



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 01:51 PM EDT

PDB ID : 1SX3
Title : GroEL14-(ATPgammaS)14
Authors : Chaudhry, C.; Horwich, A.L.; Brunger, A.T.; Adams, P.D.
Deposited on : unknown
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

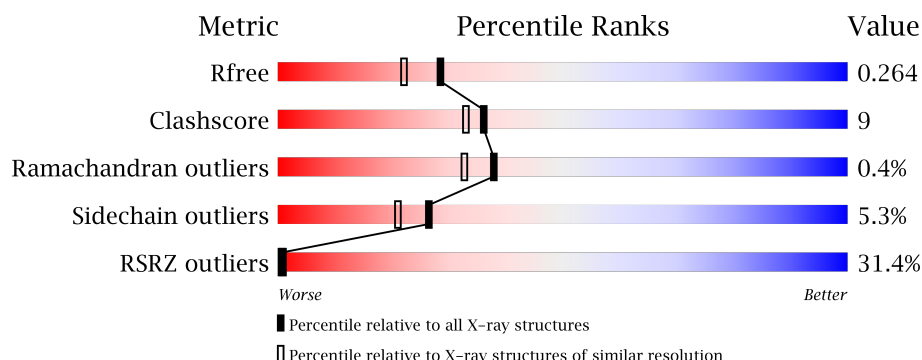
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	525	<div> <div>24%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
1	B	525	<div> <div>44%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>.</div> </div> </div>
1	C	525	<div> <div>37%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>..</div> </div> </div>
1	D	525	<div> <div>21%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>..</div> </div> </div>
1	E	525	<div> <div>38%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	525	
1	G	525	
1	H	525	
1	I	525	
1	J	525	
1	K	525	
1	L	525	
1	M	525	
1	N	525	

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	K	D	1	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 55380 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	B	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	C	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	D	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	E	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	F	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	G	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	H	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	I	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	J	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	K	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	L	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	M	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			
1	N	525	Total	C	N	O	S	0	0	0
			3855	2399	664	772	20			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	ARG	ENGINEERED	UNP P0A6F5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	126	VAL	ALA	ENGINEERED	UNP P0A6F5
B	13	GLY	ARG	ENGINEERED	UNP P0A6F5
B	126	VAL	ALA	ENGINEERED	UNP P0A6F5
C	13	GLY	ARG	ENGINEERED	UNP P0A6F5
C	126	VAL	ALA	ENGINEERED	UNP P0A6F5
D	13	GLY	ARG	ENGINEERED	UNP P0A6F5
D	126	VAL	ALA	ENGINEERED	UNP P0A6F5
E	13	GLY	ARG	ENGINEERED	UNP P0A6F5
E	126	VAL	ALA	ENGINEERED	UNP P0A6F5
F	13	GLY	ARG	ENGINEERED	UNP P0A6F5
F	126	VAL	ALA	ENGINEERED	UNP P0A6F5
G	13	GLY	ARG	ENGINEERED	UNP P0A6F5
G	126	VAL	ALA	ENGINEERED	UNP P0A6F5
H	13	GLY	ARG	ENGINEERED	UNP P0A6F5
H	126	VAL	ALA	ENGINEERED	UNP P0A6F5
I	13	GLY	ARG	ENGINEERED	UNP P0A6F5
I	126	VAL	ALA	ENGINEERED	UNP P0A6F5
J	13	GLY	ARG	ENGINEERED	UNP P0A6F5
J	126	VAL	ALA	ENGINEERED	UNP P0A6F5
K	13	GLY	ARG	ENGINEERED	UNP P0A6F5
K	126	VAL	ALA	ENGINEERED	UNP P0A6F5
L	13	GLY	ARG	ENGINEERED	UNP P0A6F5
L	126	VAL	ALA	ENGINEERED	UNP P0A6F5
M	13	GLY	ARG	ENGINEERED	UNP P0A6F5
M	126	VAL	ALA	ENGINEERED	UNP P0A6F5
N	13	GLY	ARG	ENGINEERED	UNP P0A6F5
N	126	VAL	ALA	ENGINEERED	UNP P0A6F5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	K	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0
2	I	1	Total 1	Mg 1	0	0
2	C	1	Total 1	Mg 1	0	0
2	A	1	Total 1	Mg 1	0	0
2	N	1	Total 1	Mg 1	0	0
2	L	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0
2	M	1	Total 1	Mg 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

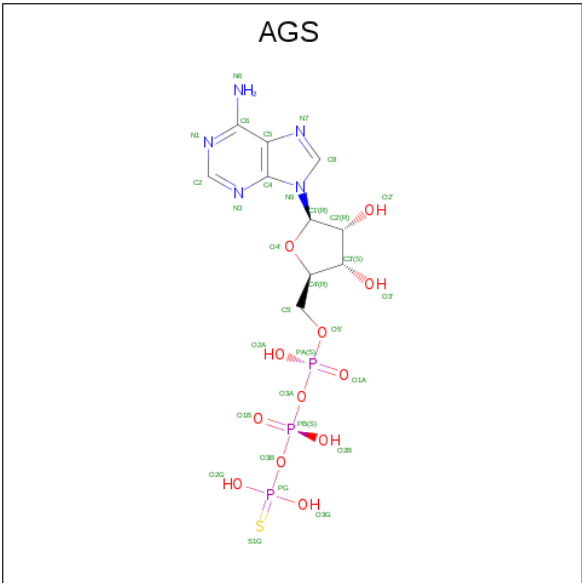
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	K 1	0	0
3	J	1	Total 1	K 1	0	0
3	D	2	Total 2	K 2	0	0
3	K	1	Total 1	K 1	0	0
3	E	2	Total 2	K 2	0	0
3	H	1	Total 1	K 1	0	0
3	B	1	Total 1	K 1	0	0
3	I	1	Total 1	K 1	0	0
3	C	1	Total 1	K 1	0	0
3	A	1	Total 1	K 1	0	0
3	N	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	K	0	0
			1	1		
3	F	1	Total	K	0	0
			1	1		
3	M	1	Total	K	0	0
			1	1		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	I	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	J	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	K	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	L	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	M	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0
4	N	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total 62	O 62	0	0
5	B	83	Total 83	O 83	0	0
5	C	57	Total 57	O 57	0	0
5	D	91	Total 91	O 91	0	0
5	E	92	Total 92	O 92	0	0
5	F	71	Total 71	O 71	0	0
5	G	83	Total 83	O 83	0	0
5	H	77	Total 77	O 77	0	0
5	I	60	Total 60	O 60	0	0
5	J	50	Total 50	O 50	0	0
5	K	47	Total 47	O 47	0	0
5	L	61	Total 61	O 61	0	0
5	M	53	Total 53	O 53	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	N	59	Total	O	0	0
			59	59		

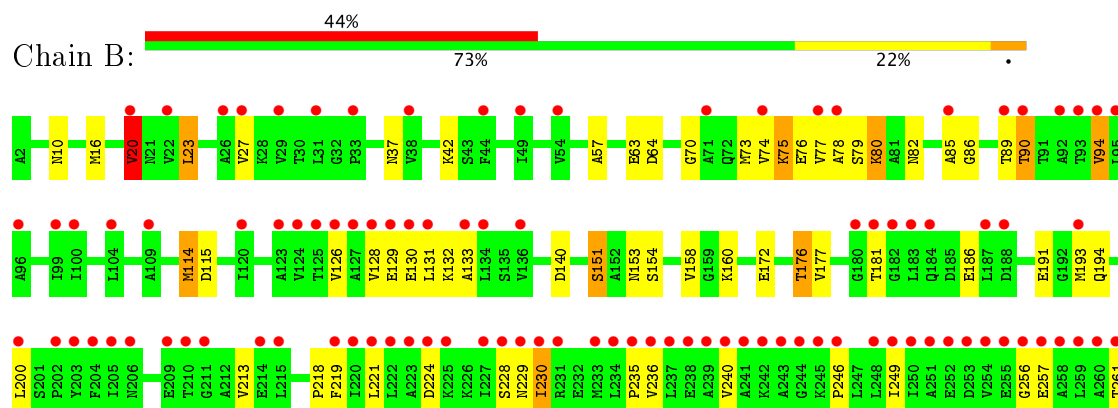
3 Residue-property plots

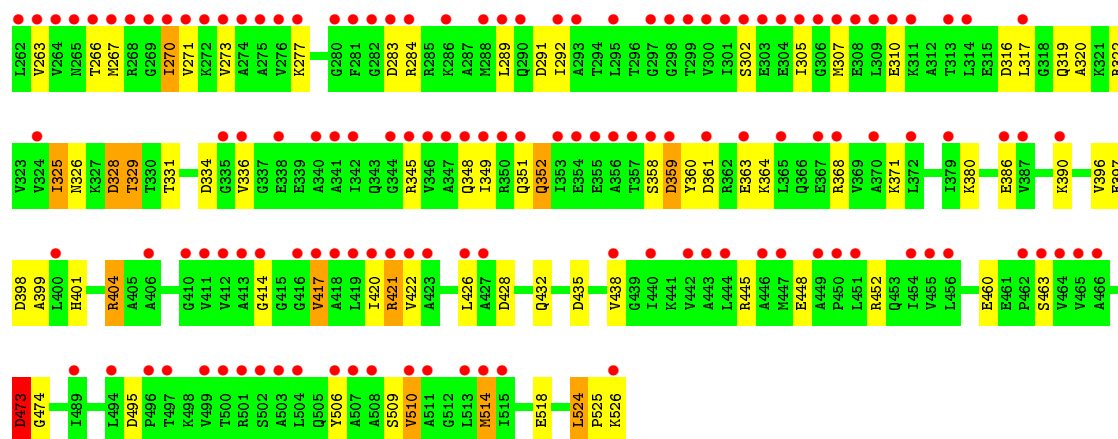
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: groEL protein

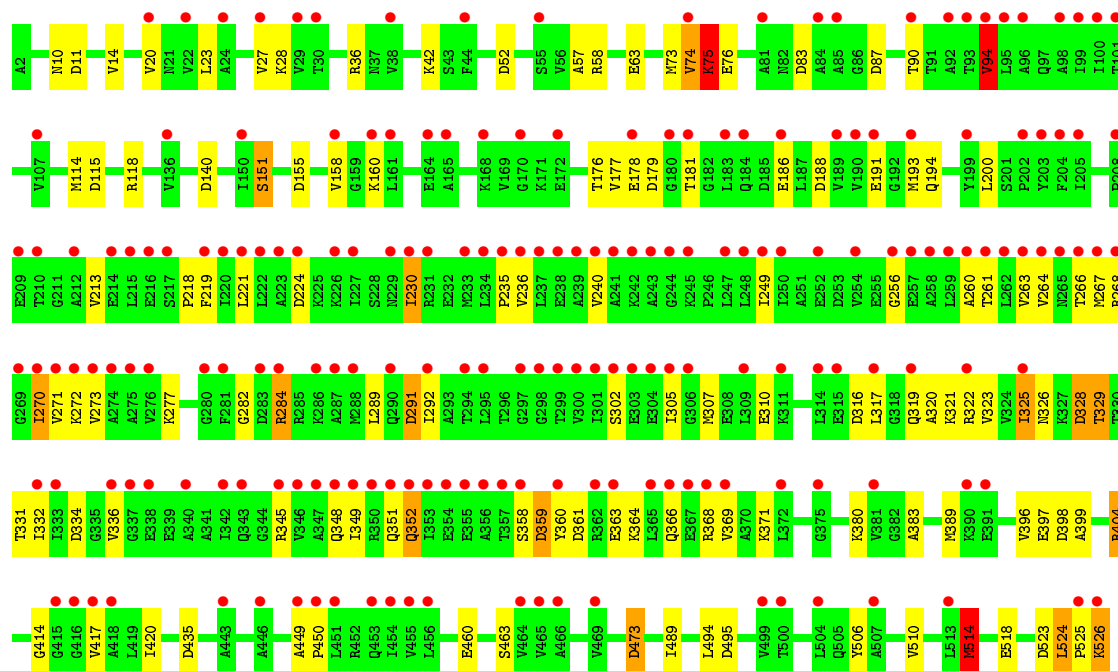
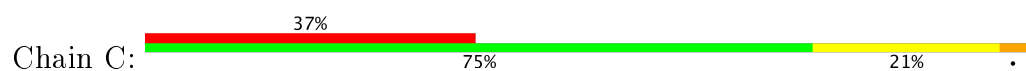


• Molecule 1: groEL protein

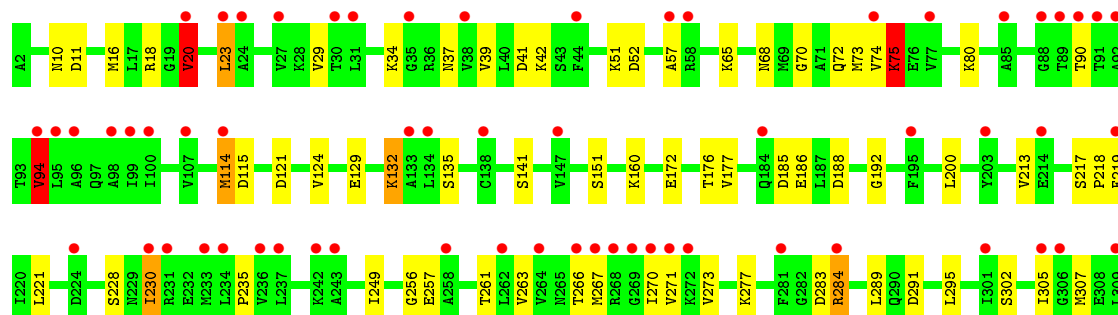
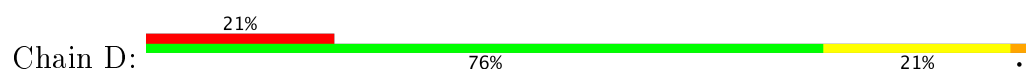


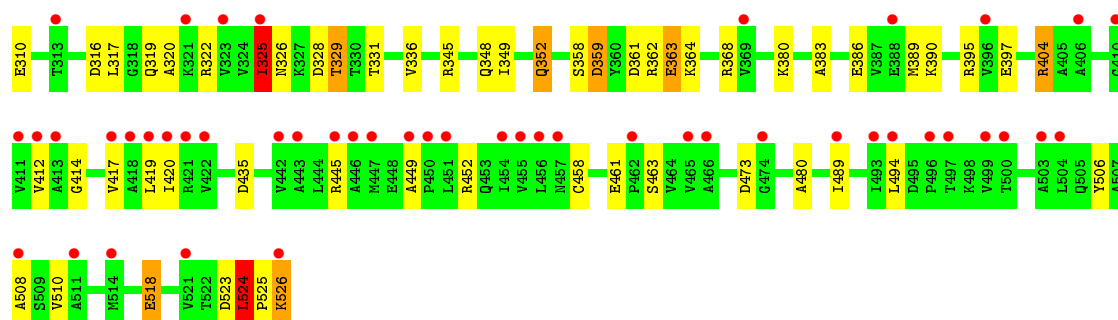


• Molecule 1: groEL protein



• Molecule 1: groEL protein

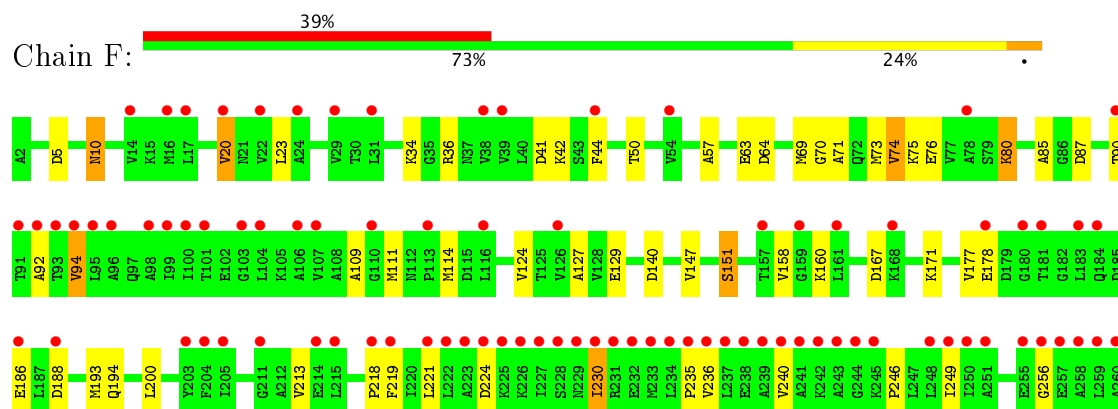


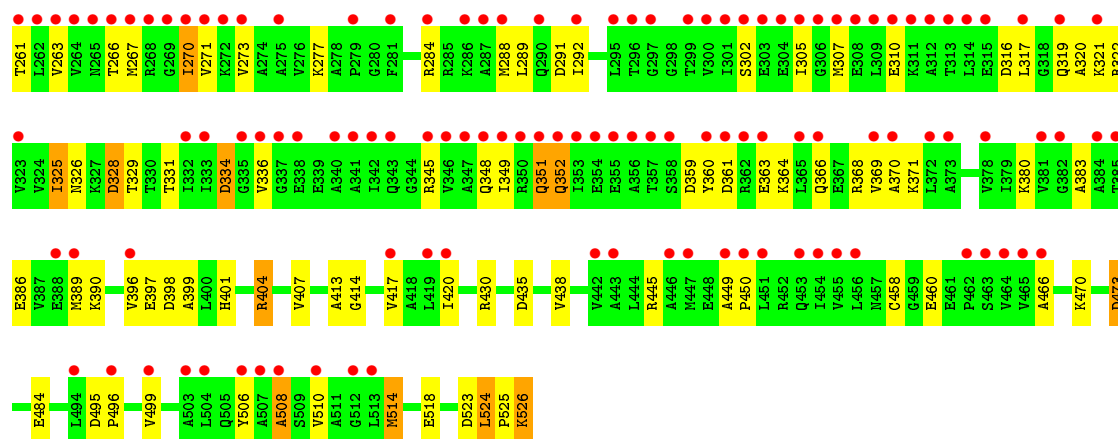


• Molecule 1: groEL protein

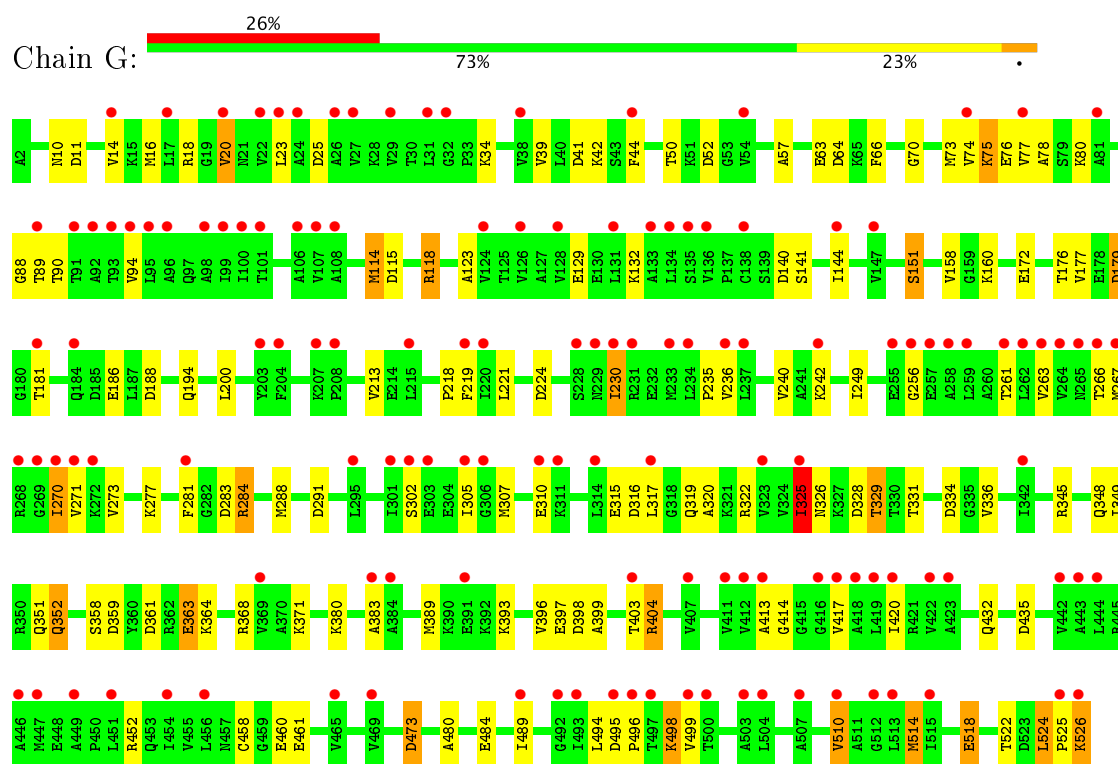


• Molecule 1: groEL protein

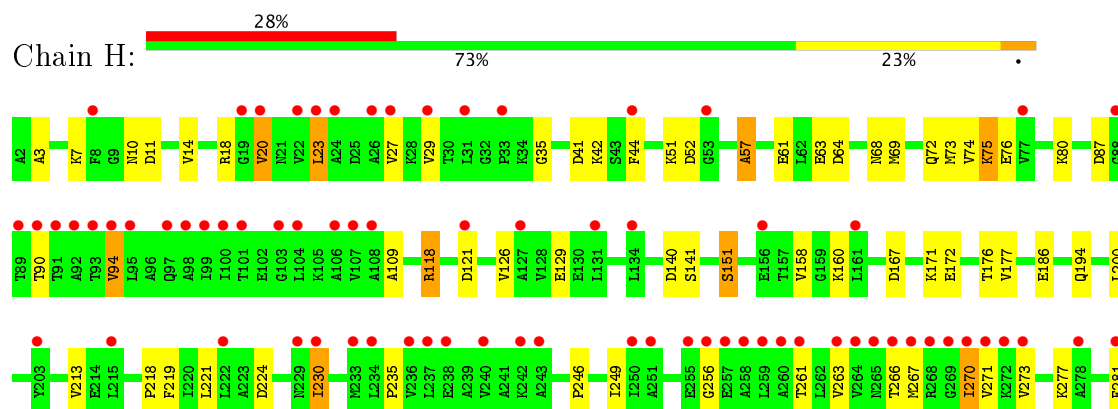


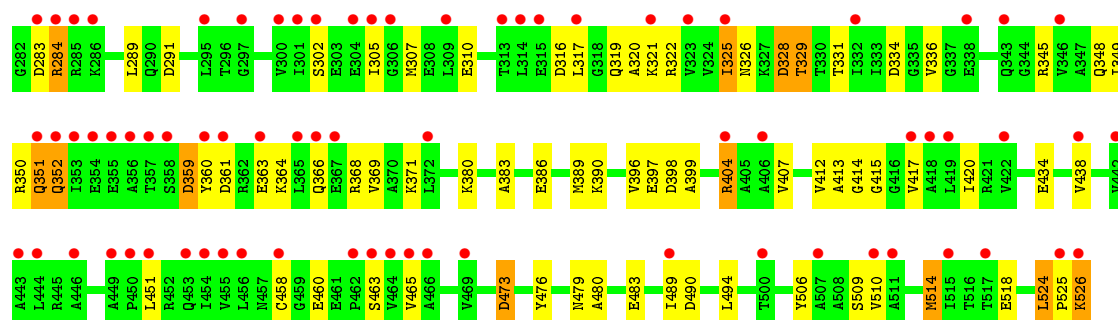


• Molecule 1: groEL protein

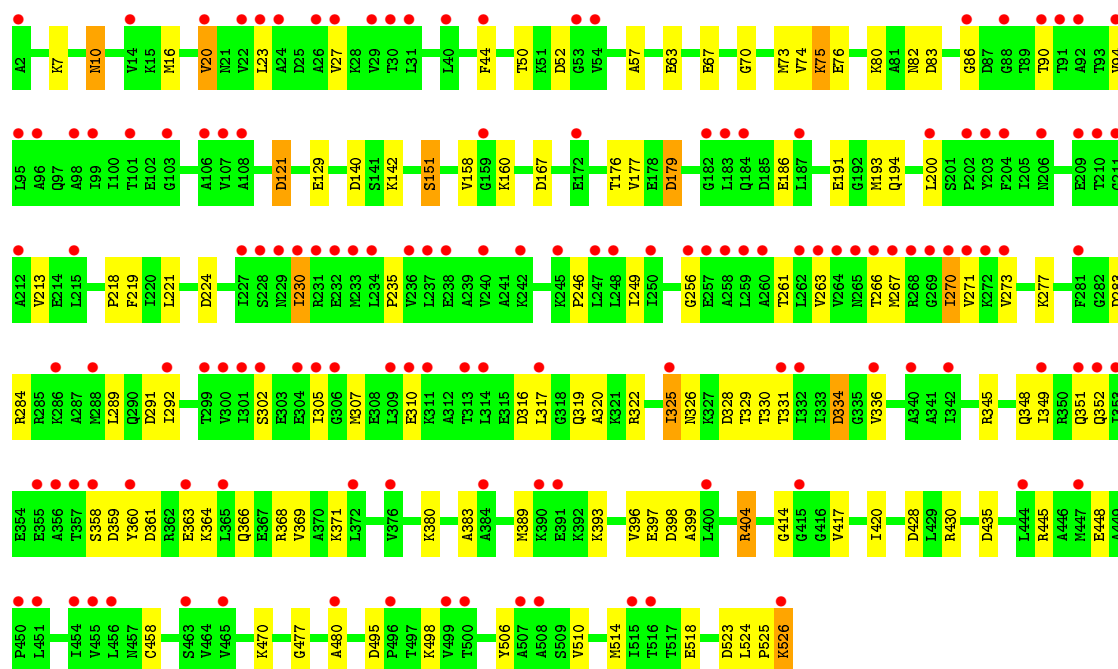
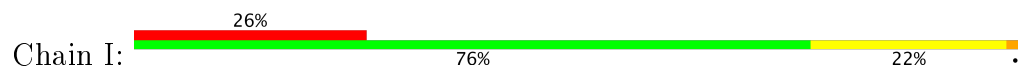


• Molecule 1: groEL protein

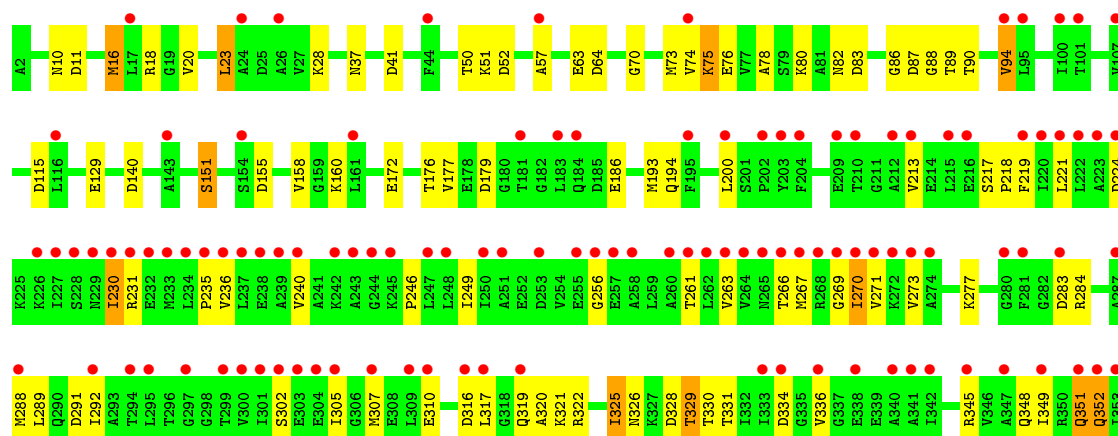
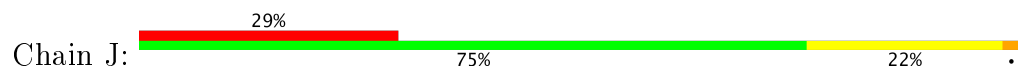


