



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:20 PM GMT

PDB ID : 1SX3
Title : GroEL14-(ATPgammaS)14
Authors : Chaudhry, C.; Horwich, A.L.; Brunger, A.T.; Adams, P.D.
Deposited on : 2004-03-30
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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

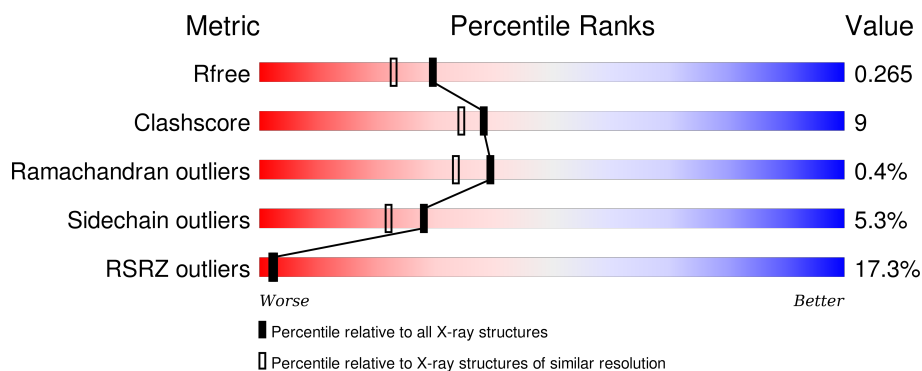
1 Overall quality at a glance

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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>13%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	B	525	<div> <div>24%</div> <div>73%</div> <div>22%</div> <div>.</div> </div>
1	C	525	<div> <div>22%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	D	525	<div> <div>6%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
1	E	525	<div> <div>18%</div> <div>72%</div> <div>23%</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

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).

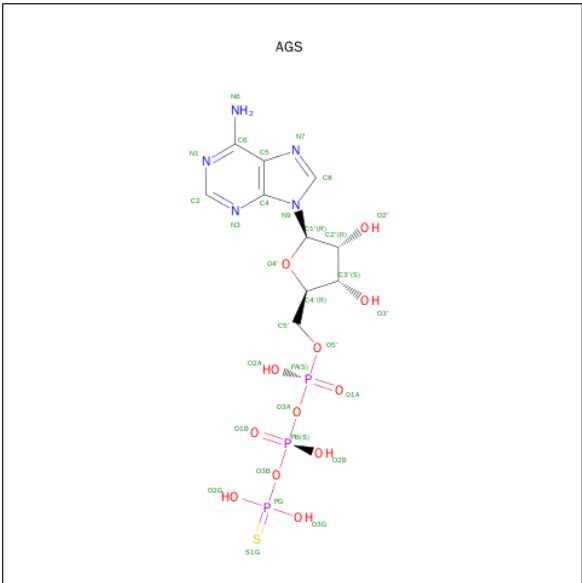
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	K 1	0	0
3	J	1	Total 1	K 1	0	0
3	D	2	Total 2	K 2	0	0
3	K	1	Total 1	K 1	0	0
3	E	2	Total 2	K 2	0	0
3	H	1	Total 1	K 1	0	0
3	B	1	Total 1	K 1	0	0
3	I	1	Total 1	K 1	0	0
3	C	1	Total 1	K 1	0	0
3	A	1	Total 1	K 1	0	0
3	N	1	Total 1	K 1	0	0

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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).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	G	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	H	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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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

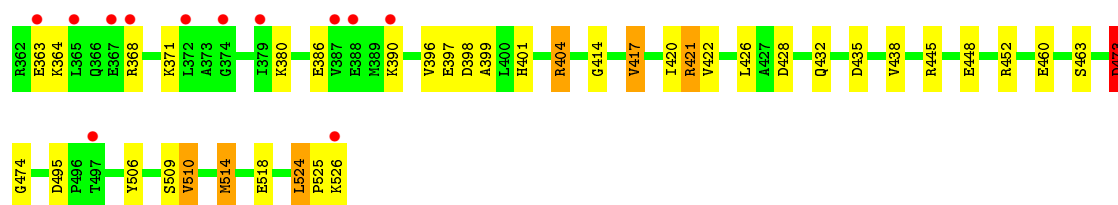
- Molecule 5 is water.

