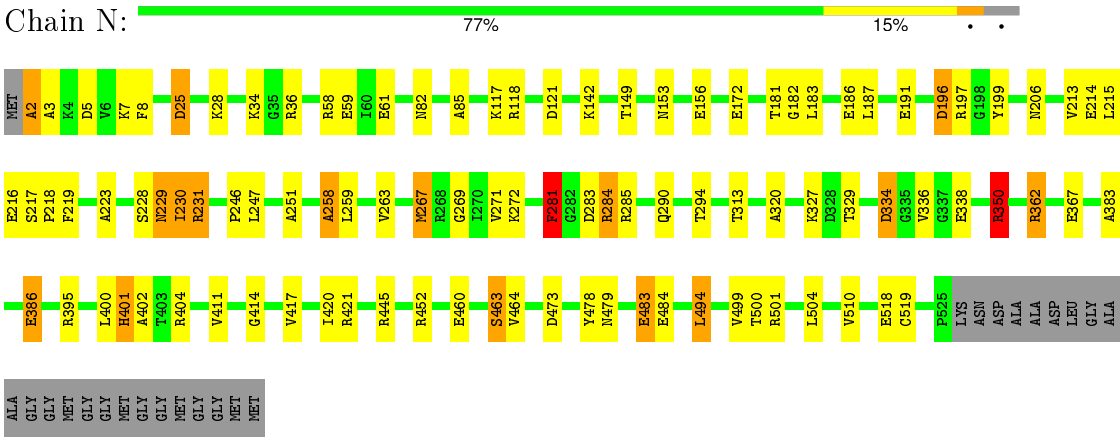
• Molecule 1: 60 KDA CHAPERONIN



• Molecule 1: 60 KDA CHAPERONIN



● Molecule 1: 60 KDA CHAPERONIN



## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	15	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN ULTRASCAN 4000 4K CCD CAM-ERA	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	1.04	3/3873 (0.1%)	1.49	73/5229 (1.4%)
1	B	1.03	3/3873 (0.1%)	1.49	74/5229 (1.4%)
1	C	1.03	3/3873 (0.1%)	1.49	73/5229 (1.4%)
1	D	1.03	2/3873 (0.1%)	1.49	76/5229 (1.5%)
1	E	1.03	2/3873 (0.1%)	1.49	74/5229 (1.4%)
1	F	1.04	3/3873 (0.1%)	1.49	75/5229 (1.4%)
1	G	1.04	3/3873 (0.1%)	1.49	74/5229 (1.4%)
1	H	0.75	4/3873 (0.1%)	1.09	22/5229 (0.4%)
1	I	0.79	3/3873 (0.1%)	1.11	26/5229 (0.5%)
1	J	0.71	4/3873 (0.1%)	1.08	20/5229 (0.4%)
1	K	0.77	2/3873 (0.1%)	1.11	25/5229 (0.5%)
1	L	0.69	2/3873 (0.1%)	1.13	26/5229 (0.5%)
1	M	0.79	2/3873 (0.1%)	1.09	23/5229 (0.4%)
1	N	0.79	4/3873 (0.1%)	1.11	28/5229 (0.5%)
All	All	0.91	40/54222 (0.1%)	1.31	689/73206 (0.9%)

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	1	10
1	B	1	10
1	C	1	10
1	D	1	10
1	E	1	10
1	F	1	10
1	G	1	10
1	H	0	11
1	I	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	9
1	K	0	10
1	L	0	9
1	M	0	10
1	N	0	9
All	All	7	137

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	400	LEU	C-N	22.64	1.86	1.34
1	K	400	LEU	C-N	20.41	1.81	1.34
1	I	400	LEU	C-N	18.68	1.77	1.34
1	N	2	ALA	N-CA	17.18	1.80	1.46
1	I	2	ALA	N-CA	16.70	1.79	1.46
1	N	401	HIS	C-N	15.85	1.70	1.34
1	M	401	HIS	C-N	-13.64	1.02	1.34
1	H	2	ALA	N-CA	13.58	1.73	1.46
1	E	401	HIS	C-N	11.37	1.60	1.34
1	F	401	HIS	C-N	11.16	1.59	1.34
1	K	2	ALA	N-CA	-11.12	1.24	1.46
1	D	401	HIS	C-N	10.42	1.58	1.34
1	H	401	HIS	C-N	10.28	1.57	1.34
1	G	401	HIS	C-N	10.03	1.57	1.34
1	H	2	ALA	CA-C	9.57	1.77	1.52
1	A	2	ALA	N-CA	9.26	1.64	1.46
1	C	401	HIS	C-N	9.00	1.54	1.34
1	N	2	ALA	CA-C	-8.85	1.29	1.52
1	A	401	HIS	C-N	8.67	1.53	1.34
1	G	2	ALA	N-CA	8.51	1.63	1.46
1	J	2	ALA	N-CA	8.41	1.63	1.46
1	L	400	LEU	C-N	8.39	1.53	1.34
1	B	401	HIS	C-N	8.25	1.53	1.34
1	B	2	ALA	N-CA	8.07	1.62	1.46
1	N	400	LEU	C-N	7.91	1.52	1.34
1	I	2	ALA	CA-C	7.68	1.73	1.52
1	J	2	ALA	CA-C	-7.47	1.33	1.52
1	H	400	LEU	C-N	7.32	1.50	1.34
1	F	50	THR	C-N	7.04	1.50	1.34
1	B	50	THR	C-N	7.02	1.50	1.34
1	C	50	THR	C-N	7.00	1.50	1.34
1	A	50	THR	C-N	7.00	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	50	THR	C-N	7.00	1.50	1.34
1	G	50	THR	C-N	6.98	1.50	1.34
1	E	50	THR	C-N	6.94	1.50	1.34
1	F	2	ALA	N-CA	6.34	1.59	1.46
1	J	401	HIS	C-N	-6.15	1.20	1.34
1	J	400	LEU	C-N	6.06	1.48	1.34
1	L	401	HIS	C-N	5.72	1.47	1.34
1	C	2	ALA	N-CA	5.70	1.57	1.46