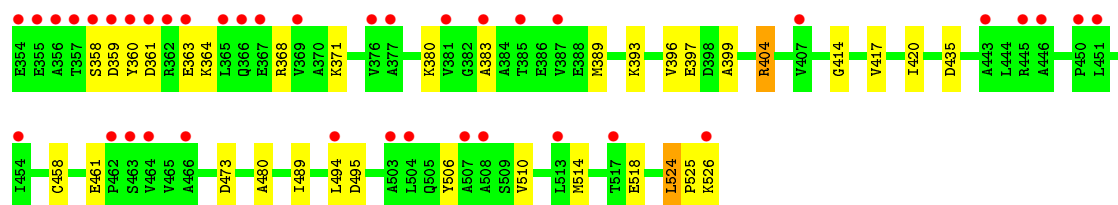


• Molecule 1: groEL protein

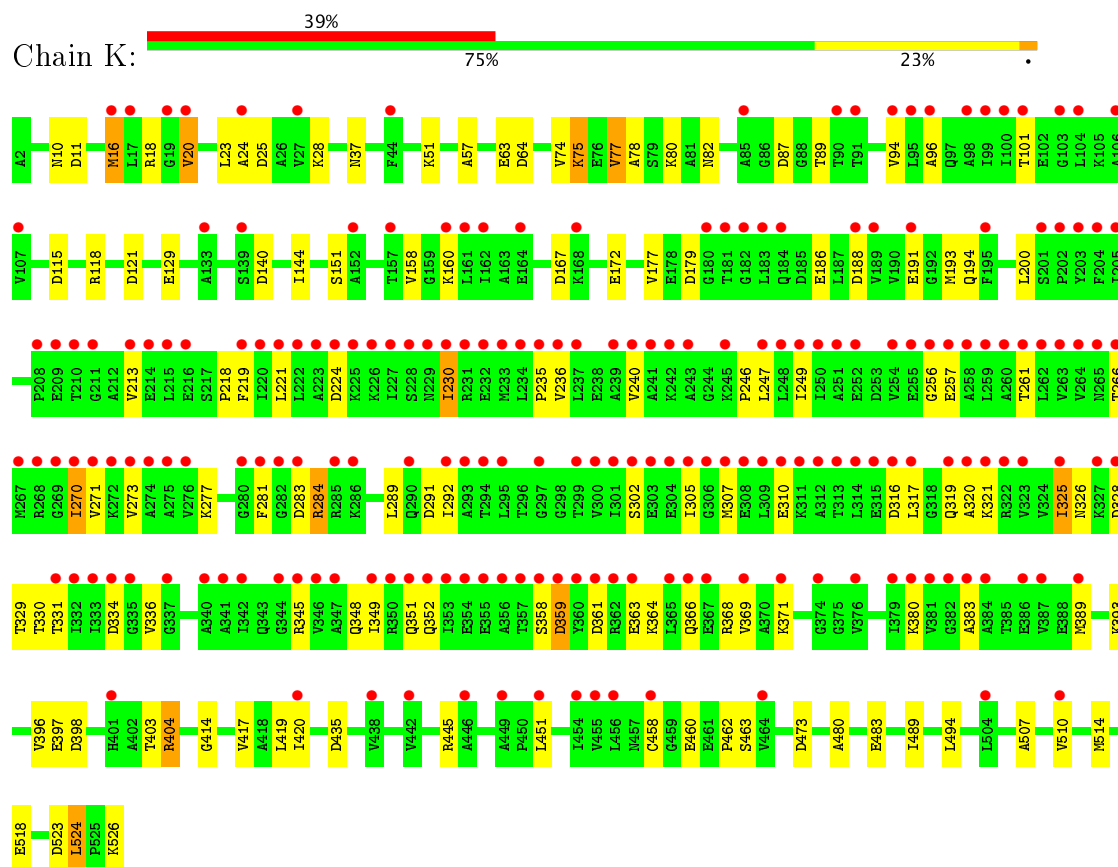


• Molecule 1: groEL protein

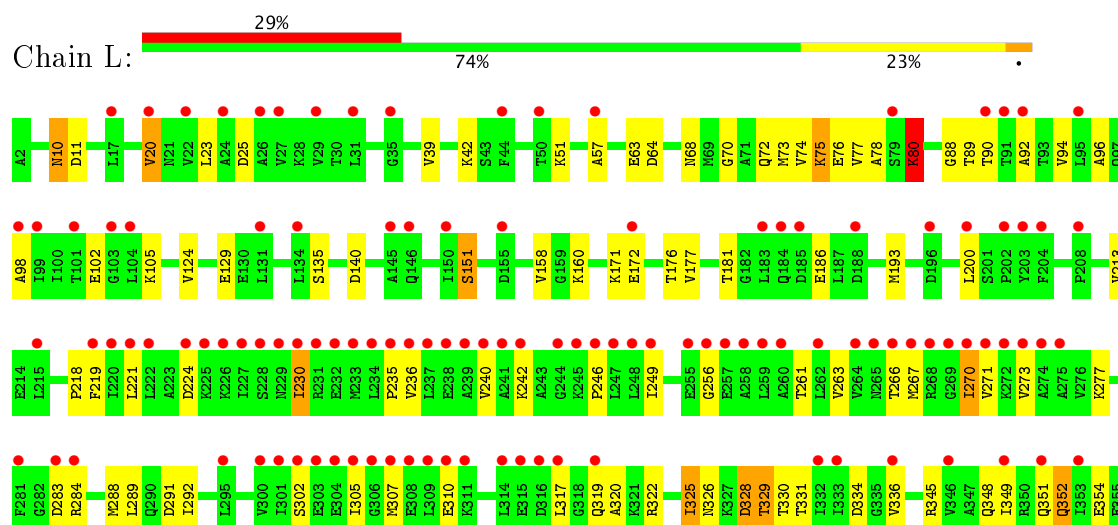


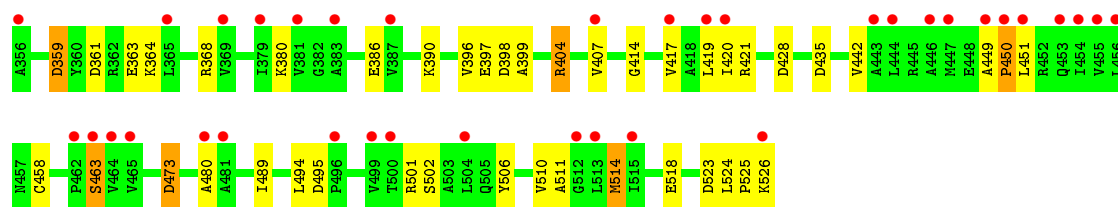


• Molecule 1: groEL protein



• Molecule 1: groEL protein

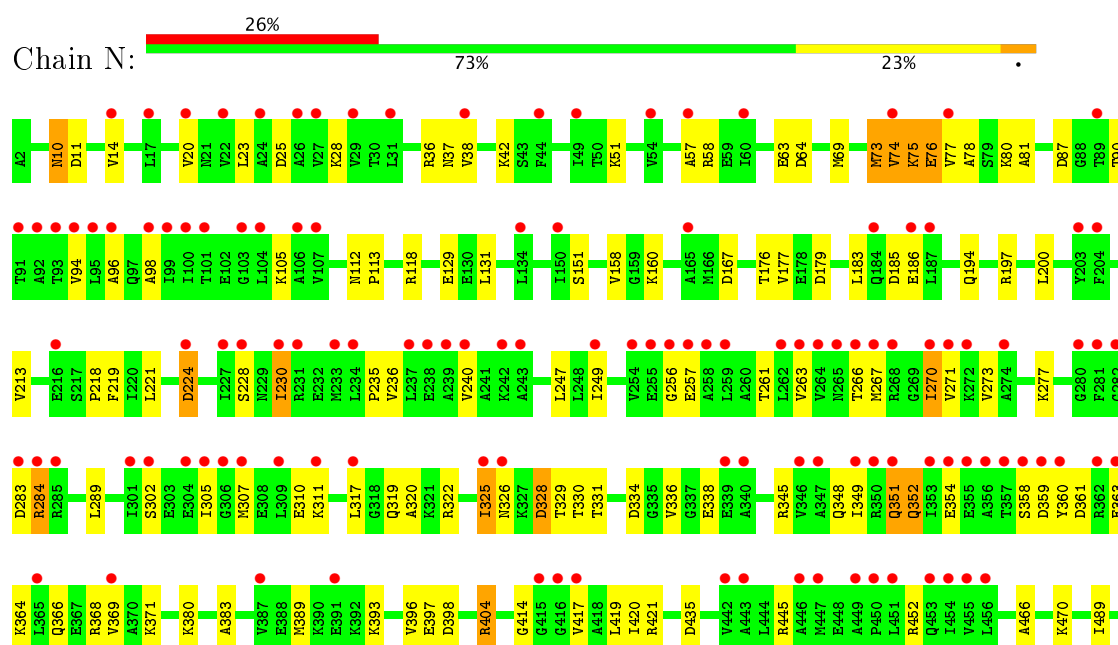


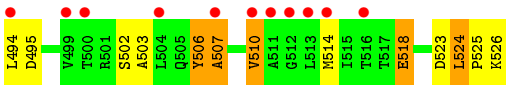


• Molecule 1: groEL protein



• Molecule 1: groEL protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.57Å 260.11Å 150.20Å 90.00° 101.14° 90.00°	Depositor
Resolution (Å)	39.84 – 2.00 39.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.84-2.00) 79.1 (39.89-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.00Å)	Xtriage
Refinement program	REFMAC refmac_5.1.19	Depositor
R, R_{free}	0.245 , 0.265 0.245 , 0.264	Depositor DCC
R_{free} test set	10651 reflections (1.97%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	55380	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.09	12/3883 (0.3%)	1.03	21/5243 (0.4%)
1	B	1.27	27/3883 (0.7%)	1.11	25/5243 (0.5%)
1	C	1.02	10/3883 (0.3%)	0.99	22/5243 (0.4%)
1	D	1.28	18/3883 (0.5%)	1.13	25/5243 (0.5%)
1	E	1.31	32/3883 (0.8%)	1.19	37/5243 (0.7%)
1	F	1.10	18/3883 (0.5%)	1.04	21/5243 (0.4%)
1	G	1.26	25/3883 (0.6%)	1.09	21/5243 (0.4%)
1	H	1.25	32/3883 (0.8%)	1.09	24/5243 (0.5%)
1	I	1.11	9/3883 (0.2%)	1.02	19/5243 (0.4%)
1	J	1.08	11/3883 (0.3%)	1.08	21/5243 (0.4%)
1	K	1.03	10/3883 (0.3%)	1.00	18/5243 (0.3%)
1	L	1.15	19/3883 (0.5%)	1.07	22/5243 (0.4%)
1	M	1.03	10/3883 (0.3%)	1.08	18/5243 (0.3%)
1	N	1.15	16/3883 (0.4%)	1.09	26/5243 (0.5%)
All	All	1.16	249/54362 (0.5%)	1.07	320/73402 (0.4%)

All (249) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	510	VAL	CB-CG2	14.81	1.83	1.52
1	B	129	GLU	CD-OE2	13.14	1.40	1.25
1	B	510	VAL	CB-CG2	12.46	1.79	1.52
1	E	490	ASP	CB-CG	-11.51	1.27	1.51
1	B	129	GLU	CG-CD	11.47	1.69	1.51
1	E	506	TYR	CD2-CE2	10.89	1.55	1.39
1	B	129	GLU	CD-OE1	10.70	1.37	1.25
1	K	510	VAL	CB-CG2	9.95	1.73	1.52
1	J	510	VAL	CB-CG2	9.69	1.73	1.52
1	F	510	VAL	CB-CG2	9.64	1.73	1.52
1	G	129	GLU	CD-OE2	9.58	1.36	1.25
1	J	506	TYR	CD1-CE1	9.37	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	506	TYR	CD1-CE1	9.29	1.53	1.39
1	E	510	VAL	CB-CG2	9.28	1.72	1.52
1	B	132	LYS	CD-CE	9.16	1.74	1.51
1	N	506	TYR	CD2-CE2	8.89	1.52	1.39
1	G	460	GLU	CD-OE1	8.89	1.35	1.25
1	D	114	MET	CG-SD	8.76	2.04	1.81
1	D	129	GLU	CD-OE2	8.54	1.35	1.25
1	L	88	GLY	C-O	8.45	1.37	1.23
1	A	129	GLU	CD-OE1	8.39	1.34	1.25
1	L	92	ALA	CA-CB	8.22	1.69	1.52
1	G	129	GLU	CG-CD	8.17	1.64	1.51
1	D	129	GLU	CD-OE1	8.07	1.34	1.25
1	D	363	GLU	CD-OE2	8.03	1.34	1.25
1	D	510	VAL	CB-CG2	8.02	1.69	1.52
1	L	172	GLU	CD-OE2	7.98	1.34	1.25
1	L	124	VAL	CB-CG2	-7.92	1.36	1.52
1	D	141	SER	CB-OG	-7.87	1.32	1.42
1	I	510	VAL	CB-CG2	7.80	1.69	1.52
1	L	511	ALA	CA-CB	-7.78	1.36	1.52
1	M	510	VAL	CB-CG2	7.77	1.69	1.52
1	N	96	ALA	CA-CB	-7.76	1.36	1.52
1	C	114	MET	CG-SD	7.74	2.01	1.81
1	H	438	VAL	CB-CG2	7.74	1.69	1.52
1	B	432	GLN	CG-CD	7.69	1.68	1.51
1	N	507	ALA	CA-CB	-7.67	1.36	1.52
1	B	130	GLU	CD-OE2	7.60	1.34	1.25
1	H	506	TYR	CD2-CE2	7.46	1.50	1.39
1	F	438	VAL	CB-CG2	7.42	1.68	1.52
1	G	510	VAL	CB-CG2	7.41	1.68	1.52
1	H	44	PHE	CD2-CE2	7.40	1.54	1.39
1	L	80	LYS	CG-CD	7.37	1.77	1.52
1	B	460	GLU	CD-OE2	7.31	1.33	1.25
1	B	90	THR	C-O	7.30	1.37	1.23
1	E	460	GLU	CD-OE2	7.30	1.33	1.25
1	G	114	MET	CG-SD	7.25	2.00	1.81
1	L	129	GLU	CD-OE2	7.24	1.33	1.25
1	J	129	GLU	CD-OE1	7.17	1.33	1.25
1	N	73	MET	SD-CE	-7.17	1.37	1.77
1	E	485	TYR	CE2-CZ	7.17	1.47	1.38
1	A	129	GLU	CD-OE2	7.16	1.33	1.25
1	H	509	SER	CB-OG	-7.16	1.32	1.42
1	I	526	LYS	CD-CE	7.16	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	98	ALA	C-O	-7.16	1.09	1.23
1	E	129	GLU	CD-OE2	7.13	1.33	1.25
1	A	81	ALA	CA-CB	-7.11	1.37	1.52
1	C	510	VAL	CB-CG2	7.09	1.67	1.52
1	L	129	GLU	CG-CD	7.08	1.62	1.51
1	D	506	TYR	CD2-CE2	7.03	1.49	1.39
1	D	445	ARG	NE-CZ	7.02	1.42	1.33
1	J	461	GLU	CD-OE2	6.97	1.33	1.25
1	I	44	PHE	CE1-CZ	6.95	1.50	1.37
1	N	506	TYR	CD1-CE1	6.95	1.49	1.39
1	B	422	VAL	CB-CG1	-6.93	1.38	1.52
1	H	129	GLU	CD-OE1	6.92	1.33	1.25
1	F	445	ARG	NE-CZ	6.91	1.42	1.33
1	G	141	SER	CB-OG	-6.90	1.33	1.42
1	I	506	TYR	CD1-CE1	6.90	1.49	1.39
1	H	415	GLY	C-O	6.87	1.34	1.23
1	K	172	GLU	CD-OE2	6.86	1.33	1.25
1	B	506	TYR	CD1-CE1	6.85	1.49	1.39
1	J	16	MET	SD-CE	6.81	2.16	1.77
1	D	412	VAL	CB-CG1	6.76	1.67	1.52
1	H	526	LYS	CB-CG	6.75	1.70	1.52
1	E	130	GLU	CD-OE2	6.73	1.33	1.25
1	B	128	VAL	CB-CG1	-6.70	1.38	1.52
1	M	483	GLU	CD-OE2	6.70	1.33	1.25
1	E	498	LYS	CE-NZ	6.63	1.65	1.49
1	H	506	TYR	CZ-OH	6.63	1.49	1.37
1	E	442	VAL	CB-CG2	-6.61	1.39	1.52
1	N	38	VAL	CB-CG2	-6.60	1.39	1.52
1	A	511	ALA	CA-CB	-6.52	1.38	1.52
1	B	114	MET	CG-SD	6.49	1.98	1.81
1	B	114	MET	CB-CG	6.49	1.72	1.51
1	H	460	GLU	CD-OE1	6.49	1.32	1.25
1	E	94	VAL	C-O	-6.48	1.11	1.23
1	L	502	SER	CB-OG	6.42	1.50	1.42
1	E	129	GLU	CD-OE1	6.42	1.32	1.25
1	E	88	GLY	C-O	6.42	1.33	1.23
1	H	126	VAL	CB-CG1	6.37	1.66	1.52
1	G	498	LYS	CE-NZ	6.36	1.65	1.49
1	B	126	VAL	CB-CG2	6.35	1.66	1.52
1	B	506	TYR	CD2-CE2	6.29	1.48	1.39
1	E	507	ALA	CA-CB	-6.29	1.39	1.52
1	H	483	GLU	CD-OE1	6.21	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	463	SER	CB-OG	6.21	1.50	1.42
1	D	449	ALA	CA-CB	6.20	1.65	1.52
1	D	129	GLU	CG-CD	6.15	1.61	1.51
1	K	24	ALA	CA-CB	6.13	1.65	1.52
1	H	526	LYS	CE-NZ	6.12	1.64	1.49
1	D	75	LYS	CE-NZ	-6.10	1.33	1.49
1	I	526	LYS	CB-CG	6.09	1.69	1.52
1	H	526	LYS	CD-CE	6.07	1.66	1.51
1	N	81	ALA	CA-CB	6.05	1.65	1.52
1	E	73	MET	SD-CE	-6.04	1.44	1.77
1	E	80	LYS	CG-CD	6.00	1.72	1.52
1	L	510	VAL	CB-CG2	6.00	1.65	1.52
1	F	80	LYS	CE-NZ	5.99	1.64	1.49
1	F	526	LYS	CE-NZ	5.97	1.64	1.49
1	J	172	GLU	CD-OE2	5.97	1.32	1.25
1	B	448	GLU	CD-OE1	5.96	1.32	1.25
1	G	526	LYS	CB-CG	5.96	1.68	1.52
1	A	129	GLU	CG-CD	5.95	1.60	1.51
1	K	483	GLU	CD-OE1	5.94	1.32	1.25
1	B	445	ARG	CG-CD	5.94	1.66	1.51
1	H	44	PHE	CE1-CZ	5.93	1.48	1.37
1	J	514	MET	CG-SD	5.92	1.96	1.81
1	E	490	ASP	CG-OD1	5.91	1.39	1.25
1	B	438	VAL	CB-CG2	5.91	1.65	1.52
1	J	461	GLU	CD-OE1	5.88	1.32	1.25
1	N	445	ARG	NE-CZ	5.88	1.40	1.33
1	D	363	GLU	CD-OE1	5.87	1.32	1.25
1	F	92	ALA	C-O	5.87	1.34	1.23
1	L	80	LYS	CE-NZ	5.86	1.63	1.49
1	F	127	ALA	CA-CB	5.84	1.64	1.52
1	L	96	ALA	CA-CB	-5.84	1.40	1.52
1	N	58	ARG	CG-CD	5.83	1.66	1.51
1	F	71	ALA	CA-CB	5.82	1.64	1.52
1	E	448	GLU	CA-CB	5.82	1.66	1.53
1	C	94	VAL	CB-CG2	-5.81	1.40	1.52
1	N	105	LYS	CE-NZ	5.81	1.63	1.49
1	K	507	ALA	CA-CB	-5.79	1.40	1.52
1	M	114	MET	CG-SD	5.79	1.96	1.81
1	F	460	GLU	CD-OE1	5.79	1.32	1.25
1	H	44	PHE	CD1-CE1	5.78	1.50	1.39
1	G	526	LYS	CE-NZ	5.77	1.63	1.49
1	L	506	TYR	CD1-CE1	5.77	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	484	GLU	CD-OE2	5.74	1.31	1.25
1	H	465	VAL	CB-CG1	5.72	1.64	1.52
1	A	506	TYR	CD2-CE2	5.71	1.48	1.39
1	L	506	TYR	CB-CG	5.71	1.60	1.51
1	J	129	GLU	CG-CD	5.70	1.60	1.51
1	C	514	MET	CG-SD	5.70	1.96	1.81
1	E	490	ASP	CA-CB	-5.69	1.41	1.53
1	H	44	PHE	CE2-CZ	5.68	1.48	1.37
1	H	510	VAL	CB-CG2	5.68	1.64	1.52
1	D	172	GLU	CG-CD	5.68	1.60	1.51
1	A	67	GLU	CD-OE1	5.67	1.31	1.25
1	G	123	ALA	CA-CB	-5.66	1.40	1.52
1	L	98	ALA	CA-CB	5.65	1.64	1.52
1	H	476	TYR	CZ-OH	5.64	1.47	1.37
1	E	101	THR	CB-CG2	5.63	1.71	1.52
1	G	432	GLN	CG-CD	5.63	1.64	1.51
1	B	474	GLY	C-O	5.62	1.32	1.23
1	B	509	SER	N-CA	-5.62	1.35	1.46
1	N	58	ARG	NE-CZ	5.61	1.40	1.33
1	A	526	LYS	CE-NZ	5.61	1.63	1.49
1	I	67	GLU	CD-OE2	5.61	1.31	1.25
1	I	498	LYS	CE-NZ	5.60	1.63	1.49
1	G	76	GLU	CD-OE2	5.60	1.31	1.25
1	M	16	MET	SD-CE	5.60	2.09	1.77
1	C	526	LYS	CD-CE	5.59	1.65	1.51
1	D	132	LYS	CD-CE	5.58	1.65	1.51
1	K	96	ALA	CA-CB	-5.58	1.40	1.52
1	E	80	LYS	CE-NZ	5.57	1.62	1.49
1	C	75	LYS	CD-CE	-5.57	1.37	1.51
1	F	44	PHE	CE1-CZ	5.56	1.48	1.37
1	E	509	SER	CB-OG	-5.56	1.35	1.42
1	M	463	SER	CB-OG	5.56	1.49	1.42
1	H	514	MET	CG-SD	5.55	1.95	1.81
1	E	85	ALA	CA-CB	5.54	1.64	1.52
1	M	461	GLU	CD-OE2	5.53	1.31	1.25
1	F	129	GLU	CD-OE2	5.51	1.31	1.25
1	H	57	ALA	CA-CB	5.51	1.64	1.52
1	G	363	GLU	CD-OE2	5.51	1.31	1.25
1	E	506	TYR	CZ-OH	5.51	1.47	1.37
1	G	172	GLU	CD-OE2	5.49	1.31	1.25
1	E	414	GLY	C-O	5.47	1.32	1.23
1	H	483	GLU	CD-OE2	5.46	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	506	TYR	CD2-CE2	5.45	1.47	1.39
1	G	44	PHE	CB-CG	5.45	1.60	1.51
1	E	114	MET	CG-SD	5.45	1.95	1.81
1	K	514	MET	CG-SD	5.44	1.95	1.81
1	C	506	TYR	CD1-CE1	5.43	1.47	1.39
1	G	20	VAL	CA-CB	5.42	1.66	1.54
1	N	129	GLU	CD-OE2	5.42	1.31	1.25
1	H	3	ALA	CA-CB	-5.41	1.41	1.52
1	E	129	GLU	CG-CD	5.40	1.60	1.51
1	M	172	GLU	CD-OE2	5.39	1.31	1.25
1	F	114	MET	CB-CG	5.38	1.68	1.51
1	H	172	GLU	CD-OE2	5.38	1.31	1.25
1	N	129	GLU	CG-CD	5.38	1.60	1.51
1	I	44	PHE	CD2-CE2	5.36	1.50	1.39
1	G	88	GLY	C-O	5.36	1.32	1.23
1	B	509	SER	CB-OG	-5.36	1.35	1.42
1	F	514	MET	CG-SD	5.34	1.95	1.81
1	G	526	LYS	CD-CE	5.33	1.64	1.51
1	G	44	PHE	CE1-CZ	5.32	1.47	1.37
1	C	463	SER	CB-OG	5.32	1.49	1.42
1	H	141	SER	CB-OG	-5.31	1.35	1.42
1	K	101	THR	C-O	-5.31	1.13	1.23
1	L	501	ARG	CG-CD	-5.29	1.38	1.51
1	C	460	GLU	CD-OE2	5.29	1.31	1.25
1	F	129	GLU	CG-CD	5.29	1.59	1.51
1	J	88	GLY	C-O	5.28	1.32	1.23
1	L	105	LYS	C-O	5.27	1.33	1.23
1	N	76	GLU	N-CA	5.25	1.56	1.46
1	C	58	ARG	NE-CZ	5.25	1.39	1.33
1	E	438	VAL	CB-CG2	5.25	1.63	1.52
1	A	509	SER	CB-OG	-5.24	1.35	1.42
1	H	61	GLU	CD-OE2	5.23	1.31	1.25
1	I	129	GLU	CG-CD	5.23	1.59	1.51
1	G	132	LYS	CD-CE	5.23	1.64	1.51
1	J	129	GLU	CD-OE2	5.23	1.31	1.25
1	G	172	GLU	CG-CD	5.22	1.59	1.51
1	H	29	VAL	CB-CG1	5.22	1.63	1.52
1	E	514	MET	CG-SD	5.22	1.94	1.81
1	L	450	PRO	CG-CD	5.20	1.67	1.50
1	A	507	ALA	CA-CB	-5.20	1.41	1.52
1	K	445	ARG	NE-CZ	5.18	1.39	1.33
1	D	172	GLU	CD-OE1	5.18	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	461	GLU	CD-OE1	5.16	1.31	1.25
1	E	473	ASP	CB-CG	-5.16	1.41	1.51
1	D	526	LYS	CD-CE	5.15	1.64	1.51
1	G	129	GLU	CD-OE1	5.14	1.31	1.25
1	F	508	ALA	CA-CB	5.14	1.63	1.52
1	B	172	GLU	CD-OE2	5.13	1.31	1.25
1	K	129	GLU	CG-CD	5.12	1.59	1.51
1	M	509	SER	CB-OG	-5.12	1.35	1.42
1	M	526	LYS	CE-NZ	5.10	1.61	1.49
1	B	80	LYS	CD-CE	5.10	1.64	1.51
1	G	473	ASP	CB-CG	-5.09	1.41	1.51
1	B	114	MET	SD-CE	5.09	2.06	1.77
1	H	27	VAL	CB-CG2	-5.09	1.42	1.52
1	E	450	PRO	CG-CD	5.08	1.67	1.50
1	F	129	GLU	CD-OE1	5.07	1.31	1.25
1	A	73	MET	SD-CE	-5.07	1.49	1.77
1	A	526	LYS	CD-CE	5.07	1.64	1.51
1	G	14	VAL	CB-CG2	-5.06	1.42	1.52
1	B	126	VAL	CB-CG1	5.06	1.63	1.52
1	M	80	LYS	CD-CE	5.05	1.63	1.51
1	E	526	LYS	CE-NZ	5.04	1.61	1.49
1	E	75	LYS	CD-CE	-5.04	1.38	1.51
1	G	484	GLU	CD-OE2	5.01	1.31	1.25
1	B	130	GLU	CD-OE1	5.01	1.31	1.25
1	H	412	VAL	CB-CG2	5.01	1.63	1.52
1	H	434	GLU	CA-CB	5.00	1.65	1.53
1	H	129	GLU	CD-OE2	5.00	1.31	1.25