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

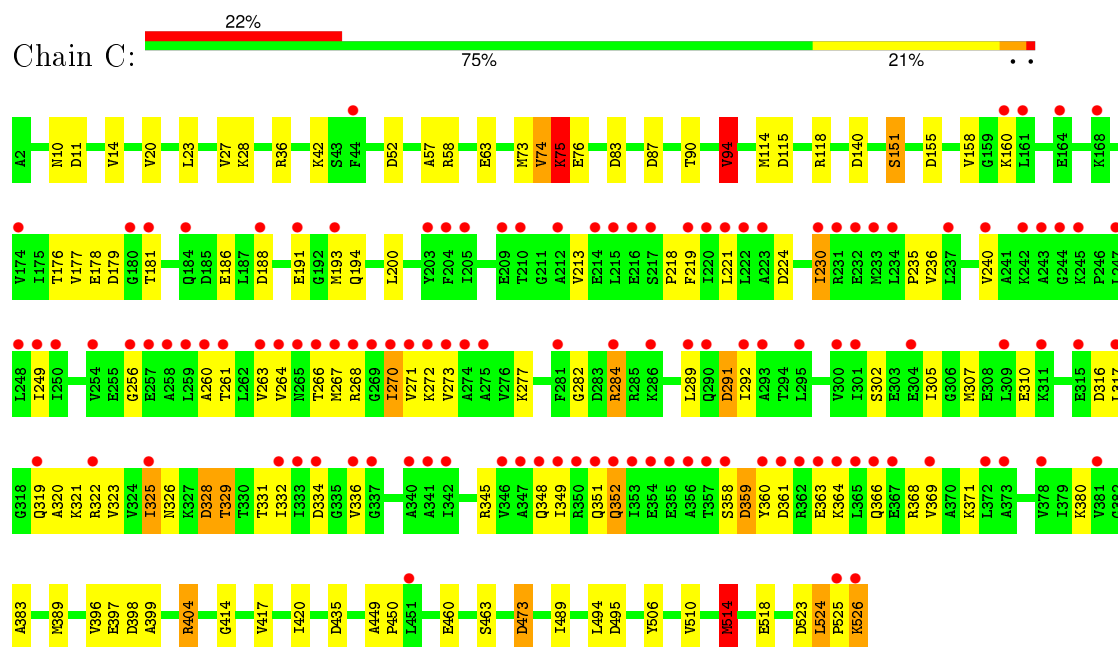
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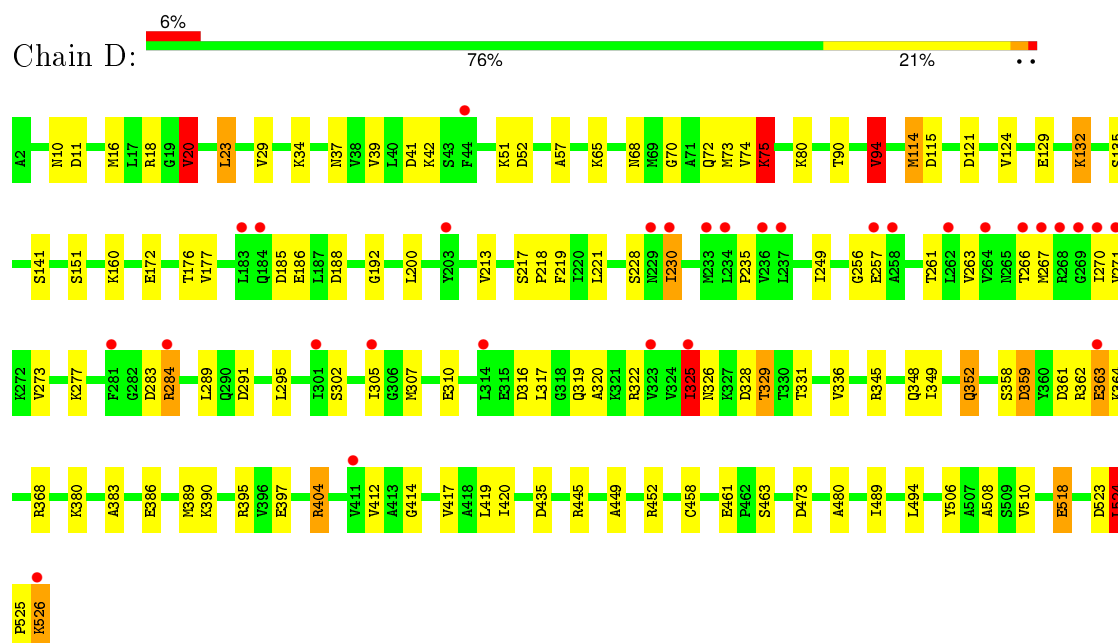
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	N	59	Total	O	0	0
			59	59		