All (689) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	THR	O-C-N	-15.61	97.73	122.70
1	F	50	THR	O-C-N	-15.58	97.77	122.70
1	D	50	THR	O-C-N	-15.57	97.79	122.70
1	G	50	THR	O-C-N	-15.57	97.79	122.70
1	C	50	THR	O-C-N	-15.55	97.81	122.70
1	B	50	THR	O-C-N	-15.54	97.84	122.70
1	E	50	THR	O-C-N	-15.52	97.87	122.70
1	L	401	HIS	O-C-N	13.79	144.76	122.70
1	N	267	MET	CG-SD-CE	12.71	120.54	100.20
1	K	267	MET	CG-SD-CE	12.69	120.50	100.20
1	D	383	ALA	N-CA-CB	11.67	126.44	110.10
1	F	383	ALA	N-CA-CB	11.66	126.42	110.10
1	B	383	ALA	N-CA-CB	11.65	126.41	110.10
1	A	383	ALA	N-CA-CB	11.63	126.38	110.10
1	G	383	ALA	N-CA-CB	11.63	126.38	110.10
1	E	383	ALA	N-CA-CB	11.61	126.35	110.10
1	C	383	ALA	N-CA-CB	11.59	126.32	110.10
1	A	391	GLU	CB-CA-C	-10.97	88.45	110.40
1	F	391	GLU	CB-CA-C	-10.96	88.47	110.40
1	C	391	GLU	CB-CA-C	-10.95	88.49	110.40
1	B	391	GLU	CB-CA-C	-10.94	88.52	110.40
1	E	391	GLU	CB-CA-C	-10.94	88.53	110.40
1	D	391	GLU	CB-CA-C	-10.93	88.53	110.40
1	G	391	GLU	CB-CA-C	-10.92	88.55	110.40
1	L	401	HIS	CA-C-N	-10.47	94.16	117.20
1	L	400	LEU	O-C-N	-10.28	106.25	122.70
1	C	334	ASP	N-CA-CB	-10.05	92.52	110.60
1	E	334	ASP	N-CA-CB	-10.02	92.57	110.60
1	A	334	ASP	N-CA-CB	-10.01	92.58	110.60
1	F	334	ASP	N-CA-CB	-10.01	92.58	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	334	ASP	N-CA-CB	-10.01	92.58	110.60
1	G	334	ASP	N-CA-CB	-10.00	92.60	110.60
1	D	334	ASP	N-CA-CB	-9.98	92.64	110.60
1	I	401	HIS	O-C-N	9.42	137.77	122.70
1	E	322	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	F	322	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	D	322	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	A	322	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	I	401	HIS	CA-C-N	-9.02	97.35	117.20
1	C	322	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	G	322	ARG	NE-CZ-NH2	-8.99	115.80	120.30
1	B	322	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	I	2	ALA	N-CA-C	-8.77	87.33	111.00
1	H	2	ALA	N-CA-C	-8.62	87.74	111.00
1	L	452	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	F	391	GLU	CA-CB-CG	8.47	132.03	113.40
1	G	494	LEU	CB-CA-C	8.46	126.28	110.20
1	D	494	LEU	CB-CA-C	8.46	126.27	110.20
1	A	494	LEU	CB-CA-C	8.45	126.26	110.20
1	B	494	LEU	CB-CA-C	8.45	126.25	110.20
1	E	494	LEU	CB-CA-C	8.45	126.25	110.20
1	C	494	LEU	CB-CA-C	8.44	126.24	110.20
1	F	494	LEU	CB-CA-C	8.43	126.21	110.20
1	B	391	GLU	CA-CB-CG	8.42	131.93	113.40
1	C	391	GLU	CA-CB-CG	8.42	131.92	113.40
1	A	391	GLU	CA-CB-CG	8.41	131.90	113.40
1	E	391	GLU	CA-CB-CG	8.40	131.88	113.40
1	M	452	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	D	391	GLU	CA-CB-CG	8.40	131.88	113.40
1	G	391	GLU	CA-CB-CG	8.40	131.88	113.40
1	I	452	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	452	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	K	452	ARG	NE-CZ-NH1	8.31	124.45	120.30
1	D	452	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	E	461	GLU	CB-CA-C	8.29	126.98	110.40
1	J	452	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	K	401	HIS	O-C-N	-8.29	109.44	122.70
1	H	452	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	F	461	GLU	CB-CA-C	8.27	126.95	110.40
1	D	461	GLU	CB-CA-C	8.27	126.94	110.40
1	F	452	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	B	452	ARG	NE-CZ-NH1	8.27	124.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	461	GLU	CB-CA-C	8.27	126.93	110.40
1	G	461	GLU	CB-CA-C	8.27	126.93	110.40
1	N	452	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	461	GLU	CB-CA-C	8.26	126.92	110.40
1	A	461	GLU	CB-CA-C	8.26	126.91	110.40
1	E	452	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	G	452	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	362	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	C	362	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	L	401	HIS	C-N-CA	-8.17	101.27	121.70
1	E	362	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	362	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	D	362	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	F	362	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	C	452	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	I	58	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	M	58	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	N	58	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	F	322	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	J	58	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	L	58	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	G	362	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	A	322	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	D	322	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	E	322	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	C	322	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	C	115	ASP	CB-CA-C	7.88	126.15	110.40
1	G	322	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	D	115	ASP	CB-CA-C	7.86	126.11	110.40
1	H	58	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	G	115	ASP	CB-CA-C	7.85	126.09	110.40
1	F	115	ASP	CB-CA-C	7.84	126.09	110.40
1	E	115	ASP	CB-CA-C	7.84	126.08	110.40
1	A	115	ASP	CB-CA-C	7.82	126.04	110.40
1	B	322	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	115	ASP	CB-CA-C	7.81	126.02	110.40
1	K	58	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	F	152	ALA	CB-CA-C	7.79	121.79	110.10
1	C	152	ALA	CB-CA-C	7.77	121.76	110.10
1	B	152	ALA	CB-CA-C	7.75	121.73	110.10
1	F	257	GLU	CB-CA-C	7.75	125.91	110.40
1	A	152	ALA	CB-CA-C	7.74	121.71	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ASN	C-N-CA	-7.72	102.41	121.70
1	G	152	ALA	CB-CA-C	7.71	121.67	110.10
1	D	152	ALA	CB-CA-C	7.71	121.66	110.10
1	A	404	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	37	ASN	C-N-CA	-7.69	102.46	121.70
1	F	404	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	E	152	ALA	CB-CA-C	7.69	121.63	110.10
1	D	37	ASN	C-N-CA	-7.68	102.50	121.70
1	C	37	ASN	C-N-CA	-7.68	102.51	121.70
1	G	404	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	G	37	ASN	C-N-CA	-7.67	102.52	121.70
1	B	257	GLU	CB-CA-C	7.67	125.74	110.40
1	F	37	ASN	C-N-CA	-7.67	102.53	121.70
1	E	37	ASN	C-N-CA	-7.67	102.54	121.70
1	A	257	GLU	CB-CA-C	7.65	125.71	110.40
1	G	257	GLU	CB-CA-C	7.65	125.69	110.40
1	D	257	GLU	CB-CA-C	7.64	125.69	110.40
1	D	404	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	C	257	GLU	CB-CA-C	7.63	125.65	110.40
1	E	257	GLU	CB-CA-C	7.61	125.61	110.40
1	E	404	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	B	153	ASN	CB-CA-C	7.59	125.58	110.40
1	A	153	ASN	CB-CA-C	7.58	125.56	110.40
1	F	153	ASN	CB-CA-C	7.58	125.56	110.40
1	D	153	ASN	CB-CA-C	7.57	125.54	110.40
1	B	404	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	G	153	ASN	CB-CA-C	7.56	125.52	110.40
1	E	153	ASN	CB-CA-C	7.56	125.51	110.40
1	C	153	ASN	CB-CA-C	7.55	125.50	110.40
1	C	404	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	C	257	GLU	N-CA-CB	7.49	124.08	110.60
1	D	257	GLU	N-CA-CB	7.47	124.05	110.60
1	A	257	GLU	N-CA-CB	7.47	124.04	110.60
1	E	257	GLU	N-CA-CB	7.46	124.03	110.60
1	G	257	GLU	N-CA-CB	7.45	124.02	110.60
1	B	257	GLU	N-CA-CB	7.44	123.99	110.60
1	B	50	THR	C-N-CA	7.38	140.16	121.70
1	A	50	THR	C-N-CA	7.38	140.14	121.70
1	F	257	GLU	N-CA-CB	7.37	123.87	110.60
1	L	36	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	E	50	THR	C-N-CA	7.37	140.12	121.70
1	M	36	ARG	NE-CZ-NH1	7.36	123.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	THR	C-N-CA	7.35	140.08	121.70
1	C	50	THR	C-N-CA	7.34	140.06	121.70
1	G	50	THR	C-N-CA	7.34	140.06	121.70
1	I	36	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	F	50	THR	C-N-CA	7.33	140.03	121.70
1	J	36	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	F	285	ARG	CB-CA-C	-7.31	95.78	110.40
1	E	50	THR	CA-C-N	7.30	133.27	117.20
1	D	50	THR	CA-C-N	7.30	133.27	117.20
1	B	50	THR	CA-C-N	7.30	133.26	117.20
1	G	50	THR	CA-C-N	7.30	133.26	117.20
1	K	36	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	C	50	THR	CA-C-N	7.29	133.24	117.20
1	G	285	ARG	CB-CA-C	-7.29	95.82	110.40
1	C	285	ARG	CB-CA-C	-7.29	95.83	110.40
1	F	50	THR	CA-C-N	7.29	133.24	117.20
1	B	285	ARG	CB-CA-C	-7.28	95.83	110.40
1	A	285	ARG	CB-CA-C	-7.27	95.86	110.40
1	D	285	ARG	CB-CA-C	-7.27	95.86	110.40
1	A	50	THR	CA-C-N	7.27	133.19	117.20
1	E	285	ARG	CB-CA-C	-7.26	95.87	110.40
1	J	367	GLU	CB-CA-C	-7.25	95.90	110.40
1	M	367	GLU	CB-CA-C	-7.25	95.91	110.40
1	N	36	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	H	367	GLU	CB-CA-C	-7.24	95.93	110.40
1	L	367	GLU	CB-CA-C	-7.24	95.93	110.40
1	N	367	GLU	CB-CA-C	-7.22	95.96	110.40
1	K	367	GLU	CB-CA-C	-7.22	95.97	110.40
1	I	367	GLU	CB-CA-C	-7.21	95.97	110.40
1	H	36	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	M	401	HIS	CA-C-N	-7.05	101.68	117.20
1	C	41	ASP	N-CA-CB	7.04	123.27	110.60
1	D	41	ASP	N-CA-CB	7.01	123.23	110.60
1	A	41	ASP	N-CA-CB	7.01	123.22	110.60
1	B	41	ASP	N-CA-CB	7.01	123.22	110.60
1	F	41	ASP	N-CA-CB	7.00	123.21	110.60
1	E	41	ASP	N-CA-CB	7.00	123.20	110.60
1	G	41	ASP	N-CA-CB	6.98	123.17	110.60
1	G	523	ASP	N-CA-CB	6.95	123.11	110.60
1	F	523	ASP	N-CA-CB	6.90	123.02	110.60
1	E	523	ASP	N-CA-CB	6.90	123.01	110.60
1	C	367	GLU	CB-CA-C	-6.74	96.92	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	367	GLU	CB-CA-C	-6.72	96.96	110.40
1	A	367	GLU	CB-CA-C	-6.71	96.98	110.40
1	M	362	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	367	GLU	CB-CA-C	-6.70	97.01	110.40
1	G	367	GLU	CB-CA-C	-6.70	97.01	110.40
1	D	367	GLU	CB-CA-C	-6.69	97.02	110.40
1	F	367	GLU	CB-CA-C	-6.69	97.03	110.40
1	E	409	GLU	N-CA-CB	6.66	122.59	110.60
1	G	409	GLU	N-CA-CB	6.66	122.58	110.60
1	A	113	PRO	CA-N-CD	-6.65	102.19	111.50
1	B	409	GLU	N-CA-CB	6.65	122.57	110.60
1	F	87	ASP	CB-CG-OD2	6.64	124.28	118.30
1	E	113	PRO	CA-N-CD	-6.64	102.20	111.50
1	D	409	GLU	N-CA-CB	6.64	122.55	110.60
1	B	113	PRO	CA-N-CD	-6.64	102.21	111.50
1	C	409	GLU	N-CA-CB	6.63	122.54	110.60
1	F	113	PRO	CA-N-CD	-6.63	102.22	111.50
1	K	362	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	F	409	GLU	N-CA-CB	6.62	122.52	110.60
1	G	113	PRO	CA-N-CD	-6.62	102.23	111.50
1	A	409	GLU	N-CA-CB	6.62	122.51	110.60
1	H	362	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	I	362	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	D	113	PRO	CA-N-CD	-6.61	102.25	111.50
1	C	113	PRO	CA-N-CD	-6.59	102.27	111.50
1	G	87	ASP	CB-CG-OD2	6.57	124.21	118.30
1	I	231	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	D	87	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	87	ASP	CB-CG-OD2	6.55	124.20	118.30
1	B	87	ASP	CB-CG-OD2	6.54	124.19	118.30
1	E	87	ASP	CB-CG-OD2	6.54	124.18	118.30
1	F	58	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	I	401	HIS	C-N-CA	-6.53	105.39	121.70
1	I	473	ASP	N-CA-CB	6.52	122.33	110.60
1	H	473	ASP	N-CA-CB	6.51	122.33	110.60
1	M	473	ASP	N-CA-CB	6.51	122.32	110.60
1	L	362	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	J	473	ASP	N-CA-CB	6.51	122.31	110.60
1	L	473	ASP	N-CA-CB	6.51	122.31	110.60
1	N	362	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	C	87	ASP	CB-CG-OD2	6.49	124.14	118.30
1	K	473	ASP	N-CA-CB	6.49	122.28	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	473	ASP	N-CA-CB	6.48	122.26	110.60
1	J	231	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	J	501	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	K	231	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	E	58	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	L	231	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	L	400	LEU	CA-C-N	6.41	131.30	117.20
1	N	231	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	H	231	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	I	501	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	J	395	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	D	482	THR	N-CA-CB	6.38	122.42	110.30
1	G	58	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	482	THR	N-CA-CB	6.38	122.42	110.30
1	E	482	THR	N-CA-CB	6.38	122.42	110.30
1	B	482	THR	N-CA-CB	6.37	122.41	110.30
1	B	58	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	F	482	THR	N-CA-CB	6.37	122.40	110.30
1	D	58	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	F	243	ALA	N-CA-CB	6.37	119.01	110.10
1	G	482	THR	N-CA-CB	6.36	122.38	110.30
1	J	362	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	H	501	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	M	501	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	C	482	THR	N-CA-CB	6.35	122.36	110.30
1	C	58	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	243	ALA	N-CA-CB	6.33	118.97	110.10
1	C	243	ALA	N-CA-CB	6.33	118.97	110.10
1	G	243	ALA	N-CA-CB	6.33	118.96	110.10
1	E	243	ALA	N-CA-CB	6.32	118.95	110.10
1	C	36	ARG	N-CA-CB	-6.32	99.23	110.60
1	B	243	ALA	N-CA-CB	6.31	118.93	110.10
1	A	58	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	B	36	ARG	N-CA-CB	-6.29	99.28	110.60
1	L	501	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	M	395	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	243	ALA	N-CA-CB	6.28	118.89	110.10
1	I	395	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	G	36	ARG	N-CA-CB	-6.27	99.31	110.60
1	D	36	ARG	N-CA-CB	-6.27	99.31	110.60
1	F	36	ARG	N-CA-CB	-6.27	99.32	110.60
1	A	36	ARG	N-CA-CB	-6.26	99.33	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	501	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	K	501	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	M	231	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	E	36	ARG	N-CA-CB	-6.24	99.36	110.60
1	H	395	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	H	2	ALA	CA-C-O	-6.21	107.05	120.10
1	D	520	MET	CG-SD-CE	-6.21	90.26	100.20
1	A	520	MET	CG-SD-CE	-6.21	90.27	100.20
1	F	520	MET	CG-SD-CE	-6.21	90.27	100.20
1	G	520	MET	CG-SD-CE	-6.19	90.29	100.20
1	N	395	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	B	41	ASP	CB-CA-C	6.19	122.78	110.40
1	E	41	ASP	CB-CA-C	6.19	122.78	110.40
1	K	395	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	F	41	ASP	CB-CA-C	6.19	122.78	110.40
1	L	395	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	520	MET	CG-SD-CE	-6.18	90.31	100.20
1	E	520	MET	CG-SD-CE	-6.18	90.31	100.20
1	G	353	ILE	CB-CA-C	-6.18	99.24	111.60
1	G	41	ASP	CB-CA-C	6.18	122.75	110.40
1	C	520	MET	CG-SD-CE	-6.17	90.33	100.20
1	C	41	ASP	CB-CA-C	6.17	122.74	110.40
1	A	353	ILE	CB-CA-C	-6.17	99.27	111.60
1	B	203	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	C	417	VAL	CA-CB-CG2	-6.17	101.65	110.90
1	C	353	ILE	CB-CA-C	-6.17	99.27	111.60
1	D	41	ASP	CB-CA-C	6.16	122.73	110.40
1	E	353	ILE	CB-CA-C	-6.16	99.28	111.60
1	F	353	ILE	CB-CA-C	-6.16	99.28	111.60
1	C	203	TYR	CB-CG-CD2	-6.16	117.31	121.00
1	G	417	VAL	CA-CB-CG2	-6.16	101.67	110.90
1	B	417	VAL	CA-CB-CG2	-6.15	101.67	110.90
1	A	41	ASP	CB-CA-C	6.15	122.70	110.40
1	B	353	ILE	CB-CA-C	-6.14	99.31	111.60
1	D	353	ILE	CB-CA-C	-6.14	99.32	111.60
1	A	391	GLU	N-CA-CB	6.14	121.64	110.60
1	F	391	GLU	N-CA-CB	6.14	121.65	110.60
1	B	391	GLU	N-CA-CB	6.13	121.64	110.60
1	C	168	LYS	N-CA-CB	-6.13	99.56	110.60
1	E	203	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	F	417	VAL	CA-CB-CG2	-6.13	101.71	110.90
1	A	417	VAL	CA-CB-CG2	-6.12	101.72	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	SER	CB-CA-C	6.12	121.72	110.10
1	A	139	SER	CB-CA-C	6.12	121.72	110.10
1	D	417	VAL	CA-CB-CG2	-6.12	101.72	110.90
1	C	391	GLU	N-CA-CB	6.12	121.61	110.60
1	E	417	VAL	CA-CB-CG2	-6.11	101.73	110.90
1	E	391	GLU	N-CA-CB	6.11	121.60	110.60
1	D	391	GLU	N-CA-CB	6.11	121.59	110.60
1	B	285	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	G	139	SER	CB-CA-C	6.11	121.70	110.10
1	A	203	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	G	285	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	G	391	GLU	N-CA-CB	6.10	121.58	110.60
1	H	5	ASP	N-CA-CB	6.10	121.57	110.60
1	F	139	SER	CB-CA-C	6.09	121.68	110.10
1	F	168	LYS	N-CA-CB	-6.09	99.63	110.60
1	A	285	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	168	LYS	N-CA-CB	-6.08	99.65	110.60
1	E	139	SER	CB-CA-C	6.08	121.65	110.10
1	K	285	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	203	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	E	168	LYS	N-CA-CB	-6.08	99.66	110.60
1	D	139	SER	CB-CA-C	6.07	121.64	110.10
1	L	285	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	L	5	ASP	N-CA-CB	6.07	121.52	110.60
1	A	168	LYS	N-CA-CB	-6.06	99.69	110.60
1	K	5	ASP	N-CA-CB	6.06	121.51	110.60
1	M	5	ASP	N-CA-CB	6.06	121.51	110.60
1	G	168	LYS	N-CA-CB	-6.06	99.69	110.60
1	N	5	ASP	N-CA-CB	6.06	121.51	110.60
1	A	141	SER	N-CA-CB	6.06	119.59	110.50
1	D	141	SER	N-CA-CB	6.06	119.58	110.50
1	B	139	SER	CB-CA-C	6.05	121.60	110.10
1	D	168	LYS	N-CA-CB	-6.05	99.70	110.60
1	I	285	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	F	141	SER	N-CA-CB	6.04	119.56	110.50
1	J	5	ASP	N-CA-CB	6.04	121.48	110.60
1	B	141	SER	N-CA-CB	6.04	119.56	110.50
1	E	294	THR	CA-CB-CG2	-6.04	103.94	112.40
1	F	203	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	G	141	SER	N-CA-CB	6.03	119.54	110.50
1	I	5	ASP	N-CA-CB	6.02	121.44	110.60
1	F	285	ARG	NE-CZ-NH1	6.02	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	H	285	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	141	SER	N-CA-CB	6.02	119.53	110.50
1	F	294	THR	CA-CB-CG2	-6.01	103.98	112.40
1	C	141	SER	N-CA-CB	6.00	119.50	110.50
1	E	285	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	294	THR	CA-CB-CG2	-6.00	104.00	112.40
1	I	196	ASP	N-CA-CB	-5.99	99.81	110.60
1	A	294	THR	CA-CB-CG2	-5.99	104.01	112.40
1	G	203	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	N	350	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	L	196	ASP	N-CA-CB	-5.99	99.83	110.60
1	M	196	ASP	N-CA-CB	-5.99	99.83	110.60
1	B	510	VAL	CB-CA-C	-5.98	100.03	111.40
1	K	196	ASP	N-CA-CB	-5.98	99.84	110.60
1	A	523	ASP	N-CA-CB	5.98	121.36	110.60
1	J	196	ASP	N-CA-CB	-5.98	99.84	110.60
1	C	294	THR	CA-CB-CG2	-5.97	104.04	112.40
1	G	294	THR	CA-CB-CG2	-5.97	104.04	112.40
1	H	196	ASP	N-CA-CB	-5.97	99.85	110.60
1	H	350	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	N	196	ASP	N-CA-CB	-5.96	99.87	110.60
1	C	510	VAL	CB-CA-C	-5.95	100.09	111.40
1	D	510	VAL	CB-CA-C	-5.95	100.09	111.40
1	J	285	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	M	285	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	G	510	VAL	CB-CA-C	-5.95	100.10	111.40
1	E	510	VAL	CB-CA-C	-5.95	100.10	111.40
1	A	510	VAL	CB-CA-C	-5.94	100.11	111.40
1	D	523	ASP	N-CA-CB	5.94	121.29	110.60
1	G	412	VAL	CB-CA-C	-5.94	100.12	111.40
1	B	294	THR	CA-CB-CG2	-5.93	104.09	112.40
1	B	523	ASP	N-CA-CB	5.92	121.26	110.60
1	F	510	VAL	CB-CA-C	-5.92	100.16	111.40
1	C	523	ASP	N-CA-CB	5.91	121.25	110.60
1	K	350	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	B	412	VAL	CB-CA-C	-5.91	100.18	111.40
1	D	412	VAL	CB-CA-C	-5.91	100.18	111.40
1	E	412	VAL	CB-CA-C	-5.90	100.19	111.40
1	F	412	VAL	CB-CA-C	-5.90	100.19	111.40
1	M	350	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	J	350	ARG	NE-CZ-NH1	5.89	123.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	THR	N-CA-CB	5.88	121.48	110.30
1	A	412	VAL	CB-CA-C	-5.88	100.22	111.40
1	F	149	THR	N-CA-CB	5.88	121.47	110.30
1	C	412	VAL	CB-CA-C	-5.87	100.25	111.40
1	D	285	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	149	THR	N-CA-CB	5.86	121.44	110.30
1	C	149	THR	N-CA-CB	5.86	121.44	110.30
1	D	149	THR	N-CA-CB	5.86	121.44	110.30
1	I	350	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	G	149	THR	N-CA-CB	5.86	121.44	110.30
1	B	149	THR	N-CA-CB	5.86	121.42	110.30
1	N	285	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	N	267	MET	N-CA-CB	-5.85	100.08	110.60
1	L	350	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	K	267	MET	CA-CB-CG	5.83	123.21	113.30
1	K	267	MET	N-CA-CB	-5.82	100.12	110.60
1	D	138	CYS	N-CA-CB	5.80	121.03	110.60
1	N	267	MET	CA-CB-CG	5.80	123.15	113.30
1	F	87	ASP	OD1-CG-OD2	-5.79	112.30	123.30
1	G	138	CYS	N-CA-CB	5.79	121.02	110.60
1	A	37	ASN	CA-C-N	-5.79	104.47	117.20
1	B	85	ALA	N-CA-CB	-5.78	102.00	110.10
1	D	87	ASP	OD1-CG-OD2	-5.78	112.31	123.30
1	C	85	ALA	N-CA-CB	-5.78	102.00	110.10
1	G	37	ASN	CA-C-N	-5.78	104.49	117.20
1	B	87	ASP	OD1-CG-OD2	-5.78	112.33	123.30
1	C	37	ASN	CA-C-N	-5.77	104.50	117.20
1	E	87	ASP	OD1-CG-OD2	-5.77	112.33	123.30
1	A	87	ASP	OD1-CG-OD2	-5.77	112.34	123.30
1	E	138	CYS	N-CA-CB	5.77	120.98	110.60
1	E	85	ALA	N-CA-CB	-5.77	102.03	110.10
1	D	37	ASN	CA-C-N	-5.76	104.52	117.20
1	F	37	ASN	CA-C-N	-5.76	104.52	117.20
1	B	138	CYS	N-CA-CB	5.76	120.97	110.60
1	F	138	CYS	N-CA-CB	5.76	120.97	110.60
1	E	37	ASN	CA-C-N	-5.76	104.53	117.20
1	F	85	ALA	N-CA-CB	-5.76	102.04	110.10
1	A	85	ALA	N-CA-CB	-5.75	102.04	110.10
1	A	138	CYS	N-CA-CB	5.75	120.96	110.60
1	D	85	ALA	N-CA-CB	-5.75	102.05	110.10
1	C	87	ASP	OD1-CG-OD2	-5.75	112.38	123.30
1	C	321	LYS	CB-CA-C	5.75	121.89	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ASN	CA-C-N	-5.74	104.57	117.20
1	E	321	LYS	CB-CA-C	5.74	121.88	110.40
1	G	321	LYS	CB-CA-C	5.74	121.88	110.40
1	D	321	LYS	CB-CA-C	5.74	121.87	110.40
1	G	87	ASP	OD1-CG-OD2	-5.73	112.42	123.30
1	A	321	LYS	CB-CA-C	5.73	121.85	110.40
1	B	321	LYS	CB-CA-C	5.72	121.85	110.40
1	C	138	CYS	N-CA-CB	5.72	120.90	110.60
1	G	85	ALA	N-CA-CB	-5.72	102.09	110.10
1	F	321	LYS	CB-CA-C	5.72	121.84	110.40
1	G	155	ASP	CB-CA-C	5.71	121.82	110.40
1	N	2	ALA	CA-C-O	5.71	132.08	120.10
1	A	371	LYS	CB-CA-C	5.70	121.80	110.40
1	F	155	ASP	CB-CA-C	5.69	121.78	110.40
1	B	155	ASP	CB-CA-C	5.69	121.78	110.40
1	D	155	ASP	CB-CA-C	5.69	121.78	110.40
1	A	155	ASP	CB-CA-C	5.68	121.77	110.40
1	C	155	ASP	CB-CA-C	5.68	121.77	110.40
1	J	59	GLU	CB-CA-C	5.68	121.76	110.40
1	B	371	LYS	CB-CA-C	5.68	121.75	110.40
1	E	155	ASP	CB-CA-C	5.68	121.75	110.40
1	F	371	LYS	CB-CA-C	5.68	121.75	110.40
1	L	59	GLU	CB-CA-C	5.66	121.73	110.40
1	E	371	LYS	CB-CA-C	5.66	121.72	110.40
1	H	59	GLU	CB-CA-C	5.66	121.71	110.40
1	M	59	GLU	CB-CA-C	5.66	121.71	110.40
1	D	371	LYS	CB-CA-C	5.65	121.71	110.40
1	G	371	LYS	CB-CA-C	5.65	121.69	110.40
1	K	59	GLU	CB-CA-C	5.65	121.69	110.40
1	C	166	MET	CG-SD-CE	-5.64	91.17	100.20
1	E	43	SER	N-CA-CB	5.64	118.97	110.50
1	C	371	LYS	CB-CA-C	5.64	121.67	110.40
1	I	59	GLU	CB-CA-C	5.63	121.67	110.40
1	N	61	GLU	N-CA-CB	-5.63	100.46	110.60
1	D	166	MET	CG-SD-CE	-5.61	91.22	100.20
1	N	2	ALA	CA-C-N	-5.61	104.86	117.20
1	E	166	MET	CG-SD-CE	-5.60	91.23	100.20
1	B	166	MET	CG-SD-CE	-5.60	91.24	100.20
1	D	43	SER	N-CA-CB	5.60	118.90	110.50
1	F	166	MET	CG-SD-CE	-5.60	91.24	100.20
1	G	166	MET	CG-SD-CE	-5.59	91.25	100.20
1	L	285	ARG	NE-CZ-NH2	-5.59	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	VAL	N-CA-CB	5.59	123.79	111.50
1	B	43	SER	N-CA-CB	5.59	118.88	110.50
1	M	401	HIS	C-N-CA	-5.58	107.74	121.70
1	L	463	SER	N-CA-CB	-5.58	102.12	110.50
1	E	369	VAL	N-CA-CB	5.58	123.77	111.50
1	J	463	SER	N-CA-CB	-5.57	102.14	110.50
1	A	166	MET	CG-SD-CE	-5.57	91.29	100.20
1	C	43	SER	N-CA-CB	5.57	118.85	110.50
1	A	126	ALA	CB-CA-C	5.56	118.44	110.10
1	I	463	SER	N-CA-CB	-5.56	102.16	110.50
1	D	126	ALA	CB-CA-C	5.56	118.44	110.10
1	A	369	VAL	N-CA-CB	5.56	123.72	111.50
1	M	463	SER	N-CA-CB	-5.56	102.17	110.50
1	N	463	SER	N-CA-CB	-5.55	102.17	110.50
1	B	73	MET	CB-CA-C	-5.55	99.30	110.40
1	F	369	VAL	N-CA-CB	5.55	123.71	111.50
1	H	463	SER	N-CA-CB	-5.55	102.18	110.50
1	B	369	VAL	N-CA-CB	5.55	123.70	111.50
1	D	73	MET	CB-CA-C	-5.55	99.31	110.40
1	B	203	TYR	CB-CG-CD1	5.54	124.33	121.00
1	N	59	GLU	CB-CA-C	5.54	121.48	110.40
1	K	463	SER	N-CA-CB	-5.54	102.19	110.50
1	F	126	ALA	CB-CA-C	5.54	118.40	110.10
1	G	73	MET	CB-CA-C	-5.53	99.33	110.40
1	E	73	MET	CB-CA-C	-5.53	99.34	110.40
1	C	369	VAL	N-CA-CB	5.53	123.66	111.50
1	G	126	ALA	CB-CA-C	5.53	118.39	110.10
1	C	73	MET	CB-CA-C	-5.52	99.36	110.40
1	E	126	ALA	CB-CA-C	5.52	118.38	110.10
1	A	73	MET	CB-CA-C	-5.52	99.36	110.40
1	B	126	ALA	CB-CA-C	5.52	118.38	110.10
1	F	73	MET	CB-CA-C	-5.51	99.37	110.40
1	G	369	VAL	N-CA-CB	5.51	123.62	111.50
1	C	126	ALA	CB-CA-C	5.51	118.36	110.10
1	K	285	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	D	203	TYR	CB-CG-CD1	5.49	124.30	121.00
1	I	285	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	C	203	TYR	CB-CG-CD1	5.48	124.29	121.00
1	G	203	TYR	CB-CG-CD1	5.47	124.28	121.00
1	F	400	LEU	O-C-N	-5.46	113.96	122.70
1	G	369	VAL	CB-CA-C	-5.46	101.03	111.40
1	F	369	VAL	CB-CA-C	-5.46	101.03	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	285	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	E	203	TYR	CB-CG-CD1	5.45	124.27	121.00
1	A	369	VAL	CB-CA-C	-5.45	101.05	111.40
1	B	369	VAL	CB-CA-C	-5.44	101.06	111.40
1	N	118	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	C	369	VAL	CB-CA-C	-5.43	101.08	111.40
1	M	61	GLU	N-CA-CB	-5.43	100.83	110.60
1	D	369	VAL	CB-CA-C	-5.42	101.09	111.40
1	E	369	VAL	CB-CA-C	-5.42	101.10	111.40
1	K	294	THR	CA-CB-CG2	-5.41	104.82	112.40
1	A	203	TYR	CB-CG-CD1	5.41	124.25	121.00
1	N	285	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	H	294	THR	CA-CB-CG2	-5.40	104.84	112.40
1	I	294	THR	CA-CB-CG2	-5.40	104.84	112.40
1	L	294	THR	CA-CB-CG2	-5.40	104.84	112.40
1	H	285	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	H	118	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	M	285	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	J	294	THR	CA-CB-CG2	-5.38	104.87	112.40
1	M	294	THR	CA-CB-CG2	-5.38	104.88	112.40
1	F	203	TYR	CB-CG-CD1	5.37	124.22	121.00
1	N	294	THR	CA-CB-CG2	-5.36	104.90	112.40
1	M	258	ALA	CB-CA-C	5.36	118.13	110.10
1	K	258	ALA	CB-CA-C	5.35	118.13	110.10
1	H	258	ALA	CB-CA-C	5.35	118.12	110.10
1	J	118	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	M	118	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	190	VAL	CB-CA-C	5.34	121.54	111.40
1	K	118	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	I	118	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	E	87	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	87	ASP	CB-CG-OD1	5.33	123.10	118.30
1	G	190	VAL	CB-CA-C	5.33	121.52	111.40
1	D	87	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	87	ASP	CB-CG-OD1	5.31	123.08	118.30
1	F	190	VAL	CB-CA-C	5.31	121.49	111.40
1	D	196	ASP	N-CA-CB	-5.30	101.05	110.60
1	A	87	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	190	VAL	CB-CA-C	5.30	121.46	111.40
1	F	267	MET	CG-SD-CE	-5.29	91.73	100.20
1	C	190	VAL	CB-CA-C	5.29	121.45	111.40
1	G	196	ASP	N-CA-CB	-5.29	101.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	118	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	368	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	196	ASP	N-CA-CB	-5.28	101.09	110.60
1	E	196	ASP	N-CA-CB	-5.28	101.10	110.60
1	F	196	ASP	N-CA-CB	-5.28	101.10	110.60
1	C	196	ASP	N-CA-CB	-5.28	101.10	110.60
1	A	190	VAL	CB-CA-C	5.28	121.42	111.40
1	B	196	ASP	N-CA-CB	-5.28	101.11	110.60
1	D	69	MET	CG-SD-CE	-5.26	91.78	100.20
1	G	69	MET	CG-SD-CE	-5.26	91.78	100.20
1	B	69	MET	CG-SD-CE	-5.26	91.78	100.20
1	B	268	ARG	CB-CA-C	5.26	120.92	110.40
1	F	87	ASP	CB-CG-OD1	5.26	123.03	118.30
1	N	267	MET	CB-CA-C	5.26	120.92	110.40
1	I	258	ALA	CB-CA-C	5.26	117.99	110.10
1	E	190	VAL	CB-CA-C	5.26	121.39	111.40
1	E	368	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	K	267	MET	CB-CA-C	5.25	120.89	110.40
1	A	69	MET	CG-SD-CE	-5.25	91.81	100.20
1	E	69	MET	CG-SD-CE	-5.24	91.82	100.20
1	E	268	ARG	CB-CA-C	5.23	120.86	110.40
1	F	268	ARG	CB-CA-C	5.23	120.86	110.40
1	G	368	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	320	ALA	N-CA-CB	5.22	117.42	110.10
1	C	268	ARG	CB-CA-C	5.22	120.85	110.40
1	E	193	MET	N-CA-CB	-5.22	101.21	110.60
1	E	320	ALA	N-CA-CB	5.22	117.41	110.10
1	F	69	MET	CG-SD-CE	-5.21	91.86	100.20
1	B	368	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	69	MET	CG-SD-CE	-5.21	91.87	100.20
1	D	104	LEU	CB-CA-C	5.20	120.08	110.20
1	F	320	ALA	N-CA-CB	5.20	117.38	110.10
1	B	193	MET	N-CA-CB	-5.20	101.25	110.60
1	C	193	MET	N-CA-CB	-5.19	101.25	110.60
1	E	104	LEU	CB-CA-C	5.19	120.07	110.20
1	G	87	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	193	MET	N-CA-CB	-5.19	101.26	110.60
1	A	193	MET	N-CA-CB	-5.18	101.27	110.60
1	F	193	MET	N-CA-CB	-5.18	101.27	110.60
1	L	61	GLU	N-CA-CB	-5.18	101.27	110.60
1	G	320	ALA	N-CA-CB	5.18	117.35	110.10
1	D	268	ARG	CB-CA-C	5.18	120.75	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	LEU	CB-CA-C	5.17	120.03	110.20
1	A	268	ARG	CB-CA-C	5.17	120.75	110.40
1	A	320	ALA	N-CA-CB	5.17	117.34	110.10
1	F	104	LEU	CB-CA-C	5.17	120.02	110.20
1	F	300	VAL	CB-CA-C	-5.17	101.58	111.40
1	G	193	MET	N-CA-CB	-5.17	101.30	110.60
1	B	104	LEU	CB-CA-C	5.17	120.02	110.20
1	D	284	ARG	CB-CA-C	-5.17	100.07	110.40
1	D	320	ALA	N-CA-CB	5.17	117.33	110.10
1	A	284	ARG	CB-CA-C	-5.16	100.07	110.40
1	B	36	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	G	104	LEU	CB-CA-C	5.16	120.00	110.20
1	F	284	ARG	CB-CA-C	-5.16	100.08	110.40
1	B	300	VAL	CB-CA-C	-5.16	101.60	111.40
1	C	320	ALA	N-CA-CB	5.16	117.32	110.10
1	G	284	ARG	CB-CA-C	-5.16	100.08	110.40
1	B	284	ARG	CB-CA-C	-5.15	100.09	110.40
1	E	300	VAL	CB-CA-C	-5.15	101.62	111.40
1	C	104	LEU	CB-CA-C	5.15	119.98	110.20
1	G	300	VAL	CB-CA-C	-5.15	101.62	111.40
1	C	284	ARG	CB-CA-C	-5.14	100.11	110.40
1	A	368	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	F	206	ASN	N-CA-CB	5.14	119.84	110.60
1	I	231	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	N	400	LEU	O-C-N	-5.13	114.49	122.70
1	D	284	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	300	VAL	CB-CA-C	-5.13	101.66	111.40
1	D	300	VAL	CB-CA-C	-5.13	101.66	111.40
1	C	300	VAL	CB-CA-C	-5.12	101.66	111.40
1	E	284	ARG	CB-CA-C	-5.12	100.16	110.40
1	C	206	ASN	N-CA-CB	5.12	119.81	110.60
1	G	206	ASN	N-CA-CB	5.12	119.81	110.60
1	E	206	ASN	N-CA-CB	5.11	119.81	110.60
1	N	258	ALA	CB-CA-C	5.11	117.77	110.10
1	A	206	ASN	N-CA-CB	5.11	119.80	110.60
1	F	368	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	F	361	ASP	CB-CA-C	5.11	120.62	110.40
1	D	361	ASP	CB-CA-C	5.10	120.60	110.40
1	A	36	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	206	ASN	N-CA-CB	5.09	119.77	110.60
1	C	368	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	J	386	GLU	CB-CA-C	-5.09	100.23	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	36	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	361	ASP	CB-CA-C	5.08	120.56	110.40
1	G	361	ASP	CB-CA-C	5.08	120.55	110.40
1	J	258	ALA	CB-CA-C	5.08	117.71	110.10
1	I	61	GLU	N-CA-CB	-5.07	101.47	110.60
1	A	361	ASP	CB-CA-C	5.07	120.54	110.40
1	M	386	GLU	CB-CA-C	-5.07	100.26	110.40
1	E	361	ASP	CB-CA-C	5.07	120.53	110.40
1	K	386	GLU	CB-CA-C	-5.07	100.27	110.40
1	D	206	ASN	N-CA-CB	5.07	119.72	110.60
1	C	361	ASP	CB-CA-C	5.06	120.52	110.40
1	D	167	ASP	CB-CA-C	5.06	120.51	110.40
1	G	268	ARG	CB-CA-C	5.05	120.51	110.40
1	I	386	GLU	CB-CA-C	-5.05	100.30	110.40
1	H	386	GLU	CB-CA-C	-5.05	100.30	110.40
1	N	386	GLU	CB-CA-C	-5.05	100.30	110.40
1	B	167	ASP	CB-CA-C	5.04	120.49	110.40
1	G	167	ASP	CB-CA-C	5.04	120.49	110.40
1	F	36	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	F	167	ASP	CB-CA-C	5.03	120.47	110.40
1	C	167	ASP	CB-CA-C	5.03	120.45	110.40
1	L	386	GLU	CB-CA-C	-5.03	100.35	110.40
1	E	167	ASP	CB-CA-C	5.02	120.45	110.40
1	E	36	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	167	ASP	CB-CA-C	5.02	120.44	110.40
1	G	284	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	D	36	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	L	258	ALA	CB-CA-C	5.01	117.61	110.10
1	D	8	PHE	CB-CA-C	-5.00	100.39	110.40