All (320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	284	ARG	NE-CZ-NH2	21.49	131.04	120.30
1	M	284	ARG	NE-CZ-NH1	-20.20	110.20	120.30
1	J	231	ARG	NE-CZ-NH2	19.91	130.25	120.30
1	J	231	ARG	NE-CZ-NH1	-18.92	110.84	120.30
1	N	368	ARG	NE-CZ-NH2	16.05	128.32	120.30
1	N	368	ARG	NE-CZ-NH1	-15.30	112.65	120.30
1	M	284	ARG	CD-NE-CZ	10.41	138.18	123.60
1	E	473	ASP	CB-CG-OD2	10.12	127.41	118.30
1	F	435	ASP	CB-CG-OD2	9.77	127.09	118.30
1	E	490	ASP	CB-CG-OD2	-9.69	109.58	118.30
1	J	52	ASP	CB-CG-OD2	9.65	126.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	428	ASP	CB-CG-OD2	9.35	126.72	118.30
1	E	421	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	J	231	ARG	CD-NE-CZ	9.31	136.63	123.60
1	E	36	ARG	NE-CZ-NH1	-9.24	115.68	120.30
1	B	428	ASP	CB-CG-OD2	9.09	126.48	118.30
1	G	435	ASP	CB-CG-OD2	9.05	126.45	118.30
1	B	132	LYS	CD-CE-NZ	8.72	131.77	111.70
1	A	41	ASP	CB-CG-OD2	8.68	126.11	118.30
1	K	435	ASP	CB-CG-OD2	8.68	126.11	118.30
1	D	328	ASP	CB-CG-OD2	8.59	126.03	118.30
1	H	167	ASP	CB-CG-OD2	8.20	125.68	118.30
1	B	473	ASP	CB-CG-OD2	8.13	125.61	118.30
1	M	495	ASP	CB-CG-OD2	8.13	125.61	118.30
1	I	435	ASP	CB-CG-OD2	8.04	125.54	118.30
1	D	11	ASP	CB-CG-OD2	7.99	125.49	118.30
1	B	64	ASP	CB-CG-OD2	7.91	125.42	118.30
1	J	140	ASP	CB-CG-OD2	7.79	125.31	118.30
1	N	368	ARG	CD-NE-CZ	7.79	134.50	123.60
1	F	495	ASP	CB-CG-OD2	7.69	125.22	118.30
1	E	523	ASP	CB-CG-OD2	7.67	125.21	118.30
1	M	52	ASP	CB-CG-OD2	7.66	125.20	118.30
1	F	20	VAL	CG1-CB-CG2	7.59	123.05	110.90
1	E	435	ASP	CB-CG-OD2	7.57	125.11	118.30
1	H	140	ASP	CB-CG-OD2	7.54	125.09	118.30
1	M	11	ASP	CB-CG-OD2	7.54	125.09	118.30
1	L	361	ASP	CB-CG-OD2	7.53	125.08	118.30
1	L	435	ASP	CB-CG-OD2	7.49	125.04	118.30
1	F	167	ASP	CB-CG-OD2	7.44	125.00	118.30
1	I	430	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	N	435	ASP	CB-CG-OD2	7.34	124.90	118.30
1	E	499	VAL	CG1-CB-CG2	7.19	122.40	110.90
1	I	121	ASP	CB-CG-OD2	7.17	124.75	118.30
1	B	398	ASP	CB-CG-OD2	7.17	124.75	118.30
1	G	328	ASP	CB-CG-OD2	7.16	124.74	118.30
1	D	435	ASP	CB-CG-OD2	7.15	124.74	118.30
1	D	121	ASP	CB-CG-OD2	7.15	124.73	118.30
1	A	167	ASP	CB-CG-OD2	7.09	124.68	118.30
1	L	20	VAL	CG1-CB-CG2	7.09	122.24	110.90
1	C	52	ASP	CB-CG-OD2	7.07	124.67	118.30
1	H	11	ASP	CB-CG-OD2	7.05	124.64	118.30
1	G	42	LYS	CD-CE-NZ	-7.03	95.53	111.70
1	K	523	ASP	CB-CG-OD2	7.02	124.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	74	VAL	CG1-CB-CG2	-6.91	99.84	110.90
1	D	283	ASP	CB-CG-OD2	6.87	124.48	118.30
1	A	52	ASP	CB-CG-OD2	6.85	124.46	118.30
1	E	121	ASP	CB-CG-OD2	6.84	124.46	118.30
1	I	523	ASP	CB-CG-OD2	6.84	124.45	118.30
1	N	328	ASP	CB-CG-OD2	6.83	124.45	118.30
1	C	140	ASP	CB-CG-OD2	6.80	124.42	118.30
1	J	41	ASP	CB-CG-OD2	6.80	124.42	118.30
1	K	11	ASP	CB-CG-OD2	6.79	124.41	118.30
1	B	140	ASP	CB-CG-OD2	6.78	124.41	118.30
1	A	20	VAL	CG1-CB-CG2	6.78	121.74	110.90
1	H	398	ASP	CB-CG-OD2	6.75	124.38	118.30
1	L	495	ASP	CB-CG-OD2	6.74	124.37	118.30
1	J	11	ASP	CB-CG-OD2	6.73	124.35	118.30
1	K	16	MET	CG-SD-CE	6.71	110.94	100.20
1	N	11	ASP	CB-CG-OD2	6.71	124.34	118.30
1	M	398	ASP	CB-CG-OD2	6.70	124.33	118.30
1	C	11	ASP	CB-CG-OD2	6.68	124.31	118.30
1	N	398	ASP	CB-CG-OD2	6.66	124.29	118.30
1	H	524	LEU	CB-CG-CD2	-6.64	99.71	111.00
1	E	421	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	K	398	ASP	CB-CG-OD2	6.59	124.24	118.30
1	G	115	ASP	CB-CG-OD2	6.59	124.23	118.30
1	J	83	ASP	CB-CG-OD2	6.58	124.22	118.30
1	E	20	VAL	CG1-CB-CG2	6.57	121.42	110.90
1	A	5	ASP	CB-CG-OD1	6.57	124.21	118.30
1	L	398	ASP	CB-CG-OD2	6.54	124.19	118.30
1	L	140	ASP	CB-CG-OD2	6.53	124.18	118.30
1	D	361	ASP	CB-CG-OD2	6.53	124.17	118.30
1	D	41	ASP	CB-CG-OD2	6.52	124.17	118.30
1	D	52	ASP	CB-CG-OD2	6.47	124.12	118.30
1	E	495	ASP	CB-CG-OD2	6.46	124.12	118.30
1	K	28	LYS	CD-CE-NZ	-6.46	96.83	111.70
1	B	361	ASP	CB-CG-OD2	6.43	124.09	118.30
1	J	87	ASP	CB-CG-OD2	6.42	124.08	118.30
1	J	495	ASP	CB-CG-OD2	6.40	124.06	118.30
1	I	179	ASP	CB-CG-OD2	6.40	124.06	118.30
1	N	523	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	64	ASP	CB-CG-OD1	6.39	124.05	118.30
1	D	523	ASP	CB-CG-OD2	6.38	124.04	118.30
1	E	52	ASP	CB-CG-OD2	6.38	124.04	118.30
1	D	445	ARG	NE-CZ-NH2	6.35	123.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	52	ASP	CB-CG-OD2	6.35	124.01	118.30
1	E	64	ASP	CB-CG-OD2	6.34	124.01	118.30
1	H	490	ASP	CB-CG-OD2	6.34	124.00	118.30
1	B	316	ASP	CB-CG-OD2	6.29	123.97	118.30
1	G	334	ASP	CB-CG-OD2	6.29	123.96	118.30
1	F	42	LYS	CD-CE-NZ	-6.28	97.25	111.70
1	I	83	ASP	CB-CG-OD2	6.28	123.95	118.30
1	D	328	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	I	398	ASP	CB-CG-OD2	6.24	123.92	118.30
1	I	140	ASP	CB-CG-OD2	6.24	123.92	118.30
1	N	361	ASP	CB-CG-OD2	6.23	123.91	118.30
1	C	328	ASP	CB-CG-OD2	6.23	123.91	118.30
1	E	451	LEU	CB-CG-CD2	-6.22	100.42	111.00
1	A	121	ASP	CB-CG-OD2	6.22	123.90	118.30
1	N	167	ASP	CB-CG-OD2	6.21	123.89	118.30
1	N	42	LYS	CD-CE-NZ	-6.20	97.44	111.70
1	E	23	LEU	CB-CG-CD2	6.20	121.53	111.00
1	J	435	ASP	CB-CG-OD2	6.17	123.86	118.30
1	F	473	ASP	CB-CG-OD2	6.17	123.85	118.30
1	E	101	THR	OG1-CB-CG2	-6.17	95.81	110.00
1	A	495	ASP	CB-CG-OD2	6.16	123.84	118.30
1	F	111	MET	CG-SD-CE	6.15	110.04	100.20
1	A	361	ASP	CB-CG-OD2	6.14	123.82	118.30
1	F	140	ASP	CB-CG-OD2	6.11	123.80	118.30
1	L	25	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	398	ASP	CB-CG-OD2	6.11	123.79	118.30
1	K	316	ASP	CB-CG-OD2	6.11	123.80	118.30
1	I	7	LYS	CD-CE-NZ	-6.10	97.67	111.70
1	B	495	ASP	CB-CG-OD2	6.08	123.77	118.30
1	I	316	ASP	CB-CG-OD2	6.07	123.76	118.30
1	G	473	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	H	328	ASP	CB-CG-OD2	6.05	123.74	118.30
1	I	361	ASP	CB-CG-OD2	6.04	123.74	118.30
1	F	430	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	D	325	ILE	CG1-CB-CG2	-6.03	98.14	111.40
1	E	490	ASP	CB-CA-C	-6.03	98.35	110.40
1	D	316	ASP	CB-CG-OD2	6.01	123.71	118.30
1	E	283	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	417	VAL	CG1-CB-CG2	6.00	120.51	110.90
1	M	361	ASP	CB-CG-OD2	6.00	123.70	118.30
1	K	167	ASP	CB-CG-OD2	6.00	123.69	118.30
1	N	74	VAL	CG1-CB-CG2	-5.96	101.37	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	495	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	316	ASP	CB-CG-OD2	5.93	123.64	118.30
1	E	167	ASP	CB-CG-OD2	5.92	123.63	118.30
1	N	25	ASP	CB-CG-OD2	5.92	123.63	118.30
1	H	283	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	20	VAL	CG1-CB-CG2	5.90	120.34	110.90
1	K	64	ASP	CB-CG-OD2	5.88	123.59	118.30
1	L	11	ASP	CB-CG-OD2	5.88	123.59	118.30
1	I	52	ASP	CB-CG-OD2	5.88	123.59	118.30
1	E	11	ASP	CB-CG-OD2	5.87	123.58	118.30
1	M	140	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	115	ASP	CB-CG-OD2	5.85	123.56	118.30
1	E	118	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	H	451	LEU	CB-CG-CD2	-5.85	101.06	111.00
1	B	115	ASP	CB-CG-OD2	5.84	123.56	118.30
1	G	283	ASP	CB-CG-OD2	5.83	123.55	118.30
1	E	452	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	K	361	ASP	CB-CG-OD2	5.82	123.53	118.30
1	H	42	LYS	CD-CE-NZ	-5.81	98.34	111.70
1	F	316	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	94	VAL	CG1-CB-CG2	5.80	120.18	110.90
1	N	131	LEU	CB-CG-CD2	-5.80	101.14	111.00
1	G	25	ASP	CB-CG-OD1	5.79	123.51	118.30
1	G	52	ASP	CB-CG-OD2	5.79	123.51	118.30
1	M	196	ASP	CB-CG-OD2	5.79	123.51	118.30
1	N	64	ASP	CB-CG-OD2	5.78	123.50	118.30
1	F	398	ASP	CB-CG-OD2	5.76	123.48	118.30
1	N	334	ASP	CB-CG-OD2	5.76	123.48	118.30
1	F	64	ASP	CB-CG-OD2	5.76	123.48	118.30
1	D	395	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	J	283	ASP	CB-CG-OD2	5.75	123.48	118.30
1	H	41	ASP	CB-CG-OD2	5.75	123.47	118.30
1	L	523	ASP	CB-CG-OD2	5.74	123.46	118.30
1	D	20	VAL	CG1-CB-CG2	5.72	120.06	110.90
1	L	64	ASP	CB-CG-OD2	5.72	123.45	118.30
1	F	41	ASP	CB-CG-OD2	5.72	123.45	118.30
1	I	328	ASP	CB-CG-OD2	5.71	123.44	118.30
1	M	473	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	398	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	74	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	M	328	ASP	CB-CG-OD2	5.70	123.42	118.30
1	L	283	ASP	CB-CG-OD2	5.69	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	115	ASP	CB-CG-OD2	5.69	123.42	118.30
1	N	452	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	E	25	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	421	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	H	64	ASP	CB-CG-OD2	5.68	123.41	118.30
1	L	514	MET	CG-SD-CE	-5.68	91.11	100.20
1	G	179	ASP	CB-CG-OD2	5.68	123.41	118.30
1	N	87	ASP	CB-CG-OD1	5.67	123.40	118.30
1	N	283	ASP	CB-CG-OD2	5.67	123.40	118.30
1	L	328	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	435	ASP	CB-CG-OD2	5.65	123.39	118.30
1	H	7	LYS	CD-CE-NZ	-5.65	98.71	111.70
1	D	188	ASP	CB-CG-OD2	5.65	123.38	118.30
1	C	495	ASP	CB-CG-OD2	5.62	123.36	118.30
1	E	359	ASP	CB-CG-OD2	5.61	123.35	118.30
1	M	155	ASP	CB-CG-OD2	5.61	123.34	118.30
1	E	20	VAL	CA-CB-CG2	5.60	119.30	110.90
1	N	421	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	E	140	ASP	CB-CG-OD2	5.59	123.33	118.30
1	G	41	ASP	CB-CG-OD2	5.58	123.33	118.30
1	H	20	VAL	CG1-CB-CG2	5.57	119.81	110.90
1	J	328	ASP	CB-CG-OD2	5.57	123.31	118.30
1	F	328	ASP	CB-CG-OD2	5.56	123.30	118.30
1	B	131	LEU	CA-CB-CG	5.56	128.08	115.30
1	M	316	ASP	CB-CG-OD2	5.55	123.30	118.30
1	H	473	ASP	CB-CG-OD2	5.55	123.30	118.30
1	H	23	LEU	CA-CB-CG	-5.54	102.55	115.30
1	C	361	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	524	LEU	CB-CG-CD1	5.54	120.41	111.00
1	C	523	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	283	ASP	CB-CG-OD2	5.53	123.28	118.30
1	E	42	LYS	CD-CE-NZ	-5.51	99.03	111.70
1	C	179	ASP	CB-CG-OD2	5.50	123.25	118.30
1	I	334	ASP	CB-CG-OD2	5.50	123.25	118.30
1	K	25	ASP	CB-CG-OD2	5.49	123.24	118.30
1	J	115	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	428	ASP	OD1-CG-OD2	-5.48	112.88	123.30
1	L	435	ASP	OD1-CG-OD2	-5.47	112.90	123.30
1	K	87	ASP	CB-CG-OD2	5.47	123.22	118.30
1	K	140	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	283	ASP	CB-CG-OD2	5.47	123.22	118.30
1	G	50	THR	OG1-CB-CG2	-5.46	97.44	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	11	ASP	CB-CG-OD2	5.44	123.20	118.30
1	H	359	ASP	CB-CG-OD2	5.44	123.20	118.30
1	D	185	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	435	ASP	CB-CG-OD2	5.44	123.19	118.30
1	J	50	THR	OG1-CB-CG2	-5.43	97.50	110.00
1	B	42	LYS	CD-CE-NZ	-5.43	99.21	111.70
1	E	489	ILE	CG1-CB-CG2	-5.43	99.45	111.40
1	G	495	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	23	LEU	CA-CB-CG	-5.41	102.85	115.30
1	N	28	LYS	CD-CE-NZ	-5.40	99.28	111.70
1	G	16	MET	CG-SD-CE	5.39	108.83	100.20
1	C	28	LYS	CD-CE-NZ	-5.38	99.32	111.70
1	N	224	ASP	CB-CG-OD2	5.38	123.15	118.30
1	J	23	LEU	CA-CB-CG	-5.37	102.95	115.30
1	A	125	THR	OG1-CB-CG2	-5.37	97.65	110.00
1	I	283	ASP	CB-CG-OD2	5.36	123.13	118.30
1	L	334	ASP	CB-CG-OD2	5.35	123.11	118.30
1	D	23	LEU	CB-CG-CD2	5.33	120.06	111.00
1	L	428	ASP	CB-CG-OD2	5.31	123.08	118.30
1	I	167	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	87	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	322	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	N	514	MET	CG-SD-CE	-5.31	91.71	100.20
1	H	87	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	359	ASP	CB-CG-OD2	5.29	123.07	118.30
1	F	361	ASP	CB-CG-OD2	5.29	123.06	118.30
1	G	325	ILE	CG1-CB-CG2	-5.29	99.76	111.40
1	E	361	ASP	CB-CG-OD2	5.29	123.06	118.30
1	K	121	ASP	CB-CG-OD2	5.29	123.06	118.30
1	J	361	ASP	CB-CG-OD2	5.29	123.06	118.30
1	I	50	THR	OG1-CB-CG2	-5.28	97.85	110.00
1	M	283	ASP	CB-CG-OD2	5.28	123.05	118.30
1	N	185	ASP	CB-CG-OD2	5.27	123.05	118.30
1	N	495	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	133	ALA	O-C-N	-5.26	114.28	122.70
1	J	64	ASP	CB-CG-OD2	5.26	123.03	118.30
1	F	334	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	253	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	291	ASP	CB-CG-OD2	5.23	123.00	118.30
1	H	361	ASP	CB-CG-OD2	5.23	123.00	118.30
1	E	490	ASP	OD1-CG-OD2	5.21	133.20	123.30
1	D	524	LEU	CB-CG-CD1	5.21	119.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	316	ASP	CB-CG-OD2	5.21	122.99	118.30
1	M	20	VAL	CG1-CB-CG2	5.20	119.22	110.90
1	C	155	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	316	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	322	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	F	5	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	140	ASP	CB-CG-OD2	5.19	122.97	118.30
1	F	87	ASP	CB-CG-OD1	5.19	122.97	118.30
1	G	361	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	42	LYS	CD-CE-NZ	-5.19	99.77	111.70
1	M	167	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	132	LYS	N-CA-C	-5.19	97.00	111.00
1	B	132	LYS	CB-CG-CD	5.18	125.07	111.60
1	L	51	LYS	CD-CE-NZ	-5.18	99.78	111.70
1	G	398	ASP	CB-CG-OD2	5.18	122.96	118.30
1	H	23	LEU	CB-CG-CD2	5.17	119.80	111.00
1	C	83	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	188	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	359	ASP	CB-CG-OD2	5.17	122.95	118.30
1	K	283	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	359	ASP	CB-CG-OD2	5.14	122.92	118.30
1	I	445	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	E	42	LYS	CB-CG-CD	-5.13	98.26	111.60
1	E	224	ASP	CB-CG-OD2	5.13	122.92	118.30
1	L	42	LYS	CD-CE-NZ	-5.12	99.92	111.70
1	L	359	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	328	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	435	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	115	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	523	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	316	ASP	CB-CG-OD2	5.09	122.89	118.30
1	H	121	ASP	CB-CG-OD2	5.09	122.88	118.30
1	J	28	LYS	CD-CE-NZ	-5.09	99.99	111.70
1	D	362	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	N	131	LEU	CA-CB-CG	5.08	126.98	115.30
1	L	20	VAL	CA-CB-CG2	5.07	118.51	110.90
1	K	115	ASP	CB-CG-OD2	5.07	122.86	118.30
1	E	473	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	G	316	ASP	CB-CG-OD2	5.05	122.84	118.30
1	D	42	LYS	CD-CE-NZ	-5.04	100.10	111.70
1	D	452	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	K	359	ASP	CB-CG-OD2	5.04	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	LEU	CA-CB-CG	-5.04	103.71	115.30
1	C	473	ASP	CB-CG-OD2	5.04	122.83	118.30
1	D	359	ASP	CB-CG-OD1	5.04	122.83	118.30
1	J	316	ASP	CB-CG-OD2	5.03	122.83	118.30
1	G	20	VAL	CG1-CB-CG2	5.03	118.95	110.90
1	L	473	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	11	ASP	CB-CG-OD2	5.03	122.82	118.30
1	E	322	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	K	328	ASP	CB-CG-OD2	5.02	122.82	118.30
1	G	64	ASP	CB-CG-OD2	5.02	122.82	118.30
1	F	50	THR	OG1-CB-CG2	-5.02	98.46	110.00
1	J	155	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	328	ASP	CB-CG-OD2	5.01	122.81	118.30
1	L	421	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	H	94	VAL	CG1-CB-CG2	5.01	118.91	110.90

There are no chirality outliers.

There are no planarity outliers.

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	3855	0	3979	74	1
1	B	3855	0	3979	76	0
1	C	3855	0	3979	71	0
1	D	3855	0	3979	75	0
1	E	3855	0	3979	68	0
1	F	3855	0	3979	77	0
1	G	3855	0	3979	82	2
1	H	3855	0	3979	68	1
1	I	3855	0	3979	64	1
1	J	3855	0	3979	66	0
1	K	3855	0	3979	67	0
1	L	3855	0	3979	75	1
1	M	3855	0	3979	77	0
1	N	3855	0	3979	70	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
4	A	31	0	12	3	0
4	B	31	0	12	4	0
4	C	31	0	12	2	0
4	D	31	0	12	4	0
4	E	31	0	12	3	0
4	F	31	0	11	3	0
4	G	31	0	12	4	0
4	H	31	0	12	4	0
4	I	31	0	12	4	0
4	J	31	0	12	5	0
4	K	31	0	12	2	0
4	L	31	0	12	3	0
4	M	31	0	12	3	0
4	N	31	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	62	0	0	3	0
5	B	83	0	0	5	0
5	C	57	0	0	3	0
5	D	91	0	0	6	0
5	E	92	0	0	4	0
5	F	71	0	0	1	0
5	G	83	0	0	8	0
5	H	77	0	0	4	0
5	I	60	0	0	3	0
5	J	50	0	0	1	0
5	K	47	0	0	3	0
5	L	61	0	0	2	0
5	M	53	0	0	3	0
5	N	59	0	0	2	0
All	All	55380	0	55873	997	5

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 9.