• Molecule 1: groEL protein

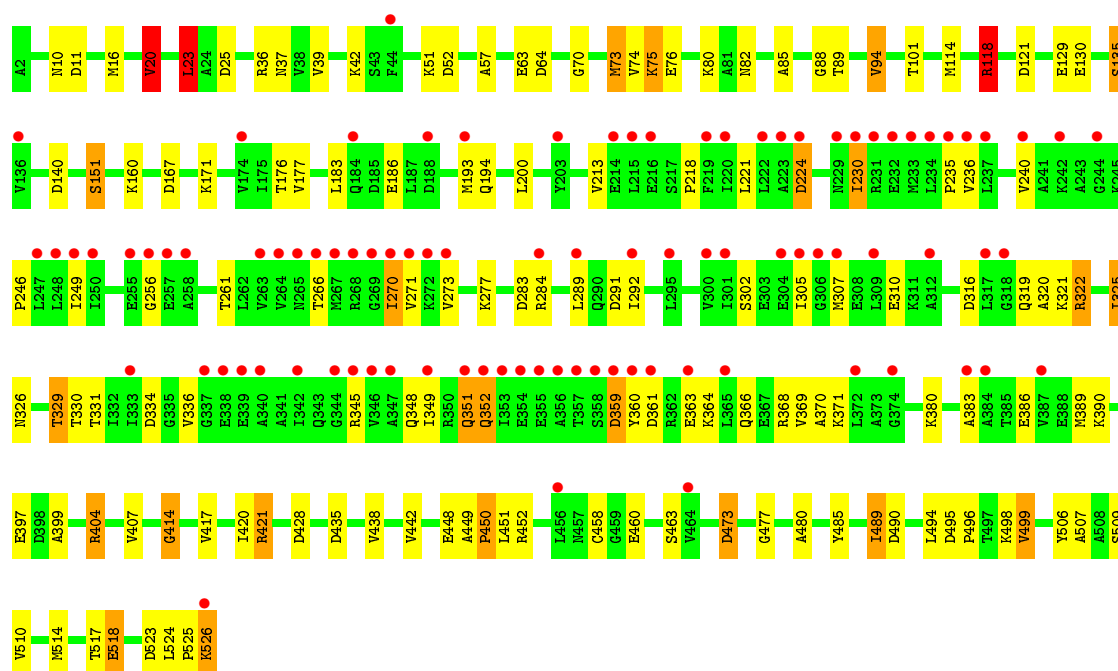


• Molecule 1: groEL protein



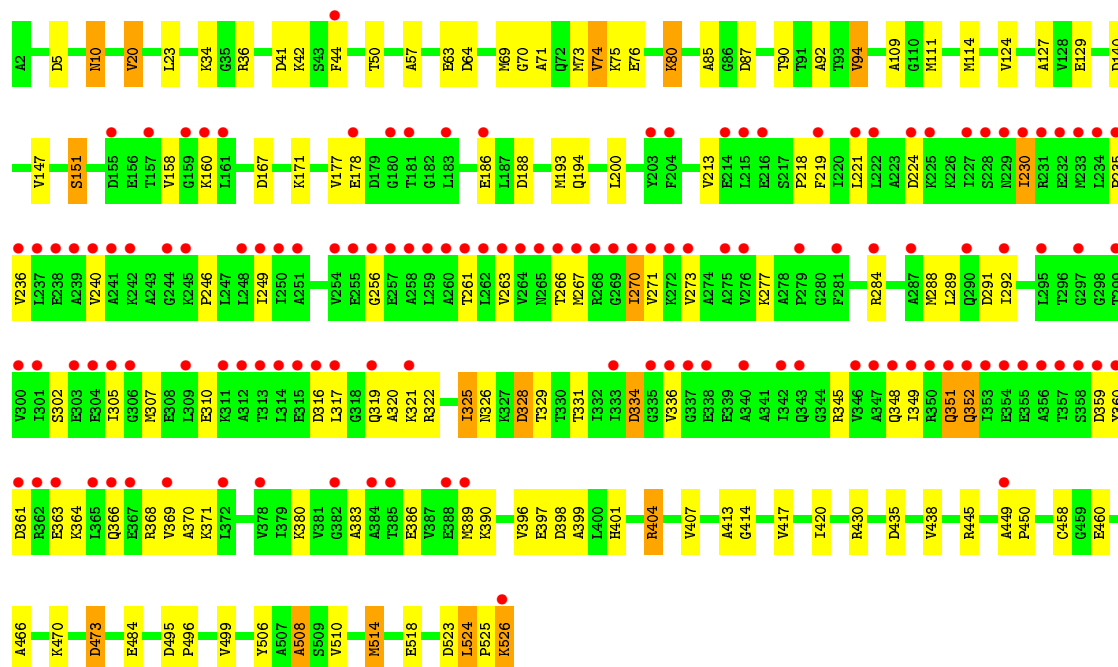
• Molecule 1: groEL protein





- Molecule 1: groEL protein

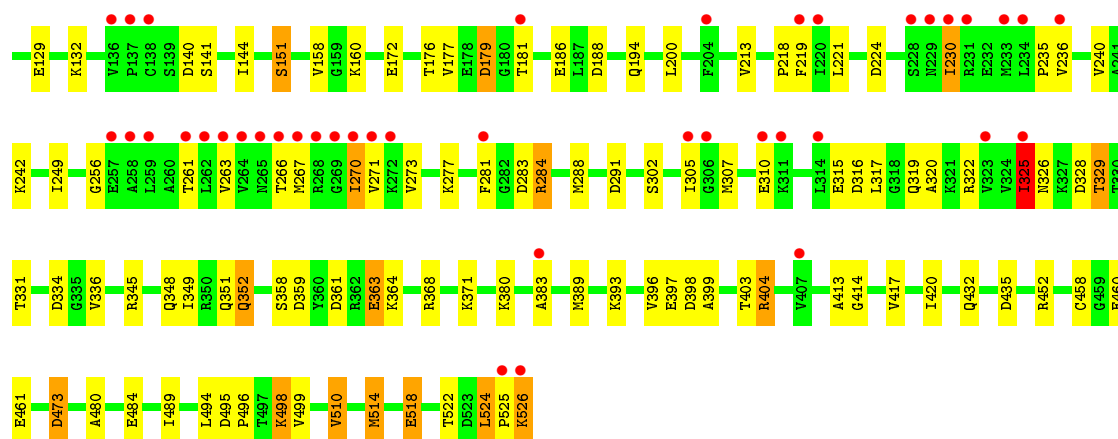
Chain F: 25% 73% 24%



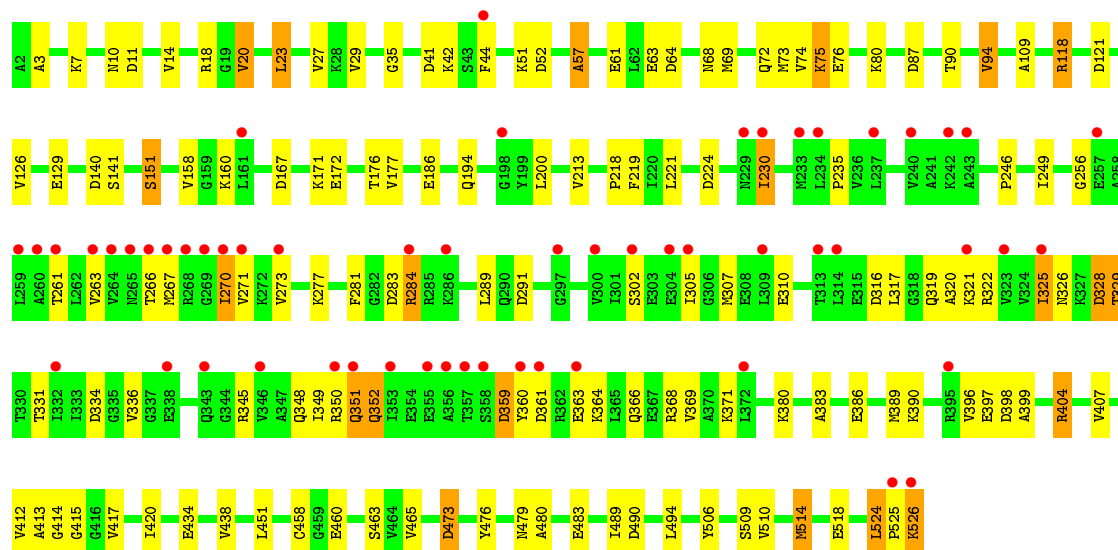