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	257	GLU	CA
1	B	257	GLU	CA
1	C	257	GLU	CA
1	D	257	GLU	CA
1	E	257	GLU	CA
1	F	257	GLU	CA
1	G	257	GLU	CA

All (137) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain
1	A	197	ARG	Sidechain
1	A	231	ARG	Sidechain
1	A	268	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	362	ARG	Sidechain
1	A	37	ASN	Mainchain
1	A	395	ARG	Sidechain
1	A	404	ARG	Sidechain
1	A	50	THR	Mainchain
1	B	118	ARG	Sidechain
1	B	197	ARG	Sidechain
1	B	231	ARG	Sidechain
1	B	268	ARG	Sidechain
1	B	350	ARG	Sidechain
1	B	362	ARG	Sidechain
1	B	37	ASN	Mainchain
1	B	395	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	50	THR	Mainchain
1	C	118	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	231	ARG	Sidechain
1	C	268	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	362	ARG	Sidechain
1	C	37	ASN	Mainchain
1	C	395	ARG	Sidechain
1	C	404	ARG	Sidechain
1	C	50	THR	Mainchain
1	D	118	ARG	Sidechain
1	D	197	ARG	Sidechain
1	D	231	ARG	Sidechain
1	D	268	ARG	Sidechain
1	D	350	ARG	Sidechain
1	D	362	ARG	Sidechain
1	D	37	ASN	Mainchain
1	D	395	ARG	Sidechain
1	D	404	ARG	Sidechain
1	D	50	THR	Mainchain
1	E	118	ARG	Sidechain
1	E	197	ARG	Sidechain
1	E	231	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	268	ARG	Sidechain
1	E	350	ARG	Sidechain
1	E	362	ARG	Sidechain
1	E	37	ASN	Mainchain
1	E	395	ARG	Sidechain
1	E	404	ARG	Sidechain
1	E	50	THR	Mainchain
1	F	118	ARG	Sidechain
1	F	197	ARG	Sidechain
1	F	231	ARG	Sidechain
1	F	268	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	362	ARG	Sidechain
1	F	37	ASN	Mainchain
1	F	395	ARG	Sidechain
1	F	404	ARG	Sidechain
1	F	50	THR	Mainchain
1	G	118	ARG	Sidechain
1	G	197	ARG	Sidechain
1	G	231	ARG	Sidechain
1	G	268	ARG	Sidechain
1	G	350	ARG	Sidechain
1	G	362	ARG	Sidechain
1	G	37	ASN	Mainchain
1	G	395	ARG	Sidechain
1	G	404	ARG	Sidechain
1	G	50	THR	Mainchain
1	H	197	ARG	Sidechain
1	H	2	ALA	Mainchain,Peptide
1	H	231	ARG	Sidechain
1	H	281	PHE	Sidechain
1	H	284	ARG	Sidechain
1	H	350	ARG	Sidechain
1	H	362	ARG	Sidechain
1	H	421	ARG	Sidechain
1	H	445	ARG	Sidechain
1	H	478	TYR	Sidechain
1	I	197	ARG	Sidechain
1	I	231	ARG	Sidechain
1	I	281	PHE	Sidechain
1	I	284	ARG	Sidechain
1	I	350	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	362	ARG	Sidechain
1	I	421	ARG	Sidechain
1	I	445	ARG	Sidechain
1	I	478	TYR	Sidechain
1	J	197	ARG	Sidechain
1	J	231	ARG	Sidechain
1	J	281	PHE	Sidechain
1	J	284	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	197	ARG	Sidechain
1	K	231	ARG	Sidechain
1	K	281	PHE	Sidechain
1	K	284	ARG	Sidechain
1	K	350	ARG	Sidechain
1	K	362	ARG	Sidechain
1	K	401	HIS	Mainchain
1	K	421	ARG	Sidechain
1	K	445	ARG	Sidechain
1	K	478	TYR	Sidechain
1	L	197	ARG	Sidechain
1	L	231	ARG	Sidechain
1	L	281	PHE	Sidechain
1	L	284	ARG	Sidechain
1	L	350	ARG	Sidechain
1	L	362	ARG	Sidechain
1	L	421	ARG	Sidechain
1	L	445	ARG	Sidechain
1	L	478	TYR	Sidechain
1	M	197	ARG	Sidechain
1	M	231	ARG	Sidechain
1	M	281	PHE	Sidechain
1	M	284	ARG	Sidechain
1	M	350	ARG	Sidechain
1	M	362	ARG	Sidechain
1	M	401	HIS	Mainchain
1	M	421	ARG	Sidechain
1	M	445	ARG	Sidechain
1	M	478	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	N	197	ARG	Sidechain
1	N	231	ARG	Sidechain
1	N	281	PHE	Sidechain
1	N	284	ARG	Sidechain
1	N	350	ARG	Sidechain
1	N	362	ARG	Sidechain
1	N	421	ARG	Sidechain
1	N	445	ARG	Sidechain
1	N	478	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3846	0	3970	102	0
1	B	3846	0	3970	101	0
1	C	3846	0	3970	103	0
1	D	3846	0	3970	103	0
1	E	3846	0	3970	101	0
1	F	3846	0	3970	99	0
1	G	3846	0	3970	105	0
1	H	3846	0	3970	31	0
1	I	3846	0	3969	32	0
1	J	3846	0	3970	29	0
1	K	3846	0	3969	31	0
1	L	3846	0	3970	29	0
1	M	3846	0	3968	29	0
1	N	3846	0	3969	34	0
2	A	31	12	12	4	0
2	B	31	12	12	4	0
2	C	31	12	12	4	0
2	D	31	12	12	4	0
2	E	31	12	12	4	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	5	0
3	C	1	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	5	0
3	E	1	0	0	5	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	55659	887	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 8.