All (997) 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:L:80:LYS:CD	1:L:80:LYS:CG	1.77	1.62
1:B:510:VAL:CG2	1:B:510:VAL:CB	1.79	1.61
4:A:1:AGS:S1G	4:A:1:AGS:PG	1.53	1.52
1:N:510:VAL:CG2	1:N:510:VAL:CB	1.83	1.51
4:B:1:AGS:PG	4:B:1:AGS:S1G	1.52	1.51
4:J:1:AGS:S1G	4:J:1:AGS:PG	1.52	1.51
4:C:1:AGS:PG	4:C:1:AGS:S1G	1.51	1.51
4:H:1:AGS:PG	4:H:1:AGS:S1G	1.51	1.51
4:K:1:AGS:S1G	4:K:1:AGS:PG	1.51	1.50
4:F:1:AGS:PG	4:F:1:AGS:S1G	1.51	1.50
4:M:1:AGS:S1G	4:M:1:AGS:PG	1.51	1.49
4:I:1:AGS:PG	4:I:1:AGS:S1G	1.50	1.49
4:D:561:AGS:PG	4:D:561:AGS:S1G	1.48	1.47
4:L:1:AGS:PG	4:L:1:AGS:S1G	1.49	1.47
1:G:114:MET:CE	1:G:114:MET:SD	2.02	1.47
4:E:1:AGS:PG	4:E:1:AGS:S1G	1.47	1.46
4:N:1:AGS:PG	4:N:1:AGS:S1G	1.47	1.46
1:E:16:MET:SD	1:E:16:MET:CE	2.03	1.46
1:L:514:MET:SD	1:L:514:MET:CE	2.04	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MET:CE	1:B:16:MET:SD	2.03	1.45
1:D:114:MET:CG	1:D:114:MET:SD	2.03	1.44
1:B:114:MET:CE	1:B:114:MET:SD	2.06	1.44
4:G:1:AGS:PG	4:G:1:AGS:S1G	1.45	1.44
1:D:114:MET:CE	1:D:114:MET:SD	2.02	1.44
1:M:16:MET:SD	1:M:16:MET:CE	2.09	1.41
3:C:560:K:K	5:C:566:HOH:O	1.34	1.34
1:J:16:MET:CE	1:J:16:MET:SD	2.16	1.33
1:H:463:SER:HB2	5:H:583:HOH:O	1.34	1.24
1:A:463:SER:HB2	5:A:570:HOH:O	1.43	1.16
1:K:463:SER:HB2	5:K:572:HOH:O	1.43	1.12
1:B:404:ARG:NH1	5:B:586:HOH:O	1.93	1.02
1:C:63:GLU:OE2	1:D:526:LYS:HE2	1.62	0.99
1:M:268:ARG:O	1:N:257:GLU:HG3	1.63	0.99
1:I:10:ASN:ND2	5:I:600:HOH:O	1.97	0.95
1:A:282:GLY:HA3	1:G:181:THR:O	1.67	0.95
4:E:1:AGS:O3B	4:E:1:AGS:S1G	2.26	0.94
1:A:231:ARG:NH1	1:G:242:LYS:HA	1.81	0.93
1:E:63:GLU:OE2	1:F:526:LYS:HE2	1.70	0.91
1:F:10:ASN:ND2	5:F:630:HOH:O	2.03	0.91
1:G:404:ARG:NH1	5:G:576:HOH:O	2.05	0.90
1:A:63:GLU:OE2	1:B:526:LYS:HE2	1.75	0.85
1:H:177:VAL:HG21	1:H:397:GLU:HG3	1.58	0.84
1:N:10:ASN:ND2	5:N:598:HOH:O	2.09	0.84
1:B:177:VAL:HG21	1:B:397:GLU:HG3	1.61	0.83
1:L:514:MET:HB3	1:L:514:MET:HE3	1.60	0.82
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.61	0.82
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.62	0.82
1:L:514:MET:HB3	1:L:514:MET:CE	2.10	0.82
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.62	0.81
1:C:177:VAL:HG21	1:C:397:GLU:HG3	1.62	0.81
4:C:1:AGS:S1G	4:C:1:AGS:O3G	2.39	0.81
1:E:345:ARG:HA	1:E:348:GLN:HE21	1.46	0.81
1:N:349:ILE:HA	1:N:352:GLN:HG3	1.63	0.80
1:L:10:ASN:ND2	5:L:586:HOH:O	2.14	0.80
1:F:177:VAL:HG21	1:F:397:GLU:HG3	1.63	0.80
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.64	0.80
1:L:514:MET:CB	1:L:514:MET:CE	2.60	0.80
1:L:80:LYS:CD	1:L:80:LYS:CB	2.60	0.79
1:A:326:ASN:HD22	1:A:329:THR:HB	1.48	0.79
1:A:177:VAL:HG21	1:A:397:GLU:HG3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.65	0.79
1:J:177:VAL:HG21	1:J:397:GLU:HG3	1.65	0.79
1:F:349:ILE:HA	1:F:352:GLN:HG3	1.64	0.78
1:L:177:VAL:HG21	1:L:397:GLU:HG3	1.62	0.78
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.64	0.78
4:L:1:AGS:O3B	4:L:1:AGS:S1G	2.41	0.78
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.65	0.78
1:E:177:VAL:HG21	1:E:397:GLU:HG3	1.66	0.78
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.66	0.78
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.65	0.78
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.66	0.78
1:E:404:ARG:NH1	5:E:604:HOH:O	2.15	0.77
1:B:349:ILE:HA	1:B:352:GLN:HG3	1.65	0.77
1:H:404:ARG:NH1	5:H:626:HOH:O	2.16	0.77
1:M:177:VAL:HG21	1:M:397:GLU:HG3	1.64	0.77
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.66	0.77
1:E:213:VAL:HB	1:E:325:ILE:HG12	1.65	0.77
1:I:177:VAL:HG21	1:I:397:GLU:HG3	1.64	0.77
4:M:1:AGS:O2G	4:M:1:AGS:S1G	2.43	0.77
4:A:1:AGS:O3B	4:A:1:AGS:S1G	2.43	0.77
4:N:1:AGS:O3G	4:N:1:AGS:S1G	2.42	0.76
1:G:57:ALA:O	1:G:75:LYS:HE3	1.85	0.76
1:A:345:ARG:HA	1:A:348:GLN:HE21	1.51	0.76
1:F:213:VAL:HB	1:F:325:ILE:HG12	1.67	0.76
4:H:1:AGS:S1G	4:H:1:AGS:O3B	2.44	0.76
1:M:213:VAL:HB	1:M:325:ILE:HG12	1.66	0.76
1:I:349:ILE:HA	1:I:352:GLN:HG3	1.66	0.76
4:F:1:AGS:O3G	4:F:1:AGS:S1G	2.43	0.76
1:K:177:VAL:HG21	1:K:397:GLU:HG3	1.67	0.75
1:K:326:ASN:HD22	1:K:329:THR:HB	1.49	0.75
1:D:177:VAL:HG21	1:D:397:GLU:HG3	1.68	0.75
1:D:345:ARG:HA	1:D:348:GLN:HE21	1.52	0.75
4:G:1:AGS:O3B	4:G:1:AGS:S1G	2.44	0.75
1:J:63:GLU:OE2	1:K:526:LYS:HE2	1.87	0.75
4:B:1:AGS:O3B	4:B:1:AGS:S1G	2.44	0.75
1:C:326:ASN:HD22	1:C:329:THR:HB	1.52	0.75
1:N:177:VAL:HG21	1:N:397:GLU:HG3	1.69	0.75
1:I:63:GLU:OE2	1:J:526:LYS:HE2	1.87	0.75
1:F:345:ARG:HA	1:F:348:GLN:HE21	1.51	0.74
1:N:73:MET:O	1:N:76:GLU:HB2	1.87	0.74
4:F:1:AGS:S1G	4:F:1:AGS:O3B	2.45	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:462:PRO:HD2	5:M:605:HOH:O	1.86	0.74
1:B:86:GLY:HA3	1:B:401:HIS:CE1	2.22	0.74
1:D:326:ASN:HD22	1:D:329:THR:HB	1.53	0.73
1:I:213:VAL:HB	1:I:325:ILE:HG12	1.70	0.73
1:B:73:MET:O	1:B:76:GLU:HB2	1.88	0.73
1:A:213:VAL:HB	1:A:325:ILE:HG12	1.70	0.73
1:J:345:ARG:HA	1:J:348:GLN:HE21	1.54	0.73
1:M:326:ASN:HD22	1:M:329:THR:HB	1.52	0.72
1:B:345:ARG:HA	1:B:348:GLN:HE21	1.53	0.72
1:C:404:ARG:HH11	1:C:404:ARG:HG2	1.55	0.72
1:B:510:VAL:CG2	1:B:510:VAL:CA	2.67	0.72
1:N:326:ASN:HD22	1:N:329:THR:HB	1.55	0.72
1:G:345:ARG:HA	1:G:348:GLN:HE21	1.55	0.71
1:A:57:ALA:O	1:A:75:LYS:HE3	1.90	0.71
1:A:268:ARG:O	1:B:257:GLU:HG3	1.90	0.71
4:J:1:AGS:S1G	4:J:1:AGS:O3B	2.49	0.71
1:K:213:VAL:HB	1:K:325:ILE:HG12	1.73	0.71
1:J:359:ASP:O	1:J:363:GLU:HG2	1.90	0.71
4:D:561:AGS:O3B	4:D:561:AGS:S1G	2.48	0.71
4:D:561:AGS:S1G	4:D:561:AGS:O3G	2.47	0.71
1:G:359:ASP:O	1:G:363:GLU:HG2	1.91	0.71
1:H:213:VAL:HB	1:H:325:ILE:HG12	1.71	0.71
1:K:345:ARG:HA	1:K:348:GLN:HE21	1.55	0.70
1:N:359:ASP:O	1:N:363:GLU:HG2	1.91	0.70
1:G:489:ILE:HD12	1:G:494:LEU:CD2	2.21	0.70
1:I:345:ARG:HA	1:I:348:GLN:HE21	1.56	0.70
1:B:510:VAL:CG2	1:B:510:VAL:CG1	2.68	0.70
1:B:359:ASP:O	1:B:363:GLU:HG2	1.91	0.70
1:G:349:ILE:HA	1:G:352:GLN:HG3	1.74	0.70
1:H:345:ARG:HA	1:H:348:GLN:HE21	1.56	0.70
1:N:345:ARG:HA	1:N:348:GLN:HE21	1.57	0.70
1:L:326:ASN:HD22	1:L:329:THR:HB	1.57	0.70
1:B:63:GLU:OE2	1:C:526:LYS:HE2	1.91	0.69
1:C:213:VAL:HB	1:C:325:ILE:HG12	1.74	0.69
1:J:213:VAL:HB	1:J:325:ILE:HG12	1.74	0.69
1:K:359:ASP:O	1:K:363:GLU:HG2	1.92	0.69
4:K:1:AGS:O3B	4:K:1:AGS:S1G	2.47	0.69
1:L:63:GLU:OE2	1:M:526:LYS:HE2	1.91	0.69
1:I:73:MET:O	1:I:76:GLU:HB2	1.92	0.69
1:N:176:THR:HG21	1:N:322:ARG:HH12	1.58	0.69
1:F:57:ALA:O	1:F:75:LYS:HE3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:1:AGS:S1G	4:G:1:AGS:O3G	2.51	0.69
1:L:73:MET:O	1:L:76:GLU:HB2	1.92	0.69
1:C:291:ASP:OD2	1:C:368:ARG:HD2	1.93	0.68
4:G:1:AGS:O2G	4:G:1:AGS:S1G	2.48	0.68
1:F:326:ASN:HD22	1:F:329:THR:HB	1.58	0.68
4:H:1:AGS:O3G	4:H:1:AGS:S1G	2.49	0.68
1:I:525:PRO:O	1:I:526:LYS:HG2	1.94	0.68
1:L:181:THR:O	1:M:282:GLY:HA3	1.93	0.68
1:M:359:ASP:O	1:M:363:GLU:HG2	1.93	0.68
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.59	0.68
1:A:231:ARG:HH11	1:G:242:LYS:HA	1.56	0.68
1:H:57:ALA:O	1:H:75:LYS:HE3	1.93	0.68
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.76	0.67
1:A:23:LEU:HD22	1:A:74:VAL:HG13	1.75	0.67
1:L:291:ASP:OD2	1:L:368:ARG:HD2	1.95	0.67
4:M:1:AGS:O3G	4:M:1:AGS:S1G	2.47	0.67
1:H:359:ASP:O	1:H:363:GLU:HG2	1.95	0.67
4:J:1:AGS:S1G	4:J:1:AGS:O2G	2.50	0.67
1:L:213:VAL:HB	1:L:325:ILE:HG12	1.77	0.67
1:D:176:THR:HG21	1:D:322:ARG:HH12	1.59	0.67
1:D:404:ARG:HG2	1:D:404:ARG:HH11	1.60	0.67
1:J:23:LEU:HD22	1:J:74:VAL:HG13	1.76	0.67
1:J:291:ASP:OD2	1:J:368:ARG:HD2	1.96	0.66
1:N:510:VAL:CG2	1:N:510:VAL:CA	2.73	0.66
1:L:359:ASP:O	1:L:363:GLU:HG2	1.95	0.66
1:M:291:ASP:OD2	1:M:368:ARG:HD2	1.95	0.66
1:M:345:ARG:HA	1:M:348:GLN:HE21	1.60	0.66
1:E:359:ASP:O	1:E:363:GLU:HG2	1.96	0.66
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.61	0.66
4:B:1:AGS:O3G	4:B:1:AGS:S1G	2.51	0.66
1:L:23:LEU:HD22	1:L:74:VAL:HG13	1.79	0.65
1:G:23:LEU:HD22	1:G:74:VAL:HG13	1.76	0.65
4:I:1:AGS:S1G	4:I:1:AGS:O3G	2.49	0.65
1:E:194:GLN:O	1:E:371:LYS:HE3	1.97	0.65
1:N:510:VAL:CG2	1:N:510:VAL:CG1	2.70	0.65
1:E:218:PRO:HD2	1:E:320:ALA:O	1.97	0.65
1:C:359:ASP:O	1:C:363:GLU:HG2	1.97	0.65
1:D:359:ASP:O	1:D:363:GLU:HG2	1.97	0.65
1:D:489:ILE:HD12	1:D:494:LEU:CD2	2.27	0.65
1:G:213:VAL:HB	1:G:325:ILE:HG12	1.79	0.65
1:M:63:GLU:OE2	1:N:526:LYS:HE2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:LYS:NZ	1:L:80:LYS:CG	2.60	0.64
1:G:291:ASP:OD2	1:G:368:ARG:HD2	1.98	0.64
1:F:63:GLU:OE2	1:G:526:LYS:HE2	1.96	0.64
1:J:326:ASN:HD22	1:J:329:THR:HB	1.62	0.64
1:D:291:ASP:OD2	1:D:368:ARG:HD2	1.98	0.64
1:A:359:ASP:O	1:A:363:GLU:HG2	1.98	0.64
1:E:489:ILE:HD12	1:E:494:LEU:CD2	2.28	0.64
1:L:266:THR:HG21	1:L:273:VAL:O	1.98	0.64
1:M:194:GLN:O	1:M:371:LYS:HE3	1.98	0.64
1:M:23:LEU:HD22	1:M:74:VAL:HG13	1.80	0.63
1:B:326:ASN:HD22	1:B:329:THR:HB	1.62	0.63
1:F:359:ASP:O	1:F:363:GLU:HG2	1.98	0.63
1:C:345:ARG:HA	1:C:348:GLN:HE21	1.62	0.63
1:G:326:ASN:HD22	1:G:329:THR:HB	1.64	0.63
1:D:213:VAL:HB	1:D:325:ILE:HG12	1.79	0.63
1:H:266:THR:CG2	1:H:273:VAL:H	2.12	0.63
1:E:326:ASN:HD22	1:E:329:THR:HB	1.63	0.63
1:K:404:ARG:HG2	1:K:404:ARG:HH11	1.62	0.63
1:D:23:LEU:HD22	1:D:74:VAL:HG13	1.81	0.63
1:I:291:ASP:OD2	1:I:368:ARG:HD2	1.98	0.63
1:K:291:ASP:OD2	1:K:368:ARG:HD2	1.98	0.63
1:E:291:ASP:OD2	1:E:368:ARG:HD2	1.99	0.62
1:G:218:PRO:HD2	1:G:320:ALA:O	1.99	0.62
4:A:1:AGS:S1G	4:A:1:AGS:O3G	2.51	0.62
1:F:291:ASP:OD2	1:F:368:ARG:HD2	1.99	0.62
1:I:326:ASN:HD22	1:I:329:THR:HB	1.65	0.62
1:N:266:THR:HG21	1:N:273:VAL:O	2.00	0.62
1:C:181:THR:N	5:C:615:HOH:O	2.29	0.62
1:M:272:LYS:NZ	1:N:228:SER:HB2	2.14	0.62
1:K:266:THR:HG21	1:K:273:VAL:O	2.00	0.62
1:L:345:ARG:HA	1:L:348:GLN:HE21	1.65	0.62
1:F:266:THR:HG21	1:F:273:VAL:O	1.99	0.61
1:G:114:MET:HB3	5:G:608:HOH:O	1.98	0.61
1:H:326:ASN:HD22	1:H:329:THR:HB	1.64	0.61
1:M:525:PRO:O	1:M:526:LYS:HG2	2.00	0.61
1:A:445:ARG:NH2	5:A:607:HOH:O	2.32	0.61
1:E:525:PRO:O	1:E:526:LYS:HG2	2.00	0.61
1:K:23:LEU:HD22	1:K:74:VAL:HG13	1.83	0.61
1:B:463:SER:HB2	5:B:601:HOH:O	1.99	0.61
4:N:1:AGS:O2G	4:N:1:AGS:S1G	2.51	0.61
1:E:414:GLY:O	1:E:417:VAL:HG13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PRO:HD2	1:B:320:ALA:O	2.00	0.61
1:B:78:ALA:HB1	1:B:89:THR:HB	1.83	0.61
4:I:1:AGS:O2G	4:I:1:AGS:S1G	2.55	0.61
1:G:498:LYS:NZ	5:G:586:HOH:O	1.97	0.61
1:F:73:MET:O	1:F:76:GLU:HB2	2.01	0.60
1:I:428:ASP:HB2	5:I:608:HOH:O	2.00	0.60
1:L:266:THR:CG2	1:L:273:VAL:H	2.14	0.60
1:M:319:GLN:HB3	1:M:336:VAL:HG21	1.82	0.60
1:B:266:THR:HG21	1:B:273:VAL:O	2.00	0.60
1:C:266:THR:CG2	1:C:273:VAL:H	2.14	0.60
1:H:414:GLY:O	1:H:417:VAL:HG13	2.01	0.60
1:I:23:LEU:HD22	1:I:74:VAL:HG13	1.83	0.60
1:G:266:THR:HG21	1:G:273:VAL:O	2.01	0.60
1:L:176:THR:HG21	1:L:322:ARG:HH12	1.67	0.60
1:D:266:THR:HG21	1:D:273:VAL:O	2.02	0.60
1:L:90:THR:OG1	4:L:1:AGS:S1G	2.59	0.60
1:M:496:PRO:HB2	1:M:499:VAL:HG13	1.83	0.60
1:N:213:VAL:HB	1:N:325:ILE:HG12	1.82	0.60
1:D:284:ARG:HH11	1:D:364:LYS:HD2	1.67	0.59
1:E:57:ALA:O	1:E:75:LYS:HE3	2.02	0.59
4:N:1:AGS:O3B	4:N:1:AGS:S1G	2.57	0.59
4:E:1:AGS:O3G	4:E:1:AGS:S1G	2.53	0.59
1:G:266:THR:CG2	1:G:273:VAL:H	2.16	0.59
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.42	0.59
1:B:23:LEU:HD22	1:B:74:VAL:HG13	1.84	0.59
1:K:414:GLY:O	1:K:417:VAL:HG13	2.02	0.59
1:L:218:PRO:HD2	1:L:320:ALA:O	2.03	0.59
1:E:266:THR:CG2	1:E:273:VAL:H	2.15	0.59
1:F:74:VAL:O	1:F:74:VAL:HG22	2.02	0.59
1:A:266:THR:HG21	1:A:273:VAL:O	2.02	0.59
1:H:266:THR:HG21	1:H:273:VAL:O	2.02	0.59
1:I:525:PRO:O	1:I:526:LYS:CG	2.51	0.59
1:E:266:THR:HG21	1:E:273:VAL:O	2.01	0.58
1:J:266:THR:CG2	1:J:273:VAL:H	2.16	0.58
1:G:18:ARG:NE	5:G:595:HOH:O	2.22	0.58
1:I:359:ASP:O	1:I:363:GLU:HG2	2.03	0.58
1:J:266:THR:HG21	1:J:273:VAL:O	2.04	0.58
1:N:218:PRO:HD2	1:N:320:ALA:O	2.03	0.58
1:D:90:THR:OG1	4:D:561:AGS:S1G	2.58	0.58
1:F:266:THR:CG2	1:F:273:VAL:H	2.16	0.58
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:PRO:O	1:B:526:LYS:HG2	2.04	0.58
1:C:194:GLN:O	1:C:371:LYS:HE3	2.02	0.58
1:I:383:ALA:HB3	1:I:389:MET:HB2	1.86	0.58
1:K:218:PRO:HD2	1:K:320:ALA:O	2.03	0.58
1:B:305:ILE:HD12	1:B:307:MET:HE2	1.86	0.57
1:J:176:THR:HG21	1:J:322:ARG:HH12	1.68	0.57
1:B:90:THR:O	1:B:94:VAL:HG13	2.03	0.57
1:I:305:ILE:HD12	1:I:307:MET:HE2	1.87	0.57
1:A:194:GLN:O	1:A:371:LYS:HE3	2.03	0.57
1:B:266:THR:CG2	1:B:273:VAL:H	2.17	0.57
1:L:57:ALA:O	1:L:75:LYS:HE3	2.05	0.57
1:I:194:GLN:O	1:I:371:LYS:HE3	2.05	0.57
1:M:266:THR:CG2	1:M:273:VAL:H	2.17	0.57
1:A:526:LYS:HE2	1:G:63:GLU:OE2	2.04	0.57
1:G:230:ILE:HD12	1:G:261:THR:HG21	1.86	0.57
1:D:132:LYS:HE2	5:D:595:HOH:O	2.04	0.57
1:J:218:PRO:HD2	1:J:320:ALA:O	2.05	0.57
1:C:266:THR:HG22	1:C:273:VAL:H	1.70	0.56
1:I:266:THR:CG2	1:I:273:VAL:H	2.18	0.56
1:L:242:LYS:HA	1:M:231:ARG:NH1	2.20	0.56
1:H:526:LYS:HE2	1:N:63:GLU:OE2	2.05	0.56
1:A:266:THR:CG2	1:A:273:VAL:H	2.18	0.56
1:B:525:PRO:O	1:B:526:LYS:CG	2.53	0.56
1:C:218:PRO:HD2	1:C:320:ALA:O	2.04	0.56
1:L:266:THR:HG22	1:L:273:VAL:H	1.69	0.56
1:L:514:MET:CG	1:L:514:MET:CE	2.83	0.56
1:C:266:THR:HG21	1:C:273:VAL:O	2.05	0.56
1:D:305:ILE:HD12	1:D:307:MET:HE2	1.86	0.56
1:E:266:THR:HG22	1:E:273:VAL:H	1.71	0.56
1:I:266:THR:HG21	1:I:273:VAL:O	2.04	0.56
1:I:448:GLU:OE2	1:I:470:LYS:NZ	2.32	0.56
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.88	0.56
1:J:23:LEU:CD2	1:J:74:VAL:HG13	2.35	0.56
1:M:266:THR:HG21	1:M:273:VAL:O	2.05	0.56
1:C:23:LEU:HD22	1:C:74:VAL:HG13	1.87	0.56
1:K:266:THR:CG2	1:K:273:VAL:H	2.18	0.56
1:M:305:ILE:HD12	1:M:307:MET:HE2	1.88	0.56
1:A:231:ARG:NH1	1:G:242:LYS:CA	2.64	0.56
1:H:525:PRO:O	1:H:526:LYS:CG	2.54	0.56
1:I:57:ALA:O	1:I:75:LYS:HE3	2.05	0.56
1:D:266:THR:CG2	1:D:273:VAL:H	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:THR:HG22	1:I:271:VAL:O	2.05	0.56
1:J:404:ARG:HH11	1:J:404:ARG:HG2	1.71	0.56
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.05	0.56
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.88	0.55
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.06	0.55
1:F:389:MET:HE3	1:G:281:PHE:CE2	2.41	0.55
1:N:23:LEU:HD22	1:N:74:VAL:HG13	1.88	0.55
1:D:218:PRO:HD2	1:D:320:ALA:O	2.05	0.55
1:G:525:PRO:O	1:G:526:LYS:CG	2.54	0.55
1:H:73:MET:O	1:H:76:GLU:HB2	2.06	0.55
1:B:85:ALA:O	1:B:401:HIS:HE1	1.89	0.55
1:M:414:GLY:O	1:M:417:VAL:HG13	2.07	0.55
1:N:266:THR:CG2	1:N:273:VAL:H	2.20	0.55
1:A:404:ARG:HG2	1:A:404:ARG:HH11	1.72	0.55
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.88	0.55
1:G:525:PRO:O	1:G:526:LYS:HG2	2.06	0.55
1:F:178:GLU:OE2	1:F:322:ARG:HD3	2.06	0.55
1:H:171:LYS:HB2	1:H:407:VAL:HG11	1.87	0.55
1:J:18:ARG:NE	5:J:572:HOH:O	2.27	0.55
1:J:194:GLN:O	1:J:371:LYS:HE3	2.05	0.55
1:M:266:THR:HG22	1:M:273:VAL:H	1.72	0.55
1:D:18:ARG:NE	5:D:587:HOH:O	2.36	0.55
1:E:345:ARG:HA	1:E:348:GLN:NE2	2.21	0.55
1:G:266:THR:HG22	1:G:271:VAL:O	2.06	0.55
1:M:200:LEU:HD21	1:M:277:LYS:HG3	1.88	0.55
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.88	0.54
1:H:23:LEU:HD22	1:H:74:VAL:HG13	1.88	0.54
1:L:80:LYS:CE	1:L:80:LYS:CG	2.79	0.54
1:M:178:GLU:OE2	1:M:322:ARG:HD3	2.06	0.54
1:A:231:ARG:HH12	1:G:242:LYS:CG	2.21	0.54
1:D:90:THR:O	1:D:94:VAL:HG13	2.07	0.54
1:B:176:THR:HG21	1:B:322:ARG:HH12	1.72	0.54
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.90	0.54
1:F:266:THR:HG22	1:F:273:VAL:H	1.72	0.54
1:G:461:GLU:OE1	5:G:630:HOH:O	2.19	0.54
1:N:404:ARG:HH11	1:N:404:ARG:HG2	1.72	0.54
1:N:319:GLN:HB3	1:N:336:VAL:HG21	1.89	0.54
1:G:305:ILE:HD12	1:G:307:MET:HE2	1.90	0.54
1:C:272:LYS:HZ3	1:D:228:SER:HB2	1.73	0.54
1:D:70:GLY:HA2	1:D:73:MET:HE3	1.90	0.54
1:A:218:PRO:HD2	1:A:320:ALA:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:ILE:HD12	1:E:307:MET:HE2	1.90	0.54
1:I:230:ILE:HD12	1:I:261:THR:HG21	1.89	0.54
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.72	0.54
1:C:73:MET:O	1:C:76:GLU:HB2	2.08	0.54
1:G:404:ARG:HG2	1:G:404:ARG:HH11	1.72	0.54
1:H:266:THR:HG22	1:H:271:VAL:O	2.06	0.54
1:B:181:THR:O	1:C:282:GLY:HA3	2.08	0.54
1:L:525:PRO:O	1:L:526:LYS:HG2	2.08	0.54
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.89	0.54
1:H:218:PRO:HD2	1:H:320:ALA:O	2.08	0.54
1:K:266:THR:HG22	1:K:273:VAL:H	1.73	0.54
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.89	0.54
1:C:305:ILE:HD12	1:C:307:MET:HE2	1.90	0.53
1:C:235:PRO:HG3	1:C:310:GLU:HA	1.91	0.53
1:K:23:LEU:CD2	1:K:74:VAL:HG13	2.37	0.53
1:F:414:GLY:O	1:F:417:VAL:HG13	2.08	0.53
1:N:305:ILE:HD12	1:N:307:MET:HE2	1.90	0.53
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.89	0.53
1:F:345:ARG:HA	1:F:348:GLN:NE2	2.21	0.53
1:N:270:ILE:HG22	1:N:271:VAL:HG23	1.91	0.53
1:E:525:PRO:O	1:E:526:LYS:CG	2.57	0.53
1:E:73:MET:O	1:E:76:GLU:HB2	2.08	0.53
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.90	0.53
1:J:266:THR:HG22	1:J:273:VAL:H	1.71	0.53
1:M:218:PRO:HD2	1:M:320:ALA:O	2.08	0.53
1:G:266:THR:HG22	1:G:273:VAL:H	1.73	0.53
1:B:57:ALA:O	1:B:75:LYS:HE3	2.08	0.53
1:E:525:PRO:HD3	5:E:594:HOH:O	2.09	0.53
1:N:158:VAL:HG13	1:N:396:VAL:HG22	1.90	0.53
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.90	0.53
1:E:496:PRO:HB2	1:E:499:VAL:HG13	1.91	0.53
1:F:305:ILE:HD12	1:F:307:MET:HE2	1.91	0.53
1:J:224:ASP:HB3	1:J:302:SER:HB3	1.91	0.53
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.90	0.53
1:A:270:ILE:HA	1:B:229:ASN:OD1	2.09	0.53
1:C:319:GLN:HB3	1:C:336:VAL:HG21	1.91	0.53
1:H:291:ASP:OD2	1:H:368:ARG:HD2	2.09	0.53
1:A:345:ARG:HA	1:A:348:GLN:NE2	2.22	0.53
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.90	0.52
1:A:231:ARG:HH12	1:G:242:LYS:HG3	1.74	0.52
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.91	0.52
1:M:319:GLN:HB3	1:M:336:VAL:CG2	2.39	0.52
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.90	0.52
1:A:414:GLY:O	1:A:417:VAL:HG13	2.09	0.52
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.91	0.52
1:I:404:ARG:HH11	1:I:404:ARG:HG2	1.75	0.52
1:K:404:ARG:HH11	1:K:404:ARG:CG	2.22	0.52
1:L:158:VAL:HG13	1:L:396:VAL:HG22	1.91	0.52
1:L:80:LYS:HZ3	1:L:80:LYS:CG	2.21	0.52
1:A:115:ASP:OD2	5:A:610:HOH:O	2.19	0.52
1:C:268:ARG:O	1:D:257:GLU:HG3	2.09	0.52
1:H:266:THR:HG22	1:H:273:VAL:H	1.74	0.52
1:H:90:THR:O	1:H:94:VAL:HG13	2.10	0.52
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.90	0.52
1:C:272:LYS:NZ	1:D:228:SER:CB	2.73	0.52
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.50	0.52
1:J:37:ASN:ND2	1:J:51:LYS:HE3	2.25	0.52
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.91	0.52
1:A:230:ILE:HD12	1:A:261:THR:HG21	1.91	0.52
1:L:414:GLY:O	1:L:417:VAL:HG13	2.09	0.52
1:A:525:PRO:O	1:A:526:LYS:HG2	2.09	0.52
1:B:16:MET:O	1:B:20:VAL:HG13	2.09	0.52
1:I:235:PRO:HG3	1:I:310:GLU:HA	1.92	0.52
1:L:200:LEU:HD21	1:L:277:LYS:HG3	1.91	0.52
1:I:218:PRO:HD2	1:I:320:ALA:O	2.11	0.51
1:L:319:GLN:HB3	1:L:336:VAL:HG21	1.91	0.51
1:M:176:THR:HG21	1:M:322:ARG:HH12	1.75	0.51
1:M:525:PRO:HD3	5:M:596:HOH:O	2.10	0.51
1:M:525:PRO:O	1:M:526:LYS:CG	2.58	0.51
1:A:272:LYS:NZ	1:B:228:SER:HB2	2.25	0.51
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.91	0.51
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.93	0.51
1:H:305:ILE:HD12	1:H:307:MET:HE2	1.92	0.51
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.93	0.51
1:B:266:THR:HG22	1:B:273:VAL:H	1.74	0.51
1:B:414:GLY:O	1:B:417:VAL:HG13	2.11	0.51
1:F:404:ARG:HG2	1:F:404:ARG:HH11	1.75	0.51
1:M:266:THR:HG22	1:M:271:VAL:O	2.10	0.51
1:J:270:ILE:HG22	1:J:271:VAL:HG23	1.92	0.51
1:F:235:PRO:HG3	1:F:310:GLU:HA	1.93	0.51
1:H:176:THR:HG21	1:H:322:ARG:HH12	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:414:GLY:O	1:N:417:VAL:HG13	2.11	0.51
1:A:224:ASP:HB3	1:A:302:SER:HB3	1.92	0.51
1:B:194:GLN:O	1:B:371:LYS:HE3	2.11	0.51
1:E:230:ILE:HD12	1:E:261:THR:HG21	1.92	0.51
1:K:57:ALA:O	1:K:75:LYS:HE3	2.11	0.51
1:B:230:ILE:HD12	1:B:261:THR:HG21	1.91	0.51
1:D:132:LYS:CE	5:D:595:HOH:O	2.58	0.51
1:G:345:ARG:HA	1:G:348:GLN:NE2	2.24	0.51
1:H:525:PRO:O	1:H:526:LYS:HG2	2.11	0.51
1:I:270:ILE:HG22	1:I:271:VAL:HG23	1.92	0.51
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.92	0.51
1:K:489:ILE:HD12	1:K:494:LEU:CD2	2.41	0.51
1:A:489:ILE:HD12	1:A:494:LEU:CD2	2.41	0.50
1:H:194:GLN:O	1:H:371:LYS:HE3	2.11	0.50
1:K:230:ILE:HD12	1:K:261:THR:HG21	1.91	0.50
1:N:489:ILE:HD12	1:N:494:LEU:CD2	2.40	0.50
1:C:525:PRO:HD3	5:C:588:HOH:O	2.11	0.50
1:D:37:ASN:ND2	1:D:51:LYS:HE3	2.27	0.50
1:F:74:VAL:O	1:F:74:VAL:CG2	2.58	0.50
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.93	0.50
1:C:272:LYS:HZ1	1:D:228:SER:HB3	1.77	0.50
1:D:458:CYS:SG	1:D:480:ALA:HB1	2.52	0.50
1:F:218:PRO:HD2	1:F:320:ALA:O	2.11	0.50
1:I:219:PHE:HB3	1:I:317:LEU:HD23	1.94	0.50
1:D:345:ARG:HA	1:D:348:GLN:NE2	2.24	0.50
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.94	0.50
1:J:266:THR:HG22	1:J:271:VAL:O	2.12	0.50
1:J:414:GLY:O	1:J:417:VAL:HG13	2.12	0.50
1:L:514:MET:HE2	1:L:514:MET:CB	2.41	0.50
1:A:266:THR:HG22	1:A:273:VAL:H	1.76	0.50
1:I:70:GLY:HA2	1:I:73:MET:HE3	1.94	0.50
1:K:305:ILE:HD12	1:K:307:MET:HE2	1.94	0.50
1:M:270:ILE:HG22	1:M:271:VAL:HG23	1.93	0.50
1:N:345:ARG:HA	1:N:348:GLN:NE2	2.24	0.50
1:B:452:ARG:HD3	5:B:594:HOH:O	2.11	0.50
1:G:176:THR:HG21	1:G:322:ARG:HH12	1.77	0.50
1:G:221:LEU:HD23	1:G:249:ILE:HD12	1.93	0.50
1:G:319:GLN:HB3	1:G:336:VAL:HG21	1.94	0.50
1:K:270:ILE:HG22	1:K:271:VAL:HG23	1.93	0.50
1:I:176:THR:HG21	1:I:322:ARG:HH12	1.76	0.49
1:N:194:GLN:O	1:N:371:LYS:HE3	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:272:LYS:HZ3	1:N:228:SER:HB2	1.77	0.49
1:D:525:PRO:O	1:D:526:LYS:HG2	2.11	0.49
1:E:266:THR:HG22	1:E:271:VAL:O	2.12	0.49
1:F:230:ILE:HD12	1:F:261:THR:HG21	1.94	0.49
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.93	0.49
1:J:179:ASP:OD1	1:J:393:LYS:HE3	2.13	0.49
1:J:525:PRO:O	1:J:526:LYS:HG2	2.11	0.49
1:K:460:GLU:HB3	5:K:586:HOH:O	2.12	0.49
1:E:23:LEU:HD22	1:E:74:VAL:HG13	1.93	0.49
1:A:305:ILE:HD12	1:A:307:MET:HE2	1.95	0.49
1:F:224:ASP:HB3	1:F:302:SER:HB3	1.93	0.49
1:F:90:THR:O	1:F:94:VAL:HG13	2.13	0.49
1:G:70:GLY:HA2	1:G:73:MET:HE3	1.93	0.49
1:C:404:ARG:NH1	1:C:404:ARG:HG2	2.25	0.49
1:F:319:GLN:HB3	1:F:336:VAL:HG21	1.93	0.49
1:L:186:GLU:HB2	1:L:380:LYS:HB2	1.95	0.49
1:L:305:ILE:HD12	1:L:307:MET:HE2	1.94	0.49
1:E:366:GLN:O	1:E:369:VAL:HG22	2.13	0.49
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.95	0.49
1:B:266:THR:HG22	1:B:271:VAL:O	2.13	0.49
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.94	0.49
1:M:458:CYS:SG	1:M:480:ALA:HB1	2.53	0.49
1:B:235:PRO:HG3	1:B:310:GLU:HA	1.94	0.49
1:C:414:GLY:O	1:C:417:VAL:HG13	2.13	0.49
1:H:68:ASN:O	1:H:72:GLN:HG2	2.13	0.49
1:I:325:ILE:HG22	1:I:330:THR:HG23	1.95	0.49
1:K:266:THR:HG22	1:K:271:VAL:O	2.13	0.49
1:N:266:THR:HG22	1:N:271:VAL:O	2.12	0.49
1:L:270:ILE:HG22	1:L:271:VAL:HG23	1.95	0.48
1:C:270:ILE:HG22	1:C:271:VAL:HG23	1.94	0.48
1:D:266:THR:HG22	1:D:273:VAL:H	1.77	0.48
1:D:192:GLY:HA2	1:D:295:LEU:HD11	1.93	0.48
1:C:36:ARG:HG3	1:D:518:GLU:HG2	1.95	0.48
1:F:151:SER:HB2	1:F:399:ALA:HA	1.96	0.48
1:B:151:SER:HB2	1:B:399:ALA:HA	1.96	0.48