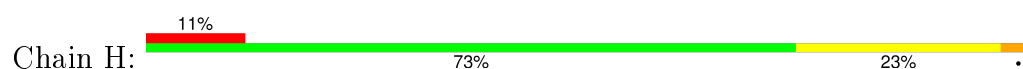
- Molecule 1: groEL protein

Chain G: 8% 73% 23%

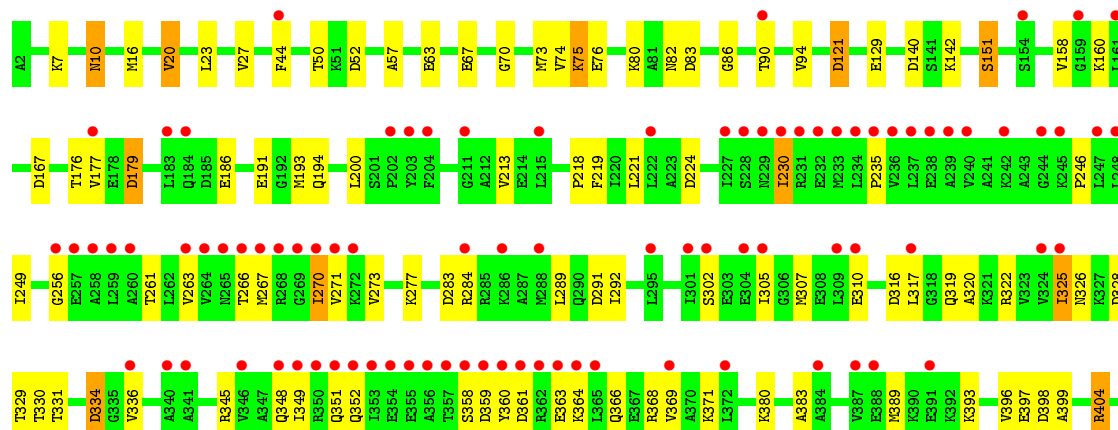
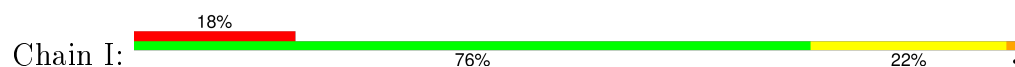




• Molecule 1: groEL protein

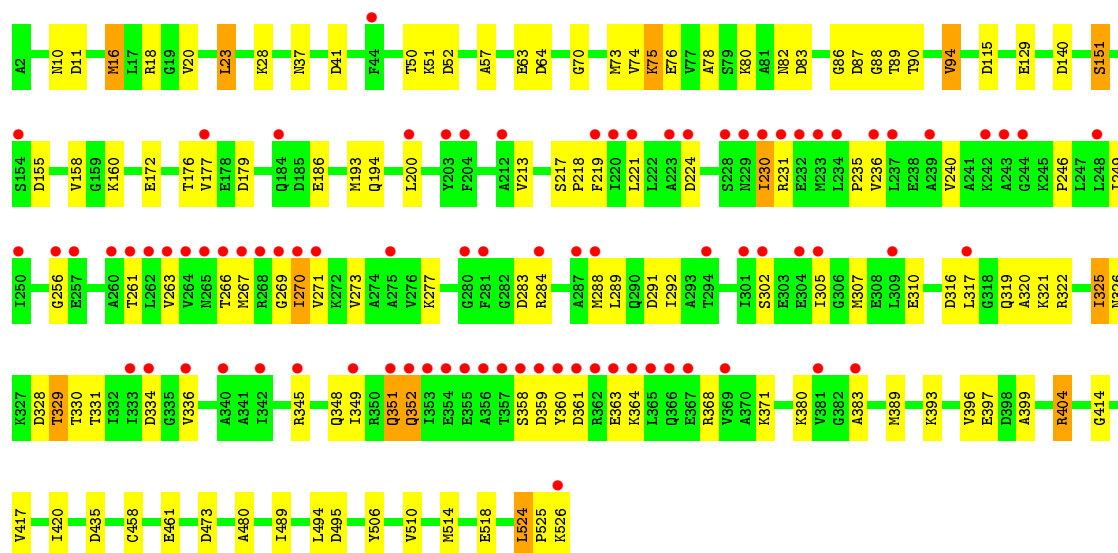
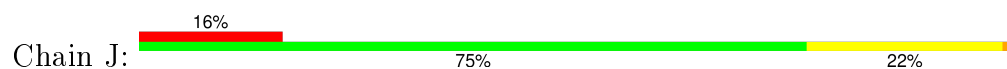