All (887) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:ALA:N	1:H:2:ALA:CA	1.73	1.51
1:H:2:ALA:C	1:H:2:ALA:CA	1.77	1.49
1:I:2:ALA:N	1:I:2:ALA:CA	1.79	1.45
1:N:2:ALA:CA	1:N:2:ALA:N	1.80	1.44
1:N:401:HIS:C	1:N:402:ALA:N	1.70	1.43
1:I:400:LEU:C	1:I:401:HIS:N	1.77	1.35
1:K:400:LEU:C	1:K:401:HIS:N	1.81	1.32
1:M:400:LEU:C	1:M:401:HIS:N	1.86	1.29
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.45	0.96
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.45	0.96
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.45	0.95
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.45	0.94
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.45	0.94
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.45	0.94
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.45	0.94
1:F:183:LEU:O	1:F:382:GLY:HA3	1.82	0.80
1:G:183:LEU:O	1:G:382:GLY:HA3	1.82	0.79
1:A:183:LEU:O	1:A:382:GLY:HA3	1.82	0.79
1:B:183:LEU:O	1:B:382:GLY:HA3	1.82	0.79
1:D:183:LEU:O	1:D:382:GLY:HA3	1.82	0.79
1:C:183:LEU:O	1:C:382:GLY:HA3	1.82	0.79
1:E:183:LEU:O	1:E:382:GLY:HA3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:HA	1:A:412:VAL:HG12	1.66	0.78
1:G:135:SER:HA	1:G:412:VAL:HG12	1.66	0.78
1:B:135:SER:HA	1:B:412:VAL:HG12	1.67	0.77
1:C:135:SER:HA	1:C:412:VAL:HG12	1.67	0.77
1:F:135:SER:HA	1:F:412:VAL:HG12	1.66	0.77
1:E:135:SER:HA	1:E:412:VAL:HG12	1.66	0.76
1:B:192:GLY:O	1:B:375:GLY:HA2	1.85	0.76
1:E:192:GLY:O	1:E:375:GLY:HA2	1.85	0.76
1:C:192:GLY:O	1:C:375:GLY:HA2	1.85	0.76
1:D:135:SER:HA	1:D:412:VAL:HG12	1.67	0.76
1:F:192:GLY:O	1:F:375:GLY:HA2	1.85	0.76
1:G:192:GLY:O	1:G:375:GLY:HA2	1.85	0.76
1:D:192:GLY:O	1:D:375:GLY:HA2	1.85	0.75
1:D:199:TYR:CD2	1:D:205:ILE:HD11	2.21	0.75
1:C:199:TYR:CD2	1:C:205:ILE:HD11	2.21	0.75
1:G:199:TYR:CD2	1:G:205:ILE:HD11	2.21	0.75
1:A:192:GLY:O	1:A:375:GLY:HA2	1.85	0.75
1:A:199:TYR:CD2	1:A:205:ILE:HD11	2.21	0.75
1:E:199:TYR:CD2	1:E:205:ILE:HD11	2.21	0.75
1:B:199:TYR:CD2	1:B:205:ILE:HD11	2.21	0.74
1:F:199:TYR:CD2	1:F:205:ILE:HD11	2.21	0.74
3:G:1525:PO4:P	2:G:1527:ATP:O1G	2.47	0.73
3:E:1526:PO4:P	2:E:1527:ATP:O1G	2.47	0.73
3:F:1525:PO4:P	2:F:1527:ATP:O1G	2.47	0.73
2:C:1526:ATP:O1G	3:C:1527:PO4:P	2.47	0.72
2:B:1525:ATP:O1G	3:B:1526:PO4:P	2.47	0.72
2:D:1525:ATP:O1G	3:D:1526:PO4:P	2.47	0.72
1:I:2:ALA:N	1:I:2:ALA:C	2.43	0.72
1:H:2:ALA:N	1:H:2:ALA:C	2.43	0.72
2:A:1525:ATP:O1G	3:A:1526:PO4:P	2.47	0.72
1:N:2:ALA:C	1:N:2:ALA:N	2.43	0.71
2:B:1525:ATP:O1A	3:B:1526:PO4:P	2.50	0.70
3:G:1525:PO4:P	2:G:1527:ATP:O1A	2.50	0.70
2:D:1525:ATP:O1A	3:D:1526:PO4:P	2.50	0.70
3:E:1526:PO4:P	2:E:1527:ATP:O1A	2.50	0.70
2:C:1526:ATP:O1A	3:C:1527:PO4:P	2.50	0.69
3:F:1525:PO4:P	2:F:1527:ATP:O1A	2.49	0.69
1:B:198:GLY:HA2	1:B:327:LYS:O	1.93	0.69
1:A:198:GLY:HA2	1:A:327:LYS:O	1.93	0.69
2:A:1525:ATP:O1A	3:A:1526:PO4:P	2.50	0.69
1:E:198:GLY:HA2	1:E:327:LYS:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:198:GLY:HA2	1:G:327:LYS:O	1.93	0.69
1:C:198:GLY:HA2	1:C:327:LYS:O	1.93	0.69
1:L:181:THR:O	1:M:283:ASP:N	2.26	0.69
1:M:181:THR:O	1:N:283:ASP:N	2.26	0.69
1:E:127:ALA:HB2	1:E:426:LEU:HD11	1.75	0.69
1:D:198:GLY:HA2	1:D:327:LYS:O	1.93	0.68
1:F:127:ALA:HB2	1:F:426:LEU:HD11	1.75	0.68
1:C:127:ALA:HB2	1:C:426:LEU:HD11	1.75	0.68
1:F:138:CYS:N	1:F:410:GLY:HA2	2.09	0.68
1:G:138:CYS:N	1:G:410:GLY:HA2	2.09	0.68
1:E:138:CYS:N	1:E:410:GLY:HA2	2.08	0.68
1:I:181:THR:O	1:J:283:ASP:N	2.26	0.68
1:A:138:CYS:N	1:A:410:GLY:HA2	2.09	0.68
1:D:138:CYS:N	1:D:410:GLY:HA2	2.09	0.68
1:D:127:ALA:HB2	1:D:426:LEU:HD11	1.76	0.68
1:F:198:GLY:HA2	1:F:327:LYS:O	1.93	0.68
1:C:138:CYS:N	1:C:410:GLY:HA2	2.09	0.68
1:J:181:THR:O	1:K:283:ASP:N	2.26	0.68
1:B:138:CYS:N	1:B:410:GLY:HA2	2.08	0.68
1:G:127:ALA:HB2	1:G:426:LEU:HD11	1.75	0.67
1:E:191:GLU:O	1:E:334:ASP:HA	1.95	0.67
1:K:181:THR:O	1:L:283:ASP:N	2.26	0.67
1:D:191:GLU:O	1:D:334:ASP:HA	1.95	0.67
1:B:127:ALA:HB2	1:B:426:LEU:HD11	1.75	0.67
1:H:283:ASP:N	1:N:181:THR:O	2.26	0.67
1:A:127:ALA:HB2	1:A:426:LEU:HD11	1.75	0.67
1:F:191:GLU:O	1:F:334:ASP:HA	1.95	0.67
1:H:181:THR:O	1:I:283:ASP:N	2.26	0.67
1:C:191:GLU:O	1:C:334:ASP:HA	1.95	0.67
1:G:214:GLU:HA	1:G:323:VAL:O	1.95	0.66
1:E:214:GLU:HA	1:E:323:VAL:O	1.95	0.66
1:G:191:GLU:O	1:G:334:ASP:HA	1.95	0.66
1:B:214:GLU:HA	1:B:323:VAL:O	1.95	0.66
1:D:27:VAL:HG12	1:D:90:THR:CG2	2.25	0.66
1:A:214:GLU:HA	1:A:323:VAL:O	1.95	0.66
1:D:214:GLU:HA	1:D:323:VAL:O	1.95	0.66
1:K:223:ALA:O	1:K:251:ALA:HA	1.96	0.66
1:A:138:CYS:CB	1:A:407:VAL:HA	2.26	0.66
1:C:214:GLU:HA	1:C:323:VAL:O	1.95	0.66
1:I:223:ALA:O	1:I:251:ALA:HA	1.96	0.66
1:B:138:CYS:CB	1:B:407:VAL:HA	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:VAL:HG12	1:E:90:THR:CG2	2.25	0.65
1:F:138:CYS:CB	1:F:407:VAL:HA	2.26	0.65
1:D:138:CYS:CB	1:D:407:VAL:HA	2.26	0.65
1:L:223:ALA:O	1:L:251:ALA:HA	1.96	0.65
1:M:223:ALA:O	1:M:251:ALA:HA	1.96	0.65
1:J:223:ALA:O	1:J:251:ALA:HA	1.96	0.65
1:E:138:CYS:CB	1:E:407:VAL:HA	2.26	0.65
1:B:191:GLU:O	1:B:334:ASP:HA	1.95	0.65
1:A:191:GLU:O	1:A:334:ASP:HA	1.95	0.65
1:F:214:GLU:HA	1:F:323:VAL:O	1.95	0.65
1:F:27:VAL:HG12	1:F:90:THR:CG2	2.25	0.65
1:C:138:CYS:CB	1:C:407:VAL:HA	2.26	0.65
1:N:223:ALA:O	1:N:251:ALA:HA	1.96	0.65
1:H:223:ALA:O	1:H:251:ALA:HA	1.96	0.65
1:G:138:CYS:CB	1:G:407:VAL:HA	2.26	0.64
1:E:138:CYS:HB2	1:E:407:VAL:HA	1.81	0.63
1:G:27:VAL:HG12	1:G:90:THR:CG2	2.25	0.63
1:D:138:CYS:HB2	1:D:407:VAL:HA	1.81	0.63
1:B:31:LEU:HB3	1:B:90:THR:HG21	1.81	0.62
1:A:31:LEU:HB3	1:A:90:THR:HG21	1.81	0.62
1:C:31:LEU:HB3	1:C:90:THR:HG21	1.81	0.62
1:D:31:LEU:HB3	1:D:90:THR:HG21	1.81	0.62
1:F:138:CYS:HB2	1:F:407:VAL:HA	1.81	0.62
1:C:138:CYS:HB2	1:C:407:VAL:HA	1.81	0.62
1:B:138:CYS:HB2	1:B:407:VAL:HA	1.81	0.62
1:G:31:LEU:HB3	1:G:90:THR:HG21	1.82	0.62
1:E:31:LEU:HB3	1:E:90:THR:HG21	1.81	0.62
1:F:31:LEU:HB3	1:F:90:THR:HG21	1.81	0.62
1:A:180:GLY:HA2	1:A:380:LYS:HB3	1.82	0.62
1:G:138:CYS:HB2	1:G:407:VAL:HA	1.81	0.61
1:H:2:ALA:O	1:H:2:ALA:CA	2.43	0.61
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.82	0.61
1:A:138:CYS:HB2	1:A:407:VAL:HA	1.81	0.61
1:G:180:GLY:HA2	1:G:380:LYS:HB3	1.82	0.61
1:A:27:VAL:HG12	1:A:90:THR:CG2	2.25	0.61
1:D:180:GLY:HA2	1:D:380:LYS:HB3	1.82	0.60
1:C:180:GLY:HA2	1:C:380:LYS:HB3	1.82	0.60
1:A:417:VAL:HG21	1:A:477:GLY:HA3	1.84	0.60
1:G:417:VAL:HG21	1:G:477:GLY:HA3	1.84	0.60
1:F:180:GLY:HA2	1:F:380:LYS:HB3	1.82	0.60
1:C:27:VAL:HG12	1:C:90:THR:CG2	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:VAL:HG21	1:B:477:GLY:HA3	1.84	0.60
1:D:417:VAL:HG21	1:D:477:GLY:HA3	1.84	0.59
1:E:180:GLY:HA2	1:E:380:LYS:HB3	1.82	0.59
1:A:60:ILE:HD12	1:G:6:VAL:HG11	1.85	0.59
1:F:6:VAL:HG11	1:G:60:ILE:HD12	1.85	0.59
1:F:417:VAL:HG21	1:F:477:GLY:HA3	1.84	0.59
1:E:417:VAL:HG21	1:E:477:GLY:HA3	1.84	0.59
1:E:6:VAL:HG11	1:F:60:ILE:HD12	1.85	0.59
1:B:27:VAL:HG12	1:B:90:THR:CG2	2.25	0.59
1:C:417:VAL:HG21	1:C:477:GLY:HA3	1.84	0.59
1:A:6:VAL:HG11	1:B:60:ILE:HD12	1.85	0.59
1:D:6:VAL:HG11	1:E:60:ILE:HD12	1.85	0.58
1:A:149:THR:HA	1:A:152:ALA:HB3	1.85	0.58
1:F:426:LEU:HB2	1:F:444:LEU:HD22	1.86	0.58
1:B:149:THR:HA	1:B:152:ALA:HB3	1.85	0.58
1:G:149:THR:HA	1:G:152:ALA:HB3	1.85	0.58
1:B:6:VAL:HG11	1:C:60:ILE:HD12	1.85	0.58
1:C:6:VAL:HG11	1:D:60:ILE:HD12	1.85	0.58
1:C:149:THR:HA	1:C:152:ALA:HB3	1.85	0.58
1:E:426:LEU:HB2	1:E:444:LEU:HD22	1.86	0.58
1:C:426:LEU:HB2	1:C:444:LEU:HD22	1.86	0.58
1:D:426:LEU:HB2	1:D:444:LEU:HD22	1.86	0.58
1:G:426:LEU:HB2	1:G:444:LEU:HD22	1.86	0.57
1:E:151:SER:HB3	1:E:399:ALA:HA	1.87	0.57
1:E:149:THR:HA	1:E:152:ALA:HB3	1.85	0.57
1:E:151:SER:CB	1:E:399:ALA:HA	2.34	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:149:THR:HA	1:D:152:ALA:HB3	1.85	0.57
1:F:149:THR:HA	1:F:152:ALA:HB3	1.85	0.57
1:D:151:SER:CB	1:D:399:ALA:HA	2.35	0.57
1:B:426:LEU:HB2	1:B:444:LEU:HD22	1.86	0.57
1:G:151:SER:CB	1:G:399:ALA:HA	2.35	0.57
1:F:151:SER:CB	1:F:399:ALA:HA	2.35	0.57
1:A:426:LEU:HB2	1:A:444:LEU:HD22	1.86	0.57
1:L:229:ASN:HA	1:L:258:ALA:HB3	1.87	0.57
1:D:151:SER:HB3	1:D:399:ALA:HA	1.87	0.57
1:F:151:SER:HB3	1:F:399:ALA:HA	1.87	0.57
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.86	0.56
1:G:151:SER:HB3	1:G:399:ALA:HA	1.87	0.56
1:C:151:SER:HB3	1:C:399:ALA:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.86	0.56
1:A:151:SER:CB	1:A:399:ALA:HA	2.35	0.56
1:C:151:SER:CB	1:C:399:ALA:HA	2.35	0.56
1:J:229:ASN:HA	1:J:258:ALA:HB3	1.87	0.56
1:B:151:SER:HB3	1:B:399:ALA:HA	1.87	0.56
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.56
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.86	0.56
1:N:229:ASN:HA	1:N:258:ALA:HB3	1.88	0.56
1:A:151:SER:HB3	1:A:399:ALA:HA	1.87	0.56
1:B:212:ALA:HA	1:B:325:ILE:O	2.06	0.56
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.86	0.56
1:B:151:SER:CB	1:B:399:ALA:HA	2.35	0.56
1:G:212:ALA:HA	1:G:325:ILE:O	2.07	0.55
1:E:212:ALA:HA	1:E:325:ILE:O	2.06	0.55
1:G:218:PRO:HG2	1:G:320:ALA:HB3	1.89	0.55
1:D:212:ALA:HA	1:D:325:ILE:O	2.06	0.55
1:M:229:ASN:HA	1:M:258:ALA:HB3	1.89	0.55
1:A:427:ALA:HA	1:A:444:LEU:HD11	1.89	0.55
1:C:217:SER:HA	1:C:320:ALA:O	2.07	0.55
1:C:218:PRO:HG2	1:C:320:ALA:HB3	1.89	0.55
1:D:218:PRO:HG2	1:D:320:ALA:HB3	1.89	0.55
1:G:217:SER:HA	1:G:320:ALA:O	2.07	0.55
1:A:212:ALA:HA	1:A:325:ILE:O	2.06	0.55
1:F:212:ALA:HA	1:F:325:ILE:O	2.06	0.55
1:F:218:PRO:HG2	1:F:320:ALA:HB3	1.89	0.55
2:A:1525:ATP:O3B	3:A:1526:PO4:P	2.66	0.55
1:D:427:ALA:HA	1:D:444:LEU:HD11	1.89	0.55
1:C:212:ALA:HA	1:C:325:ILE:O	2.06	0.55
1:D:31:LEU:CB	1:D:90:THR:HG21	2.37	0.54
1:E:427:ALA:HA	1:E:444:LEU:HD11	1.89	0.54
1:E:31:LEU:CB	1:E:90:THR:HG21	2.37	0.54
1:B:427:ALA:HA	1:B:444:LEU:HD11	1.89	0.54
1:D:217:SER:HA	1:D:320:ALA:O	2.07	0.54
1:B:218:PRO:HG2	1:B:320:ALA:HB3	1.89	0.54
1:G:427:ALA:HA	1:G:444:LEU:HD11	1.89	0.54
1:E:247:LEU:O	1:E:273:VAL:HA	2.07	0.54
3:F:1525:PO4:P	2:F:1527:ATP:O3B	2.66	0.54
1:A:218:PRO:HG2	1:A:320:ALA:HB3	1.89	0.54
1:E:218:PRO:HG2	1:E:320:ALA:HB3	1.89	0.54
1:K:229:ASN:HA	1:K:258:ALA:HB3	1.90	0.54
2:B:1525:ATP:O3B	3:B:1526:PO4:P	2.66	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LEU:CB	1:C:90:THR:HG21	2.38	0.54
1:D:523:ASP:H	1:E:43:SER:HB3	1.73	0.54
1:H:229:ASN:HA	1:H:258:ALA:HB3	1.89	0.54
3:E:1526:PO4:P	2:E:1527:ATP:O3B	2.66	0.54
2:C:1526:ATP:O3B	3:C:1527:PO4:P	2.66	0.54
1:F:31:LEU:CB	1:F:90:THR:HG21	2.37	0.54
1:A:247:LEU:O	1:A:273:VAL:HA	2.07	0.54
1:I:229:ASN:HA	1:I:258:ALA:HB3	1.89	0.54
1:B:247:LEU:O	1:B:273:VAL:HA	2.08	0.54
1:F:217:SER:HA	1:F:320:ALA:O	2.07	0.54
1:A:217:SER:HA	1:A:320:ALA:O	2.07	0.54
1:E:217:SER:HA	1:E:320:ALA:O	2.07	0.54
1:A:523:ASP:H	1:B:43:SER:HB3	1.73	0.54
1:H:25:ASP:CG	1:H:28:LYS:HZ3	2.11	0.54
1:B:31:LEU:CB	1:B:90:THR:HG21	2.37	0.54
3:G:1525:PO4:P	2:G:1527:ATP:O3B	2.66	0.54
1:B:523:ASP:H	1:C:43:SER:HB3	1.73	0.54
1:B:217:SER:HA	1:B:320:ALA:O	2.07	0.53
1:F:247:LEU:O	1:F:273:VAL:HA	2.08	0.53
1:D:247:LEU:O	1:D:273:VAL:HA	2.08	0.53
1:A:31:LEU:CB	1:A:90:THR:HG21	2.38	0.53
2:D:1525:ATP:O3B	3:D:1526:PO4:P	2.65	0.53
1:F:427:ALA:HA	1:F:444:LEU:HD11	1.89	0.53
1:C:427:ALA:HA	1:C:444:LEU:HD11	1.89	0.53
1:J:25:ASP:CG	1:J:28:LYS:HZ3	2.12	0.53
1:C:130:GLU:HB3	1:C:422:VAL:HG12	1.91	0.53
1:G:31:LEU:CB	1:G:90:THR:HG21	2.38	0.53
1:C:247:LEU:O	1:C:273:VAL:HA	2.07	0.53
1:K:400:LEU:C	1:K:401:HIS:CA	2.73	0.53
1:N:25:ASP:CG	1:N:28:LYS:HZ3	2.12	0.53
1:E:523:ASP:H	1:F:43:SER:HB3	1.74	0.53
1:D:130:GLU:HB3	1:D:422:VAL:HG12	1.91	0.53
1:G:247:LEU:O	1:G:273:VAL:HA	2.08	0.53
1:L:25:ASP:CG	1:L:28:LYS:HZ3	2.11	0.53
1:A:43:SER:HB3	1:G:523:ASP:H	1.74	0.53
1:A:411:VAL:HB	1:A:494:LEU:HB2	1.91	0.53
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:C:523:ASP:H	1:D:43:SER:HB3	1.73	0.52
1:B:130:GLU:HB3	1:B:422:VAL:HG12	1.91	0.52
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:GLU:HB3	1:E:422:VAL:HG12	1.91	0.52
1:B:6:VAL:HG13	1:B:521:VAL:HG22	1.92	0.52
1:F:523:ASP:H	1:G:43:SER:HB3	1.74	0.52
1:F:411:VAL:HB	1:F:494:LEU:HB2	1.91	0.52
1:D:6:VAL:HG13	1:D:521:VAL:HG22	1.92	0.52
1:G:31:LEU:HA	3:G:1525:PO4:P	2.50	0.52
1:C:31:LEU:HA	3:C:1527:PO4:P	2.50	0.52
1:D:144:ILE:HG23	1:D:403:THR:CG2	2.40	0.52
1:D:411:VAL:HB	1:D:494:LEU:HB2	1.91	0.52
1:C:411:VAL:HB	1:C:494:LEU:HB2	1.91	0.52
1:G:144:ILE:HG23	1:G:403:THR:CG2	2.40	0.52
1:G:106:ALA:CB	1:G:116:LEU:HD21	2.40	0.52
1:A:31:LEU:HA	3:A:1526:PO4:P	2.50	0.52
1:A:130:GLU:HB3	1:A:422:VAL:HG12	1.91	0.52
1:E:406:ALA:HB2	1:E:496:PRO:HG3	1.92	0.52
1:D:31:LEU:HA	3:D:1526:PO4:P	2.50	0.51
1:C:186:GLU:H	1:C:380:LYS:HB2	1.75	0.51
1:A:6:VAL:HG13	1:A:521:VAL:HG22	1.92	0.51
1:G:411:VAL:HB	1:G:494:LEU:HB2	1.91	0.51
1:F:130:GLU:HB3	1:F:422:VAL:HG12	1.91	0.51
1:G:130:GLU:HB3	1:G:422:VAL:HG12	1.91	0.51
1:F:106:ALA:CB	1:F:116:LEU:HD21	2.40	0.51
1:E:144:ILE:HG23	1:E:403:THR:CG2	2.40	0.51
1:F:406:ALA:HB2	1:F:496:PRO:HG3	1.93	0.51
1:B:411:VAL:HB	1:B:494:LEU:HB2	1.91	0.51
1:F:31:LEU:HA	3:F:1525:PO4:P	2.50	0.51
1:E:6:VAL:HG13	1:E:521:VAL:HG22	1.92	0.51
1:A:106:ALA:CB	1:A:116:LEU:HD21	2.40	0.51
1:E:172:GLU:H	1:E:172:GLU:CD	2.14	0.51
1:B:31:LEU:HA	3:B:1526:PO4:P	2.50	0.51
1:B:186:GLU:H	1:B:380:LYS:HB2	1.75	0.51
1:G:406:ALA:HB2	1:G:496:PRO:HG3	1.92	0.51
1:E:411:VAL:HB	1:E:494:LEU:HB2	1.91	0.51
1:E:31:LEU:HA	3:E:1526:PO4:P	2.50	0.51