1:B:74:VAL:O	1:B:77:VAL:HB	2.12	0.48
1:H:319:GLN:HB3	1:H:336:VAL:HG21	1.95	0.48
1:N:77:VAL:O	1:N:78:ALA:C	2.51	0.48
1:I:266:THR:HG22	1:I:273:VAL:H	1.79	0.48
1:J:345:ARG:HA	1:J:348:GLN:NE2	2.26	0.48
1:D:177:VAL:CG2	1:D:397:GLU:HG3	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:325:ILE:HG22	1:L:330:THR:HG23	1.95	0.48
1:M:90:THR:O	1:M:94:VAL:HG13	2.13	0.48
1:I:121:ASP:OD1	5:I:594:HOH:O	2.20	0.48
1:K:460:GLU:O	1:K:462:PRO:HD3	2.14	0.48
1:L:404:ARG:HG2	1:L:404:ARG:HH11	1.78	0.48
1:C:236:VAL:O	1:C:240:VAL:HG23	2.13	0.48
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.96	0.48
1:E:82:ASN:HB2	1:E:89:THR:HG21	1.95	0.48
1:E:325:ILE:HG22	1:E:330:THR:HG23	1.94	0.48
1:G:489:ILE:HD12	1:G:494:LEU:HD22	1.95	0.48
1:H:266:THR:HG21	1:H:273:VAL:H	1.78	0.48
1:M:404:ARG:CG	1:M:404:ARG:HH11	2.26	0.48
1:N:74:VAL:HG22	1:N:74:VAL:O	2.13	0.48
1:A:178:GLU:OE2	1:A:322:ARG:HD3	2.13	0.48
1:B:176:THR:HG22	1:B:177:VAL:H	1.78	0.48
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.96	0.48
1:I:345:ARG:HA	1:I:348:GLN:NE2	2.26	0.48
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.95	0.48
1:F:194:GLN:O	1:F:371:LYS:HE3	2.13	0.47
1:G:194:GLN:O	1:G:371:LYS:HE3	2.14	0.47
1:I:23:LEU:CD2	1:I:74:VAL:HG13	2.43	0.47
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.95	0.47
1:M:321:LYS:HB2	1:M:334:ASP:HB3	1.96	0.47
1:N:266:THR:HG22	1:N:273:VAL:H	1.78	0.47
1:G:179:ASP:OD1	1:G:393:LYS:HE3	2.14	0.47
1:G:452:ARG:HD3	5:G:585:HOH:O	2.15	0.47
1:G:90:THR:O	1:G:94:VAL:HG13	2.13	0.47
1:L:80:LYS:HB2	1:L:80:LYS:CD	2.43	0.47
1:D:414:GLY:O	1:D:417:VAL:HG13	2.13	0.47
1:M:224:ASP:HB3	1:M:302:SER:HB3	1.95	0.47
1:D:404:ARG:HH11	1:D:404:ARG:CG	2.25	0.47
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.96	0.47
1:F:63:GLU:HB2	1:G:524:LEU:CD2	2.45	0.47
1:J:236:VAL:O	1:J:240:VAL:HG23	2.14	0.47
1:M:78:ALA:HB1	1:M:89:THR:HB	1.97	0.47
1:F:85:ALA:O	1:F:401:HIS:HE1	1.98	0.47
1:F:525:PRO:O	1:F:526:LYS:HG2	2.14	0.47
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.96	0.47
1:G:458:CYS:SG	1:G:480:ALA:HB1	2.54	0.47
1:D:29:VAL:HG11	1:E:518:GLU:HG3	1.97	0.47
1:E:82:ASN:HB2	1:E:89:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:383:ALA:HB3	1:N:389:MET:HB2	1.95	0.47
1:H:345:ARG:HA	1:H:348:GLN:NE2	2.29	0.47
1:K:345:ARG:HA	1:K:348:GLN:NE2	2.26	0.47
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.96	0.47
1:A:73:MET:O	1:A:76:GLU:HB2	2.15	0.47
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.95	0.47
1:H:479:ASN:C	1:H:479:ASN:OD1	2.53	0.47
1:I:221:LEU:HD23	1:I:249:ILE:HD12	1.96	0.47
1:D:263:VAL:O	1:D:267:MET:HB2	2.14	0.47
1:E:319:GLN:HB3	1:E:336:VAL:CG2	2.44	0.47
1:E:489:ILE:HD12	1:E:494:LEU:HD22	1.97	0.47
1:I:319:GLN:HB3	1:I:336:VAL:HG21	1.96	0.47
1:J:305:ILE:HD12	1:J:307:MET:HE2	1.96	0.47
1:L:77:VAL:O	1:L:78:ALA:C	2.53	0.47
1:G:236:VAL:O	1:G:240:VAL:HG23	2.13	0.47
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.97	0.47
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.97	0.47
1:A:74:VAL:HG22	1:A:74:VAL:O	2.14	0.47
1:B:319:GLN:HB3	1:B:336:VAL:HG21	1.97	0.46
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.96	0.46
1:G:18:ARG:NH2	5:G:595:HOH:O	2.41	0.46
1:K:194:GLN:O	1:K:371:LYS:HE3	2.15	0.46
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.96	0.46
1:N:525:PRO:O	1:N:526:LYS:HG2	2.14	0.46
1:G:263:VAL:O	1:G:267:MET:HB2	2.15	0.46
1:K:236:VAL:O	1:K:240:VAL:HG23	2.15	0.46
1:N:90:THR:OG1	4:N:1:AGS:S1G	2.63	0.46
1:A:124:VAL:HG21	1:A:508:ALA:HB2	1.97	0.46
1:C:319:GLN:HB3	1:C:336:VAL:CG2	2.45	0.46
1:F:389:MET:CE	1:G:281:PHE:CE2	2.97	0.46
1:G:77:VAL:HG23	1:G:510:VAL:HG21	1.98	0.46
1:I:177:VAL:CG2	1:I:397:GLU:HG3	2.40	0.46
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.98	0.46
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.98	0.46
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.97	0.46
1:M:218:PRO:HB3	1:M:246:PRO:HG2	1.97	0.46
1:N:348:GLN:O	1:N:352:GLN:HG2	2.15	0.46
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.95	0.46
1:H:90:THR:OG1	4:H:1:AGS:S1G	2.69	0.46
1:L:319:GLN:HB3	1:L:336:VAL:CG2	2.45	0.46
1:B:77:VAL:HG23	1:B:510:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:ASP:HB3	1:G:302:SER:HB3	1.96	0.46
1:I:364:LYS:HA	1:I:364:LYS:HD3	1.70	0.46
1:I:360:TYR:CE1	1:I:364:LYS:HE3	2.51	0.46
1:D:57:ALA:O	1:D:75:LYS:CE	2.63	0.46
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.97	0.46
1:E:151:SER:HB2	1:E:399:ALA:HA	1.98	0.46
1:H:151:SER:HB2	1:H:399:ALA:HA	1.98	0.46
1:J:193:MET:CE	1:J:292:ILE:HG12	2.46	0.46
1:K:319:GLN:HB3	1:K:336:VAL:HG21	1.96	0.46
1:L:102:GLU:HB2	1:L:442:VAL:HG13	1.98	0.46
1:A:404:ARG:HH11	1:A:404:ARG:CG	2.28	0.46
1:D:34:LYS:HE2	1:E:118:ARG:HH22	1.80	0.46
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.97	0.46
1:I:179:ASP:OD1	1:I:393:LYS:HE3	2.16	0.46
1:K:404:ARG:NH1	1:K:404:ARG:CG	2.79	0.46
1:L:221:LEU:HD23	1:L:249:ILE:HD12	1.98	0.46
1:M:360:TYR:CE1	1:M:364:LYS:HE3	2.51	0.46
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.98	0.46
1:C:323:VAL:HG12	1:C:332:ILE:HA	1.98	0.46
1:G:284:ARG:HH12	1:G:364:LYS:NZ	2.14	0.46
1:J:489:ILE:HD12	1:J:494:LEU:CD2	2.46	0.46
1:K:451:LEU:C	1:K:451:LEU:HD23	2.36	0.46
1:N:263:VAL:O	1:N:267:MET:HB2	2.16	0.46
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.98	0.46
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.97	0.46
1:B:191:GLU:O	1:B:334:ASP:HA	2.14	0.46
1:H:489:ILE:HD12	1:H:494:LEU:CD2	2.45	0.46
1:I:151:SER:HB2	1:I:399:ALA:HA	1.98	0.46
1:J:218:PRO:HB3	1:J:246:PRO:HG2	1.97	0.46
1:M:57:ALA:O	1:M:75:LYS:CE	2.63	0.46
1:D:68:ASN:O	1:D:72:GLN:HG2	2.16	0.46
1:E:176:THR:HG21	1:E:322:ARG:HH12	1.81	0.46
1:I:57:ALA:O	1:I:75:LYS:CE	2.64	0.46
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.98	0.46
1:L:68:ASN:O	1:L:72:GLN:HG2	2.15	0.46
1:A:171:LYS:HB2	1:A:407:VAL:HG11	1.98	0.45
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.98	0.45
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.98	0.45
1:C:321:LYS:HB2	1:C:334:ASP:HB3	1.97	0.45
1:E:193:MET:CE	1:E:292:ILE:HG12	2.47	0.45
1:F:449:ALA:N	1:F:450:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:176:THR:HG22	1:M:177:VAL:H	1.80	0.45
1:M:236:VAL:O	1:M:240:VAL:HG23	2.17	0.45
1:N:360:TYR:CE1	1:N:364:LYS:HE3	2.52	0.45
1:C:266:THR:HG22	1:C:271:VAL:O	2.16	0.45
1:E:463:SER:HB2	5:E:649:HOH:O	2.16	0.45
1:G:284:ARG:HH11	1:G:364:LYS:HD2	1.80	0.45
1:N:351:GLN:HE21	1:N:351:GLN:HB3	1.65	0.45
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.98	0.45
1:F:386:GLU:O	1:F:390:LYS:HG2	2.16	0.45
1:H:35:GLY:O	1:H:51:LYS:HE2	2.16	0.45
1:B:263:VAL:O	1:B:267:MET:HB2	2.17	0.45
1:B:345:ARG:HA	1:B:348:GLN:NE2	2.27	0.45
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.82	0.45
1:H:63:GLU:OE2	1:I:526:LYS:HE2	2.16	0.45
1:B:90:THR:OG1	4:B:1:AGS:S1G	2.66	0.45
1:F:171:LYS:HB2	1:F:407:VAL:HG11	1.97	0.45
1:F:360:TYR:CE1	1:F:364:LYS:HE3	2.52	0.45
1:H:263:VAL:O	1:H:267:MET:HB2	2.17	0.45
1:H:177:VAL:CG2	1:H:397:GLU:HG3	2.40	0.45
1:K:77:VAL:O	1:K:78:ALA:C	2.55	0.45
1:L:177:VAL:CG2	1:L:397:GLU:HG3	2.42	0.45
1:L:80:LYS:HG2	1:L:80:LYS:NZ	2.32	0.45
1:D:221:LEU:HD23	1:D:249:ILE:HD12	1.98	0.45
1:D:57:ALA:O	1:D:75:LYS:HE3	2.16	0.45
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.99	0.45
1:G:413:ALA:HB3	1:G:417:VAL:HG22	1.99	0.45
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.98	0.45
1:I:82:ASN:O	1:I:86:GLY:N	2.45	0.45
1:L:193:MET:CE	1:L:292:ILE:HG12	2.46	0.45
1:L:224:ASP:HB3	1:L:302:SER:HB3	1.98	0.45
1:B:158:VAL:HG13	1:B:396:VAL:HG22	1.99	0.45
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.98	0.45
1:E:224:ASP:HB3	1:E:302:SER:HB3	1.97	0.45
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.99	0.45
1:H:360:TYR:CE1	1:H:364:LYS:HE3	2.52	0.45
1:J:57:ALA:O	1:J:75:LYS:CE	2.65	0.45
1:K:221:LEU:HD23	1:K:249:ILE:HD12	1.98	0.45
1:K:321:LYS:HB2	1:K:334:ASP:HB3	1.98	0.45
1:L:78:ALA:HB1	1:L:89:THR:HB	1.99	0.45
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.99	0.45
1:C:449:ALA:N	1:C:450:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:ILE:HD13	1:D:325:ILE:HG23	1.67	0.45
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.97	0.45
1:F:413:ALA:CB	1:F:417:VAL:HG22	2.47	0.45
1:L:449:ALA:N	1:L:450:PRO:CD	2.79	0.45
1:C:57:ALA:O	1:C:75:LYS:HE3	2.17	0.45
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.99	0.45
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.98	0.45
1:L:386:GLU:O	1:L:390:LYS:HG2	2.16	0.45
1:I:193:MET:CE	1:I:292:ILE:HG12	2.47	0.44
1:J:158:VAL:HG13	1:J:396:VAL:HG22	1.99	0.44
1:J:82:ASN:O	1:J:86:GLY:N	2.49	0.44
1:A:386:GLU:O	1:A:390:LYS:HG2	2.16	0.44
1:A:489:ILE:HD12	1:A:494:LEU:HD22	1.98	0.44
1:E:458:CYS:SG	1:E:480:ALA:HB1	2.57	0.44
1:F:221:LEU:HD23	1:F:249:ILE:HD12	1.98	0.44
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.99	0.44
1:G:514:MET:HB3	1:G:514:MET:HE3	1.92	0.44
1:I:366:GLN:O	1:I:369:VAL:HG22	2.17	0.44
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.99	0.44
1:M:36:ARG:HG3	1:N:518:GLU:HG2	1.98	0.44
1:E:449:ALA:N	1:E:450:PRO:CD	2.80	0.44
1:F:236:VAL:O	1:F:240:VAL:HG23	2.17	0.44
1:F:266:THR:HG22	1:F:271:VAL:O	2.18	0.44
1:K:186:GLU:HB2	1:K:380:LYS:HB2	2.00	0.44
1:K:218:PRO:HB3	1:K:246:PRO:HG2	1.99	0.44
1:K:224:ASP:HB3	1:K:302:SER:HB3	1.99	0.44
1:M:68:ASN:O	1:M:72:GLN:HG2	2.17	0.44
1:C:57:ALA:O	1:C:75:LYS:CE	2.66	0.44
1:G:288:MET:HG2	1:G:368:ARG:HD3	1.98	0.44
1:G:414:GLY:O	1:G:417:VAL:HG13	2.17	0.44
1:J:319:GLN:HB3	1:J:336:VAL:HG21	1.99	0.44
1:C:383:ALA:HB3	1:C:389:MET:HB2	1.99	0.44
1:F:193:MET:CE	1:F:292:ILE:HG12	2.48	0.44
1:G:496:PRO:HB2	1:G:499:VAL:HG13	1.99	0.44
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.99	0.44
1:H:224:ASP:HB3	1:H:302:SER:HB3	2.00	0.44
1:I:348:GLN:O	1:I:352:GLN:HG2	2.17	0.44
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.58	0.44
1:J:90:THR:O	1:J:94:VAL:HG13	2.17	0.44
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.98	0.44
1:K:179:ASP:OD1	1:K:393:LYS:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:463:SER:HB2	5:L:612:HOH:O	2.17	0.44
1:D:217:SER:N	1:D:218:PRO:HD3	2.33	0.44
1:D:404:ARG:NH1	1:D:404:ARG:CG	2.79	0.44
1:F:36:ARG:HG3	1:G:518:GLU:HG2	1.98	0.44
1:H:386:GLU:O	1:H:390:LYS:HG2	2.17	0.44
1:I:186:GLU:HB2	1:I:380:LYS:HB2	1.99	0.44
1:K:82:ASN:HB2	1:K:89:THR:HG21	1.99	0.44
1:L:451:LEU:C	1:L:451:LEU:HD23	2.38	0.44
1:N:236:VAL:O	1:N:240:VAL:HG23	2.17	0.44
1:F:524:LEU:O	1:F:526:LYS:N	2.51	0.44
1:I:514:MET:HE3	1:I:514:MET:HB3	1.94	0.44
1:J:325:ILE:HG22	1:J:330:THR:HG23	2.00	0.44
1:J:151:SER:HB2	1:J:399:ALA:HA	1.99	0.44
1:J:404:ARG:CG	1:J:404:ARG:HH11	2.29	0.44
1:J:63:GLU:HB2	1:K:524:LEU:HD21	2.00	0.44
1:K:193:MET:CE	1:K:292:ILE:HG12	2.47	0.44
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.98	0.44
1:N:69:MET:O	1:N:73:MET:HE2	2.17	0.44
1:B:186:GLU:HB2	1:B:380:LYS:HB2	2.00	0.44
1:C:178:GLU:OE2	1:C:322:ARG:HD3	2.18	0.44
1:E:369:VAL:HG23	1:E:370:ALA:N	2.33	0.44
1:I:351:GLN:HE21	1:I:351:GLN:HB3	1.69	0.44
1:I:417:VAL:HG11	1:I:477:GLY:HA3	1.99	0.44
1:N:37:ASN:ND2	1:N:51:LYS:HE3	2.33	0.44
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.99	0.43
1:C:151:SER:HB2	1:C:399:ALA:HA	2.00	0.43
1:G:151:SER:HB2	1:G:399:ALA:HA	1.99	0.43
1:J:364:LYS:HA	1:J:364:LYS:HD3	1.84	0.43
1:L:263:VAL:O	1:L:267:MET:HB2	2.18	0.43
1:F:263:VAL:O	1:F:267:MET:HB2	2.18	0.43
1:J:263:VAL:O	1:J:267:MET:HB2	2.18	0.43
1:M:158:VAL:HG13	1:M:396:VAL:HG22	1.99	0.43
1:N:319:GLN:HB3	1:N:336:VAL:CG2	2.48	0.43
1:A:525:PRO:O	1:A:526:LYS:CG	2.65	0.43
1:B:78:ALA:O	1:B:79:SER:C	2.55	0.43
1:B:82:ASN:HB2	1:B:89:THR:HG21	2.00	0.43
1:F:23:LEU:HD22	1:F:74:VAL:HG13	2.00	0.43
1:F:369:VAL:HG23	1:F:370:ALA:N	2.33	0.43
1:K:524:LEU:O	1:K:526:LYS:N	2.51	0.43
1:N:506:TYR:O	1:N:507:ALA:C	2.56	0.43
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:ASP:HB2	5:B:599:HOH:O	2.19	0.43
1:D:524:LEU:O	1:D:526:LYS:N	2.51	0.43
1:E:386:GLU:O	1:E:390:LYS:HG2	2.17	0.43
1:F:147:VAL:O	1:F:151:SER:OG	2.36	0.43
1:J:235:PRO:HG3	1:J:310:GLU:HA	2.00	0.43
1:F:514:MET:HE3	1:F:514:MET:HB3	1.85	0.43
1:K:144:ILE:HG23	1:K:403:THR:HG21	2.00	0.43
1:L:151:SER:HB2	1:L:399:ALA:HA	2.00	0.43
1:L:489:ILE:HD12	1:L:494:LEU:CD2	2.49	0.43
1:A:151:SER:HB2	1:A:399:ALA:HA	2.01	0.43
1:A:514:MET:HB3	1:A:514:MET:HE3	1.73	0.43
1:C:23:LEU:O	1:C:23:LEU:HG	2.11	0.43
1:C:514:MET:HB3	1:C:514:MET:HE3	1.93	0.43
1:D:284:ARG:HH12	1:D:364:LYS:NZ	2.16	0.43
1:A:118:ARG:HH22	1:G:34:LYS:HE2	1.84	0.43
1:H:218:PRO:HB3	1:H:246:PRO:HG2	2.00	0.43
1:B:221:LEU:HD23	1:B:249:ILE:HD12	2.01	0.43
1:B:193:MET:HE1	1:B:292:ILE:HG12	2.00	0.43
1:E:186:GLU:HB2	1:E:380:LYS:HB2	2.00	0.43
1:E:37:ASN:ND2	1:E:51:LYS:HE3	2.33	0.43
1:F:351:GLN:HB3	1:F:351:GLN:HE21	1.64	0.43
1:H:366:GLN:O	1:H:369:VAL:HG22	2.18	0.43
1:J:351:GLN:HE21	1:J:351:GLN:HB3	1.66	0.43
1:B:224:ASP:HB3	1:B:302:SER:HB3	1.99	0.43
1:C:191:GLU:O	1:C:334:ASP:HA	2.18	0.43
1:D:325:ILE:HG21	1:D:325:ILE:HD12	1.64	0.43
1:H:351:GLN:HB3	1:H:351:GLN:HE21	1.68	0.43
1:K:364:LYS:HD3	1:K:364:LYS:HA	1.83	0.43
1:L:266:THR:HG22	1:L:271:VAL:O	2.18	0.43
1:M:178:GLU:HG2	1:M:322:ARG:NH1	2.33	0.43
1:A:186:GLU:HB2	1:A:380:LYS:HB2	2.01	0.43
1:B:82:ASN:HB2	1:B:89:THR:CG2	2.49	0.43
1:C:284:ARG:HH11	1:C:364:LYS:HD2	1.84	0.43
1:H:158:VAL:HG13	1:H:396:VAL:HG22	2.00	0.43
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.58	0.43
1:I:224:ASP:HB3	1:I:302:SER:HB3	2.01	0.43
1:J:186:GLU:HB2	1:J:380:LYS:HB2	2.01	0.43
1:K:366:GLN:O	1:K:369:VAL:HG22	2.19	0.43
1:M:404:ARG:CG	1:M:404:ARG:NH1	2.82	0.43
1:A:466:ALA:O	1:A:470:LYS:HG3	2.19	0.43
1:E:236:VAL:O	1:E:240:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:39:VAL:HG12	1:M:69:MET:CE	2.49	0.43
1:A:364:LYS:HD3	1:A:364:LYS:HA	1.85	0.42
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.49	0.42
1:C:364:LYS:HA	1:C:364:LYS:HD3	1.82	0.42
1:D:186:GLU:HB2	1:D:380:LYS:HB2	2.01	0.42
1:F:366:GLN:O	1:F:369:VAL:HG22	2.18	0.42
1:G:325:ILE:HD13	1:G:325:ILE:HG23	1.78	0.42
1:K:284:ARG:HH11	1:K:364:LYS:HD2	1.84	0.42
1:K:63:GLU:OE2	1:L:526:LYS:HE2	2.18	0.42
1:B:193:MET:CE	1:B:292:ILE:HG12	2.49	0.42
1:B:218:PRO:HB3	1:B:246:PRO:HG2	2.01	0.42
1:C:272:LYS:NZ	1:D:228:SER:HB2	2.34	0.42
1:F:177:VAL:CG2	1:F:397:GLU:HG3	2.43	0.42
1:H:219:PHE:HB3	1:H:317:LEU:HD23	2.00	0.42
1:J:389:MET:HE3	1:K:281:PHE:CD2	2.54	0.42
1:L:345:ARG:HA	1:L:348:GLN:NE2	2.34	0.42
1:N:179:ASP:OD1	1:N:393:LYS:HE3	2.19	0.42
1:N:284:ARG:HH11	1:N:364:LYS:HD2	1.84	0.42
1:B:514:MET:HE3	1:B:514:MET:HB3	1.71	0.42
1:M:186:GLU:HB2	1:M:380:LYS:HB2	2.01	0.42
1:N:240:VAL:HG11	1:N:247:LEU:HB2	2.01	0.42
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.01	0.42
1:C:263:VAL:O	1:C:267:MET:HB2	2.19	0.42
1:E:135:SER:HB3	5:E:618:HOH:O	2.18	0.42
1:F:319:GLN:HB3	1:F:336:VAL:CG2	2.50	0.42
1:F:413:ALA:HB3	1:F:417:VAL:HG22	2.00	0.42
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.32	0.42
1:J:360:TYR:CE1	1:J:364:LYS:HE3	2.54	0.42
1:K:37:ASN:ND2	1:K:51:LYS:HE3	2.34	0.42
1:A:263:VAL:O	1:A:267:MET:HB2	2.18	0.42
1:C:404:ARG:CG	1:C:404:ARG:NH1	2.81	0.42
1:D:404:ARG:HG2	1:D:404:ARG:NH1	2.30	0.42
1:F:288:MET:HG2	1:F:368:ARG:HD3	2.00	0.42
1:F:383:ALA:HB3	1:F:389:MET:HB2	2.01	0.42
1:H:364:LYS:HA	1:H:364:LYS:HD3	1.86	0.42
1:B:386:GLU:O	1:B:390:LYS:HG2	2.19	0.42
1:C:489:ILE:HD12	1:C:494:LEU:CD2	2.49	0.42
1:F:389:MET:CE	1:G:281:PHE:HE2	2.33	0.42
1:F:158:VAL:HG13	1:F:396:VAL:HG22	2.01	0.42
1:F:466:ALA:O	1:F:470:LYS:HG3	2.20	0.42
1:G:18:ARG:CZ	5:G:595:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ALA:HB2	1:H:109:ALA:HB2	2.02	0.42
1:I:218:PRO:HB3	1:I:246:PRO:HG2	2.01	0.42
1:J:217:SER:N	1:J:218:PRO:HD3	2.35	0.42
1:J:288:MET:HG2	1:J:368:ARG:HD3	2.02	0.42
1:N:57:ALA:O	1:N:75:LYS:CE	2.68	0.42
1:B:153:ASN:O	1:B:154:SER:HB2	2.20	0.42
1:C:63:GLU:HB2	1:D:524:LEU:HD21	2.01	0.42
1:E:171:LYS:HB2	1:E:407:VAL:HG11	2.02	0.42
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.49	0.42
1:G:144:ILE:HG23	1:G:403:THR:HG21	2.02	0.42
1:G:158:VAL:HG13	1:G:396:VAL:HG22	2.02	0.42
1:H:118:ARG:HG3	5:H:587:HOH:O	2.18	0.42
1:N:404:ARG:HH11	1:N:404:ARG:CG	2.32	0.42
1:C:272:LYS:NZ	1:D:228:SER:HB3	2.35	0.42
1:E:351:GLN:HB3	1:E:351:GLN:HE21	1.66	0.42
1:F:348:GLN:O	1:F:352:GLN:HG2	2.20	0.42
1:G:118:ARG:HE	1:G:118:ARG:HB2	1.78	0.42
1:G:489:ILE:HD12	1:G:494:LEU:HD21	2.01	0.42
1:H:305:ILE:O	1:H:305:ILE:HG22	2.20	0.42
1:H:413:ALA:HB3	1:H:417:VAL:HG22	2.01	0.42
1:H:514:MET:HB3	1:H:514:MET:HE3	1.80	0.42
1:J:489:ILE:HD12	1:J:494:LEU:HD22	2.00	0.42
1:D:65:LYS:HG2	5:D:646:HOH:O	2.19	0.42
1:E:421:ARG:HD3	1:E:421:ARG:HH11	1.60	0.42
1:I:158:VAL:HG13	1:I:396:VAL:HG22	2.01	0.42
1:I:414:GLY:O	1:I:417:VAL:HG13	2.20	0.42
1:J:221:LEU:HD23	1:J:249:ILE:HD12	2.01	0.42
1:K:18:ARG:NE	5:K:590:HOH:O	2.47	0.42
1:L:171:LYS:HB2	1:L:407:VAL:HG11	2.02	0.42
1:L:218:PRO:HB3	1:L:246:PRO:HG2	2.00	0.42
1:M:325:ILE:HG22	1:M:330:THR:HG23	2.01	0.42
1:E:118:ARG:HB2	1:E:118:ARG:HE	1.80	0.42
1:E:321:LYS:HB2	1:E:334:ASP:HB3	2.02	0.42
1:F:188:ASP:OD1	1:F:188:ASP:N	2.53	0.42
1:H:270:ILE:HG22	1:H:271:VAL:HG23	2.02	0.42
1:H:383:ALA:HB3	1:H:389:MET:HB2	2.01	0.42
1:A:236:VAL:O	1:A:240:VAL:HG23	2.20	0.41
1:A:37:ASN:ND2	1:A:51:LYS:HE3	2.35	0.41
1:F:321:LYS:HB2	1:F:334:ASP:HB3	2.02	0.41
1:H:18:ARG:NE	5:H:584:HOH:O	2.32	0.41
1:H:284:ARG:HH11	1:H:364:LYS:HD2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:319:GLN:HB3	1:K:336:VAL:CG2	2.50	0.41
1:L:288:MET:HG2	1:L:368:ARG:HD3	2.02	0.41
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.60	0.41
1:M:366:GLN:O	1:M:369:VAL:HG22	2.20	0.41
1:M:409:GLU:OE1	5:M:578:HOH:O	2.22	0.41
1:N:489:ILE:HD12	1:N:494:LEU:HD22	2.00	0.41
1:N:502:SER:O	1:N:503:ALA:C	2.59	0.41
1:F:218:PRO:HB3	1:F:246:PRO:HG2	2.03	0.41
1:F:305:ILE:HG22	1:F:305:ILE:O	2.20	0.41
1:H:69:MET:O	1:H:73:MET:HG3	2.20	0.41
1:M:179:ASP:OD1	1:M:393:LYS:HE3	2.20	0.41
1:M:263:VAL:O	1:M:267:MET:HB2	2.20	0.41
1:M:23:LEU:CD2	1:M:74:VAL:HG13	2.49	0.41
1:N:224:ASP:HB3	1:N:302:SER:HB3	2.02	0.41
1:A:319:GLN:HB3	1:A:336:VAL:HG21	2.02	0.41
1:B:27:VAL:HG12	1:B:90:THR:HG23	2.02	0.41
1:C:118:ARG:HE	1:C:118:ARG:HB2	1.79	0.41
1:C:193:MET:CE	1:C:292:ILE:HG12	2.51	0.41
1:D:16:MET:O	1:D:20:VAL:HG13	2.21	0.41
1:A:351:GLN:HB3	1:A:351:GLN:HE21	1.65	0.41
1:N:219:PHE:HB3	1:N:317:LEU:HD23	2.02	0.41
1:B:219:PHE:HB3	1:B:317:LEU:HD23	2.02	0.41
1:D:419:LEU:HD23	1:D:419:LEU:HA	1.82	0.41
1:E:417:VAL:HG11	1:E:477:GLY:HA3	2.01	0.41
1:H:281:PHE:CD2	1:N:389:MET:HE3	2.54	0.41
4:I:1:AGS:O3B	4:I:1:AGS:S1G	2.59	0.41
1:J:269:GLY:HA3	1:K:257:GLU:HG3	2.03	0.41
1:M:221:LEU:HD23	1:M:249:ILE:HD12	2.02	0.41
1:M:360:TYR:CZ	1:M:364:LYS:HE3	2.55	0.41
1:A:266:THR:HG22	1:A:271:VAL:O	2.20	0.41
1:A:366:GLN:O	1:A:369:VAL:HG22	2.20	0.41
1:C:524:LEU:O	1:C:526:LYS:N	2.53	0.41
1:J:90:THR:OG1	4:J:1:AGS:S1G	2.68	0.41
1:M:205:ILE:HA	1:M:213:VAL:HG22	2.03	0.41
1:N:366:GLN:O	1:N:369:VAL:HG22	2.21	0.41
1:B:37:ASN:ND2	5:B:628:HOH:O	2.47	0.41
1:G:266:THR:HG21	1:G:273:VAL:H	1.86	0.41
1:K:219:PHE:O	1:K:247:LEU:HD12	2.20	0.41
1:L:236:VAL:O	1:L:240:VAL:HG23	2.21	0.41
1:L:419:LEU:HD23	1:L:419:LEU:HA	1.96	0.41
1:M:305:ILE:O	1:M:305:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:345:ARG:HA	1:M:348:GLN:NE2	2.32	0.41
1:N:419:LEU:HD23	1:N:419:LEU:HA	1.91	0.41
1:A:158:VAL:HG13	1:A:396:VAL:HG22	2.02	0.41
1:B:426:LEU:HA	1:B:426:LEU:HD23	1.82	0.41
1:C:158:VAL:HG13	1:C:396:VAL:HG22	2.03	0.41
1:C:260:ALA:O	1:C:264:VAL:HG23	2.20	0.41
1:C:90:THR:O	1:C:94:VAL:HG13	2.21	0.41
1:D:39:VAL:HG23	1:E:517:THR:CG2	2.51	0.41
1:G:319:GLN:HB3	1:G:336:VAL:CG2	2.50	0.41
1:I:235:PRO:CG	1:I:310:GLU:HA	2.51	0.41
4:J:1:AGS:S1G	4:J:1:AGS:O3G	2.57	0.41
1:J:73:MET:O	1:J:76:GLU:HB2	2.20	0.41
1:J:78:ALA:HB1	1:J:89:THR:HB	2.03	0.41
1:K:177:VAL:CG2	1:K:397:GLU:HG3	2.44	0.41
1:M:57:ALA:O	1:M:75:LYS:HE2	2.21	0.41
1:N:112:ASN:HA	1:N:113:PRO:HD3	1.96	0.41
1:N:221:LEU:HD23	1:N:249:ILE:HD12	2.02	0.41
1:C:224:ASP:HB3	1:C:302:SER:HB3	2.03	0.41
1:C:345:ARG:HA	1:C:348:GLN:NE2	2.31	0.41
1:D:18:ARG:NH2	5:D:587:HOH:O	2.51	0.41
1:A:69:MET:CE	1:G:39:VAL:HG12	2.50	0.41
1:I:16:MET:O	1:I:20:VAL:HG13	2.21	0.41
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.33	0.41
1:E:16:MET:O	1:E:20:VAL:HG13	2.21	0.41
1:E:39:VAL:HG12	1:F:69:MET:CE	2.51	0.41
1:G:78:ALA:HB1	1:G:89:THR:HB	2.03	0.41
1:I:191:GLU:O	1:I:334:ASP:HA	2.21	0.41
1:I:263:VAL:O	1:I:267:MET:HB2	2.21	0.41
1:K:348:GLN:O	1:K:352:GLN:HG2	2.20	0.41
1:L:364:LYS:HA	1:L:364:LYS:HD3	1.73	0.41
1:C:176:THR:HG21	1:C:322:ARG:HH12	1.86	0.41
1:C:366:GLN:O	1:C:369:VAL:HG22	2.21	0.41
1:D:124:VAL:HG21	1:D:508:ALA:HB2	2.03	0.41
1:D:302:SER:H	1:D:307:MET:CE	2.34	0.41
1:D:319:GLN:HB3	1:D:336:VAL:HG21	2.02	0.41
1:D:386:GLU:O	1:D:390:LYS:HG2	2.20	0.41
1:D:463:SER:HB2	5:D:644:HOH:O	2.20	0.41
1:F:34:LYS:HG3	1:F:458:CYS:SG	2.61	0.41
1:H:321:LYS:HB2	1:H:334:ASP:HB3	2.02	0.41
1:K:16:MET:O	1:K:20:VAL:HG13	2.21	0.41
1:K:325:ILE:HG22	1:K:330:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:197:ARG:HD2	1:N:277:LYS:HB2	2.03	0.41
1:A:348:GLN:O	1:A:352:GLN:HG2	2.22	0.40
1:B:236:VAL:O	1:B:240:VAL:HG23	2.21	0.40
1:C:193:MET:HE1	1:C:292:ILE:HG12	2.01	0.40
1:D:266:THR:HG22	1:D:271:VAL:O	2.21	0.40
1:F:496:PRO:HB2	1:F:499:VAL:HG13	2.03	0.40
1:K:188:ASP:N	1:K:188:ASP:OD1	2.54	0.40
1:K:191:GLU:O	1:K:334:ASP:HA	2.22	0.40
1:M:364:LYS:HA	1:M:364:LYS:HD3	1.86	0.40
1:E:360:TYR:CE1	1:E:364:LYS:HE3	2.56	0.40
1:F:178:GLU:HG2	1:F:322:ARG:NH1	2.36	0.40
1:A:231:ARG:NH1	1:G:242:LYS:CG	2.83	0.40
1:G:66:PHE:CZ	1:G:522:THR:HG22	2.57	0.40
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.61	0.40
1:M:16:MET:O	1:M:20:VAL:HG13	2.21	0.40
1:N:466:ALA:O	1:N:470:LYS:HG3	2.21	0.40
1:A:284:ARG:HH11	1:A:364:LYS:HD2	1.87	0.40
1:J:57:ALA:O	1:J:75:LYS:HE3	2.20	0.40
1:M:124:VAL:HG21	1:M:508:ALA:CB	2.51	0.40
1:N:325:ILE:HG22	1:N:330:THR:HG23	2.02	0.40
1:C:360:TYR:CE1	1:C:364:LYS:HE3	2.56	0.40
1:H:404:ARG:CG	1:H:404:ARG:NH1	2.83	0.40
1:I:63:GLU:HB2	1:J:524:LEU:HD21	2.04	0.40
1:K:419:LEU:HD23	1:K:419:LEU:HA	1.94	0.40
1:L:348:GLN:O	1:L:352:GLN:HG2	2.21	0.40
1:M:176:THR:HG22	1:M:177:VAL:N	2.36	0.40
1:M:57:ALA:O	1:M:75:LYS:HE3	2.20	0.40
1:A:404:ARG:CG	1:A:404:ARG:NH1	2.84	0.40
1:B:360:TYR:CE1	1:B:364:LYS:HE3	2.57	0.40
1:C:221:LEU:HD23	1:C:249:ILE:HD12	2.03	0.40
1:D:114:MET:CG	1:D:114:MET:CE	2.99	0.40
1:J:321:LYS:HB2	1:J:334:ASP:HB3	2.03	0.40
1:M:369:VAL:HG23	1:M:370:ALA:N	2.36	0.40
1:M:63:GLU:HB2	1:N:524:LEU:CD2	2.52	0.40
1:N:36:ARG:HD2	5:N:614:HOH:O	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:142:LYS:NZ	1:N:354:GLU:O[2_646]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:315:GLU:OE2	1:N:338:GLU:OE1[1_554]	2.05	0.15
1:A:311:LYS:NZ	1:N:311:LYS:O[1_554]	2.09	0.11
1:H:350:ARG:NH1	1:L:354:GLU:OE1[1_455]	2.11	0.09
1:G:315:GLU:OE1	1:N:338:GLU:OE2[1_554]	2.14	0.06