• Molecule 1: groEL protein

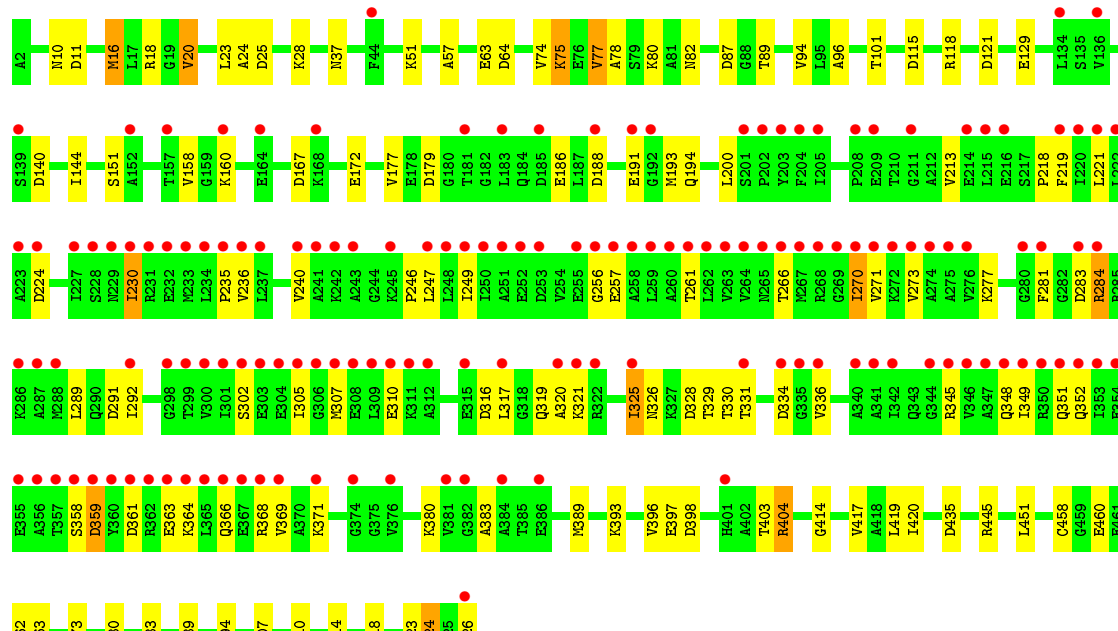
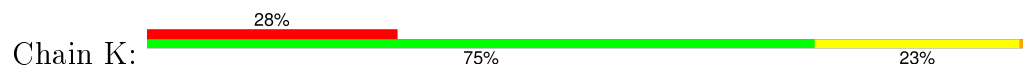