1:C:205:ILE:HD12	1:C:211:GLY:O	2.10	0.51
1:A:205:ILE:HD12	1:A:211:GLY:O	2.10	0.51
1:G:186:GLU:H	1:G:380:LYS:HB2	1.75	0.51
1:D:172:GLU:CD	1:D:172:GLU:H	2.14	0.51
1:G:205:ILE:HD12	1:G:211:GLY:O	2.10	0.51
1:B:205:ILE:HD12	1:B:211:GLY:O	2.10	0.51
1:F:186:GLU:H	1:F:380:LYS:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:ALA:CB	1:E:116:LEU:HD21	2.40	0.51
1:B:172:GLU:CD	1:B:172:GLU:H	2.14	0.51
1:C:106:ALA:CB	1:C:116:LEU:HD21	2.40	0.51
1:D:205:ILE:HD12	1:D:211:GLY:O	2.10	0.51
1:E:186:GLU:H	1:E:380:LYS:HB2	1.75	0.51
1:B:406:ALA:HB2	1:B:496:PRO:HG3	1.93	0.51
1:D:106:ALA:CB	1:D:116:LEU:HD21	2.40	0.51
1:G:463:SER:OG	1:N:464:VAL:HG22	2.11	0.51
1:I:25:ASP:CG	1:I:28:LYS:HZ3	2.15	0.51
1:A:172:GLU:CD	1:A:172:GLU:H	2.14	0.51
1:B:106:ALA:CB	1:B:116:LEU:HD21	2.40	0.51
1:C:463:SER:OG	1:J:464:VAL:HG22	2.11	0.51
1:D:406:ALA:HB2	1:D:496:PRO:HG3	1.92	0.51
1:F:144:ILE:HG23	1:F:403:THR:CG2	2.40	0.51
1:F:205:ILE:HD12	1:F:211:GLY:O	2.10	0.50
1:G:6:VAL:HG13	1:G:521:VAL:HG22	1.92	0.50
1:C:6:VAL:HG13	1:C:521:VAL:HG22	1.92	0.50
1:A:463:SER:OG	1:H:464:VAL:HG22	2.11	0.50
1:K:25:ASP:CG	1:K:28:LYS:HZ3	2.14	0.50
1:D:196:ASP:HA	1:D:329:THR:HA	1.94	0.50
1:D:463:SER:OG	1:K:464:VAL:HG22	2.11	0.50
1:E:196:ASP:HA	1:E:329:THR:HA	1.94	0.50
1:F:196:ASP:HA	1:F:329:THR:HA	1.93	0.50
1:F:6:VAL:HG13	1:F:521:VAL:HG22	1.92	0.50
1:G:152:ALA:HB1	1:G:155:ASP:HB3	1.94	0.50
1:A:152:ALA:HB1	1:A:155:ASP:HB3	1.94	0.50
1:C:406:ALA:HB2	1:C:496:PRO:HG3	1.93	0.50
1:C:196:ASP:HA	1:C:329:THR:HA	1.94	0.50
1:E:205:ILE:HD12	1:E:211:GLY:O	2.10	0.50
1:A:186:GLU:H	1:A:380:LYS:HB2	1.75	0.50
1:D:279:PRO:HG3	1:D:292:ILE:HD11	1.94	0.50
1:G:172:GLU:H	1:G:172:GLU:CD	2.14	0.50
1:E:463:SER:OG	1:L:464:VAL:HG22	2.11	0.49
1:F:463:SER:OG	1:M:464:VAL:HG22	2.11	0.49
1:A:406:ALA:HB2	1:A:496:PRO:HG3	1.92	0.49
1:E:279:PRO:HG3	1:E:292:ILE:HD11	1.94	0.49
1:E:39:VAL:HG22	1:E:49:ILE:HG23	1.95	0.49
1:G:196:ASP:HA	1:G:329:THR:HA	1.94	0.49
1:B:463:SER:OG	1:I:464:VAL:HG22	2.11	0.49
1:C:279:PRO:HG3	1:C:292:ILE:HD11	1.94	0.49
1:D:186:GLU:H	1:D:380:LYS:HB2	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ALA:HB1	1:B:155:ASP:HB3	1.94	0.49
1:C:172:GLU:H	1:C:172:GLU:CD	2.14	0.49
1:F:152:ALA:HB1	1:F:155:ASP:HB3	1.94	0.49
1:F:39:VAL:HG22	1:F:49:ILE:HG23	1.95	0.49
1:M:25:ASP:CG	1:M:28:LYS:HZ3	2.16	0.49
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.95	0.49
1:B:196:ASP:HA	1:B:329:THR:HA	1.94	0.49
1:B:39:VAL:HG22	1:B:49:ILE:HG23	1.95	0.49
1:C:39:VAL:HG22	1:C:49:ILE:HG23	1.95	0.49
1:F:172:GLU:CD	1:F:172:GLU:H	2.14	0.49
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.43	0.49
1:E:124:VAL:HG21	1:E:508:ALA:CB	2.43	0.49
1:G:39:VAL:HG22	1:G:49:ILE:HG23	1.95	0.49
1:A:196:ASP:HA	1:A:329:THR:HA	1.94	0.49
1:I:182:GLY:HA2	1:I:284:ARG:HH22	1.78	0.49
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.95	0.49
1:C:152:ALA:HB1	1:C:155:ASP:HB3	1.94	0.49
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.95	0.49
1:K:386:GLU:HA	1:L:281:PHE:CG	2.48	0.49
1:D:124:VAL:HG21	1:D:508:ALA:CB	2.43	0.49
1:G:279:PRO:HG3	1:G:292:ILE:HD11	1.94	0.49
1:B:279:PRO:HG3	1:B:292:ILE:HD11	1.94	0.49
1:E:152:ALA:HB1	1:E:155:ASP:HB3	1.94	0.48
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.43	0.48
1:D:152:ALA:HB1	1:D:155:ASP:HB3	1.94	0.48
1:M:386:GLU:HA	1:N:281:PHE:CG	2.48	0.48
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.43	0.48
1:A:213:VAL:HG13	1:A:325:ILE:HB	1.96	0.48
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.43	0.48
1:K:182:GLY:HA2	1:L:284:ARG:HH22	1.78	0.48
1:F:279:PRO:HG3	1:F:292:ILE:HD11	1.94	0.48
1:A:279:PRO:HG3	1:A:292:ILE:HD11	1.94	0.48
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.43	0.48
1:A:39:VAL:HG22	1:A:49:ILE:HG23	1.95	0.48
1:G:213:VAL:HG13	1:G:325:ILE:HB	1.96	0.48
1:D:106:ALA:HB3	1:D:116:LEU:HD21	1.96	0.48
1:M:182:GLY:HA2	1:N:284:ARG:HH22	1.78	0.48
1:C:106:ALA:HB3	1:C:116:LEU:HD21	1.96	0.48
1:H:386:GLU:HA	1:I:281:PHE:CG	2.49	0.48
1:E:144:ILE:HG23	1:E:403:THR:HG21	1.95	0.48
1:D:39:VAL:HG22	1:D:49:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:386:GLU:HA	1:K:281:PHE:CG	2.48	0.48
1:B:213:VAL:HG13	1:B:325:ILE:HB	1.96	0.48
1:I:386:GLU:HA	1:J:281:PHE:CG	2.49	0.48
1:J:182:GLY:HA2	1:K:284:ARG:HH22	1.78	0.48
1:L:182:GLY:HA2	1:M:284:ARG:HH22	1.78	0.48
1:D:144:ILE:HG23	1:D:403:THR:HG21	1.96	0.47
1:C:240:VAL:HA	1:C:314:LEU:HD21	1.96	0.47
1:H:284:ARG:HH22	1:N:182:GLY:HA2	1.78	0.47
1:H:182:GLY:HA2	1:I:284:ARG:HH22	1.78	0.47
1:H:281:PHE:CG	1:N:386:GLU:HA	2.49	0.47
1:G:240:VAL:HA	1:G:314:LEU:HD21	1.96	0.47
1:B:144:ILE:HG23	1:B:403:THR:HG21	1.95	0.47
1:F:144:ILE:HG23	1:F:403:THR:HG21	1.96	0.47
1:C:40:LEU:HD11	1:C:55:SER:HB3	1.96	0.47
1:D:240:VAL:HA	1:D:314:LEU:HD21	1.96	0.47
1:A:240:VAL:HA	1:A:314:LEU:HD21	1.97	0.47
1:F:213:VAL:HG13	1:F:325:ILE:HB	1.96	0.47
1:A:144:ILE:HG23	1:A:403:THR:HG21	1.96	0.47
1:B:240:VAL:HA	1:B:314:LEU:HD21	1.96	0.47
1:N:230:ILE:HG23	1:N:259:LEU:HD12	1.96	0.47
1:F:383:ALA:HB3	1:F:389:MET:HB2	1.95	0.47
1:L:386:GLU:HA	1:M:281:PHE:CG	2.49	0.47
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.95	0.47
1:E:106:ALA:HB3	1:E:116:LEU:HD21	1.96	0.47
1:E:40:LEU:HD11	1:E:55:SER:HB3	1.96	0.47
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.95	0.47
1:D:40:LEU:HD11	1:D:55:SER:HB3	1.96	0.47
1:F:240:VAL:HA	1:F:314:LEU:HD21	1.97	0.47
1:E:213:VAL:HG13	1:E:325:ILE:HB	1.96	0.47
1:C:213:VAL:HG13	1:C:325:ILE:HB	1.96	0.47
1:G:144:ILE:HG23	1:G:403:THR:HG21	1.96	0.47
1:K:320:ALA:HA	1:K:334:ASP:O	2.15	0.47
1:E:240:VAL:HA	1:E:314:LEU:HD21	1.96	0.47
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.95	0.47
1:J:320:ALA:HA	1:J:334:ASP:O	2.15	0.47
1:L:320:ALA:HA	1:L:334:ASP:O	2.15	0.47
1:M:320:ALA:HA	1:M:334:ASP:O	2.15	0.47
1:D:213:VAL:HG13	1:D:325:ILE:HB	1.96	0.47
1:C:144:ILE:HG23	1:C:403:THR:HG21	1.96	0.47
1:B:106:ALA:HB3	1:B:116:LEU:HD21	1.96	0.47
1:B:113:PRO:HD2	1:C:36:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:320:ALA:HA	1:I:334:ASP:O	2.15	0.47
1:H:320:ALA:HA	1:H:334:ASP:O	2.15	0.47
1:D:417:VAL:HG13	1:D:476:TYR:O	2.15	0.47
1:G:106:ALA:HB3	1:G:116:LEU:HD21	1.96	0.47
1:N:479:ASN:O	1:N:483:GLU:N	2.48	0.47
1:C:113:PRO:HD2	1:D:36:ARG:HD2	1.97	0.47
1:N:320:ALA:HA	1:N:334:ASP:O	2.15	0.47
1:J:230:ILE:HG23	1:J:259:LEU:HD12	1.97	0.46
1:B:40:LEU:HD11	1:B:55:SER:HB3	1.96	0.46
1:K:400:LEU:CA	1:K:401:HIS:N	2.72	0.46
1:E:417:VAL:HG13	1:E:476:TYR:O	2.15	0.46
1:L:230:ILE:HG23	1:L:259:LEU:HD12	1.97	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:B:158:VAL:HG22	1:B:396:VAL:HG22	1.97	0.46
1:F:180:GLY:HA3	1:F:381:VAL:O	2.16	0.46
1:C:226:LYS:HA	1:C:253:ASP:O	2.16	0.46
1:M:183:LEU:HA	1:M:383:ALA:O	2.15	0.46
1:A:113:PRO:HD2	1:B:36:ARG:HD2	1.97	0.46
1:B:417:VAL:HG13	1:B:476:TYR:O	2.15	0.46
1:J:183:LEU:HA	1:J:383:ALA:O	2.15	0.46
1:A:66:PHE:CZ	1:A:522:THR:HG22	2.50	0.46
1:D:113:PRO:HD2	1:E:36:ARG:HD2	1.97	0.46
1:D:66:PHE:CZ	1:D:522:THR:HG22	2.51	0.46
1:M:398:ALA:O	1:M:401:HIS:N	2.49	0.46
1:G:180:GLY:HA3	1:G:381:VAL:O	2.16	0.46
1:A:417:VAL:HG13	1:A:476:TYR:O	2.15	0.46
1:F:287:ALA:HB1	1:F:368:ARG:CZ	2.46	0.46
1:G:287:ALA:HB1	1:G:368:ARG:CZ	2.46	0.46
1:M:479:ASN:O	1:M:483:GLU:N	2.48	0.46
1:N:183:LEU:HA	1:N:383:ALA:O	2.15	0.46
1:H:183:LEU:HA	1:H:383:ALA:O	2.16	0.46
1:E:180:GLY:HA3	1:E:381:VAL:O	2.16	0.46
1:F:417:VAL:HG13	1:F:476:TYR:O	2.15	0.46
1:F:40:LEU:HD11	1:F:55:SER:HB3	1.97	0.46
1:E:66:PHE:CZ	1:E:522:THR:HG22	2.51	0.46
1:F:520:MET:HA	1:G:41:ASP:HB2	1.97	0.46
1:A:180:GLY:HA3	1:A:381:VAL:O	2.16	0.46
1:F:106:ALA:HB3	1:F:116:LEU:HD21	1.96	0.46
1:C:520:MET:HA	1:D:41:ASP:HB2	1.97	0.46
1:C:158:VAL:HG22	1:C:396:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:ALA:HB1	1:E:361:ASP:HB2	1.98	0.46
1:G:356:ALA:HB1	1:G:361:ASP:HB2	1.98	0.46
1:C:180:GLY:HA3	1:C:381:VAL:O	2.16	0.46
1:C:417:VAL:HG13	1:C:476:TYR:O	2.15	0.46
1:F:158:VAL:HG22	1:F:396:VAL:HG22	1.97	0.46
1:A:287:ALA:HB1	1:A:368:ARG:CZ	2.46	0.46
1:A:158:VAL:HG22	1:A:396:VAL:HG22	1.97	0.46
1:C:287:ALA:HB1	1:C:368:ARG:CZ	2.46	0.46
1:A:106:ALA:HB3	1:A:116:LEU:HD21	1.96	0.46
1:A:356:ALA:HB1	1:A:361:ASP:HB2	1.98	0.46
1:K:414:GLY:N	1:K:494:LEU:HA	2.31	0.46
1:D:356:ALA:HB1	1:D:361:ASP:HB2	1.98	0.46
1:I:414:GLY:N	1:I:494:LEU:HA	2.31	0.46
1:B:520:MET:HA	1:C:41:ASP:HB2	1.97	0.46
1:B:226:LYS:HA	1:B:253:ASP:O	2.15	0.46
1:E:520:MET:HA	1:F:41:ASP:HB2	1.97	0.46
1:B:287:ALA:HB1	1:B:368:ARG:CZ	2.46	0.46
1:B:66:PHE:CZ	1:B:522:THR:HG22	2.50	0.46
1:H:414:GLY:N	1:H:494:LEU:HA	2.31	0.45
1:E:113:PRO:HD2	1:F:36:ARG:HD2	1.97	0.45
1:I:246:PRO:HB3	1:I:272:LYS:HB2	1.99	0.45
1:D:287:ALA:HB1	1:D:368:ARG:CZ	2.46	0.45
1:A:226:LYS:HA	1:A:253:ASP:O	2.16	0.45
1:G:417:VAL:HG13	1:G:476:TYR:O	2.15	0.45
1:E:120:ILE:O	1:E:124:VAL:HG23	2.17	0.45
1:D:120:ILE:O	1:D:124:VAL:HG23	2.17	0.45
1:D:520:MET:HA	1:E:41:ASP:HB2	1.97	0.45
1:F:356:ALA:HB1	1:F:361:ASP:HB2	1.98	0.45
1:H:246:PRO:HB3	1:H:272:LYS:HB2	1.99	0.45
1:J:149:THR:CG2	1:J:156:GLU:HA	2.47	0.45
1:J:246:PRO:HB3	1:J:272:LYS:HB2	1.99	0.45
1:A:36:ARG:HD2	1:G:113:PRO:HD2	1.97	0.45
1:M:414:GLY:N	1:M:494:LEU:HA	2.31	0.45
1:B:206:ASN:HB2	1:B:213:VAL:HA	1.98	0.45
1:B:120:ILE:O	1:B:124:VAL:HG23	2.17	0.45
1:C:120:ILE:O	1:C:124:VAL:HG23	2.17	0.45
1:N:414:GLY:N	1:N:494:LEU:HA	2.31	0.45
1:G:40:LEU:HD11	1:G:55:SER:HB3	1.96	0.45
1:N:246:PRO:HB3	1:N:272:LYS:HB2	1.99	0.45
1:C:356:ALA:HB1	1:C:361:ASP:HB2	1.98	0.45
1:D:180:GLY:HA3	1:D:381:VAL:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASN:HB2	1:C:213:VAL:HA	1.98	0.45
1:M:217:SER:HA	1:M:320:ALA:O	2.16	0.45
1:N:217:SER:HA	1:N:320:ALA:O	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:A:41:ASP:HB2	1:G:520:MET:HA	1.97	0.45
1:B:356:ALA:HB1	1:B:361:ASP:HB2	1.98	0.45
1:A:40:LEU:HD11	1:A:55:SER:HB3	1.96	0.45
1:K:271:VAL:HG12	1:K:272:LYS:H	1.82	0.45
1:L:149:THR:CG2	1:L:156:GLU:HA	2.47	0.45
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.33	0.45
1:A:206:ASN:HB2	1:A:213:VAL:HA	1.99	0.45
1:A:120:ILE:O	1:A:124:VAL:HG23	2.17	0.45
1:I:217:SER:HA	1:I:320:ALA:O	2.17	0.45
1:E:158:VAL:HG22	1:E:396:VAL:HG22	1.97	0.45
1:F:113:PRO:HD2	1:G:36:ARG:HD2	1.97	0.45
1:F:66:PHE:CZ	1:F:522:THR:HG22	2.51	0.45
1:G:206:ASN:HB2	1:G:213:VAL:HA	1.98	0.45
1:B:112:ASN:HA	1:B:113:PRO:HD2	1.88	0.45
1:C:65:LYS:HZ2	1:C:525:PRO:N	2.14	0.45
1:G:158:VAL:HG22	1:G:396:VAL:HG22	1.97	0.45
1:K:479:ASN:O	1:K:483:GLU:N	2.48	0.45
1:F:226:LYS:HA	1:F:253:ASP:O	2.16	0.45
1:I:183:LEU:HA	1:I:383:ALA:O	2.15	0.45
1:F:120:ILE:O	1:F:124:VAL:HG23	2.17	0.45
1:J:217:SER:HA	1:J:320:ALA:O	2.16	0.45
1:G:66:PHE:CZ	1:G:522:THR:HG22	2.51	0.45
1:K:149:THR:CG2	1:K:156:GLU:HA	2.47	0.45
1:I:479:ASN:O	1:I:483:GLU:N	2.49	0.45
1:B:180:GLY:HA3	1:B:381:VAL:O	2.16	0.45
1:N:271:VAL:HG12	1:N:272:LYS:H	1.82	0.45
1:K:246:PRO:HB3	1:K:272:LYS:HB2	1.99	0.45
1:M:246:PRO:HB3	1:M:272:LYS:HB2	1.99	0.45
1:C:66:PHE:CZ	1:C:522:THR:HG22	2.50	0.45
1:L:414:GLY:N	1:L:494:LEU:HA	2.31	0.45
1:G:120:ILE:O	1:G:124:VAL:HG23	2.17	0.45
1:A:244:GLY:O	1:G:257:GLU:HB3	2.17	0.45
1:G:226:LYS:HA	1:G:253:ASP:O	2.16	0.45
1:A:257:GLU:HB3	1:B:244:GLY:O	2.17	0.45
1:H:149:THR:CG2	1:H:156:GLU:HA	2.46	0.45
1:B:257:GLU:HB3	1:C:244:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:GLU:HB3	1:E:244:GLY:O	2.17	0.45
1:H:217:SER:HA	1:H:320:ALA:O	2.16	0.45
1:M:271:VAL:HG12	1:M:272:LYS:H	1.82	0.45
1:I:149:THR:CG2	1:I:156:GLU:HA	2.47	0.45
1:E:226:LYS:HA	1:E:253:ASP:O	2.16	0.45
1:E:257:GLU:HB3	1:F:244:GLY:O	2.17	0.45
1:A:520:MET:HA	1:B:41:ASP:HB2	1.97	0.44
1:B:190:VAL:HG11	1:B:333:ILE:HG23	2.00	0.44
1:D:226:LYS:HA	1:D:253:ASP:O	2.16	0.44
1:A:190:VAL:HG11	1:A:333:ILE:HG23	2.00	0.44
1:F:206:ASN:HB2	1:F:213:VAL:HA	1.98	0.44
1:M:149:THR:CG2	1:M:156:GLU:HA	2.46	0.44
1:F:257:GLU:HB3	1:G:244:GLY:O	2.17	0.44
1:M:417:VAL:HA	1:M:420:ILE:HG22	2.00	0.44
1:L:246:PRO:HB3	1:L:272:LYS:HB2	1.99	0.44
1:D:293:ALA:HB2	1:D:300:VAL:CG2	2.47	0.44
1:F:293:ALA:HB2	1:F:300:VAL:CG2	2.47	0.44
1:E:293:ALA:HB2	1:E:300:VAL:CG2	2.48	0.44
1:N:8:PHE:HA	1:N:518:GLU:O	2.18	0.44
1:D:461:GLU:HA	1:D:462:PRO:HD2	1.78	0.44
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.33	0.44
1:A:293:ALA:HB2	1:A:300:VAL:CG2	2.47	0.44
1:J:414:GLY:N	1:J:494:LEU:HA	2.31	0.44
1:G:293:ALA:HB2	1:G:300:VAL:CG2	2.48	0.44
1:J:8:PHE:HA	1:J:518:GLU:O	2.18	0.44
1:N:417:VAL:HA	1:N:420:ILE:HG22	2.00	0.44
1:K:8:PHE:HA	1:K:518:GLU:O	2.18	0.44
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.33	0.44
1:D:206:ASN:HB2	1:D:213:VAL:HA	1.99	0.44
1:J:191:GLU:O	1:J:334:ASP:HA	2.18	0.44
1:H:479:ASN:O	1:H:483:GLU:N	2.48	0.44
1:N:149:THR:CG2	1:N:156:GLU:HA	2.47	0.44
1:H:8:PHE:HA	1:H:518:GLU:O	2.18	0.44
1:C:190:VAL:HG11	1:C:333:ILE:HG23	2.00	0.44
1:M:8:PHE:HA	1:M:518:GLU:O	2.18	0.44
1:D:349:ILE:HG22	1:D:369:VAL:HG13	1.99	0.44
1:L:8:PHE:HA	1:L:518:GLU:O	2.18	0.44
1:C:412:VAL:HG22	1:C:495:ASP:O	2.18	0.44
1:E:206:ASN:HB2	1:E:213:VAL:HA	1.98	0.44
1:K:217:SER:HA	1:K:320:ALA:O	2.16	0.44
1:D:158:VAL:HG22	1:D:396:VAL:HG22	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:191:GLU:O	1:I:334:ASP:HA	2.18	0.44
1:D:190:VAL:HG11	1:D:333:ILE:HG23	1.99	0.44
1:G:190:VAL:HG11	1:G:333:ILE:HG23	2.00	0.44
1:I:8:PHE:HA	1:I:518:GLU:O	2.18	0.44