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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/525 (100%)	509 (97%)	12 (2%)	2 (0%)	38	33
1	B	523/525 (100%)	506 (97%)	15 (3%)	2 (0%)	38	33
1	C	523/525 (100%)	505 (97%)	16 (3%)	2 (0%)	38	33
1	D	523/525 (100%)	509 (97%)	13 (2%)	1 (0%)	51	48
1	E	523/525 (100%)	507 (97%)	14 (3%)	2 (0%)	38	33
1	F	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	38	33
1	G	523/525 (100%)	511 (98%)	10 (2%)	2 (0%)	38	33
1	H	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	38	33
1	I	523/525 (100%)	511 (98%)	10 (2%)	2 (0%)	38	33
1	J	523/525 (100%)	509 (97%)	12 (2%)	2 (0%)	38	33
1	K	523/525 (100%)	505 (97%)	15 (3%)	3 (1%)	28	21
1	L	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	38	33
1	M	523/525 (100%)	512 (98%)	9 (2%)	2 (0%)	38	33
1	N	523/525 (100%)	503 (96%)	18 (3%)	2 (0%)	38	33
All	All	7322/7350 (100%)	7111 (97%)	183 (2%)	28 (0%)	38	33

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	GLY
1	A	256	GLY
1	B	256	GLY
1	C	256	GLY
1	E	256	GLY
1	F	256	GLY
1	G	256	GLY
1	H	256	GLY
1	I	256	GLY
1	J	256	GLY
1	K	256	GLY
1	L	256	GLY
1	M	256	GLY
1	N	256	GLY
1	N	270	ILE
1	I	270	ILE
1	H	270	ILE
1	K	270	ILE
1	L	270	ILE
1	M	270	ILE
1	B	270	ILE
1	C	270	ILE
1	E	270	ILE
1	F	270	ILE
1	G	270	ILE
1	K	77	VAL
1	A	270	ILE
1	J	270	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	404/405 (100%)	383 (95%)	21 (5%)	27	22
1	B	404/405 (100%)	379 (94%)	25 (6%)	21	16
1	C	404/405 (100%)	381 (94%)	23 (6%)	24	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	404/405 (100%)	383 (95%)	21 (5%)	27	22
1	E	404/405 (100%)	382 (95%)	22 (5%)	26	20
1	F	404/405 (100%)	385 (95%)	19 (5%)	30	26
1	G	404/405 (100%)	381 (94%)	23 (6%)	24	18
1	H	404/405 (100%)	382 (95%)	22 (5%)	26	20
1	I	404/405 (100%)	387 (96%)	17 (4%)	34	30
1	J	404/405 (100%)	383 (95%)	21 (5%)	27	22
1	K	404/405 (100%)	384 (95%)	20 (5%)	28	23
1	L	404/405 (100%)	382 (95%)	22 (5%)	26	20
1	M	404/405 (100%)	384 (95%)	20 (5%)	28	23
1	N	404/405 (100%)	381 (94%)	23 (6%)	24	18
All	All	5656/5670 (100%)	5357 (95%)	299 (5%)	26	21

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	14	VAL
1	A	20	VAL
1	A	75	LYS
1	A	80	LYS
1	A	118	ARG
1	A	151	SER
1	A	160	LYS
1	A	230	ILE
1	A	284	ARG
1	A	289	LEU
1	A	325	ILE
1	A	328	ASP
1	A	331	THR
1	A	351	GLN
1	A	352	GLN
1	A	404	ARG
1	A	420	ILE
1	A	473	ASP
1	A	518	GLU
1	A	524	LEU
1	B	10	ASN

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Mol	Chain	Res	Type
1	B	20	VAL
1	B	75	LYS
1	B	80	LYS
1	B	94	VAL
1	B	151	SER
1	B	160	LYS
1	B	176	THR
1	B	230	ILE
1	B	284	ARG
1	B	289	LEU
1	B	325	ILE
1	B	328	ASP
1	B	329	THR
1	B	331	THR
1	B	351	GLN
1	B	352	GLN
1	B	358	SER
1	B	404	ARG
1	B	420	ILE
1	B	421	ARG
1	B	473	ASP
1	B	514	MET
1	B	518	GLU
1	B	524	LEU
1	C	10	ASN
1	C	14	VAL
1	C	20	VAL
1	C	75	LYS
1	C	94	VAL
1	C	151	SER
1	C	160	LYS
1	C	230	ILE
1	C	284	ARG
1	C	289	LEU
1	C	325	ILE
1	C	328	ASP
1	C	329	THR
1	C	331	THR
1	C	351	GLN
1	C	352	GLN
1	C	358	SER
1	C	404	ARG

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Mol	Chain	Res	Type
1	C	420	ILE
1	C	473	ASP
1	C	514	MET
1	C	518	GLU
1	C	524	LEU
1	D	10	ASN
1	D	20	VAL
1	D	75	LYS
1	D	80	LYS
1	D	94	VAL
1	D	135	SER
1	D	151	SER
1	D	160	LYS
1	D	230	ILE
1	D	284	ARG
1	D	289	LEU
1	D	325	ILE
1	D	329	THR
1	D	331	THR
1	D	352	GLN
1	D	358	SER
1	D	404	ARG
1	D	420	ILE
1	D	473	ASP
1	D	518	GLU
1	D	524	LEU
1	E	10	ASN
1	E	20	VAL
1	E	23	LEU
1	E	94	VAL
1	E	118	ARG
1	E	135	SER
1	E	151	SER
1	E	160	LYS
1	E	183	LEU
1	E	230	ILE
1	E	284	ARG
1	E	289	LEU
1	E	325	ILE
1	E	329	THR
1	E	331	THR
1	E	351	GLN

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Mol	Chain	Res	Type
1	E	352	GLN
1	E	404	ARG
1	E	420	ILE
1	E	473	ASP
1	E	518	GLU
1	E	524	LEU
1	F	10	ASN
1	F	20	VAL
1	F	80	LYS
1	F	94	VAL
1	F	151	SER
1	F	160	LYS
1	F	230	ILE
1	F	284	ARG
1	F	289	LEU
1	F	325	ILE
1	F	328	ASP
1	F	331	THR
1	F	351	GLN
1	F	352	GLN
1	F	404	ARG
1	F	420	ILE
1	F	473	ASP
1	F	518	GLU
1	F	524	LEU
1	G	10	ASN
1	G	20	VAL
1	G	75	LYS
1	G	80	LYS
1	G	118	ARG
1	G	140	ASP
1	G	151	SER
1	G	160	LYS
1	G	188	ASP
1	G	230	ILE
1	G	284	ARG
1	G	325	ILE
1	G	329	THR
1	G	331	THR
1	G	351	GLN
1	G	352	GLN
1	G	358	SER

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Mol	Chain	Res	Type
1	G	404	ARG
1	G	420	ILE
1	G	473	ASP
1	G	514	MET
1	G	518	GLU
1	G	524	LEU
1	H	10	ASN
1	H	14	VAL
1	H	20	VAL
1	H	75	LYS
1	H	80	LYS
1	H	118	ARG
1	H	151	SER
1	H	160	LYS
1	H	230	ILE
1	H	284	ARG
1	H	289	LEU
1	H	325	ILE
1	H	328	ASP
1	H	329	THR
1	H	331	THR
1	H	351	GLN
1	H	352	GLN
1	H	404	ARG
1	H	420	ILE
1	H	473	ASP
1	H	518	GLU
1	H	524	LEU
1	I	10	ASN
1	I	20	VAL
1	I	75	LYS
1	I	80	LYS
1	I	94	VAL
1	I	151	SER
1	I	160	LYS
1	I	230	ILE
1	I	284	ARG
1	I	289	LEU
1	I	325	ILE
1	I	331	THR
1	I	358	SER
1	I	404	ARG

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Mol	Chain	Res	Type
1	I	420	ILE
1	I	518	GLU
1	I	524	LEU
1	J	10	ASN
1	J	20	VAL
1	J	75	LYS
1	J	80	LYS
1	J	94	VAL
1	J	151	SER
1	J	160	LYS
1	J	230	ILE
1	J	284	ARG
1	J	289	LEU
1	J	325	ILE
1	J	329	THR
1	J	331	THR
1	J	351	GLN
1	J	352	GLN
1	J	358	SER
1	J	404	ARG
1	J	420	ILE
1	J	473	ASP
1	J	518	GLU
1	J	524	LEU
1	K	10	ASN
1	K	20	VAL
1	K	75	LYS
1	K	80	LYS
1	K	94	VAL
1	K	118	ARG
1	K	151	SER
1	K	160	LYS
1	K	230	ILE
1	K	284	ARG
1	K	289	LEU
1	K	325	ILE
1	K	331	THR
1	K	351	GLN
1	K	358	SER
1	K	404	ARG
1	K	420	ILE
1	K	473	ASP

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Mol	Chain	Res	Type
1	K	518	GLU
1	K	524	LEU
1	L	10	ASN
1	L	20	VAL
1	L	75	LYS
1	L	80	LYS
1	L	94	VAL
1	L	135	SER
1	L	151	SER
1	L	160	LYS
1	L	230	ILE
1	L	284	ARG
1	L	289	LEU
1	L	325	ILE
1	L	328	ASP
1	L	329	THR
1	L	331	THR
1	L	351	GLN
1	L	352	GLN
1	L	404	ARG
1	L	420	ILE
1	L	473	ASP
1	L	518	GLU
1	L	524	LEU
1	M	10	ASN
1	M	20	VAL
1	M	75	LYS
1	M	151	SER
1	M	160	LYS
1	M	230	ILE
1	M	284	ARG
1	M	289	LEU
1	M	325	ILE
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	351	GLN
1	M	352	GLN
1	M	358	SER
1	M	404	ARG
1	M	420	ILE
1	M	473	ASP