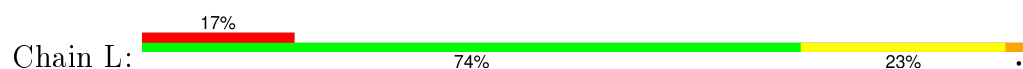
• Molecule 1: groEL protein

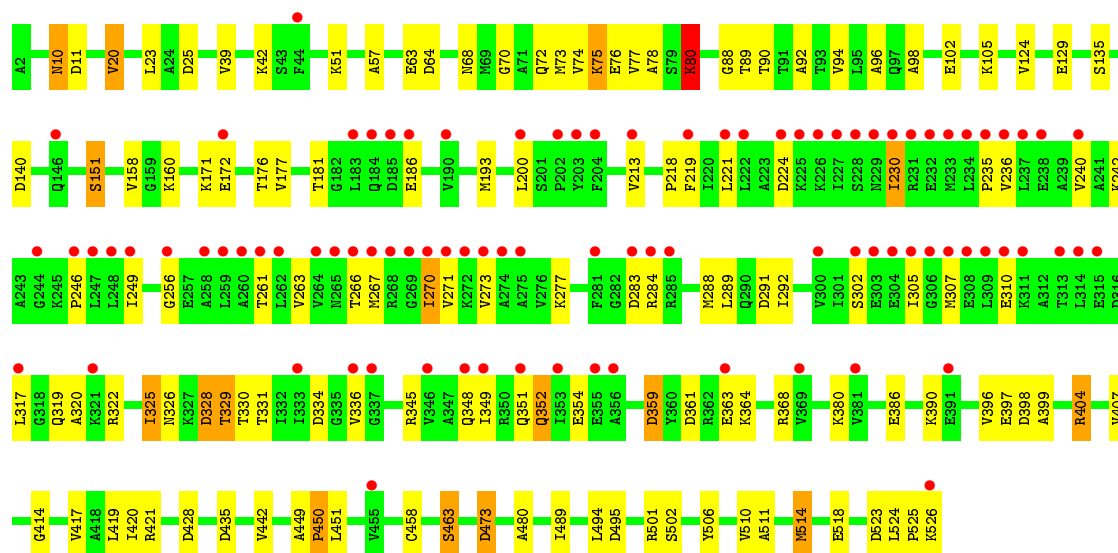


• Molecule 1: groEL protein

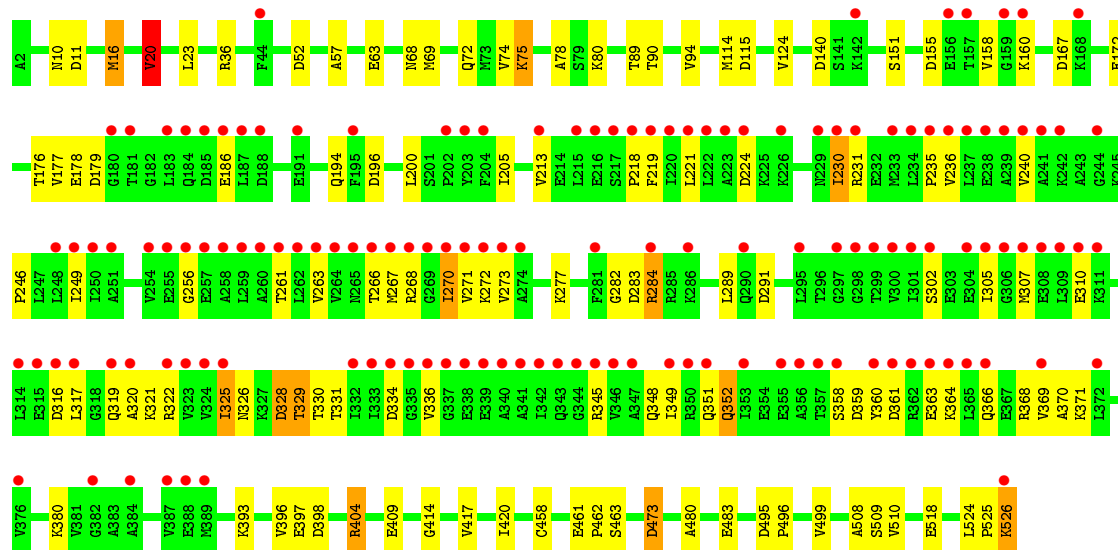
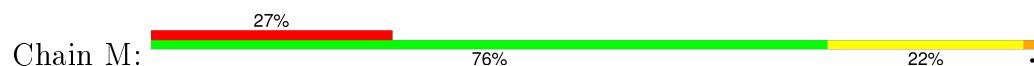