1:N:2:ALA:CB	1:N:2:ALA:N	2.74	0.44
1:D:23:LEU:O	1:D:27:VAL:HG23	2.18	0.44
1:D:412:VAL:HG22	1:D:495:ASP:O	2.18	0.44
1:E:199:TYR:CE2	1:E:327:LYS:HB3	2.53	0.44
1:C:152:ALA:HB1	1:C:155:ASP:CA	2.48	0.44
1:D:152:ALA:HB1	1:D:155:ASP:CA	2.48	0.44
1:L:217:SER:HA	1:L:320:ALA:O	2.17	0.44
1:D:111:MET:O	1:D:113:PRO:HD3	2.18	0.44
1:B:293:ALA:HB2	1:B:300:VAL:CG2	2.48	0.44
1:A:65:LYS:HZ2	1:A:525:PRO:N	2.15	0.44
1:C:23:LEU:O	1:C:27:VAL:HG23	2.18	0.44
1:E:412:VAL:HG22	1:E:495:ASP:O	2.18	0.44
1:G:199:TYR:CE2	1:G:327:LYS:HB3	2.53	0.44
1:F:349:ILE:HG22	1:F:369:VAL:HG13	1.99	0.44
1:L:479:ASN:O	1:L:483:GLU:N	2.49	0.44
1:L:417:VAL:HA	1:L:420:ILE:HG22	2.00	0.44
1:B:412:VAL:HG22	1:B:495:ASP:O	2.18	0.43
1:B:6:VAL:HG11	1:C:60:ILE:CD1	2.48	0.43
1:B:111:MET:O	1:B:113:PRO:HD3	2.18	0.43
1:E:111:MET:O	1:E:113:PRO:HD3	2.18	0.43
1:F:111:MET:O	1:F:113:PRO:HD3	2.18	0.43
1:E:294:THR:HG21	1:E:345:ARG:HG3	2.00	0.43
1:G:349:ILE:HG22	1:G:369:VAL:HG13	1.99	0.43
1:D:127:ALA:CB	1:D:426:LEU:HD11	2.47	0.43
1:E:6:VAL:HG11	1:F:60:ILE:CD1	2.49	0.43
1:K:191:GLU:O	1:K:334:ASP:HA	2.18	0.43
1:E:190:VAL:HG11	1:E:333:ILE:HG23	1.99	0.43
1:D:65:LYS:HZ2	1:D:525:PRO:N	2.16	0.43
1:F:23:LEU:O	1:F:27:VAL:HG23	2.18	0.43
1:C:135:SER:CA	1:C:412:VAL:HG12	2.45	0.43
1:C:199:TYR:CE2	1:C:327:LYS:HB3	2.53	0.43
1:A:126:ALA:HB3	1:A:426:LEU:HD22	2.01	0.43
1:L:215:LEU:O	1:L:218:PRO:HD3	2.18	0.43
1:B:23:LEU:O	1:B:27:VAL:HG23	2.18	0.43
1:A:60:ILE:CD1	1:G:6:VAL:HG11	2.49	0.43
1:B:152:ALA:HB1	1:B:155:ASP:CA	2.48	0.43
1:E:152:ALA:HB1	1:E:155:ASP:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:417:VAL:HA	1:H:420:ILE:HG22	2.00	0.43
1:C:257:GLU:HB3	1:D:244:GLY:O	2.17	0.43
1:M:215:LEU:O	1:M:218:PRO:HD3	2.18	0.43
1:M:117:LYS:HZ2	1:M:121:ASP:CG	2.21	0.43
1:C:349:ILE:HG22	1:C:369:VAL:HG13	2.00	0.43
1:H:117:LYS:HZ2	1:H:121:ASP:CG	2.21	0.43
1:F:412:VAL:HG22	1:F:495:ASP:O	2.18	0.43
1:D:199:TYR:CE2	1:D:327:LYS:HB3	2.53	0.43
1:B:126:ALA:HB3	1:B:426:LEU:HD22	2.01	0.43
1:H:191:GLU:O	1:H:334:ASP:HA	2.18	0.43
1:J:7:LYS:O	1:J:519:CYS:HA	2.18	0.43
1:C:293:ALA:HB2	1:C:300:VAL:CG2	2.47	0.43
1:C:82:ASN:HB2	1:C:89:THR:HG23	2.01	0.43
1:M:7:LYS:O	1:M:519:CYS:HA	2.18	0.43
1:G:82:ASN:HB2	1:G:89:THR:HG23	2.01	0.43
1:F:190:VAL:HG11	1:F:333:ILE:HG23	2.00	0.43
1:E:23:LEU:O	1:E:27:VAL:HG23	2.18	0.43
1:A:412:VAL:HG22	1:A:495:ASP:O	2.18	0.43
1:G:126:ALA:HB3	1:G:426:LEU:HD22	2.01	0.43
1:G:111:MET:O	1:G:113:PRO:HD3	2.18	0.43
1:F:294:THR:HG21	1:F:345:ARG:HG3	2.00	0.43
1:A:294:THR:HG21	1:A:345:ARG:HG3	2.00	0.43
1:A:199:TYR:CE2	1:A:327:LYS:HB3	2.53	0.43
1:G:152:ALA:HB1	1:G:155:ASP:CA	2.48	0.43
1:F:152:ALA:HB1	1:F:155:ASP:CA	2.48	0.43
1:D:112:ASN:HA	1:D:113:PRO:HD2	1.88	0.43
1:A:349:ILE:HG22	1:A:369:VAL:HG13	1.99	0.43
1:K:215:LEU:O	1:K:218:PRO:HD3	2.18	0.43
1:J:417:VAL:HA	1:J:420:ILE:HG22	1.99	0.43
1:E:126:ALA:HB3	1:E:426:LEU:HD22	2.01	0.43
1:F:126:ALA:HB3	1:F:426:LEU:HD22	2.01	0.43
1:M:191:GLU:O	1:M:334:ASP:HA	2.18	0.43
1:B:82:ASN:HB2	1:B:89:THR:HG23	2.01	0.43
1:E:349:ILE:HG22	1:E:369:VAL:HG13	1.99	0.43
1:I:215:LEU:O	1:I:218:PRO:HD3	2.18	0.43
1:B:349:ILE:HG22	1:B:369:VAL:HG13	1.99	0.43
1:D:506:TYR:O	1:D:510:VAL:HG23	2.19	0.43
1:L:219:PHE:O	1:L:247:LEU:HD12	2.19	0.43
1:N:7:LYS:O	1:N:519:CYS:HA	2.18	0.43
1:B:294:THR:HG21	1:B:345:ARG:HG3	2.00	0.43
1:A:90:THR:HG22	1:A:94:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:LEU:O	1:G:27:VAL:HG23	2.18	0.43
1:G:412:VAL:HG22	1:G:495:ASP:O	2.18	0.43
1:B:199:TYR:CE2	1:B:327:LYS:HB3	2.53	0.43
1:A:127:ALA:CB	1:A:426:LEU:HD11	2.47	0.43
1:D:294:THR:HG21	1:D:345:ARG:HG3	2.00	0.43
1:J:206:ASN:HB2	1:J:213:VAL:HG23	2.01	0.43
1:I:417:VAL:HA	1:I:420:ILE:HG22	2.00	0.43
1:C:251:ALA:O	1:C:277:LYS:HA	2.19	0.43
1:H:7:LYS:O	1:H:519:CYS:HA	2.18	0.43
1:H:215:LEU:O	1:H:218:PRO:HD3	2.19	0.43
1:A:152:ALA:HB1	1:A:155:ASP:CA	2.48	0.43
1:D:194:GLN:HE21	1:D:329:THR:HG21	1.84	0.43
1:L:191:GLU:O	1:L:334:ASP:HA	2.18	0.43
1:C:111:MET:O	1:C:113:PRO:HD3	2.18	0.43
1:A:111:MET:O	1:A:113:PRO:HD3	2.18	0.43
1:F:506:TYR:O	1:F:510:VAL:HG23	2.19	0.43
1:J:117:LYS:HZ2	1:J:121:ASP:CG	2.22	0.43
1:L:7:LYS:O	1:L:519:CYS:HA	2.18	0.43
1:J:219:PHE:O	1:J:247:LEU:HD12	2.19	0.43
1:D:251:ALA:O	1:D:277:LYS:HA	2.19	0.43
1:K:417:VAL:HA	1:K:420:ILE:HG22	2.00	0.43
1:A:82:ASN:HB2	1:A:89:THR:HG23	2.01	0.43
1:N:215:LEU:O	1:N:218:PRO:HD3	2.18	0.43
1:G:127:ALA:CB	1:G:426:LEU:HD11	2.47	0.42
1:F:383:ALA:HB3	1:F:389:MET:N	2.34	0.42
1:H:271:VAL:HG12	1:H:272:LYS:H	1.85	0.42
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.49	0.42
1:B:19:GLY:HA2	1:B:62:LEU:CD1	2.49	0.42
1:B:90:THR:HG22	1:B:94:VAL:HG23	2.01	0.42
1:A:23:LEU:O	1:A:27:VAL:HG23	2.18	0.42
1:D:6:VAL:HG11	1:E:60:ILE:CD1	2.49	0.42
1:G:383:ALA:HB3	1:G:389:MET:N	2.34	0.42
1:C:190:VAL:HG12	1:C:376:VAL:O	2.19	0.42
1:E:190:VAL:HG12	1:E:376:VAL:O	2.19	0.42
1:I:206:ASN:HB2	1:I:213:VAL:HG23	2.01	0.42
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.49	0.42
1:C:294:THR:HG21	1:C:345:ARG:HG3	2.00	0.42
1:C:90:THR:HG22	1:C:94:VAL:HG23	2.01	0.42
1:C:126:ALA:HB3	1:C:426:LEU:HD22	2.01	0.42
1:C:194:GLN:HE21	1:C:329:THR:HG21	1.84	0.42
1:B:194:GLN:HE21	1:B:329:THR:HG21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:ALA:HB3	1:A:389:MET:N	2.34	0.42
1:D:190:VAL:HG12	1:D:376:VAL:O	2.19	0.42
1:F:190:VAL:HG12	1:F:376:VAL:O	2.20	0.42
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.49	0.42
1:G:506:TYR:O	1:G:510:VAL:HG23	2.19	0.42
1:A:506:TYR:O	1:A:510:VAL:HG23	2.19	0.42
1:G:251:ALA:O	1:G:277:LYS:HA	2.19	0.42
1:G:90:THR:HG22	1:G:94:VAL:HG23	2.01	0.42
1:D:90:THR:HG22	1:D:94:VAL:HG23	2.01	0.42
1:F:199:TYR:CE2	1:F:327:LYS:HB3	2.53	0.42
1:E:194:GLN:HE21	1:E:329:THR:HG21	1.85	0.42
1:E:383:ALA:HB3	1:E:389:MET:N	2.35	0.42
1:I:117:LYS:HZ2	1:I:121:ASP:CG	2.23	0.42
1:B:506:TYR:O	1:B:510:VAL:HG23	2.19	0.42
1:K:206:ASN:HB2	1:K:213:VAL:HG23	2.01	0.42
1:N:117:LYS:HZ2	1:N:121:ASP:CG	2.23	0.42
1:G:294:THR:HG21	1:G:345:ARG:HG3	2.00	0.42
1:I:271:VAL:HG12	1:I:272:LYS:H	1.85	0.42
1:B:190:VAL:HG12	1:B:376:VAL:O	2.19	0.42
1:G:190:VAL:HG12	1:G:376:VAL:O	2.19	0.42
1:J:215:LEU:O	1:J:218:PRO:HD3	2.18	0.42
1:F:82:ASN:HB2	1:F:89:THR:HG23	2.01	0.42
1:I:7:LYS:O	1:I:519:CYS:HA	2.18	0.42
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.33	0.42
1:E:90:THR:HG22	1:E:94:VAL:HG23	2.01	0.42
1:F:194:GLN:HE21	1:F:329:THR:HG21	1.85	0.42
1:G:194:GLN:HE21	1:G:329:THR:HG21	1.85	0.42
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.49	0.42
1:H:206:ASN:HB2	1:H:213:VAL:HG23	2.01	0.42
1:D:383:ALA:HB3	1:D:389:MET:N	2.34	0.42
1:G:112:ASN:HA	1:G:113:PRO:HD2	1.88	0.42
1:A:236:VAL:HG22	1:A:309:LEU:O	2.20	0.42
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.49	0.42
1:A:6:VAL:HG11	1:B:60:ILE:CD1	2.49	0.42
1:B:383:ALA:HB3	1:B:389:MET:N	2.34	0.42
1:K:7:LYS:O	1:K:519:CYS:HA	2.18	0.42
1:C:234:LEU:HB2	1:C:235:PRO:HD3	2.01	0.42
1:E:82:ASN:HB2	1:E:89:THR:HG23	2.01	0.42
1:E:506:TYR:O	1:E:510:VAL:HG23	2.19	0.42
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.49	0.42
1:F:127:ALA:CB	1:F:426:LEU:HD11	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ALA:CB	1:B:426:LEU:HD11	2.47	0.42
1:B:234:LEU:HB2	1:B:235:PRO:HD3	2.02	0.42
1:K:117:LYS:HZ2	1:K:121:ASP:CG	2.23	0.42
1:A:251:ALA:O	1:A:277:LYS:HA	2.19	0.42
1:K:219:PHE:O	1:K:247:LEU:HD12	2.20	0.42
1:D:126:ALA:HB3	1:D:426:LEU:HD22	2.01	0.42
1:F:6:VAL:HG11	1:G:60:ILE:CD1	2.49	0.42
1:A:213:VAL:CG1	1:A:325:ILE:HB	2.50	0.42
1:M:206:ASN:HB2	1:M:213:VAL:HG23	2.01	0.42
1:F:251:ALA:O	1:F:277:LYS:HA	2.19	0.42
1:N:206:ASN:HB2	1:N:213:VAL:HG23	2.00	0.42
1:G:213:VAL:CG1	1:G:325:ILE:HB	2.50	0.41
1:N:191:GLU:O	1:N:334:ASP:HA	2.18	0.41
1:J:271:VAL:HG12	1:J:272:LYS:H	1.85	0.41
1:F:234:LEU:HB2	1:F:235:PRO:HD3	2.01	0.41
1:C:506:TYR:O	1:C:510:VAL:HG23	2.19	0.41
1:D:82:ASN:HB2	1:D:89:THR:HG23	2.01	0.41
1:L:117:LYS:HZ2	1:L:121:ASP:CG	2.23	0.41
1:N:219:PHE:O	1:N:247:LEU:HD12	2.20	0.41
1:C:383:ALA:HB3	1:C:389:MET:N	2.34	0.41
1:A:194:GLN:HE21	1:A:329:THR:HG21	1.84	0.41
1:A:190:VAL:HG12	1:A:376:VAL:O	2.20	0.41
1:L:271:VAL:HG12	1:L:272:LYS:H	1.85	0.41
1:G:220:ILE:HD12	1:G:248:LEU:HD23	2.03	0.41
1:C:236:VAL:HG22	1:C:309:LEU:O	2.20	0.41
1:E:236:VAL:HG22	1:E:309:LEU:O	2.20	0.41
1:A:182:GLY:O	1:A:382:GLY:HA2	2.21	0.41
1:B:213:VAL:CG1	1:B:325:ILE:HB	2.50	0.41
1:E:251:ALA:O	1:E:277:LYS:HA	2.19	0.41
1:B:251:ALA:O	1:B:277:LYS:HA	2.19	0.41
1:F:220:ILE:HD12	1:F:248:LEU:HD23	2.03	0.41
1:H:2:ALA:O	1:H:3:ALA:C	2.58	0.41
1:F:323:VAL:HG22	1:F:332:ILE:HA	2.03	0.41
1:F:213:VAL:CG1	1:F:325:ILE:HB	2.50	0.41
1:D:383:ALA:HB3	1:D:389:MET:CA	2.51	0.41
1:I:219:PHE:O	1:I:247:LEU:HD12	2.20	0.41
1:D:236:VAL:HG22	1:D:309:LEU:O	2.20	0.41
1:E:220:ILE:HD12	1:E:248:LEU:HD23	2.03	0.41
1:N:2:ALA:O	1:N:3:ALA:C	2.59	0.41
1:F:90:THR:HG22	1:F:94:VAL:HG23	2.01	0.41
1:E:182:GLY:O	1:E:382:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:SER:CA	1:B:412:VAL:HG12	2.45	0.41
1:E:323:VAL:HG22	1:E:332:ILE:HA	2.03	0.41
1:L:2:ALA:O	1:L:3:ALA:C	2.59	0.41
1:G:182:GLY:O	1:G:382:GLY:HA2	2.21	0.41
1:G:323:VAL:HG22	1:G:332:ILE:HA	2.03	0.41
1:D:323:VAL:HG22	1:D:332:ILE:HA	2.03	0.41
1:E:383:ALA:HB3	1:E:389:MET:CA	2.51	0.41
1:A:461:GLU:HA	1:A:462:PRO:HD2	1.78	0.41
2:D:1525:ATP:PG	3:D:1526:PO4:P	3.19	0.41
1:C:202:PRO:O	1:C:205:ILE:HB	2.21	0.41
1:G:205:ILE:HG23	1:G:211:GLY:HA2	2.03	0.41
1:A:202:PRO:O	1:A:205:ILE:HB	2.21	0.41
1:E:127:ALA:CB	1:E:426:LEU:HD11	2.47	0.41
1:F:383:ALA:HB3	1:F:389:MET:CA	2.51	0.41
1:A:383:ALA:HB3	1:A:389:MET:CA	2.51	0.41
1:B:102:GLU:HB2	1:B:442:VAL:HG13	2.03	0.41
1:G:236:VAL:HG22	1:G:309:LEU:O	2.20	0.41
1:F:236:VAL:HG22	1:F:309:LEU:O	2.20	0.41
1:D:220:ILE:HD12	1:D:248:LEU:HD23	2.02	0.41
1:A:102:GLU:HB2	1:A:442:VAL:HG13	2.03	0.41
2:C:1526:ATP:PG	3:C:1527:PO4:P	3.19	0.41
1:B:182:GLY:O	1:B:382:GLY:HA2	2.21	0.41
1:D:205:ILE:HG23	1:D:211:GLY:HA2	2.03	0.41
1:B:202:PRO:O	1:B:205:ILE:HB	2.21	0.41
1:D:213:VAL:CG1	1:D:325:ILE:HB	2.50	0.41
1:A:234:LEU:HB2	1:A:235:PRO:HD3	2.03	0.41
1:A:220:ILE:HD12	1:A:248:LEU:HD23	2.03	0.41
1:G:102:GLU:HB2	1:G:442:VAL:HG13	2.03	0.41
1:L:206:ASN:HB2	1:L:213:VAL:HG23	2.01	0.41
2:A:1525:ATP:PG	3:A:1526:PO4:P	3.19	0.41
3:E:1526:PO4:P	2:E:1527:ATP:PG	3.19	0.41
1:F:182:GLY:O	1:F:382:GLY:HA2	2.21	0.41
1:D:182:GLY:O	1:D:382:GLY:HA2	2.21	0.41
1:D:202:PRO:O	1:D:205:ILE:HB	2.21	0.41
1:G:202:PRO:O	1:G:205:ILE:HB	2.21	0.41
1:E:205:ILE:HG23	1:E:211:GLY:HA2	2.03	0.41
1:F:205:ILE:HG23	1:F:211:GLY:HA2	2.03	0.41
1:C:127:ALA:N	1:C:426:LEU:HD21	2.36	0.41
1:C:213:VAL:CG1	1:C:325:ILE:HB	2.50	0.41
1:G:383:ALA:HB3	1:G:389:MET:CA	2.51	0.41
1:D:4:LYS:HA	1:D:522:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:VAL:HG22	1:B:309:LEU:O	2.20	0.41
1:N:263:VAL:O	1:N:267:MET:HB3	2.21	0.41
1:B:65:LYS:HZ2	1:B:525:PRO:N	2.19	0.41
1:J:2:ALA:O	1:J:3:ALA:C	2.59	0.41
1:E:234:LEU:HB2	1:E:235:PRO:HD3	2.02	0.41
3:G:1525:PO4:P	2:G:1527:ATP:PG	3.19	0.41
3:F:1525:PO4:P	2:F:1527:ATP:PG	3.19	0.41
1:E:127:ALA:N	1:E:426:LEU:HD21	2.36	0.41
1:B:127:ALA:N	1:B:426:LEU:HD21	2.36	0.41
1:C:383:ALA:HB3	1:C:389:MET:CA	2.51	0.41
1:B:383:ALA:HB3	1:B:389:MET:CA	2.51	0.41
1:F:4:LYS:HA	1:F:522:THR:O	2.21	0.41
1:I:230:ILE:HG23	1:I:259:LEU:HD12	2.02	0.41
1:M:230:ILE:HG23	1:M:259:LEU:HD12	2.03	0.41
1:I:2:ALA:O	1:I:3:ALA:C	2.59	0.40
1:A:152:ALA:HB1	1:A:155:ASP:O	2.21	0.40
1:G:4:LYS:HA	1:G:522:THR:O	2.22	0.40
1:G:34:LYS:HZ1	1:G:483:GLU:CD	2.25	0.40
1:K:263:VAL:O	1:K:267:MET:HB3	2.21	0.40
2:B:1525:ATP:PG	3:B:1526:PO4:P	3.19	0.40
1:C:205:ILE:HG23	1:C:211:GLY:HA2	2.03	0.40
1:G:127:ALA:N	1:G:426:LEU:HD21	2.36	0.40
1:A:323:VAL:HG22	1:A:332:ILE:HA	2.03	0.40
1:C:6:VAL:HG11	1:D:60:ILE:CD1	2.48	0.40
1:D:152:ALA:HB1	1:D:155:ASP:O	2.22	0.40
1:E:213:VAL:CG1	1:E:325:ILE:HB	2.51	0.40
1:G:234:LEU:HB2	1:G:235:PRO:HD3	2.02	0.40
1:C:220:ILE:HD12	1:C:248:LEU:HD23	2.03	0.40
1:B:220:ILE:HD12	1:B:248:LEU:HD23	2.03	0.40
1:A:205:ILE:HG23	1:A:211:GLY:HA2	2.03	0.40
1:C:323:VAL:HG22	1:C:332:ILE:HA	2.03	0.40
1:A:378:VAL:HG11	1:A:380:LYS:HZ2	1.86	0.40
1:G:213:VAL:O	1:G:324:VAL:HA	2.22	0.40
1:E:206:ASN:HB2	1:E:213:VAL:CB	2.52	0.40
1:D:206:ASN:HB2	1:D:213:VAL:CB	2.52	0.40
1:F:213:VAL:O	1:F:324:VAL:HA	2.22	0.40
1:C:206:ASN:HB2	1:C:213:VAL:CB	2.52	0.40
1:E:4:LYS:HA	1:E:522:THR:O	2.21	0.40
1:G:152:ALA:HB1	1:G:155:ASP:O	2.22	0.40
1:F:102:GLU:HB2	1:F:442:VAL:HG13	2.03	0.40
1:C:102:GLU:HB2	1:C:442:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:PRO:O	1:E:205:ILE:HB	2.21	0.40
1:E:213:VAL:O	1:E:324:VAL:HA	2.22	0.40
1:C:4:LYS:HA	1:C:522:THR:O	2.21	0.40
1:C:34:LYS:HZ1	1:C:483:GLU:CD	2.25	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%)	516 (99%)	5 (1%)	1 (0%)	52	86
1	B	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	52	86
1	C	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	52	86
1	D	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	52	86
1	E	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	52	86
1	F	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	52	86
1	G	522/548 (95%)	516 (99%)	5 (1%)	1 (0%)	52	86
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
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%)	7098 (97%)	189 (3%)	21 (0%)	50	83