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Mol	Chain	Res	Type
1	M	518	GLU
1	M	524	LEU
1	N	10	ASN
1	N	14	VAL
1	N	20	VAL
1	N	75	LYS
1	N	80	LYS
1	N	94	VAL
1	N	118	ARG
1	N	151	SER
1	N	160	LYS
1	N	183	LEU
1	N	230	ILE
1	N	284	ARG
1	N	289	LEU
1	N	325	ILE
1	N	328	ASP
1	N	331	THR
1	N	351	GLN
1	N	352	GLN
1	N	358	SER
1	N	404	ARG
1	N	420	ILE
1	N	518	GLU
1	N	524	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	146	GLN
1	A	229	ASN
1	A	265	ASN
1	A	326	ASN
1	A	348	GLN
1	A	351	GLN
1	A	366	GLN
1	A	453	GLN
1	A	475	ASN
1	B	37	ASN
1	B	146	GLN
1	B	265	ASN

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Mol	Chain	Res	Type
1	B	326	ASN
1	B	348	GLN
1	B	351	GLN
1	B	366	GLN
1	B	401	HIS
1	B	453	GLN
1	B	475	ASN
1	C	37	ASN
1	C	146	GLN
1	C	265	ASN
1	C	326	ASN
1	C	348	GLN
1	C	351	GLN
1	C	366	GLN
1	C	401	HIS
1	C	453	GLN
1	C	475	ASN
1	D	37	ASN
1	D	146	GLN
1	D	265	ASN
1	D	326	ASN
1	D	348	GLN
1	D	351	GLN
1	D	366	GLN
1	D	453	GLN
1	E	37	ASN
1	E	146	GLN
1	E	265	ASN
1	E	326	ASN
1	E	348	GLN
1	E	351	GLN
1	E	366	GLN
1	E	475	ASN
1	F	37	ASN
1	F	146	GLN
1	F	265	ASN
1	F	326	ASN
1	F	348	GLN
1	F	351	GLN
1	F	366	GLN
1	F	401	HIS
1	F	453	GLN

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Mol	Chain	Res	Type
1	F	475	ASN
1	G	37	ASN
1	G	146	GLN
1	G	265	ASN
1	G	326	ASN
1	G	348	GLN
1	G	351	GLN
1	G	366	GLN
1	G	453	GLN
1	G	475	ASN
1	H	37	ASN
1	H	146	GLN
1	H	265	ASN
1	H	326	ASN
1	H	348	GLN
1	H	351	GLN
1	H	366	GLN
1	H	401	HIS
1	H	453	GLN
1	H	475	ASN
1	I	37	ASN
1	I	146	GLN
1	I	265	ASN
1	I	326	ASN
1	I	348	GLN
1	I	351	GLN
1	I	366	GLN
1	I	401	HIS
1	I	453	GLN
1	I	475	ASN
1	J	37	ASN
1	J	146	GLN
1	J	265	ASN
1	J	326	ASN
1	J	348	GLN
1	J	351	GLN
1	J	366	GLN
1	J	453	GLN
1	J	475	ASN
1	K	37	ASN
1	K	146	GLN
1	K	265	ASN

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Mol	Chain	Res	Type
1	K	326	ASN
1	K	348	GLN
1	K	351	GLN
1	K	366	GLN
1	K	453	GLN
1	K	475	ASN
1	L	10	ASN
1	L	37	ASN
1	L	146	GLN
1	L	229	ASN
1	L	265	ASN
1	L	326	ASN
1	L	348	GLN
1	L	351	GLN
1	L	401	HIS
1	L	453	GLN
1	M	37	ASN
1	M	146	GLN
1	M	265	ASN
1	M	326	ASN
1	M	348	GLN
1	M	351	GLN
1	M	366	GLN
1	M	453	GLN
1	M	475	ASN
1	N	37	ASN
1	N	146	GLN
1	N	265	ASN
1	N	326	ASN
1	N	348	GLN
1	N	351	GLN
1	N	366	GLN
1	N	401	HIS
1	N	453	GLN
1	N	475	ASN

5.3.3 RNA ⓘ

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 44 ligands modelled in this entry, 30 are monoatomic - leaving 14 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$
4	AGS	A	1	3,2	26,33,33	4.02	4 (15%)	22,52,52	3.35	8 (36%)
4	AGS	B	1	3,2	26,33,33	4.17	5 (19%)	22,52,52	2.61	5 (22%)
4	AGS	C	1	3,2	26,33,33	4.23	4 (15%)	22,52,52	3.41	3 (13%)
4	AGS	D	561	3,2	26,33,33	4.65	7 (26%)	22,52,52	2.05	7 (31%)
4	AGS	E	1	3,2	26,33,33	4.75	5 (19%)	22,52,52	2.65	8 (36%)
4	AGS	F	1	3,2	26,33,33	4.27	4 (15%)	22,52,52	2.12	6 (27%)
4	AGS	G	1	3,2	26,33,33	4.88	5 (19%)	22,52,52	2.63	10 (45%)
4	AGS	H	1	3,2	26,33,33	4.31	5 (19%)	22,52,52	2.57	6 (27%)
4	AGS	I	1	3,2	26,33,33	4.39	5 (19%)	22,52,52	2.25	4 (18%)
4	AGS	J	1	3,2	26,33,33	4.09	3 (11%)	22,52,52	2.26	4 (18%)
4	AGS	K	1	3,2	26,33,33	4.32	6 (23%)	22,52,52	2.12	3 (13%)
4	AGS	L	1	3,2	26,33,33	4.41	6 (23%)	22,52,52	3.65	5 (22%)
4	AGS	M	1	3,2	26,33,33	4.27	5 (19%)	22,52,52	3.74	3 (13%)
4	AGS	N	1	3,2	26,33,33	4.72	5 (19%)	22,52,52	3.14	9 (40%)

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
4	AGS	A	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	B	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	C	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	D	561	3,2	-	0/17/38/38	0/3/3/3
4	AGS	E	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	F	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	G	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	H	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	I	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	J	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	K	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	L	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	M	1	3,2	-	0/17/38/38	0/3/3/3
4	AGS	N	1	3,2	-	0/17/38/38	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	AGS	PG-S1G	-23.56	1.45	1.90
4	E	1	AGS	PG-S1G	-22.84	1.47	1.90
4	N	1	AGS	PG-S1G	-22.82	1.47	1.90
4	D	561	AGS	PG-S1G	-21.90	1.48	1.90
4	L	1	AGS	PG-S1G	-21.45	1.49	1.90
4	I	1	AGS	PG-S1G	-21.03	1.50	1.90
4	F	1	AGS	PG-S1G	-20.77	1.51	1.90
4	C	1	AGS	PG-S1G	-20.75	1.51	1.90
4	H	1	AGS	PG-S1G	-20.73	1.51	1.90
4	K	1	AGS	PG-S1G	-20.66	1.51	1.90
4	M	1	AGS	PG-S1G	-20.60	1.51	1.90
4	B	1	AGS	PG-S1G	-20.18	1.52	1.90
4	J	1	AGS	PG-S1G	-20.07	1.52	1.90
4	A	1	AGS	PG-S1G	-19.45	1.53	1.90
4	N	1	AGS	O4'-C1'	-4.32	1.35	1.41
4	E	1	AGS	PA-O1A	-3.86	1.36	1.50
4	M	1	AGS	C2'-C1'	-3.68	1.47	1.53
4	F	1	AGS	O3'-C3'	-3.42	1.35	1.43
4	F	1	AGS	PA-O1A	-3.31	1.38	1.50
4	G	1	AGS	PA-O1A	-2.93	1.39	1.50
4	I	1	AGS	C2'-C1'	-2.85	1.49	1.53
4	K	1	AGS	PB-O1B	-2.85	1.40	1.50
4	L	1	AGS	PA-O1A	-2.78	1.40	1.50
4	I	1	AGS	O4'-C4'	-2.76	1.38	1.45
4	A	1	AGS	O4'-C1'	-2.71	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	AGS	O3'-C3'	-2.54	1.37	1.43
4	N	1	AGS	PA-O1A	-2.54	1.41	1.50
4	B	1	AGS	O4'-C1'	-2.52	1.37	1.41
4	H	1	AGS	O2'-C2'	-2.50	1.37	1.43
4	L	1	AGS	C2'-C1'	-2.50	1.49	1.53
4	B	1	AGS	PA-O1A	-2.42	1.41	1.50
4	M	1	AGS	O2'-C2'	-2.33	1.37	1.43
4	E	1	AGS	PB-O1B	-2.30	1.42	1.50
4	H	1	AGS	O4'-C1'	-2.27	1.38	1.41
4	D	561	AGS	PA-O1A	-2.22	1.42	1.50
4	J	1	AGS	O4'-C4'	-2.18	1.40	1.45
4	H	1	AGS	C4-N3	-2.16	1.32	1.35
4	K	1	AGS	O2'-C2'	-2.12	1.38	1.43
4	C	1	AGS	PA-O1A	-2.08	1.43	1.50
4	L	1	AGS	C5-C4	-2.07	1.35	1.40
4	D	561	AGS	O4'-C1'	-2.05	1.38	1.41
4	K	1	AGS	C2-N1	2.03	1.37	1.33
4	E	1	AGS	C5-N7	2.05	1.46	1.39
4	M	1	AGS	C8-N7	2.08	1.38	1.34
4	I	1	AGS	PA-O2A	2.09	1.65	1.55
4	L	1	AGS	C2-N3	2.14	1.35	1.32
4	A	1	AGS	C8-N7	2.25	1.38	1.34
4	N	1	AGS	C2-N1	2.26	1.38	1.33
4	C	1	AGS	C2-N1	2.35	1.38	1.33
4	F	1	AGS	C2-N3	2.36	1.36	1.32
4	B	1	AGS	C2'-C1'	2.45	1.57	1.53
4	D	561	AGS	PG-O2G	2.56	1.64	1.55
4	J	1	AGS	C2-N3	2.63	1.36	1.32
4	G	1	AGS	C2-N1	2.75	1.39	1.33
4	L	1	AGS	C2-N1	2.78	1.39	1.33
4	B	1	AGS	C2-N3	2.98	1.37	1.32
4	C	1	AGS	C2-N3	3.23	1.37	1.32
4	H	1	AGS	C2-N3	3.26	1.37	1.32
4	M	1	AGS	C2-N3	3.32	1.37	1.32
4	D	561	AGS	C2-N1	3.46	1.40	1.33
4	I	1	AGS	C2-N3	3.63	1.38	1.32
4	K	1	AGS	C2-N3	3.70	1.38	1.32
4	K	1	AGS	O4'-C1'	3.83	1.46	1.41
4	A	1	AGS	C2-N3	3.97	1.38	1.32
4	N	1	AGS	C2-N3	4.01	1.38	1.32
4	G	1	AGS	C2-N3	4.52	1.39	1.32
4	D	561	AGS	C2-N3	4.62	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1	AGS	C2-N3	4.69	1.40	1.32
4	D	561	AGS	C4-N3	4.85	1.42	1.35

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1	AGS	N3-C2-N1	-16.13	114.81	128.86
4	L	1	AGS	N3-C2-N1	-15.18	115.64	128.86
4	C	1	AGS	N3-C2-N1	-15.03	115.77	128.86
4	A	1	AGS	N3-C2-N1	-13.01	117.53	128.86
4	N	1	AGS	N3-C2-N1	-10.45	119.75	128.86
4	E	1	AGS	N3-C2-N1	-9.68	120.43	128.86
4	B	1	AGS	N3-C2-N1	-9.64	120.46	128.86
4	G	1	AGS	N3-C2-N1	-8.90	121.11	128.86
4	J	1	AGS	N3-C2-N1	-8.56	121.40	128.86
4	H	1	AGS	N3-C2-N1	-8.43	121.51	128.86
4	I	1	AGS	N3-C2-N1	-8.14	121.77	128.86
4	K	1	AGS	N3-C2-N1	-7.92	121.96	128.86
4	F	1	AGS	N3-C2-N1	-7.07	122.70	128.86
4	D	561	AGS	N3-C2-N1	-6.30	123.37	128.86
4	A	1	AGS	O3'-C3'-C4'	-4.75	97.21	111.09
4	H	1	AGS	O5'-PA-O1A	-4.73	90.15	109.25
4	N	1	AGS	O5'-PA-O1A	-4.72	90.20	109.25
4	N	1	AGS	C4-C5-N7	-4.46	105.10	109.41
4	G	1	AGS	C1'-N9-C4	-4.46	118.93	126.64
4	N	1	AGS	C1'-N9-C4	-4.43	118.98	126.64
4	L	1	AGS	C1'-N9-C4	-4.41	119.02	126.64
4	I	1	AGS	C1'-N9-C4	-3.91	119.88	126.64
4	B	1	AGS	C4'-O4'-C1'	-3.88	105.63	109.77
4	M	1	AGS	C1'-N9-C4	-3.76	120.14	126.64
4	J	1	AGS	C4-C5-N7	-3.72	105.82	109.41
4	K	1	AGS	PB-O3B-PG	-3.70	120.39	132.35
4	F	1	AGS	C5'-C4'-C3'	-3.65	101.38	115.29
4	B	1	AGS	C1'-N9-C4	-3.46	120.65	126.64
4	E	1	AGS	C1'-N9-C4	-3.44	120.69	126.64
4	H	1	AGS	PB-O3B-PG	-3.37	121.47	132.35
4	A	1	AGS	C1'-N9-C4	-3.33	120.88	126.64
4	N	1	AGS	C5'-C4'-C3'	-3.31	102.68	115.29
4	N	1	AGS	PB-O3B-PG	-3.23	121.90	132.35
4	L	1	AGS	O3'-C3'-C4'	-3.20	101.75	111.09
4	D	561	AGS	O5'-PA-O1A	-3.18	96.44	109.25
4	E	1	AGS	C5'-C4'-C3'	-3.02	103.79	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	AGS	C1'-N9-C4	-3.00	121.46	126.64
4	H	1	AGS	C4'-O4'-C1'	-2.89	106.69	109.77
4	G	1	AGS	C4'-O4'-C1'	-2.89	106.69	109.77
4	M	1	AGS	N6-C6-N1	-2.87	113.08	118.77
4	D	561	AGS	C5'-C4'-C3'	-2.76	104.75	115.29
4	I	1	AGS	PB-O3B-PG	-2.70	123.63	132.35
4	G	1	AGS	PB-O3B-PG	-2.65	123.77	132.35
4	I	1	AGS	C5'-C4'-C3'	-2.64	105.22	115.29
4	D	561	AGS	C1'-N9-C4	-2.63	122.09	126.64
4	E	1	AGS	PB-O3B-PG	-2.62	123.90	132.35
4	L	1	AGS	C5'-C4'-C3'	-2.61	105.34	115.29
4	C	1	AGS	C5'-C4'-C3'	-2.60	105.39	115.29
4	B	1	AGS	C5'-C4'-C3'	-2.57	105.49	115.29
4	F	1	AGS	C1'-N9-C4	-2.45	122.41	126.64
4	A	1	AGS	O5'-PA-O1A	-2.34	99.82	109.25
4	F	1	AGS	C4-C5-N7	-2.34	107.15	109.41
4	E	1	AGS	O4'-C4'-C3'	-2.32	100.55	105.17
4	N	1	AGS	C4'-O4'-C1'	-2.28	107.34	109.77
4	J	1	AGS	N6-C6-N1	-2.27	114.26	118.77
4	F	1	AGS	C4'-O4'-C1'	-2.27	107.35	109.77
4	F	1	AGS	O3'-C3'-C4'	-2.21	104.64	111.09
4	G	1	AGS	C4-C5-N7	-2.20	107.29	109.41
4	D	561	AGS	O3'-C3'-C4'	-2.20	104.67	111.09
4	L	1	AGS	C4'-O4'-C1'	-2.19	107.44	109.77
4	G	1	AGS	O3'-C3'-C4'	-2.12	104.89	111.09
4	A	1	AGS	N6-C6-N1	-2.11	114.58	118.77
4	E	1	AGS	C4'-O4'-C1'	-2.08	107.55	109.77
4	G	1	AGS	N6-C6-N1	-2.08	114.64	118.77
4	A	1	AGS	PB-O3B-PG	-2.07	125.67	132.35
4	D	561	AGS	PB-O3B-PG	-2.06	125.70	132.35
4	H	1	AGS	O3'-C3'-C4'	-2.05	105.09	111.09
4	G	1	AGS	C5'-C4'-C3'	-2.02	107.58	115.29
4	N	1	AGS	O5'-C5'-C4'	2.02	116.17	109.00
4	A	1	AGS	C5-C6-N6	2.04	124.63	120.47
4	A	1	AGS	O2A-PA-O5'	2.07	117.93	108.14
4	B	1	AGS	O4'-C4'-C3'	2.09	109.32	105.17
4	G	1	AGS	C5-C6-N6	2.10	124.75	120.47
4	G	1	AGS	O2A-PA-O5'	2.11	118.10	108.14
4	E	1	AGS	C2'-C3'-C4'	2.14	106.79	102.62
4	J	1	AGS	C5-C6-N6	2.15	124.85	120.47
4	K	1	AGS	O2A-PA-O5'	2.33	119.12	108.14
4	N	1	AGS	O2A-PA-O1A	2.39	124.67	112.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	561	AGS	O2B-PB-O1B	2.57	125.59	112.28
4	C	1	AGS	C2-N1-C6	2.62	123.36	118.77
4	E	1	AGS	O2A-PA-O5'	3.00	122.31	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	AGS	3	0
4	B	1	AGS	4	0
4	C	1	AGS	2	0
4	D	561	AGS	4	0
4	E	1	AGS	3	0
4	F	1	AGS	3	0
4	G	1	AGS	4	0
4	H	1	AGS	4	0
4	I	1	AGS	4	0
4	J	1	AGS	5	0
4	K	1	AGS	2	0
4	L	1	AGS	3	0
4	M	1	AGS	3	0
4	N	1	AGS	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	525/525 (100%)	1.39	124 (23%) 1 1	10, 14, 16, 20	0
1	B	525/525 (100%)	2.10	232 (44%) 0 1	10, 14, 16, 20	0
1	C	525/525 (100%)	1.80	196 (37%) 0 1	10, 14, 16, 20	0
1	D	525/525 (100%)	1.27	109 (20%) 1 1	10, 14, 16, 20	0
1	E	525/525 (100%)	1.82	198 (37%) 0 1	9, 14, 16, 20	0
1	F	525/525 (100%)	2.05	204 (38%) 0 1	10, 14, 16, 20	0
1	G	525/525 (100%)	1.37	135 (25%) 1 1	10, 14, 16, 20	0
1	H	525/525 (100%)	1.39	146 (27%) 1 1	9, 14, 16, 20	0
1	I	525/525 (100%)	1.52	139 (26%) 1 1	9, 14, 16, 20	0
1	J	525/525 (100%)	1.61	152 (28%) 1 1	10, 14, 16, 20	0
1	K	525/525 (100%)	1.99	203 (38%) 0 1	10, 14, 16, 20	0
1	L	525/525 (100%)	1.58	152 (28%) 1 1	10, 14, 16, 20	0
1	M	525/525 (100%)	1.92	180 (34%) 0 1	10, 14, 16, 20	0
1	N	525/525 (100%)	1.39	135 (25%) 1 1	10, 14, 16, 20	0
All	All	7350/7350 (100%)	1.66	2305 (31%) 0 1	9, 14, 16, 20	0

All (2305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	269	GLY	11.1
1	F	240	VAL	10.0
1	K	305	ILE	10.0
1	E	234	LEU	9.8
1	M	270	ILE	9.8
1	M	309	LEU	9.5
1	L	234	LEU	9.3
1	J	271	VAL	9.2

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Mol	Chain	Res	Type	RSRZ
1	M	267	MET	9.1
1	I	305	ILE	9.0
1	C	244	GLY	9.0
1	K	236	VAL	8.9
1	E	353	ILE	8.9
1	K	264	VAL	8.9
1	F	309	LEU	8.8
1	F	353	ILE	8.6
1	F	227	ILE	8.6
1	B	349	ILE	8.6
1	B	353	ILE	8.6
1	F	236	VAL	8.6
1	F	256	GLY	8.5
1	F	349	ILE	8.4
1	F	314	LEU	8.4
1	B	281	PHE	8.4
1	M	353	ILE	8.3
1	M	237	LEU	8.3
1	K	271	VAL	8.3
1	K	356	ALA	8.2
1	K	335	GLY	8.1
1	C	353	ILE	8.1
1	B	230	ILE	8.1
1	K	270	ILE	8.1
1	F	263	VAL	8.0
1	E	349	ILE	7.9
1	F	219	PHE	7.9
1	K	260	ALA	7.8
1	K	267	MET	7.8
1	B	233	MET	7.8
1	K	349	ILE	7.7
1	J	44	PHE	7.7
1	M	264	VAL	7.6
1	B	227	ILE	7.5
1	J	264	VAL	7.5
1	F	222	LEU	7.5
1	L	270	ILE	7.5
1	J	237	LEU	7.4
1	F	270	ILE	7.4
1	K	353	ILE	7.4
1	K	228	SER	7.4
1	L	266	THR	7.3

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Mol	Chain	Res	Type	RSRZ
1	B	264	VAL	7.3
1	J	357	THR	7.3
1	E	356	ALA	7.3
1	J	305	ILE	7.3
1	M	301	ILE	7.2
1	B	357	THR	7.2
1	F	317	LEU	7.2
1	K	203	TYR	7.1
1	I	270	ILE	7.1
1	M	251	ALA	7.1
1	M	223	ALA	7.0
1	M	357	THR	7.0
1	E	271	VAL	7.0
1	F	234	LEU	7.0
1	C	360	TYR	7.0
1	B	258	ALA	6.9
1	F	312	ALA	6.9
1	I	271	VAL	6.9
1	F	237	LEU	6.9
1	C	270	ILE	6.9
1	M	340	ALA	6.8
1	M	203	TYR	6.8
1	F	357	THR	6.8
1	J	248	LEU	6.8
1	L	258	ALA	6.8
1	C	365	LEU	6.8
1	M	356	ALA	6.8
1	M	263	VAL	6.8
1	N	263	VAL	6.8
1	E	309	LEU	6.8
1	C	349	ILE	6.8
1	I	237	LEU	6.7
1	K	309	LEU	6.7
1	M	268	ARG	6.7
1	B	355	GLU	6.7
1	F	305	ILE	6.7
1	L	227	ILE	6.7
1	N	349	ILE	6.7
1	F	203	TYR	6.7
1	K	259	LEU	6.7
1	D	271	VAL	6.7
1	B	257	GLU	6.7