• Molecule 1: groEL protein

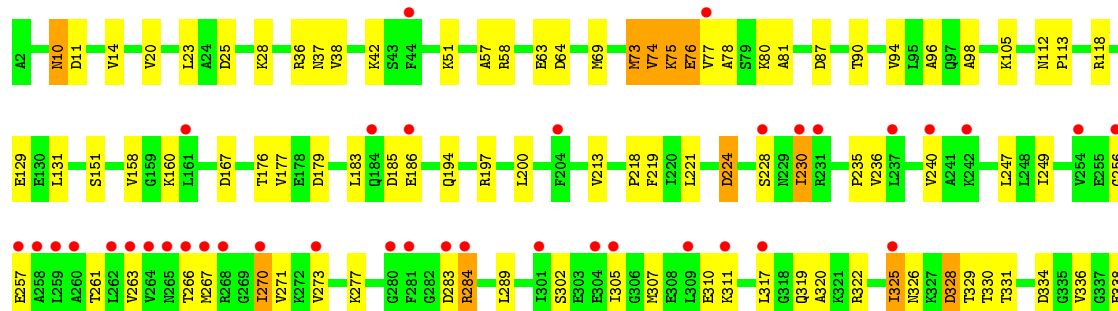


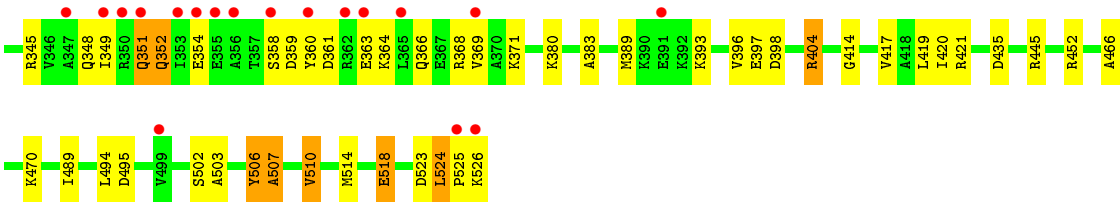


• Molecule 1: groEL protein



• 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 5	Depositor
R, R_{free}	0.245 , 0.265 0.246 , 0.265	Depositor DCC
R_{free} test set	10672 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 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 645898 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.94	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, 0.375 respectively for untwinned datasets, and 0.333, 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:J:1:AGS:S1G	4:J:1:AGS:PG	1.52	1.51
4:B:1:AGS:PG	4:B:1:AGS:S1G	1.52	1.51
4:H:1:AGS:PG	4:H:1:AGS:S1G	1.51	1.51
4:C:1:AGS:PG	4:C: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:L:1:AGS:PG	4:L:1:AGS:S1G	1.49	1.47
4:D:561:AGS:PG	4:D:561:AGS:S1G	1.48	1.47
1:G:114:MET:CE	1:G:114:MET:SD	2.02	1.47
4:N:1:AGS:PG	4:N:1:AGS:S1G	1.47	1.46
4:E:1:AGS:PG	4:E: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:L:514:MET:CB	1:L:514:MET:CE	2.60	0.80
1:C:349:ILE:HA	1:C:352:GLN:HG3	1.64	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
4:L:1:AGS:O3B	4:L:1:AGS:S1G	2.41	0.78
1:B:213:VAL:HB	1:B:325:ILE:HG12	1.64	0.78
1:E:349:ILE:HA	1:E:352:GLN:HG3	1.65	0.78
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.66	0.78
1:E:177:VAL:HG21	1:E:397:GLU:HG3	1.66	0.78
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.66	0.78
1:A:349:ILE:HA	1:A:352:GLN:HG3	1.65	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:I:177:VAL:HG21	1:I:397:GLU:HG3	1.64	0.77
1:E:213:VAL:HB	1:E:325:ILE:HG12	1.65	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
4:G:1:AGS:O3B	4:G:1:AGS:S1G	2.44	0.75
1:D:345:ARG:HA	1:D:348:GLN:HE21	1.52	0.75
1:J:63:GLU:OE2	1:K:526:LYS:HE2	1.87	0.75
4:B:1:AGS:S1G	4:B:1:AGS:O3B	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:I:213:VAL:HB	1:I:325:ILE:HG12	1.70	0.73
1:D:326:ASN:HD22	1:D:329:THR:HB	1.53	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
4:J:1:AGS:O3B	4:J:1:AGS:S1G	2.49	0.71
1:A:268:ARG:O	1:B:257:GLU:HG3	1.90	0.71
1:A:57:ALA:O	1:A:75:LYS:HE3	1.90	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:H:213:VAL:HB	1:H:325:ILE:HG12	1.71	0.71
1:G:359:ASP:O	1:G:363:GLU:HG2	1.91	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:I:345:ARG:HA	1:I:348:GLN:HE21	1.56	0.70
1:G:489:ILE:HD12	1:G:494:LEU:CD2	2.21	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:N:345:ARG:HA	1:N:348:GLN:HE21	1.57	0.70
1:H:345:ARG:HA	1:H:348:GLN:HE21	1.56	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:K:359:ASP:O	1:K:363:GLU:HG2	1.92	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
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
4:G:1:AGS:S1G	4:G:1:AGS:O3G	2.51	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ALA:O	1:F:75:LYS:HE3	1.92	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
4:M:1:AGS:O3G	4:M:1:AGS:S1G	2.47	0.67
1:L:291:ASP:OD2	1:L:368:ARG:HD2	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:H:359:ASP:O	1:H:363:GLU:HG2	1.95	0.67
1:D:176:THR:HG21	1:D:322:ARG:HH12	1.59	0.67
1:J:23:LEU:HD22	1:J:74:VAL:HG13	1.76	0.67
1:D:404:ARG:HG2	1:D:404:ARG:HH11	1.60	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:345:ARG:HA	1:M:348:GLN:HE21	1.60	0.66
1:M:291:ASP:OD2	1:M:368:ARG:HD2	1.95	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:N:510:VAL:CG2	1:N:510:VAL:CG1	2.70	0.65
1:E:194:GLN:O	1:E:371:LYS:HE3	1.97	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:G:213:VAL:HB	1:G:325:ILE:HG12	1.79	0.65
1:D:489:ILE:HD12	1:D:494:LEU:CD2	2.27	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:J:326:ASN:HD22	1:J:329:THR:HB	1.62	0.64
1:F:63:GLU:OE2	1:G:526:LYS:HE2	1.96	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:F:359:ASP:O	1:F:363:GLU:HG2	1.98	0.63
1:B:326:ASN:HD22	1:B:329:THR:HB	1.62	0.63
1:G:326:ASN:HD22	1:G:329:THR:HB	1.64	0.63
1:C:345:ARG:HA	1:C:348:GLN:HE21	1.62	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:K:291:ASP:OD2	1:K:368:ARG:HD2	1.98	0.63
1:I:291:ASP:OD2	1:I:368:ARG:HD2	1.98	0.63
1:G:218:PRO:HD2	1:G:320:ALA:O	1.99	0.62
1:E:291:ASP:OD2	1:E:368:ARG:HD2	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:M:272:LYS:NZ	1:N:228:SER:HB2	2.14	0.62