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ALA
1	B	243	ALA
1	C	243	ALA
1	D	243	ALA
1	E	243	ALA
1	F	243	ALA
1	G	243	ALA
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 ⓘ

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%)	365 (91%)	37 (9%)	11	43
1	B	402/414 (97%)	365 (91%)	37 (9%)	11	43
1	C	402/414 (97%)	365 (91%)	37 (9%)	11	43
1	D	402/414 (97%)	365 (91%)	37 (9%)	11	43
1	E	402/414 (97%)	365 (91%)	37 (9%)	11	43
1	F	402/414 (97%)	365 (91%)	37 (9%)	11	43
1	G	402/414 (97%)	365 (91%)	37 (9%)	11	43
1	H	402/414 (97%)	369 (92%)	33 (8%)	14	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	402/414 (97%)	369 (92%)	33 (8%)	14	49
1	J	402/414 (97%)	369 (92%)	33 (8%)	14	49
1	K	402/414 (97%)	369 (92%)	33 (8%)	14	49
1	L	402/414 (97%)	369 (92%)	33 (8%)	14	49
1	M	402/414 (97%)	368 (92%)	34 (8%)	13	48
1	N	402/414 (97%)	369 (92%)	33 (8%)	14	49
All	All	5628/5796 (97%)	5137 (91%)	491 (9%)	17	45