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Mol	Chain	Res	Type	RSRZ
1	L	305	ILE	6.6
1	K	230	ILE	6.6
1	J	356	ALA	6.6
1	L	264	VAL	6.6
1	A	263	VAL	6.6
1	B	301	ILE	6.6
1	J	269	GLY	6.6
1	E	268	ARG	6.6
1	B	240	VAL	6.5
1	M	358	SER	6.5
1	C	356	ALA	6.5
1	I	301	ILE	6.5
1	M	317	LEU	6.5
1	A	353	ILE	6.5
1	F	356	ALA	6.4
1	F	360	TYR	6.4
1	B	242	LYS	6.4
1	B	286	LYS	6.4
1	J	270	ILE	6.4
1	M	305	ILE	6.4
1	M	271	VAL	6.4
1	E	233	MET	6.4
1	J	267	MET	6.4
1	I	356	ALA	6.4
1	C	215	LEU	6.3
1	J	353	ILE	6.3
1	K	188	ASP	6.3
1	F	271	VAL	6.3
1	L	230	ILE	6.3
1	N	281	PHE	6.3
1	H	233	MET	6.2
1	B	203	TYR	6.2
1	E	223	ALA	6.2
1	I	240	VAL	6.2
1	L	309	LEU	6.2
1	B	215	LEU	6.2
1	M	262	LEU	6.2
1	M	230	ILE	6.2
1	K	237	LEU	6.2
1	C	249	ILE	6.1
1	B	234	LEU	6.1
1	M	266	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	M	336	VAL	6.1
1	J	349	ILE	6.1
1	L	307	MET	6.1
1	K	360	TYR	6.1
1	B	44	PHE	6.1
1	I	211	GLY	6.1
1	E	231	ARG	6.1
1	F	259	LEU	6.0
1	F	260	ALA	6.0
1	C	259	LEU	6.0
1	F	264	VAL	6.0
1	H	263	VAL	6.0
1	J	230	ILE	6.0
1	B	309	LEU	6.0
1	K	215	LEU	6.0
1	K	358	SER	6.0
1	E	270	ILE	6.0
1	F	230	ILE	6.0
1	M	306	GLY	5.9
1	M	204	PHE	5.9
1	F	233	MET	5.9
1	M	233	MET	5.9
1	B	260	ALA	5.9
1	M	221	LEU	5.9
1	M	236	VAL	5.9
1	K	231	ARG	5.9
1	H	353	ILE	5.9
1	C	292	ILE	5.9
1	I	268	ARG	5.9
1	M	240	VAL	5.8
1	N	280	GLY	5.8
1	N	230	ILE	5.8
1	L	231	ARG	5.8
1	J	342	ILE	5.8
1	F	268	ARG	5.8
1	J	351	GLN	5.8
1	H	309	LEU	5.8
1	M	314	LEU	5.8
1	J	233	MET	5.7
1	F	244	GLY	5.7
1	K	227	ILE	5.7
1	K	265	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
1	K	223	ALA	5.6
1	E	305	ILE	5.6
1	C	268	ARG	5.6
1	J	266	THR	5.6
1	M	234	LEU	5.6
1	F	204	PHE	5.6
1	E	357	THR	5.6
1	A	187	LEU	5.6
1	K	234	LEU	5.6
1	K	266	THR	5.6
1	C	234	LEU	5.6
1	K	204	PHE	5.6
1	B	265	ASN	5.5
1	B	365	LEU	5.5
1	M	235	PRO	5.5
1	G	269	GLY	5.5
1	E	266	THR	5.5
1	K	299	THR	5.5
1	I	265	ASN	5.5
1	M	265	ASN	5.5
1	C	340	ALA	5.5
1	L	317	LEU	5.5
1	M	300	VAL	5.4
1	J	317	LEU	5.4
1	B	268	ARG	5.4
1	I	264	VAL	5.4
1	M	186	GLU	5.4
1	J	268	ARG	5.4
1	B	266	THR	5.4
1	J	309	LEU	5.3
1	E	272	LYS	5.3
1	K	325	ILE	5.3
1	F	215	LEU	5.3
1	B	223	ALA	5.3
1	C	212	ALA	5.3
1	M	222	LEU	5.3
1	F	269	GLY	5.3
1	A	356	ALA	5.3
1	L	233	MET	5.3
1	E	256	GLY	5.3
1	E	230	ILE	5.3
1	K	302	SER	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	181	THR	5.3
1	B	314	LEU	5.3
1	B	77	VAL	5.2
1	B	262	LEU	5.2
1	M	180	GLY	5.2
1	N	305	ILE	5.2
1	A	44	PHE	5.2
1	K	181	THR	5.2
1	C	230	ILE	5.2
1	I	353	ILE	5.2
1	K	219	PHE	5.2
1	I	234	LEU	5.2
1	G	230	ILE	5.2
1	K	268	ARG	5.2
1	J	256	GLY	5.2
1	M	259	LEU	5.2
1	D	264	VAL	5.2
1	M	238	GLU	5.2
1	F	225	LYS	5.1
1	H	242	LYS	5.1
1	K	160	LYS	5.1
1	N	231	ARG	5.1
1	E	456	LEU	5.1
1	M	376	VAL	5.1
1	J	229	ASN	5.1
1	B	248	LEU	5.1
1	M	365	LEU	5.1
1	I	230	ILE	5.1
1	L	259	LEU	5.1
1	B	236	VAL	5.1
1	D	268	ARG	5.1
1	C	242	LYS	5.1
1	F	44	PHE	5.1
1	L	267	MET	5.1
1	K	44	PHE	5.0
1	L	356	ALA	5.0
1	J	234	LEU	5.0
1	C	44	PHE	5.0
1	C	204	PHE	5.0
1	J	387	VAL	5.0
1	J	231	ARG	5.0
1	E	351	GLN	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	44	PHE	5.0
1	C	233	MET	5.0
1	A	270	ILE	5.0
1	E	301	ILE	5.0
1	H	234	LEU	5.0
1	I	351	GLN	5.0
1	N	256	GLY	5.0
1	F	346	VAL	5.0
1	M	273	VAL	5.0
1	L	268	ARG	5.0
1	C	203	TYR	5.0
1	C	369	VAL	4.9
1	G	263	VAL	4.9
1	M	244	GLY	4.9
1	M	219	PHE	4.9
1	B	304	GLU	4.9
1	B	231	ARG	4.9
1	H	259	LEU	4.9
1	B	251	ALA	4.9
1	G	229	ASN	4.9
1	M	320	ALA	4.9
1	H	268	ARG	4.9
1	F	358	SER	4.9
1	F	249	ILE	4.9
1	B	270	ILE	4.8
1	K	233	MET	4.8
1	L	237	LEU	4.8
1	L	203	TYR	4.8
1	F	250	ILE	4.8
1	B	273	VAL	4.8
1	F	336	VAL	4.8
1	I	44	PHE	4.8
1	E	263	VAL	4.8
1	L	336	VAL	4.8
1	M	350	ARG	4.8
1	M	248	LEU	4.7
1	E	360	TYR	4.7
1	J	262	LEU	4.7
1	K	232	GLU	4.7
1	C	264	VAL	4.7
1	K	275	ALA	4.7
1	H	265	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	204	PHE	4.7
1	K	276	VAL	4.7
1	J	301	ILE	4.7
1	B	307	MET	4.7
1	M	307	MET	4.7
1	C	256	GLY	4.7
1	C	263	VAL	4.7
1	K	369	VAL	4.7
1	B	272	LYS	4.7
1	G	267	MET	4.7
1	K	340	ALA	4.7
1	K	350	ARG	4.7
1	K	272	LYS	4.7
1	I	233	MET	4.7
1	C	362	ARG	4.6
1	I	263	VAL	4.6
1	C	301	ILE	4.6
1	D	301	ILE	4.6
1	F	221	LEU	4.6
1	K	262	LEU	4.6
1	M	269	GLY	4.6
1	C	261	THR	4.6
1	M	333	ILE	4.6
1	F	365	LEU	4.6
1	J	219	PHE	4.6
1	L	244	GLY	4.6
1	M	310	GLU	4.6
1	I	266	THR	4.6
1	F	228	SER	4.6
1	J	526	LYS	4.6
1	F	238	GLU	4.5
1	J	333	ILE	4.5
1	B	229	ASN	4.5
1	I	363	GLU	4.5
1	F	241	ALA	4.5
1	J	358	SER	4.5
1	H	270	ILE	4.5
1	A	384	ALA	4.5
1	K	241	ALA	4.5
1	K	341	ALA	4.5
1	J	203	TYR	4.5
1	B	206	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	222	LEU	4.5
1	M	249	ILE	4.5
1	L	240	VAL	4.5
1	N	240	VAL	4.5
1	M	258	ALA	4.5
1	F	232	GLU	4.5
1	C	305	ILE	4.5
1	E	307	MET	4.5
1	B	354	GLU	4.5
1	D	305	ILE	4.5
1	A	357	THR	4.5
1	C	266	THR	4.5
1	L	271	VAL	4.5
1	C	223	ALA	4.5
1	M	44	PHE	4.5
1	M	202	PRO	4.4
1	A	273	VAL	4.4
1	C	273	VAL	4.4
1	C	274	ALA	4.4
1	F	258	ALA	4.4
1	L	306	GLY	4.4
1	K	365	LEU	4.4
1	E	258	ALA	4.4
1	L	262	LEU	4.4
1	C	271	VAL	4.4
1	J	257	GLU	4.4
1	M	218	PRO	4.4
1	F	251	ALA	4.4
1	M	242	LYS	4.4
1	C	333	ILE	4.4
1	H	264	VAL	4.4
1	A	306	GLY	4.4
1	M	335	GLY	4.4
1	I	267	MET	4.4
1	B	259	LEU	4.4
1	D	262	LEU	4.4
1	K	342	ILE	4.4
1	J	381	VAL	4.4
1	K	263	VAL	4.4
1	H	266	THR	4.4
1	K	357	THR	4.4
1	M	347	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	K	317	LEU	4.3
1	E	273	VAL	4.3
1	I	336	VAL	4.3
1	A	260	ALA	4.3
1	B	372	LEU	4.3
1	M	342	ILE	4.3
1	B	271	VAL	4.3
1	C	357	THR	4.3
1	B	297	GLY	4.3
1	H	297	GLY	4.3
1	B	134	LEU	4.3
1	F	267	MET	4.3
1	C	351	GLN	4.3
1	K	202	PRO	4.3
1	B	237	LEU	4.3
1	K	224	ASP	4.3
1	C	355	GLU	4.3
1	D	281	PHE	4.3
1	B	255	GLU	4.3
1	J	365	LEU	4.3
1	I	342	ILE	4.3
1	K	274	ALA	4.3
1	K	281	PHE	4.2
1	K	256	GLY	4.2
1	H	357	THR	4.2
1	A	349	ILE	4.2
1	C	336	VAL	4.2
1	E	354	GLU	4.2
1	F	186	GLU	4.2
1	F	255	GLU	4.2
1	I	360	TYR	4.2
1	G	268	ARG	4.2
1	G	270	ILE	4.2
1	K	312	ALA	4.2
1	E	215	LEU	4.2
1	E	358	SER	4.2
1	B	356	ALA	4.2
1	N	270	ILE	4.2
1	L	255	GLU	4.2
1	I	215	LEU	4.2
1	A	271	VAL	4.2
1	K	273	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	L	224	ASP	4.2
1	J	360	TYR	4.2
1	L	273	VAL	4.2
1	C	227	ILE	4.2
1	C	303	GLU	4.2
1	K	354	GLU	4.2
1	F	281	PHE	4.1
1	K	345	ARG	4.1
1	E	384	ALA	4.1
1	G	259	LEU	4.1
1	B	324	VAL	4.1
1	N	283	ASP	4.1
1	F	347	ALA	4.1
1	L	311	LYS	4.1
1	F	262	LEU	4.1
1	N	264	VAL	4.1
1	A	305	ILE	4.1
1	B	351	GLN	4.1
1	I	204	PHE	4.1
1	E	242	LYS	4.1
1	K	250	ILE	4.1
1	M	181	THR	4.1
1	I	310	GLU	4.1
1	M	231	ARG	4.1
1	E	236	VAL	4.1
1	B	204	PHE	4.1
1	H	44	PHE	4.1
1	F	372	LEU	4.1
1	B	211	GLY	4.1
1	F	279	PRO	4.1
1	F	273	VAL	4.1
1	D	266	THR	4.1
1	E	355	GLU	4.0
1	C	247	LEU	4.0
1	C	372	LEU	4.0
1	A	361	ASP	4.0
1	F	300	VAL	4.0
1	I	184	GLN	4.0
1	C	295	LEU	4.0
1	A	257	GLU	4.0
1	C	184	GLN	4.0
1	J	263	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	N	304	GLU	4.0
1	B	249	ILE	4.0
1	E	267	MET	4.0
1	F	306	GLY	4.0
1	K	235	PRO	4.0
1	B	302	SER	4.0
1	L	455	VAL	4.0
1	K	208	PRO	4.0
1	A	231	ARG	4.0
1	E	312	ALA	4.0
1	N	233	MET	4.0
1	F	384	ALA	4.0
1	F	231	ARG	4.0
1	M	220	ILE	4.0
1	M	250	ILE	4.0
1	F	242	LYS	3.9
1	K	251	ALA	3.9
1	B	300	VAL	3.9
1	K	310	GLU	3.9
1	E	333	ILE	3.9
1	L	249	ILE	3.9
1	F	178	GLU	3.9
1	K	247	LEU	3.9
1	J	383	ALA	3.9
1	A	264	VAL	3.9
1	N	266	THR	3.9
1	F	362	ARG	3.9
1	A	359	ASP	3.9
1	F	224	ASP	3.9
1	F	351	GLN	3.9
1	I	365	LEU	3.9
1	N	451	LEU	3.9
1	K	255	GLU	3.9
1	C	217	SER	3.9
1	H	351	GLN	3.9
1	A	223	ALA	3.9
1	I	355	GLU	3.9
1	M	355	GLU	3.9
1	H	286	LYS	3.9
1	L	44	PHE	3.9
1	F	229	ASN	3.9
1	K	306	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	292	ILE	3.9
1	K	304	GLU	3.9
1	K	242	LYS	3.9
1	J	281	PHE	3.9
1	K	351	GLN	3.9
1	B	305	ILE	3.9
1	E	249	ILE	3.9
1	F	100	ILE	3.9
1	B	243	ALA	3.8
1	C	267	MET	3.8
1	F	337	GLY	3.8
1	A	240	VAL	3.8
1	I	231	ARG	3.8
1	D	230	ILE	3.8
1	J	363	GLU	3.8
1	L	275	ALA	3.8
1	L	226	LYS	3.8
1	A	183	LEU	3.8
1	M	372	LEU	3.8
1	D	44	PHE	3.8
1	F	226	LYS	3.8
1	J	243	ALA	3.8
1	A	182	GLY	3.8
1	A	304	GLU	3.8
1	F	214	GLU	3.8
1	K	257	GLU	3.8
1	K	248	LEU	3.8
1	B	261	THR	3.8
1	J	224	ASP	3.8
1	C	240	VAL	3.8
1	B	133	ALA	3.8
1	J	274	ALA	3.8
1	K	301	ILE	3.8
1	F	361	ASP	3.8
1	C	248	LEU	3.8
1	F	235	PRO	3.8
1	N	309	LEU	3.8
1	J	265	ASN	3.8
1	G	264	VAL	3.8
1	C	304	GLU	3.8
1	N	255	GLU	3.8
1	C	250	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	526	LYS	3.8
1	C	231	ARG	3.8
1	C	237	LEU	3.8
1	J	367	GLU	3.8
1	N	356	ALA	3.8
1	E	238	GLU	3.7
1	B	235	PRO	3.7
1	M	213	VAL	3.7
1	C	229	ASN	3.7
1	F	342	ILE	3.7
1	I	526	LYS	3.7
1	M	349	ILE	3.7
1	M	351	GLN	3.7
1	A	284	ARG	3.7
1	K	213	VAL	3.7
1	K	347	ALA	3.7
1	L	272	LYS	3.7
1	N	44	PHE	3.7
1	G	257	GLU	3.7
1	J	253	ASP	3.7
1	M	299	THR	3.7
1	K	362	ARG	3.7
1	B	183	LEU	3.7
1	C	161	LEU	3.7
1	F	389	MET	3.7
1	J	287	ALA	3.7
1	C	281	PHE	3.7
1	B	256	GLY	3.7
1	B	497	THR	3.7
1	D	234	LEU	3.7
1	E	232	GLU	3.7
1	J	355	GLU	3.7
1	M	200	LEU	3.7
1	B	224	ASP	3.7
1	C	322	ARG	3.7
1	C	337	GLY	3.7
1	I	352	GLN	3.7
1	J	221	LEU	3.7
1	K	311	LYS	3.7
1	N	347	ALA	3.7
1	L	208	PRO	3.7
1	B	313	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	237	LEU	3.6
1	F	248	LEU	3.6
1	A	346	VAL	3.6
1	B	124	VAL	3.6
1	E	264	VAL	3.6
1	G	311	LYS	3.6
1	B	342	ILE	3.6
1	F	315	GLU	3.6
1	F	332	ILE	3.6
1	M	304	GLU	3.6
1	B	246	PRO	3.6
1	K	243	ALA	3.6
1	G	306	GLY	3.6
1	E	247	LEU	3.6
1	J	494	LEU	3.6
1	C	160	LYS	3.6
1	K	240	VAL	3.6
1	G	305	ILE	3.6
1	K	307	MET	3.6
1	J	223	ALA	3.6
1	L	269	GLY	3.6
1	E	257	GLU	3.6
1	E	289	LEU	3.6
1	F	354	GLU	3.6
1	M	257	GLU	3.6
1	J	226	LYS	3.6
1	C	358	SER	3.6
1	N	204	PHE	3.6
1	B	202	PRO	3.6
1	B	335	GLY	3.6
1	B	274	ALA	3.6
1	E	449	ALA	3.6
1	B	99	ILE	3.6
1	I	349	ILE	3.6
1	B	221	LEU	3.6
1	I	203	TYR	3.6
1	H	526	LYS	3.6
1	G	525	PRO	3.6
1	M	344	GLY	3.6
1	F	449	ALA	3.6
1	G	418	ALA	3.6
1	F	99	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	311	LYS	3.6
1	F	95	LEU	3.6
1	I	357	THR	3.6
1	L	265	ASN	3.6
1	E	300	VAL	3.6
1	B	293	ALA	3.5
1	E	99	ILE	3.5
1	K	220	ILE	3.5
1	K	313	THR	3.5
1	K	222	LEU	3.5
1	C	236	VAL	3.5
1	H	355	GLU	3.5
1	I	250	ILE	3.5
1	C	180	GLY	3.5
1	D	456	LEU	3.5
1	A	363	GLU	3.5
1	H	360	TYR	3.5
1	K	191	GLU	3.5
1	N	354	GLU	3.5
1	N	391	GLU	3.5
1	J	376	VAL	3.5
1	K	381	VAL	3.5
1	B	449	ALA	3.5
1	H	243	ALA	3.5
1	F	101	THR	3.5
1	G	135	SER	3.5
1	H	358	SER	3.5
1	J	232	GLU	3.5
1	G	95	LEU	3.5
1	K	183	LEU	3.5
1	D	267	MET	3.5
1	B	417	VAL	3.5
1	C	346	VAL	3.5
1	D	417	VAL	3.5
1	M	346	VAL	3.5
1	K	152	ALA	3.5
1	L	239	ALA	3.5
1	F	257	GLU	3.5
1	B	219	PHE	3.5
1	F	261	THR	3.5
1	C	272	LYS	3.5
1	J	362	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	131	LEU	3.5
1	E	262	LEU	3.5
1	A	449	ALA	3.5
1	G	271	VAL	3.5
1	B	311	LYS	3.5
1	B	526	LYS	3.5
1	G	219	PHE	3.5
1	D	270	ILE	3.5
1	E	229	ASN	3.5
1	C	317	LEU	3.5
1	G	317	LEU	3.5
1	I	451	LEU	3.5
1	F	94	VAL	3.5
1	I	391	GLU	3.4
1	F	299	THR	3.4
1	B	225	LYS	3.4
1	B	451	LEU	3.4
1	D	494	LEU	3.4
1	M	260	ALA	3.4
1	N	262	LEU	3.4
1	A	244	GLY	3.4
1	C	209	GLU	3.4
1	C	306	GLY	3.4
1	L	303	GLU	3.4
1	B	387	VAL	3.4
1	D	411	VAL	3.4
1	E	462	PRO	3.4
1	F	91	THR	3.4
1	F	307	MET	3.4
1	E	95	LEU	3.4
1	I	258	ALA	3.4
1	M	239	ALA	3.4
1	C	300	VAL	3.4
1	D	526	LYS	3.4
1	E	464	VAL	3.4
1	H	261	THR	3.4
1	F	355	GLU	3.4
1	B	284	ARG	3.4
1	G	44	PHE	3.4
1	L	256	GLY	3.4
1	N	258	ALA	3.4
1	B	209	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	27	VAL	3.4
1	E	94	VAL	3.4
1	L	236	VAL	3.4
1	L	346	VAL	3.4
1	B	447	MET	3.4
1	C	219	PHE	3.4
1	J	228	SER	3.4
1	K	383	ALA	3.4
1	L	304	GLU	3.4
1	M	384	ALA	3.4
1	I	317	LEU	3.4
1	A	94	VAL	3.4
1	A	266	THR	3.4
1	G	417	VAL	3.4
1	H	313	THR	3.4
1	H	323	VAL	3.4
1	I	299	THR	3.4
1	F	272	LYS	3.4
1	M	290	GLN	3.4
1	F	239	ALA	3.4
1	J	345	ARG	3.4
1	E	451	LEU	3.4
1	J	242	LYS	3.4
1	M	168	LYS	3.4
1	G	74	VAL	3.4
1	B	180	GLY	3.4
1	I	358	SER	3.3
1	L	284	ARG	3.3
1	L	449	ALA	3.3
1	M	160	LYS	3.3
1	M	272	LYS	3.3
1	C	315	GLU	3.3
1	N	353	ILE	3.3
1	B	210	THR	3.3
1	H	161	LEU	3.3
1	K	95	LEU	3.3
1	M	187	LEU	3.3
1	N	365	LEU	3.3
1	C	375	GLY	3.3
1	A	268	ARG	3.3
1	N	254	VAL	3.3
1	L	228	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	188	ASP	3.3
1	J	212	ALA	3.3
1	J	361	ASP	3.3
1	L	283	ASP	3.3
1	M	216	GLU	3.3
1	N	446	ALA	3.3
1	A	95	LEU	3.3
1	B	244	GLY	3.3
1	F	333	ILE	3.3
1	E	526	LYS	3.3
1	M	183	LEU	3.3
1	E	174	VAL	3.3
1	E	455	VAL	3.3
1	G	412	VAL	3.3
1	H	465	VAL	3.3
1	E	446	ALA	3.3
1	M	360	TYR	3.3
1	L	238	GLU	3.3
1	N	363	GLU	3.3
1	I	228	SER	3.3
1	K	205	ILE	3.3
1	M	217	SER	3.3
1	B	95	LEU	3.3
1	F	161	LEU	3.3
1	C	290	GLN	3.3
1	D	236	VAL	3.3
1	M	319	GLN	3.3
1	B	367	GLU	3.3
1	J	294	THR	3.3
1	H	305	ILE	3.3
1	L	332	ILE	3.3
1	A	267	MET	3.3
1	B	390	LYS	3.3
1	K	168	LYS	3.3
1	K	322	ARG	3.3
1	N	268	ARG	3.3
1	B	303	GLU	3.3
1	B	363	GLU	3.3
1	C	94	VAL	3.3
1	K	107	VAL	3.3
1	K	346	VAL	3.3
1	B	92	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	258	ALA	3.3
1	L	24	ALA	3.3
1	A	184	GLN	3.3
1	K	226	LYS	3.3
1	M	245	LYS	3.3
1	H	304	GLU	3.3
1	L	204	PHE	3.3
1	E	295	LEU	3.3
1	G	451	LEU	3.3
1	H	451	LEU	3.3
1	H	456	LEU	3.3
1	L	183	LEU	3.3
1	L	451	LEU	3.3
1	E	346	VAL	3.3
1	B	446	ALA	3.3
1	C	241	ALA	3.3
1	F	223	ALA	3.3
1	I	242	LYS	3.2
1	K	214	GLU	3.2
1	E	458	CYS	3.2
1	C	325	ILE	3.2
1	C	456	LEU	3.2
1	I	202	PRO	3.2
1	K	221	LEU	3.2
1	N	99	ILE	3.2
1	B	510	VAL	3.2
1	G	77	VAL	3.2
1	M	503	ALA	3.2
1	N	98	ALA	3.2
1	C	101	THR	3.2
1	N	91	THR	3.2
1	E	420	ILE	3.2
1	N	234	LEU	3.2
1	A	81	ALA	3.2
1	B	78	ALA	3.2
1	G	446	ALA	3.2
1	E	417	VAL	3.2
1	N	499	VAL	3.2
1	K	225	LYS	3.2
1	K	229	ASN	3.2
1	L	462	PRO	3.2
1	E	203	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	365	LEU	3.2
1	H	314	LEU	3.2
1	L	219	PHE	3.2
1	F	24	ALA	3.2
1	F	292	ILE	3.2
1	F	507	ALA	3.2
1	G	106	ALA	3.2
1	L	221	LEU	3.2
1	E	22	VAL	3.2
1	J	236	VAL	3.2
1	K	20	VAL	3.2
1	B	283	ASP	3.2
1	G	403	THR	3.2
1	F	180	GLY	3.2
1	F	286	LYS	3.2
1	G	228	SER	3.2
1	E	241	ALA	3.2
1	E	304	GLU	3.2
1	L	383	ALA	3.2
1	F	295	LEU	3.2
1	J	513	LEU	3.2
1	E	342	ILE	3.2
1	D	455	VAL	3.2
1	H	240	VAL	3.2
1	D	272	LYS	3.2
1	D	496	PRO	3.2
1	H	267	MET	3.2
1	B	130	GLU	3.2
1	C	363	GLU	3.2
1	E	24	ALA	3.2
1	C	221	LEU	3.2
1	E	284	ARG	3.2
1	I	227	ILE	3.2
1	B	411	VAL	3.2
1	B	500	THR	3.2
1	C	526	LYS	3.2
1	H	27	VAL	3.2
1	B	280	GLY	3.1
1	B	306	GLY	3.1
1	J	202	PRO	3.1
1	C	319	GLN	3.1
1	B	423	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	384	ALA	3.1
1	J	260	ALA	3.1
1	J	215	LEU	3.1
1	L	314	LEU	3.1
1	M	195	PHE	3.1
1	B	93	THR	3.1
1	G	493	ILE	3.1
1	K	292	ILE	3.1
1	G	499	VAL	3.1
1	H	300	VAL	3.1
1	M	159	GLY	3.1
1	F	388	GLU	3.1
1	M	241	ALA	3.1
1	N	243	ALA	3.1
1	B	456	LEU	3.1
1	I	256	GLY	3.1
1	I	309	LEU	3.1
1	K	261	THR	3.1
1	N	134	LEU	3.1
1	D	454	ILE	3.1
1	L	353	ILE	3.1
1	F	54	VAL	3.1
1	F	378	VAL	3.1
1	H	29	VAL	3.1
1	H	229	ASN	3.1
1	E	418	ALA	3.1
1	H	356	ALA	3.1
1	N	92	ALA	3.1
1	C	245	LYS	3.1
1	E	306	GLY	3.1
1	M	311	LYS	3.1
1	A	181	THR	3.1
1	E	91	THR	3.1
1	F	157	THR	3.1
1	L	215	LEU	3.1
1	N	237	LEU	3.1
1	A	360	TYR	3.1
1	B	292	ILE	3.1
1	C	99	ILE	3.1
1	E	184	GLN	3.1
1	F	370	ALA	3.1
1	I	340	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	308	GLU	3.1
1	C	202	PRO	3.1
1	C	181	THR	3.1
1	F	90	THR	3.1
1	J	181	THR	3.1
1	K	210	THR	3.1
1	F	31	LEU	3.1
1	C	455	VAL	3.1
1	G	54	VAL	3.1
1	N	27	VAL	3.1
1	B	418	ALA	3.1
1	M	341	ALA	3.1
1	E	450	PRO	3.1
1	G	496	PRO	3.1
1	C	302	SER	3.1
1	E	463	SER	3.1
1	G	207	LYS	3.1
1	B	267	MET	3.1
1	D	451	LEU	3.1
1	K	451	LEU	3.1
1	B	499	VAL	3.1
1	F	107	VAL	3.1
1	F	323	VAL	3.1
1	E	274	ALA	3.0
1	F	78	ALA	3.0
1	F	106	ALA	3.0
1	I	269	GLY	3.0
1	K	446	ALA	3.0
1	N	24	ALA	3.0
1	F	168	LYS	3.0
1	A	358	SER	3.0
1	D	500	THR	3.0
1	G	497	THR	3.0
1	K	252	GLU	3.0
1	A	288	MET	3.0
1	D	309	LEU	3.0
1	N	259	LEU	3.0
1	B	440	ILE	3.0
1	H	99	ILE	3.0
1	G	383	ALA	3.0
1	K	96	ALA	3.0
1	B	496	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	302	SER	3.0
1	A	500	THR	3.0
1	G	266	THR	3.0
1	B	187	LEU	3.0
1	B	295	LEU	3.0
1	C	216	GLU	3.0
1	C	354	GLU	3.0
1	C	504	LEU	3.0
1	F	363	GLU	3.0
1	L	247	LEU	3.0
1	B	96	ALA	3.0
1	E	29	VAL	3.0
1	F	442	VAL	3.0
1	M	302	SER	3.0
1	M	261	THR	3.0
1	I	272	LYS	3.0
1	E	255	GLU	3.0
1	H	257	GLU	3.0
1	I	229	ASN	3.0
1	D	95	LEU	3.0
1	I	259	LEU	3.0
1	E	362	ARG	3.0
1	C	449	ALA	3.0
1	D	27	VAL	3.0
1	E	107	VAL	3.0
1	H	258	ALA	3.0
1	H	273	VAL	3.0
1	N	311	LYS	3.0
1	C	238	GLU	3.0
1	C	265	ASN	3.0
1	F	343	GLN	3.0
1	A	339	GLU	3.0
1	B	289	LEU	3.0
1	C	191	GLU	3.0
1	E	444	LEU	3.0
1	L	222	LEU	3.0
1	C	342	ILE	3.0
1	C	454	ILE	3.0
1	E	281	PHE	3.0
1	H	230	ILE	3.0
1	N	22	VAL	3.0
1	N	346	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	203	TYR	3.0
1	L	91	THR	3.0
1	I	159	GLY	3.0
1	K	382	GLY	3.0
1	M	362	ARG	3.0
1	G	303	GLU	3.0
1	C	222	LEU	3.0
1	D	258	ALA	3.0
1	E	98	ALA	3.0
1	H	24	ALA	3.0
1	K	24	ALA	3.0
1	M	274	ALA	3.0
1	D	412	VAL	2.9
1	F	417	VAL	2.9
1	J	336	VAL	2.9
1	K	27	VAL	2.9
1	K	379	ILE	2.9
1	N	60	ILE	2.9
1	N	357	THR	2.9
1	B	129	GLU	2.9
1	E	214	GLU	2.9
1	I	238	GLU	2.9
1	K	355	GLU	2.9
1	L	257	GLU	2.9
1	M	316	ASP	2.9
1	N	512	GLY	2.9
1	M	229	ASN	2.9
1	L	260	ALA	2.9
1	M	243	ALA	2.9
1	A	295	LEU	2.9
1	G	237	LEU	2.9
1	M	286	LYS	2.9
1	A	74	VAL	2.9
1	A	261	THR	2.9
1	D	269	GLY	2.9
1	F	313	THR	2.9
1	H	500	THR	2.9
1	K	328	ASP	2.9
1	N	94	VAL	2.9
1	A	99	ILE	2.9
1	C	332	ILE	2.9
1	J	307	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	351	GLN	2.9
1	I	302	SER	2.9
1	D	231	ARG	2.9
1	M	388	GLU	2.9
1	N	285	ARG	2.9
1	B	127	ALA	2.9
1	E	260	ALA	2.9
1	F	446	ALA	2.9
1	F	503	ALA	2.9
1	K	320	ALA	2.9
1	E	361	ASP	2.9
1	A	262	LEU	2.9
1	C	451	LEU	2.9
1	F	504	LEU	2.9
1	H	31	LEU	2.9
1	L	248	LEU	2.9
1	B	263	VAL	2.9
1	E	20	VAL	2.9
1	G	411	VAL	2.9
1	H	20	VAL	2.9
1	A	281	PHE	2.9
1	E	100	ILE	2.9
1	M	389	MET	2.9
1	F	265	ASN	2.9
1	H	302	SER	2.9
1	J	302	SER	2.9
1	M	185	ASP	2.9
1	E	466	ALA	2.9
1	L	274	ALA	2.9
1	E	299	THR	2.9
1	I	262	LEU	2.9
1	A	388	GLU	2.9
1	C	168	LYS	2.9
1	K	209	GLU	2.9
1	K	352	GLN	2.9
1	M	339	GLU	2.9
1	B	74	VAL	2.9
1	C	417	VAL	2.9
1	E	422	VAL	2.9
1	G	265	ASN	2.9
1	H	271	VAL	2.9
1	H	442	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	229	ASN	2.9
1	H	454	ILE	2.9
1	K	162	ILE	2.9
1	K	249	ILE	2.9
1	M	205	ILE	2.9
1	N	454	ILE	2.9
1	L	450	PRO	2.9
1	C	260	ALA	2.9
1	C	286	LYS	2.9
1	C	366	GLN	2.9
1	C	284	ARG	2.9
1	B	419	LEU	2.9
1	B	426	LEU	2.9
1	F	451	LEU	2.9
1	E	193	MET	2.9
1	N	267	MET	2.9
1	C	29	VAL	2.9
1	E	240	VAL	2.9
1	K	361	ASP	2.9
1	G	99	ILE	2.9
1	L	281	PHE	2.9
1	G	256	GLY	2.9
1	B	71	ALA	2.9
1	B	241	ALA	2.9
1	A	400	LEU	2.9
1	B	200	LEU	2.9
1	D	134	LEU	2.9
1	E	317	LEU	2.9
1	H	95	LEU	2.9
1	H	215	LEU	2.9
1	K	245	LYS	2.9
1	I	300	VAL	2.8
1	E	350	ARG	2.8
1	A	24	ALA	2.8
1	A	503	ALA	2.8
1	F	92	ALA	2.8
1	G	133	ALA	2.8
1	L	98	ALA	2.8
1	E	188	ASP	2.8
1	K	283	ASP	2.8
1	A	286	LYS	2.8
1	F	245	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	228	SER	2.8
1	E	222	LEU	2.8
1	G	314	LEU	2.8
1	I	183	LEU	2.8
1	D	499	VAL	2.8
1	F	22	VAL	2.8
1	G	38	VAL	2.8
1	G	407	VAL	2.8
1	L	300	VAL	2.8
1	E	265	ASN	2.8
1	C	347	ALA	2.8
1	F	338	GLU	2.8
1	F	443	ALA	2.8
1	H	272	LYS	2.8
1	I	24	ALA	2.8
1	J	238	GLU	2.8
1	E	93	THR	2.8
1	F	385	THR	2.8
1	N	351	GLN	2.8
1	B	104	LEU	2.8
1	F	494	LEU	2.8
1	N	17	LEU	2.8
1	E	374	GLY	2.8
1	E	338	GLU	2.8
1	B	346	VAL	2.8
1	D	77	VAL	2.8
1	C	275	ALA	2.8
1	D	493	ILE	2.8
1	G	26	ALA	2.8
1	N	96	ALA	2.8
1	D	91	THR	2.8
1	F	447	MET	2.8
1	A	355	GLU	2.8
1	F	321	LYS	2.8
1	M	226	LYS	2.8
1	J	280	GLY	2.8
1	A	237	LEU	2.8
1	B	188	ASP	2.8
1	G	134	LEU	2.8
1	J	316	ASP	2.8
1	E	453	GLN	2.8
1	H	107	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	455	VAL	2.8
1	I	499	VAL	2.8
1	K	510	VAL	2.8
1	E	92	ALA	2.8
1	H	251	ALA	2.8
1	B	338	GLU	2.8
1	H	462	PRO	2.8
1	K	157	THR	2.8
1	K	308	GLU	2.8
1	K	331	THR	2.8
1	E	269	GLY	2.8
1	M	256	GLY	2.8
1	N	360	TYR	2.8
1	G	262	LEU	2.8
1	K	456	LEU	2.8
1	L	419	LEU	2.8
1	N	317	LEU	2.8
1	A	177	VAL	2.8
1	D	94	VAL	2.8
1	F	275	ALA	2.8
1	H	346	VAL	2.8
1	K	189	VAL	2.8
1	K	376	VAL	2.8
1	L	302	SER	2.8
1	L	381	VAL	2.8
1	M	383	ALA	2.8
1	M	446	ALA	2.8
1	C	283	ASP	2.8
1	F	266	THR	2.8
1	L	333	ILE	2.8
1	L	454	ILE	2.8
1	A	256	GLY	2.8
1	F	159	GLY	2.8
1	H	306	GLY	2.8
1	J	244	GLY	2.8
1	B	308	GLU	2.8
1	A	451	LEU	2.8
1	A	513	LEU	2.8
1	G	31	LEU	2.8
1	D	443	ALA	2.7
1	E	96	ALA	2.7
1	G	96	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	423	ALA	2.7
1	H	98	ALA	2.7
1	K	300	VAL	2.7
1	L	387	VAL	2.7
1	N	510	VAL	2.7
1	B	450	PRO	2.7
1	I	313	THR	2.7
1	M	313	THR	2.7
1	C	205	ILE	2.7
1	F	290	GLN	2.7
1	K	211	GLY	2.7
1	B	386	GLU	2.7
1	C	350	ARG	2.7
1	G	231	ARG	2.7
1	K	216	GLU	2.7
1	A	444	LEU	2.7
1	B	361	ASP	2.7
1	B	504	LEU	2.7
1	D	419	LEU	2.7
1	E	17	LEU	2.7
1	H	237	LEU	2.7
1	H	365	LEU	2.7
1	B	466	ALA	2.7
1	D	85	ALA	2.7
1	A	107	VAL	2.7
1	B	348	GLN	2.7
1	A	311	LYS	2.7
1	B	94	VAL	2.7
1	I	29	VAL	2.7
1	J	407	VAL	2.7
1	L	27	VAL	2.7
1	N	257	GLU	2.7
1	E	345	ARG	2.7
1	E	497	THR	2.7
1	A	301	ILE	2.7
1	B	420	ILE	2.7
1	K	100	ILE	2.7
1	K	333	ILE	2.7
1	L	349	ILE	2.7
1	K	334	ASP	2.7
1	M	361	ASP	2.7
1	N	358	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	371	LYS	2.7
1	C	165	ALA	2.7
1	C	199	TYR	2.7
1	E	372	LEU	2.7
1	F	450	PRO	2.7
1	G	131	LEU	2.7
1	H	444	LEU	2.7
1	H	466	ALA	2.7
1	J	504	LEU	2.7
1	L	456	LEU	2.7
1	K	280	GLY	2.7
1	A	417	VAL	2.7
1	B	126	VAL	2.7
1	B	465	VAL	2.7
1	K	94	VAL	2.7
1	B	220	ILE	2.7
1	E	454	ILE	2.7
1	H	361	ASP	2.7
1	M	188	ASP	2.7
1	I	286	LYS	2.7
1	A	462	PRO	2.7
1	C	450	PRO	2.7
1	D	474	GLY	2.7
1	K	449	ALA	2.7
1	M	297	GLY	2.7
1	B	31	LEU	2.7
1	C	309	LEU	2.7
1	D	23	LEU	2.7
1	F	183	LEU	2.7
1	I	248	LEU	2.7
1	K	295	LEU	2.7
1	L	134	LEU	2.7
1	M	95	LEU	2.7
1	M	161	LEU	2.7
1	M	90	THR	2.7
1	I	22	VAL	2.7
1	N	184	GLN	2.7
1	G	325	ILE	2.7
1	H	100	ILE	2.7
1	J	220	ILE	2.7
1	L	99	ILE	2.7
1	M	325	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	N	150	ILE	2.7
1	A	450	PRO	2.7
1	K	19	GLY	2.7
1	D	98	ALA	2.7
1	E	106	ALA	2.7
1	H	26	ALA	2.7
1	B	245	LYS	2.7
1	E	101	THR	2.7
1	G	234	LEU	2.7
1	J	95	LEU	2.7
1	M	155	ASP	2.7
1	M	247	LEU	2.7
1	K	290	GLN	2.7
1	E	323	VAL	2.7
1	E	387	VAL	2.7
1	G	94	VAL	2.7
1	M	254	VAL	2.7
1	N	77	VAL	2.7
1	B	358	SER	2.7
1	A	420	ILE	2.7
1	D	99	ILE	2.7
1	J	100	ILE	2.7
1	C	367	GLU	2.7
1	F	496	PRO	2.7
1	J	297	GLY	2.7
1	N	242	LYS	2.7
1	D	503	ALA	2.7
1	K	316	ASP	2.7
1	M	343	GLN	2.7
1	A	91	THR	2.7
1	C	90	THR	2.7
1	E	30	THR	2.7
1	G	419	LEU	2.7
1	H	104	LEU	2.7
1	I	288	MET	2.7
1	N	504	LEU	2.7
1	A	442	VAL	2.6
1	B	455	VAL	2.6
1	C	381	VAL	2.6
1	C	465	VAL	2.6
1	N	387	VAL	2.6
1	I	306	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	332	ILE	2.6
1	N	100	ILE	2.6
1	E	97	GLN	2.6
1	M	106	ALA	2.6
1	M	281	PHE	2.6
1	N	350	ARG	2.6
1	F	288	MET	2.6
1	G	500	THR	2.6
1	I	209	GLU	2.6
1	M	232	GLU	2.6
1	B	317	LEU	2.6
1	B	463	SER	2.6
1	D	237	LEU	2.6
1	F	513	LEU	2.6
1	B	412	VAL	2.6
1	H	236	VAL	2.6
1	K	254	VAL	2.6
1	B	282	GLY	2.6
1	I	86	GLY	2.6
1	F	345	ARG	2.6
1	L	420	ILE	2.6
1	L	515	ILE	2.6
1	A	92	ALA	2.6
1	B	252	GLU	2.6
1	I	257	GLU	2.6
1	M	255	GLU	2.6
1	G	272	LYS	2.6
1	B	181	THR	2.6
1	E	31	LEU	2.6
1	F	350	ARG	2.6
1	A	455	VAL	2.6
1	B	506	TYR	2.6
1	D	450	PRO	2.6
1	E	478	TYR	2.6
1	F	113	PRO	2.6
1	F	303	GLU	2.6
1	G	236	VAL	2.6
1	I	496	PRO	2.6
1	J	240	VAL	2.6
1	K	164	GLU	2.6
1	G	92	ALA	2.6
1	G	138	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	514	MET	2.6
1	F	93	THR	2.6
1	N	228	SER	2.6
1	E	290	GLN	2.6
1	J	359	ASP	2.6
1	K	319	GLN	2.6
1	L	184	GLN	2.6
1	A	255	GLU	2.6
1	A	416	GLY	2.6
1	C	164	GLU	2.6
1	J	216	GLU	2.6
1	M	363	GLU	2.6
1	E	23	LEU	2.6
1	H	134	LEU	2.6
1	I	400	LEU	2.6
1	K	286	LYS	2.6
1	A	510	VAL	2.6
1	B	438	VAL	2.6
1	F	499	VAL	2.6
1	I	54	VAL	2.6
1	N	265	ASN	2.6
1	C	98	ALA	2.6
1	A	516	THR	2.6
1	J	209	GLU	2.6
1	N	284	ARG	2.6
1	C	390	LYS	2.6
1	E	311	LYS	2.6
1	G	204	PHE	2.6
1	L	103	GLY	2.6
1	A	259	LEU	2.6
1	E	504	LEU	2.6
1	F	104	LEU	2.6
1	I	314	LEU	2.6
1	K	314	LEU	2.6
1	M	295	LEU	2.6
1	N	513	LEU	2.6
1	F	510	VAL	2.6
1	G	136	VAL	2.6
1	I	20	VAL	2.6
1	I	27	VAL	2.6
1	M	29	VAL	2.6
1	M	422	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	352	GLN	2.6
1	K	363	GLU	2.6
1	L	316	ASP	2.6
1	A	98	ALA	2.6
1	C	226	LYS	2.6
1	D	406	ALA	2.6
1	E	347	ALA	2.6
1	L	446	ALA	2.6
1	B	125	THR	2.6
1	C	288	MET	2.6
1	H	515	ILE	2.6
1	K	99	ILE	2.6
1	B	269	GLY	2.6
1	F	335	GLY	2.6
1	C	172	GLU	2.6
1	G	391	GLU	2.6
1	K	303	GLU	2.6
1	M	315	GLU	2.6
1	A	350	ARG	2.5
1	C	314	LEU	2.6
1	K	104	LEU	2.6
1	I	245	LYS	2.5
1	D	107	VAL	2.5
1	G	469	VAL	2.5
1	I	96	ALA	2.5
1	J	340	ALA	2.5
1	L	26	ALA	2.5
1	B	299	THR	2.5
1	F	297	GLY	2.5
1	N	93	THR	2.5
1	K	454	ILE	2.5
1	N	301	ILE	2.5
1	K	184	GLN	2.5
1	H	121	ASP	2.5
1	H	404	ARG	2.5
1	B	444	LEU	2.5
1	B	513	LEU	2.5
1	C	262	LEU	2.5
1	J	295	LEU	2.5
1	M	456	LEU	2.5
1	A	507	ALA	2.5
1	B	22	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	107	VAL	2.5
1	C	243	ALA	2.5
1	F	126	VAL	2.5
1	F	287	ALA	2.5
1	F	508	ALA	2.5
1	J	107	VAL	2.5
1	K	98	ALA	2.5
1	M	323	VAL	2.5
1	N	106	ALA	2.5
1	N	507	ALA	2.5
1	C	257	GLU	2.5
1	H	256	GLY	2.5
1	A	93	THR	2.5
1	D	497	THR	2.5
1	J	261	THR	2.5
1	A	342	ILE	2.5
1	A	454	ILE	2.5
1	H	301	ILE	2.5
1	K	332	ILE	2.5
1	D	31	LEU	2.5
1	E	513	LEU	2.5
1	F	310	GLU	2.5
1	L	295	LEU	2.5
1	N	355	GLU	2.5
1	D	446	ALA	2.5
1	F	110	GLY	2.5
1	H	418	ALA	2.5
1	I	507	ALA	2.5
1	N	272	LYS	2.5
1	B	20	VAL	2.5
1	B	422	VAL	2.5
1	E	469	VAL	2.5
1	G	184	GLN	2.5
1	G	323	VAL	2.5
1	K	323	VAL	2.5
1	L	20	VAL	2.5
1	N	29	VAL	2.5
1	E	500	THR	2.5
1	G	181	THR	2.5
1	H	90	THR	2.5
1	I	90	THR	2.5
1	I	101	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	203	TYR	2.5
1	B	205	ILE	2.5
1	B	454	ILE	2.5
1	H	238	GLU	2.5
1	H	332	ILE	2.5
1	L	301	ILE	2.5
1	N	216	GLU	2.5
1	A	269	GLY	2.5
1	A	504	LEU	2.5
1	B	350	ARG	2.5
1	E	416	GLY	2.5
1	J	366	GLN	2.5
1	G	456	LEU	2.5
1	K	103	GLY	2.5
1	B	239	ALA	2.5
1	J	334	ASP	2.5
1	K	106	ALA	2.5
1	L	185	ASP	2.5
1	B	89	THR	2.5
1	C	20	VAL	2.5
1	C	210	THR	2.5
1	F	369	VAL	2.5
1	G	261	THR	2.5
1	L	465	VAL	2.5
1	N	54	VAL	2.5
1	I	232	GLU	2.5
1	M	354	GLU	2.5
1	H	321	LYS	2.5
1	C	220	ILE	2.5
1	D	420	ILE	2.5
1	I	99	ILE	2.5
1	I	454	ILE	2.5
1	A	209	GLU	2.5
1	A	216	GLU	2.5
1	A	446	ALA	2.5
1	B	123	ALA	2.5
1	B	494	LEU	2.5
1	D	24	ALA	2.5
1	E	134	LEU	2.5
1	E	507	ALA	2.5
1	I	304	GLU	2.5
1	J	143	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	85	ALA	2.5
1	K	258	ALA	2.5
1	N	340	ALA	2.5
1	N	511	ALA	2.5
1	C	299	THR	2.5
1	B	128	VAL	2.5
1	C	158	VAL	2.5
1	C	276	VAL	2.5
1	G	20	VAL	2.5
1	H	417	VAL	2.5
1	H	464	VAL	2.5
1	I	94	VAL	2.5
1	J	273	VAL	2.5
1	M	27	VAL	2.5
1	F	319	GLN	2.5
1	A	265	ASN	2.5
1	N	203	TYR	2.5
1	B	416	GLY	2.5
1	E	250	ILE	2.5
1	G	301	ILE	2.5
1	K	420	ILE	2.5
1	K	321	LYS	2.5
1	A	341	ALA	2.5
1	D	92	ALA	2.5
1	F	243	ALA	2.5
1	G	81	ALA	2.5
1	G	98	ALA	2.5
1	G	215	LEU	2.4
1	H	419	LEU	2.4
1	I	247	LEU	2.4
1	N	95	LEU	2.4
1	N	450	PRO	2.4
1	D	184	GLN	2.4
1	B	254	VAL	2.4
1	B	276	VAL	2.4
1	B	336	VAL	2.4
1	D	147	VAL	2.4
1	F	396	VAL	2.4
1	H	77	VAL	2.4
1	I	465	VAL	2.4
1	C	338	GLU	2.4
1	D	306	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	226	LYS	2.4
1	F	420	ILE	2.4
1	M	292	ILE	2.4
1	M	454	ILE	2.4
1	B	413	ALA	2.4
1	B	427	ALA	2.4
1	C	239	ALA	2.4
1	D	133	ALA	2.4
1	D	511	ALA	2.4
1	H	449	ALA	2.4
1	B	462	PRO	2.4
1	G	233	MET	2.4
1	J	352	GLN	2.4
1	L	90	THR	2.4
1	M	345	ARG	2.4
1	A	456	LEU	2.4
1	B	238	GLU	2.4
1	C	214	GLU	2.4
1	G	444	LEU	2.4
1	N	187	LEU	2.4
1	A	22	VAL	2.4
1	A	499	VAL	2.4
1	C	38	VAL	2.4
1	C	469	VAL	2.4
1	G	242	LYS	2.4
1	N	20	VAL	2.4
1	I	103	GLY	2.4
1	N	306	GLY	2.4
1	A	100	ILE	2.4
1	D	100	ILE	2.4
1	L	146	GLN	2.4
1	N	249	ILE	2.4
1	D	449	ALA	2.4
1	J	507	ALA	2.4
1	E	224	ASP	2.4
1	G	101	THR	2.4
1	K	327	LYS	2.4
1	F	419	LEU	2.4
1	J	222	LEU	2.4
1	K	282	GLY	2.4
1	G	422	VAL	2.4
1	H	22	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	14	VAL	2.4
1	B	184	GLN	2.4
1	I	172	GLU	2.4
1	J	338	GLU	2.4
1	L	308	GLU	2.4
1	B	253	ASP	2.4
1	B	120	ILE	2.4
1	B	275	ALA	2.4
1	H	203	TYR	2.4
1	H	525	PRO	2.4
1	J	235	PRO	2.4
1	L	202	PRO	2.4
1	M	92	ALA	2.4
1	L	500	THR	2.4
1	G	281	PHE	2.4
1	I	463	SER	2.4
1	G	504	LEU	2.4
1	H	156	GLU	2.4
1	I	40	LEU	2.4
1	I	95	LEU	2.4
1	J	200	LEU	2.4
1	J	451	LEU	2.4
1	K	504	LEU	2.4
1	N	104	LEU	2.4
1	N	282	GLY	2.4
1	D	445	ARG	2.4
1	K	366	GLN	2.4
1	E	465	VAL	2.4
1	B	347	ALA	2.4
1	C	85	ALA	2.4
1	I	108	ALA	2.4
1	E	111	MET	2.4
1	B	228	SER	2.4
1	F	301	ILE	2.4
1	G	220	ILE	2.4
1	H	101	THR	2.4
1	K	294	THR	2.4
1	N	49	ILE	2.4
1	N	89	THR	2.4
1	N	339	GLU	2.4
1	C	368	ARG	2.4
1	K	182	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	116	LEU	2.4
1	F	456	LEU	2.4
1	A	283	ASP	2.4
1	B	27	VAL	2.4
1	B	54	VAL	2.4
1	E	324	VAL	2.4
1	F	20	VAL	2.4
1	F	29	VAL	2.4
1	I	273	VAL	2.4
1	L	417	VAL	2.4
1	L	464	VAL	2.4
1	M	465	VAL	2.4
1	N	326	ASN	2.4
1	D	243	ALA	2.4
1	I	260	ALA	2.4
1	I	508	ALA	2.4
1	J	446	ALA	2.4
1	K	384	ALA	2.4
1	M	108	ALA	2.4
1	E	261	THR	2.4
1	E	474	GLY	2.4
1	J	385	THR	2.4
1	G	454	ILE	2.4
1	N	325	ILE	2.4
1	E	359	ASP	2.4
1	H	338	GLU	2.3
1	H	458	CYS	2.3
1	I	372	LEU	2.3
1	J	255	GLU	2.3
1	J	304	GLU	2.3
1	C	22	VAL	2.3
1	C	499	VAL	2.3
1	D	521	VAL	2.3
1	F	14	VAL	2.3
1	I	236	VAL	2.3
1	L	22	VAL	2.3
1	L	499	VAL	2.3
1	M	136	VAL	2.3
1	N	369	VAL	2.3
1	B	290	GLN	2.3
1	F	218	PRO	2.3
1	K	401	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	453	GLN	2.3
1	B	443	ALA	2.3
1	K	337	GLY	2.3
1	L	447	MET	2.3
1	B	90	THR	2.3
1	D	30	THR	2.3
1	H	91	THR	2.3
1	M	296	THR	2.3
1	M	298	GLY	2.3
1	B	515	ILE	2.3
1	D	489	ILE	2.3
1	E	252	GLU	2.3
1	E	515	ILE	2.3
1	F	304	GLU	2.3
1	H	363	GLU	2.3
1	E	321	LYS	2.3
1	J	272	LYS	2.3
1	B	345	ARG	2.3
1	C	343	GLN	2.3
1	F	348	GLN	2.3
1	K	285	ARG	2.3
1	L	104	LEU	2.3
1	A	519	CYS	2.3
1	C	208	PRO	2.3
1	C	189	VAL	2.3
1	C	464	VAL	2.3
1	D	38	VAL	2.3
1	G	22	VAL	2.3
1	M	189	VAL	2.3
1	B	503	ALA	2.3
1	F	512	GLY	2.3
1	G	447	MET	2.3
1	H	269	GLY	2.3
1	I	88	GLY	2.3
1	I	92	ALA	2.3
1	N	165	ALA	2.3
1	N	447	MET	2.3
1	G	93	THR	2.3
1	K	90	THR	2.3
1	K	91	THR	2.3
1	C	311	LYS	2.3
1	L	526	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	285	ARG	2.3
1	J	227	ILE	2.3
1	M	322	ARG	2.3
1	E	62	LEU	2.3
1	G	23	LEU	2.3
1	H	131	LEU	2.3
1	H	222	LEU	2.3
1	I	450	PRO	2.3
1	C	186	GLU	2.3
1	C	252	GLU	2.3
1	L	310	GLU	2.3
1	M	338	GLU	2.3
1	F	463	SER	2.3
1	J	463	SER	2.3
1	L	155	ASP	2.3
1	L	463	SER	2.3
1	N	224	ASP	2.3
1	D	20	VAL	2.3
1	E	136	VAL	2.3
1	F	38	VAL	2.3
1	K	387	VAL	2.3
1	B	26	ALA	2.3
1	B	507	ALA	2.3
1	D	96	ALA	2.3
1	E	383	ALA	2.3
1	E	90	THR	2.3
1	E	519	CYS	2.3
1	G	24	ALA	2.3
1	K	458	CYS	2.3
1	L	480	ALA	2.3
1	G	89	THR	2.3
1	A	515	ILE	2.3
1	J	250	ILE	2.3
1	L	188	ASP	2.3
1	A	104	LEU	2.3
1	E	168	LYS	2.3
1	F	382	GLY	2.3
1	K	161	LEU	2.3
1	K	201	SER	2.3
1	K	297	GLY	2.3
1	K	344	GLY	2.3
1	N	415	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	85	ALA	2.3
1	C	84	ALA	2.3
1	D	74	VAL	2.3
1	D	284	ARG	2.3
1	E	508	ALA	2.3
1	G	108	ALA	2.3
1	H	284	ARG	2.3
1	I	26	ALA	2.3
1	I	455	VAL	2.3
1	L	29	VAL	2.3
1	L	443	ALA	2.3
1	M	24	ALA	2.3
1	G	91	THR	2.3
1	A	214	GLU	2.3
1	G	310	GLU	2.3
1	B	379	ILE	2.3
1	C	280	GLY	2.3
1	E	244	GLY	2.3
1	M	318	GLY	2.3
1	C	258	ALA	2.3
1	E	303	GLU	2.3
1	G	507	ALA	2.3
1	I	106	ALA	2.3
1	J	341	ALA	2.3
1	J	354	GLU	2.3
1	E	27	VAL	2.3
1	H	510	VAL	2.3
1	M	142	LYS	2.3
1	A	229	ASN	2.3
1	D	457	ASN	2.3
1	E	217	SER	2.3
1	J	450	PRO	2.3
1	J	462	PRO	2.3
1	M	113	PRO	2.3
1	M	450	PRO	2.3
1	F	284	ARG	2.3
1	K	386	GLU	2.3
1	L	232	GLU	2.3
1	L	319	GLN	2.3
1	B	85	ALA	2.2
1	B	406	ALA	2.2
1	C	193	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	406	ALA	2.2
1	G	449	ALA	2.2
1	G	503	ALA	2.2
1	H	446	ALA	2.2
1	J	503	ALA	2.2
1	N	307	MET	2.2
1	N	456	LEU	2.2
1	A	497	THR	2.2
1	H	93	THR	2.2
1	J	195	PHE	2.2
1	E	381	VAL	2.2
1	J	464	VAL	2.2
1	N	417	VAL	2.2
1	A	172	GLU	2.2
1	D	214	GLU	2.2
1	E	352	GLN	2.2
1	F	453	GLN	2.2
1	G	255	GLU	2.2
1	N	238	GLU	2.2
1	E	135	SER	2.2
1	G	32	GLY	2.2
1	I	311	LYS	2.2
1	B	100	ILE	2.2
1	G	100	ILE	2.2
1	B	340	ALA	2.2
1	C	24	ALA	2.2
1	C	287	ALA	2.2
1	C	466	ALA	2.2
1	E	127	ALA	2.2
1	E	447	MET	2.2
1	G	495	ASP	2.2
1	K	359	ASP	2.2
1	C	513	LEU	2.2
1	E	503	ALA	2.2
1	H	372	LEU	2.2
1	H	406	ALA	2.2
1	K	293	ALA	2.2
1	N	274	ALA	2.2
1	E	313	THR	2.2
1	J	299	THR	2.2
1	E	204	PHE	2.2
1	L	315	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	164	GLU	2.2
1	M	209	GLU	2.2
1	B	38	VAL	2.2
1	B	442	VAL	2.2
1	E	510	VAL	2.2
1	F	39	VAL	2.2
1	F	455	VAL	2.2
1	J	94	VAL	2.2
1	J	184	GLN	2.2
1	J	319	GLN	2.2
1	N	107	VAL	2.2
1	N	453	GLN	2.2
1	B	502	SER	2.2
1	F	103	GLY	2.2
1	K	374	GLY	2.2
1	C	224	ASP	2.2
1	M	224	ASP	2.2
1	A	447	MET	2.2
1	B	193	MET	2.2
1	E	391	GLU	2.2
1	B	508	ALA	2.2
1	F	16	MET	2.2
1	H	325	ILE	2.2
1	D	421	ARG	2.2
1	F	98	ALA	2.2
1	F	184	GLN	2.2
1	H	517	THR	2.2
1	C	95	LEU	2.2
1	D	242	LYS	2.2
1	E	104	LEU	2.2
1	G	17	LEU	2.2
1	I	444	LEU	2.2
1	M	400	LEU	2.2
1	E	14	VAL	2.2
1	E	302	SER	2.2
1	F	302	SER	2.2
1	G	107	VAL	2.2
1	G	126	VAL	2.2
1	J	213	VAL	2.2
1	K	195	PHE	2.2
1	N	359	ASP	2.2
1	H	354	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	N	362	ARG	2.2
1	A	96	ALA	2.2
1	B	370	ALA	2.2
1	C	446	ALA	2.2
1	D	466	ALA	2.2
1	E	21	ASN	2.2
1	E	511	ALA	2.2
1	F	373	ALA	2.2
1	H	489	ILE	2.2
1	J	466	ALA	2.2
1	L	92	ALA	2.2
1	C	500	THR	2.2
1	I	500	THR	2.2
1	J	517	THR	2.2
1	N	227	ILE	2.2
1	B	414	GLY	2.2
1	C	269	GLY	2.2
1	C	298	GLY	2.2
1	C	415	GLY	2.2
1	D	138	CYS	2.2
1	E	494	LEU	2.2
1	G	513	LEU	2.2
1	I	31	LEU	2.2
1	L	95	LEU	2.2
1	A	188	ASP	2.2
1	A	354	GLU	2.2
1	C	235	PRO	2.2
1	F	462	PRO	2.2
1	H	450	PRO	2.2
1	M	178	GLU	2.2
1	D	369	VAL	2.2
1	D	396	VAL	2.2
1	D	422	VAL	2.2
1	E	336	VAL	2.2
1	E	442	VAL	2.2
1	G	369	VAL	2.2
1	K	442	VAL	2.2
1	K	380	LYS	2.2
1	L	351	GLN	2.2
1	A	127	ALA	2.2
1	B	511	ALA	2.2
1	C	81	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	93	THR	2.2
1	D	313	THR	2.2
1	E	212	ALA	2.2
1	E	517	THR	2.2
1	F	340	ALA	2.2
1	I	91	THR	2.2
1	I	212	ALA	2.2
1	J	210	THR	2.2
1	L	50	THR	2.2
1	L	481	ALA	2.2
1	B	250	ILE	2.2
1	E	227	ILE	2.2
1	E	318	GLY	2.2
1	E	459	GLY	2.2
1	H	103	GLY	2.2
1	I	182	GLY	2.2
1	K	180	GLY	2.2
1	A	224	ASP	2.2
1	N	302	SER	2.2
1	H	317	LEU	2.2
1	I	200	LEU	2.2
1	L	17	LEU	2.2
1	L	365	LEU	2.2
1	A	58	ARG	2.2
1	I	390	LYS	2.2
1	C	348	GLN	2.2
1	F	366	GLN	2.2
1	A	219	PHE	2.2
1	D	195	PHE	2.2
1	D	219	PHE	2.2
1	D	323	VAL	2.2
1	F	506	TYR	2.2
1	J	300	VAL	2.2
1	M	56	VAL	2.2
1	J	310	GLU	2.2
1	C	507	ALA	2.2
1	E	19	GLY	2.2
1	E	490	ASP	2.2
1	F	341	ALA	2.2
1	G	413	ALA	2.2
1	G	443	ALA	2.2
1	H	511	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	384	ALA	2.2
1	J	57	ALA	2.2
1	J	239	ALA	2.2
1	J	258	ALA	2.2
1	J	377	ALA	2.2
1	L	145	ALA	2.2
1	L	512	GLY	2.2
1	C	55	SER	2.2
1	E	327	LYS	2.2
1	G	526	LYS	2.2
1	D	58	ARG	2.2
1	E	452	ARG	2.2
1	C	100	ILE	2.1
1	F	205	ILE	2.1
1	H	250	ILE	2.1
1	I	515	ILE	2.1
1	B	400	LEU	2.1
1	E	131	LEU	2.1
1	F	17	LEU	2.1
1	J	161	LEU	2.1
1	L	31	LEU	2.1
1	L	504	LEU	2.1
1	L	513	LEU	2.1
1	B	310	GLU	2.1
1	C	136	VAL	2.1
1	E	499	VAL	2.1
1	F	381	VAL	2.1
1	G	14	VAL	2.1
1	H	315	GLU	2.1
1	K	455	VAL	2.1
1	G	203	TYR	2.1
1	H	283	ASP	2.1
1	M	225	LYS	2.1
1	N	514	MET	2.1
1	D	35	GLY	2.1
1	C	30	THR	2.1
1	C	92	ALA	2.1
1	C	170	GLY	2.1
1	D	89	THR	2.1
1	E	443	ALA	2.1
1	H	108	ALA	2.1
1	H	507	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	53	GLY	2.1
1	L	241	ALA	2.1
1	N	103	GLY	2.1
1	I	210	THR	2.1
1	N	500	THR	2.1
1	L	496	PRO	2.1
1	C	178	GLU	2.1
1	J	454	ILE	2.1
1	L	150	ILE	2.1
1	M	420	ILE	2.1
1	D	504	LEU	2.1
1	J	116	LEU	2.1
1	L	131	LEU	2.1
1	C	190	VAL	2.1
1	C	254	VAL	2.1
1	J	283	ASP	2.1
1	J	369	VAL	2.1
1	L	407	VAL	2.1
1	M	167	ASP	2.1
1	M	442	VAL	2.1
1	N	74	VAL	2.1
1	A	453	GLN	2.1
1	C	297	GLY	2.1
1	D	514	MET	2.1
1	G	416	GLY	2.1
1	H	88	GLY	2.1
1	I	447	MET	2.1
1	A	71	ALA	2.1
1	H	92	ALA	2.1
1	H	443	ALA	2.1
1	H	463	SER	2.1
1	C	294	THR	2.1
1	D	462	PRO	2.1
1	F	296	THR	2.1
1	J	101	THR	2.1
1	M	156	GLU	2.1
1	N	449	ALA	2.1
1	B	49	ILE	2.1
1	D	325	ILE	2.1
1	E	493	ILE	2.1
1	F	454	ILE	2.1
1	G	144	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	220	ILE	2.1
1	I	23	LEU	2.1
1	J	183	LEU	2.1
1	J	445	ARG	2.1
1	L	200	LEU	2.1
1	M	513	LEU	2.1
1	G	27	VAL	2.1
1	G	29	VAL	2.1
1	G	492	GLY	2.1
1	G	512	GLY	2.1
1	H	422	VAL	2.1
1	K	367	GLU	2.1
1	K	438	VAL	2.1
1	L	35	GLY	2.1
1	N	186	GLU	2.1
1	K	389	MET	2.1
1	D	57	ALA	2.1
1	E	468	THR	2.1
1	H	106	ALA	2.1
1	J	26	ALA	2.1
1	K	239	ALA	2.1
1	L	57	ALA	2.1
1	N	57	ALA	2.1
1	I	206	ASN	2.1
1	D	224	ASP	2.1
1	M	172	GLU	2.1
1	G	420	ILE	2.1
1	A	234	LEU	2.1
1	B	344	GLY	2.1
1	E	221	LEU	2.1
1	I	456	LEU	2.1
1	K	17	LEU	2.1
1	J	245	LYS	2.1
1	K	139	SER	2.1
1	B	136	VAL	2.1
1	B	464	VAL	2.1
1	D	447	MET	2.1
1	D	465	VAL	2.1
1	E	190	VAL	2.1
1	A	84	ALA	2.1
1	D	508	ALA	2.1
1	E	239	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	96	ALA	2.1
1	H	8	PHE	2.1
1	H	127	ALA	2.1
1	I	98	ALA	2.1
1	I	281	PHE	2.1
1	I	480	ALA	2.1
1	J	24	ALA	2.1
1	K	101	THR	2.1
1	K	133	ALA	2.1
1	M	91	THR	2.1
1	N	516	THR	2.1
1	A	362	ARG	2.1
1	B	368	ARG	2.1
1	C	352	GLN	2.1
1	C	391	GLU	2.1
1	F	308	GLU	2.1
1	B	277	LYS	2.1
1	H	53	GLY	2.1
1	L	225	LYS	2.1
1	C	150	ILE	2.1
1	G	489	ILE	2.1
1	I	325	ILE	2.1
1	G	295	LEU	2.1
1	I	187	LEU	2.1
1	J	288	MET	2.1
1	B	359	ASP	2.1
1	G	465	VAL	2.1
1	H	367	GLU	2.1
1	I	107	VAL	2.1
1	L	172	GLU	2.1
1	L	196	ASP	2.1
1	L	369	VAL	2.1
1	N	271	VAL	2.1
1	N	442	VAL	2.1
1	N	455	VAL	2.1
1	A	243	ALA	2.1
1	B	109	ALA	2.1
1	H	97	GLN	2.1
1	H	343	GLN	2.1
1	H	366	GLN	2.1
1	H	453	GLN	2.1
1	J	508	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	26	ALA	2.1
1	N	443	ALA	2.1
1	B	182	GLY	2.1
1	H	255	GLU	2.0
1	J	303	GLU	2.0
1	K	315	GLU	2.0
1	B	288	MET	2.0
1	C	183	LEU	2.0
1	H	23	LEU	2.0
1	I	292	ILE	2.0
1	I	332	ILE	2.0
1	C	525	PRO	2.0
1	D	114	MET	2.0
1	E	235	PRO	2.0
1	H	33	PRO	2.0
1	J	247	LEU	2.0
1	L	246	PRO	2.0
1	M	451	LEU	2.0
1	N	31	LEU	2.0
1	D	442	VAL	2.0
1	F	466	ALA	2.0
1	G	147	VAL	2.0
1	H	89	THR	2.0
1	H	260	ALA	2.0
1	I	30	THR	2.0
1	I	516	THR	2.0
1	J	347	ALA	2.0
1	M	324	VAL	2.0
1	N	101	THR	2.0
1	H	281	PHE	2.0
1	D	388	GLU	2.0
1	D	410	GLY	2.0
1	E	415	GLY	2.0
1	F	211	GLY	2.0
1	I	415	GLY	2.0
1	N	416	GLY	2.0
1	B	421	ARG	2.0
1	B	501	ARG	2.0
1	E	502	SER	2.0
1	L	79	SER	2.0
1	M	141	SER	2.0
1	C	453	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	168	LYS	2.0
1	L	242	LYS	2.0
1	L	245	LYS	2.0
1	D	233	MET	2.0
1	G	342	ILE	2.0
1	G	515	ILE	2.0
1	J	292	ILE	2.0
1	K	16	MET	2.0
1	L	379	ILE	2.0
1	N	494	LEU	2.0
1	A	443	ALA	2.0
1	B	341	ALA	2.0
1	C	443	ALA	2.0
1	D	90	THR	2.0
1	D	418	ALA	2.0
1	I	2	ALA	2.0
1	J	443	ALA	2.0
1	L	101	THR	2.0
1	M	275	ALA	2.0
1	G	124	VAL	2.0
1	G	442	VAL	2.0
1	G	510	VAL	2.0
1	H	94	VAL	2.0
1	H	438	VAL	2.0
1	H	469	VAL	2.0
1	J	74	VAL	2.0
1	M	22	VAL	2.0
1	M	369	VAL	2.0
1	N	38	VAL	2.0
1	B	298	GLY	2.0
1	B	410	GLY	2.0
1	C	345	ARG	2.0
1	D	88	GLY	2.0
1	H	19	GLY	2.0
1	G	302	SER	2.0
1	H	352	GLN	2.0
1	J	154	SER	2.0
1	B	33	PRO	2.0
1	G	208	PRO	2.0
1	L	235	PRO	2.0
1	E	488	MET	2.0
1	B	214	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	252	GLU	2.0
1	A	150	ILE	2.0
1	A	402	ALA	2.0
1	B	489	ILE	2.0
1	C	96	ALA	2.0
1	C	418	ALA	2.0
1	D	413	ALA	2.0
1	E	325	ILE	2.0
1	H	278	ALA	2.0
1	H	295	LEU	2.0
1	I	331	THR	2.0
1	J	17	LEU	2.0
1	J	251	ALA	2.0
1	L	444	LEU	2.0
1	M	162	ILE	2.0
1	N	239	ALA	2.0
1	A	97	GLN	2.0
1	B	29	VAL	2.0
1	C	74	VAL	2.0
1	C	416	GLY	2.0
1	D	321	LYS	2.0
1	E	286	LYS	2.0
1	E	486	GLY	2.0
1	F	464	VAL	2.0
1	F	465	VAL	2.0
1	G	128	VAL	2.0
1	I	14	VAL	2.0
1	I	376	VAL	2.0
1	K	464	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	K	D	1	1/1	0.98	0.36	2.52	29,29,29,29	0
3	K	E	527	1/1	0.94	0.32	1.42	31,31,31,31	0
3	K	D	560	1/1	0.98	0.24	0.66	16,16,16,16	0
4	AGS	M	1	31/31	0.94	0.20	0.26	5,12,18,21	0
4	AGS	D	561	31/31	0.94	0.23	0.26	2,11,18,21	0
4	AGS	K	1	31/31	0.95	0.18	0.25	6,14,21,24	0
4	AGS	F	1	31/31	0.95	0.22	0.24	2,11,22,23	0
4	AGS	C	1	31/31	0.94	0.20	0.13	8,13,19,20	0
4	AGS	I	1	31/31	0.94	0.20	-0.08	5,12,16,20	0
4	AGS	A	1	31/31	0.96	0.19	-0.15	4,11,16,20	0
4	AGS	L	1	31/31	0.95	0.19	-0.19	2,8,11,18	0
4	AGS	G	1	31/31	0.95	0.21	-0.19	4,9,16,16	0
4	AGS	N	1	31/31	0.96	0.20	-0.20	4,10,17,19	0
3	K	E	560	1/1	0.98	0.21	-0.24	11,11,11,11	0
4	AGS	E	1	31/31	0.95	0.21	-0.26	2,11,19,20	0
4	AGS	J	1	31/31	0.93	0.17	-0.33	2,7,14,15	0
4	AGS	B	1	31/31	0.96	0.20	-0.59	8,13,21,24	0
4	AGS	H	1	31/31	0.95	0.18	-0.91	3,9,15,17	0
3	K	F	560	1/1	0.99	0.14	-1.14	13,13,13,13	0
3	K	B	560	1/1	0.98	0.18	-1.17	13,13,13,13	0
3	K	H	560	1/1	0.97	0.15	-1.65	15,15,15,15	0
3	K	M	560	1/1	0.97	0.17	-1.75	14,14,14,14	0
3	K	C	560	1/1	0.93	0.16	-1.82	19,19,19,19	0
3	K	N	560	1/1	0.98	0.14	-2.04	11,11,11,11	0
3	K	G	560	1/1	0.97	0.15	-2.35	16,16,16,16	0
3	K	J	560	1/1	0.94	0.14	-2.53	11,11,11,11	0
3	K	L	560	1/1	0.98	0.15	-2.61	6,6,6,6	0
3	K	A	560	1/1	0.98	0.16	-2.64	13,13,13,13	0
3	K	K	560	1/1	0.97	0.11	-2.64	11,11,11,11	0
3	K	I	560	1/1	0.98	0.15	-3.39	11,11,11,11	0
2	MG	J	550	1/1	0.93	0.23	-	8,8,8,8	0
2	MG	L	550	1/1	0.92	0.23	-	9,9,9,9	0
2	MG	G	550	1/1	0.94	0.25	-	9,9,9,9	0
2	MG	I	550	1/1	0.93	0.24	-	9,9,9,9	0
2	MG	D	550	1/1	0.95	0.21	-	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	E	550	1/1	0.95	0.18	-	6,6,6,6	0
2	MG	H	550	1/1	0.95	0.21	-	4,4,4,4	0
2	MG	F	550	1/1	0.92	0.24	-	7,7,7,7	0
2	MG	C	550	1/1	0.98	0.16	-	9,9,9,9	0
2	MG	B	550	1/1	0.90	0.22	-	8,8,8,8	0
2	MG	A	550	1/1	0.93	0.21	-	7,7,7,7	0
2	MG	N	550	1/1	0.96	0.21	-	7,7,7,7	0
2	MG	M	550	1/1	0.93	0.23	-	7,7,7,7	0
2	MG	K	550	1/1	0.98	0.14	-	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.