All (491) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	25	ASP
1	A	31	LEU
1	A	38	VAL
1	A	41	ASP
1	A	55	SER
1	A	65	LYS
1	A	115	ASP
1	A	140	ASP
1	A	142	LYS
1	A	156	GLU
1	A	169	VAL
1	A	171	LYS
1	A	186	GLU
1	A	205	ILE
1	A	207	LYS
1	A	213	VAL
1	A	214	GLU
1	A	219	PHE
1	A	231	ARG
1	A	238	GLU
1	A	261	THR
1	A	268	ARG
1	A	290	GLN
1	A	321	LYS
1	A	327	LYS
1	A	328	ASP
1	A	338	GLU
1	A	339	GLU

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Mol	Chain	Res	Type
1	A	350	ARG
1	A	358	SER
1	A	421	ARG
1	A	430	ARG
1	A	460	GLU
1	A	484	GLU
1	A	494	LEU
1	A	504	LEU
1	B	13	ARG
1	B	25	ASP
1	B	31	LEU
1	B	38	VAL
1	B	41	ASP
1	B	55	SER
1	B	65	LYS
1	B	115	ASP
1	B	140	ASP
1	B	142	LYS
1	B	156	GLU
1	B	169	VAL
1	B	171	LYS
1	B	186	GLU
1	B	205	ILE
1	B	207	LYS
1	B	213	VAL
1	B	214	GLU
1	B	219	PHE
1	B	231	ARG
1	B	238	GLU
1	B	261	THR
1	B	268	ARG
1	B	290	GLN
1	B	321	LYS
1	B	327	LYS
1	B	328	ASP
1	B	338	GLU
1	B	339	GLU
1	B	350	ARG
1	B	358	SER
1	B	421	ARG
1	B	430	ARG
1	B	460	GLU

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Mol	Chain	Res	Type
1	B	484	GLU
1	B	494	LEU
1	B	504	LEU
1	C	13	ARG
1	C	25	ASP
1	C	31	LEU
1	C	38	VAL
1	C	41	ASP
1	C	55	SER
1	C	65	LYS
1	C	115	ASP
1	C	140	ASP
1	C	142	LYS
1	C	156	GLU
1	C	169	VAL
1	C	171	LYS
1	C	186	GLU
1	C	205	ILE
1	C	207	LYS
1	C	213	VAL
1	C	214	GLU
1	C	219	PHE
1	C	231	ARG
1	C	238	GLU
1	C	261	THR
1	C	268	ARG
1	C	290	GLN
1	C	321	LYS
1	C	327	LYS
1	C	328	ASP
1	C	338	GLU
1	C	339	GLU
1	C	350	ARG
1	C	358	SER
1	C	421	ARG
1	C	430	ARG
1	C	460	GLU
1	C	484	GLU
1	C	494	LEU
1	C	504	LEU
1	D	13	ARG
1	D	25	ASP

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Mol	Chain	Res	Type
1	D	31	LEU
1	D	38	VAL
1	D	41	ASP
1	D	55	SER
1	D	65	LYS
1	D	115	ASP
1	D	140	ASP
1	D	142	LYS
1	D	156	GLU
1	D	169	VAL
1	D	171	LYS
1	D	186	GLU
1	D	205	ILE
1	D	207	LYS
1	D	213	VAL
1	D	214	GLU
1	D	219	PHE
1	D	231	ARG
1	D	238	GLU
1	D	261	THR
1	D	268	ARG
1	D	290	GLN
1	D	321	LYS
1	D	327	LYS
1	D	328	ASP
1	D	338	GLU
1	D	339	GLU
1	D	350	ARG
1	D	358	SER
1	D	421	ARG
1	D	430	ARG
1	D	460	GLU
1	D	484	GLU
1	D	494	LEU
1	D	504	LEU
1	E	13	ARG
1	E	25	ASP
1	E	31	LEU
1	E	38	VAL
1	E	41	ASP
1	E	55	SER
1	E	65	LYS

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Mol	Chain	Res	Type
1	E	115	ASP
1	E	140	ASP
1	E	142	LYS
1	E	156	GLU
1	E	169	VAL
1	E	171	LYS
1	E	186	GLU
1	E	205	ILE
1	E	207	LYS
1	E	213	VAL
1	E	214	GLU
1	E	219	PHE
1	E	231	ARG
1	E	238	GLU
1	E	261	THR
1	E	268	ARG
1	E	290	GLN
1	E	321	LYS
1	E	327	LYS
1	E	328	ASP
1	E	338	GLU
1	E	339	GLU
1	E	350	ARG
1	E	358	SER
1	E	421	ARG
1	E	430	ARG
1	E	460	GLU
1	E	484	GLU
1	E	494	LEU
1	E	504	LEU
1	F	13	ARG
1	F	25	ASP
1	F	31	LEU
1	F	38	VAL
1	F	41	ASP
1	F	55	SER
1	F	65	LYS
1	F	115	ASP
1	F	140	ASP
1	F	142	LYS
1	F	156	GLU
1	F	169	VAL

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Mol	Chain	Res	Type
1	F	171	LYS
1	F	186	GLU
1	F	205	ILE
1	F	207	LYS
1	F	213	VAL
1	F	214	GLU
1	F	219	PHE
1	F	231	ARG
1	F	238	GLU
1	F	261	THR
1	F	268	ARG
1	F	290	GLN
1	F	321	LYS
1	F	327	LYS
1	F	328	ASP
1	F	338	GLU
1	F	339	GLU
1	F	350	ARG
1	F	358	SER
1	F	421	ARG
1	F	430	ARG
1	F	460	GLU
1	F	484	GLU
1	F	494	LEU
1	F	504	LEU
1	G	13	ARG
1	G	25	ASP
1	G	31	LEU
1	G	38	VAL
1	G	41	ASP
1	G	55	SER
1	G	65	LYS
1	G	115	ASP
1	G	140	ASP
1	G	142	LYS
1	G	156	GLU
1	G	169	VAL
1	G	171	LYS
1	G	186	GLU
1	G	205	ILE
1	G	207	LYS
1	G	213	VAL

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Mol	Chain	Res	Type
1	G	214	GLU
1	G	219	PHE
1	G	231	ARG
1	G	238	GLU
1	G	261	THR
1	G	268	ARG
1	G	290	GLN
1	G	321	LYS
1	G	327	LYS
1	G	328	ASP
1	G	338	GLU
1	G	339	GLU
1	G	350	ARG
1	G	358	SER
1	G	421	ARG
1	G	430	ARG
1	G	460	GLU
1	G	484	GLU
1	G	494	LEU
1	G	504	LEU
1	H	25	ASP
1	H	34	LYS
1	H	82	ASN
1	H	142	LYS
1	H	153	ASN
1	H	172	GLU
1	H	186	GLU
1	H	187	LEU
1	H	196	ASP
1	H	199	TYR
1	H	214	GLU
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	313	THR
1	H	327	LYS
1	H	329	THR
1	H	334	ASP
1	H	338	GLU

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Mol	Chain	Res	Type
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	142	LYS
1	I	153	ASN
1	I	172	GLU
1	I	186	GLU
1	I	187	LEU
1	I	196	ASP
1	I	199	TYR
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	313	THR
1	I	327	LYS
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

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Mol	Chain	Res	Type
1	I	504	LEU
1	I	510	VAL
1	J	25	ASP
1	J	34	LYS
1	J	82	ASN
1	J	142	LYS
1	J	153	ASN
1	J	172	GLU
1	J	186	GLU
1	J	187	LEU
1	J	196	ASP
1	J	199	TYR
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	313	THR
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
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	142	LYS
1	K	153	ASN
1	K	172	GLU
1	K	186	GLU

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Mol	Chain	Res	Type
1	K	187	LEU
1	K	196	ASP
1	K	199	TYR
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	313	THR
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
1	L	25	ASP
1	L	34	LYS
1	L	82	ASN
1	L	142	LYS
1	L	153	ASN
1	L	172	GLU
1	L	186	GLU
1	L	187	LEU
1	L	196	ASP
1	L	199	TYR
1	L	214	GLU
1	L	216	GLU
1	L	228	SER
1	L	229	ASN
1	L	230	ILE
1	L	281	PHE

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Mol	Chain	Res	Type
1	L	290	GLN
1	L	313	THR
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	142	LYS
1	M	153	ASN
1	M	172	GLU
1	M	186	GLU
1	M	187	LEU
1	M	196	ASP
1	M	199	TYR
1	M	214	GLU
1	M	216	GLU
1	M	228	SER
1	M	229	ASN
1	M	230	ILE
1	M	267	MET
1	M	281	PHE
1	M	290	GLN
1	M	313	THR
1	M	327	LYS
1	M	329	THR
1	M	334	ASP
1	M	338	GLU
1	M	350	ARG
1	M	404	ARG

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Mol	Chain	Res	Type
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	142	LYS
1	N	153	ASN
1	N	172	GLU
1	N	186	GLU
1	N	187	LEU
1	N	196	ASP
1	N	199	TYR
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	313	THR
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	453	GLN
1	B	453	GLN
1	C	453	GLN
1	D	453	GLN
1	E	453	GLN
1	F	453	GLN
1	G	453	GLN
1	H	68	ASN
1	I	68	ASN
1	J	68	ASN
1	K	68	ASN
1	L	68	ASN
1	M	68	ASN
1	N	68	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	0.97	1 (3%)	26,52,52	1.34	5 (19%)
2	ATP	B	1525	4	26,33,33	0.97	1 (3%)	26,52,52	1.34	5 (19%)
2	ATP	C	1526	4	26,33,33	0.97	1 (3%)	26,52,52	1.34	5 (19%)
2	ATP	D	1525	4	26,33,33	0.97	1 (3%)	26,52,52	1.34	5 (19%)
2	ATP	E	1527	4	26,33,33	0.97	1 (3%)	26,52,52	1.34	5 (19%)
2	ATP	F	1527	4	26,33,33	0.96	1 (3%)	26,52,52	1.34	5 (19%)
2	ATP	G	1527	4	26,33,33	0.97	1 (3%)	26,52,52	1.34	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	A	1525	ATP	C2'-C1'	-3.32	1.48	1.53
2	B	1525	ATP	C2'-C1'	-3.32	1.48	1.53
2	E	1527	ATP	C2'-C1'	-3.31	1.48	1.53
2	C	1526	ATP	C2'-C1'	-3.28	1.48	1.53
2	D	1525	ATP	C2'-C1'	-3.28	1.48	1.53
2	G	1527	ATP	C2'-C1'	-3.26	1.48	1.53
2	F	1527	ATP	C2'-C1'	-3.25	1.48	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1527	ATP	C4'-O4'-C1'	-2.33	107.17	109.64
2	G	1527	ATP	C4'-O4'-C1'	-2.33	107.17	109.64
2	C	1526	ATP	C4'-O4'-C1'	-2.33	107.18	109.64
2	B	1525	ATP	C4'-O4'-C1'	-2.31	107.19	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1527	ATP	C4'-O4'-C1'	-2.31	107.20	109.64
2	D	1525	ATP	C4'-O4'-C1'	-2.30	107.20	109.64
2	A	1525	ATP	C4'-O4'-C1'	-2.28	107.23	109.64
2	A	1525	ATP	C1'-N9-C4	-2.26	124.28	126.81
2	D	1525	ATP	C1'-N9-C4	-2.24	124.31	126.81
2	E	1527	ATP	C1'-N9-C4	-2.23	124.32	126.81
2	G	1527	ATP	C1'-N9-C4	-2.22	124.33	126.81
2	B	1525	ATP	C1'-N9-C4	-2.21	124.33	126.81
2	C	1526	ATP	C1'-N9-C4	-2.21	124.34	126.81
2	F	1527	ATP	C1'-N9-C4	-2.19	124.36	126.81
2	F	1527	ATP	O2A-PA-O3A	2.25	114.91	105.27
2	C	1526	ATP	O2A-PA-O3A	2.26	114.94	105.27
2	A	1525	ATP	O2A-PA-O3A	2.26	114.95	105.27
2	D	1525	ATP	O2A-PA-O3A	2.26	114.95	105.27
2	B	1525	ATP	O2A-PA-O3A	2.26	114.96	105.27
2	G	1527	ATP	O2A-PA-O3A	2.27	114.98	105.27
2	E	1527	ATP	O2A-PA-O3A	2.27	114.98	105.27
2	B	1525	ATP	O4'-C1'-N9	2.38	112.60	108.11
2	E	1527	ATP	O4'-C1'-N9	2.38	112.61	108.11
2	A	1525	ATP	O4'-C1'-N9	2.39	112.62	108.11
2	D	1525	ATP	O4'-C1'-N9	2.39	112.63	108.11
2	C	1526	ATP	O4'-C1'-N9	2.40	112.64	108.11
2	F	1527	ATP	O4'-C1'-N9	2.40	112.64	108.11
2	G	1527	ATP	O4'-C1'-N9	2.40	112.64	108.11
2	B	1525	ATP	O3G-PG-O2G	2.44	116.41	107.44
2	E	1527	ATP	O3G-PG-O2G	2.44	116.41	107.44
2	A	1525	ATP	O3G-PG-O2G	2.45	116.43	107.44
2	F	1527	ATP	O3G-PG-O2G	2.45	116.44	107.44
2	C	1526	ATP	O3G-PG-O2G	2.45	116.44	107.44
2	D	1525	ATP	O3G-PG-O2G	2.46	116.47	107.44
2	G	1527	ATP	O3G-PG-O2G	2.46	116.49	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1525	ATP	4	0
2	B	1525	ATP	4	0
2	C	1526	ATP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1525	ATP	4	0
2	E	1527	ATP	4	0
2	F	1527	ATP	4	0
2	G	1527	ATP	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.