1:C:181:THR:N	5:C:615:HOH:O	2.29	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:G:114:MET:HB3	5:G:608:HOH:O	1.98	0.61
1:M:525:PRO:O	1:M:526:LYS:HG2	2.00	0.61
1:H:326:ASN:HD22	1:H:329:THR:HB	1.64	0.61
1:F:266:THR:HG21	1:F:273:VAL:O	1.99	0.61
1:A:445:ARG:NH2	5:A:607:HOH:O	2.32	0.61
1:K:23:LEU:HD22	1:K:74:VAL:HG13	1.83	0.61
1:E:525:PRO:O	1:E:526:LYS:HG2	2.00	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:78:ALA:HB1	1:B:89:THR:HB	1.83	0.61
1:B:218:PRO:HD2	1:B:320:ALA:O	2.00	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: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:I:428:ASP:HB2	5:I:608:HOH:O	2.00	0.60
1:F:73:MET:O	1:F:76:GLU:HB2	2.01	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:I:23:LEU:HD22	1:I:74:VAL:HG13	1.83	0.60
1:H:414:GLY:O	1:H:417:VAL:HG13	2.01	0.60
1:L:176:THR:HG21	1:L:322:ARG:HH12	1.67	0.60
1:G:266:THR:HG21	1:G:273:VAL:O	2.01	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
4:N:1:AGS:O3B	4:N:1:AGS:S1G	2.57	0.59
1:E:57:ALA:O	1:E:75:LYS:HE3	2.02	0.59
1:D:284:ARG:HH11	1:D:364:LYS:HD2	1.67	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:B:23:LEU:HD22	1:B:74:VAL:HG13	1.84	0.59
1:L:218:PRO:HD2	1:L:320:ALA:O	2.03	0.59
1:K:414:GLY:O	1:K:417:VAL:HG13	2.02	0.59
1:A:458:CYS:SG	1:A:480:ALA:HB1	2.42	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:I:525:PRO:O	1:I:526:LYS:CG	2.51	0.59
1:H:266:THR:HG21	1:H:273:VAL:O	2.02	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:J:266:THR:HG21	1:J:273:VAL:O	2.04	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: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:B:266:THR:CG2	1:B:273:VAL:H	2.17	0.57
1:A:194:GLN:O	1:A:371:LYS:HE3	2.03	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:G:230:ILE:HD12	1:G:261:THR:HG21	1.86	0.57
1:A:526:LYS:HE2	1:G:63:GLU:OE2	2.04	0.57
1:J:218:PRO:HD2	1:J:320:ALA:O	2.05	0.57
1:D:132:LYS:HE2	5:D:595:HOH:O	2.04	0.57
1:C:266:THR:HG22	1:C:273:VAL:H	1.70	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:I:266:THR:CG2	1:I:273:VAL:H	2.18	0.56
1:L:514:MET:CG	1:L:514:MET:CE	2.83	0.56
1:B:525:PRO:O	1:B:526:LYS:CG	2.53	0.56
1:L:266:THR:HG22	1:L:273:VAL:H	1.69	0.56
1:C:266:THR:HG21	1:C:273:VAL:O	2.05	0.56
1:E:266:THR:HG22	1:E:273:VAL:H	1.71	0.56
1:A:266:THR:CG2	1:A:273:VAL:H	2.18	0.56
1:I:266:THR:HG21	1:I:273:VAL:O	2.04	0.56
1:C:218:PRO:HD2	1:C:320:ALA:O	2.04	0.56
1:D:305:ILE:HD12	1:D:307:MET:HE2	1.86	0.56
1:I:448:GLU:OE2	1:I:470:LYS:NZ	2.32	0.56
1:J:23:LEU:CD2	1:J:74:VAL:HG13	2.35	0.56
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.88	0.56
1:M:266:THR:HG21	1:M:273:VAL:O	2.05	0.56
1:K:266:THR:CG2	1:K:273:VAL:H	2.18	0.56
1:C:23:LEU:HD22	1:C:74:VAL:HG13	1.87	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: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:A:291:ASP:OD2	1:A:368:ARG:HD2	2.06	0.55
1:G:525:PRO:O	1:G:526:LYS:CG	2.54	0.55
1:D:218:PRO:HD2	1:D:320:ALA:O	2.05	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:N:266:THR:CG2	1:N:273:VAL:H	2.20	0.55
1:M:414:GLY:O	1:M:417:VAL:HG13	2.07	0.55
1:G:525:PRO:O	1:G:526:LYS:HG2	2.06	0.55
1:C:230:ILE:HD12	1:C:261:THR:HG21	1.88	0.55
1:A:404:ARG:HH11	1:A:404:ARG:HG2	1.72	0.55
1:M:266:THR:HG22	1:M:273:VAL:H	1.72	0.55
1:J:194:GLN:O	1:J:371:LYS:HE3	2.05	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: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:18:ARG:NE	5:D:587:HOH:O	2.36	0.55
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: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:D:90:THR:O	1:D:94:VAL:HG13	2.07	0.54
1:A:231:ARG:HH12	1:G:242:LYS:CG	2.21	0.54
1:B:176:THR:HG21	1:B:322:ARG:HH12	1.72	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:C:200:LEU:HD21	1:C:277:LYS:HG3	1.90	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:D:70:GLY:HA2	1:D:73:MET:HE3	1.90	0.54
1:C:272:LYS:HZ3	1:D:228:SER:HB2	1.73	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:I:230:ILE:HD12	1:I:261:THR:HG21	1.89	0.54
1:E:305:ILE:HD12	1:E:307:MET:HE2	1.90	0.54
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.72	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:C:73:MET:O	1:C:76:GLU:HB2	2.08	0.54
1:L:525:PRO:O	1:L:526:LYS:HG2	2.08	0.54
1:B:181:THR:O	1:C:282:GLY:HA3	2.08	0.54
1:K:266:THR:HG22	1:K:273:VAL:H	1.73	0.54
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.89	0.54
1:M:230:ILE:HD12	1:M:261:THR:HG21	1.89	0.54
1:H:218:PRO:HD2	1:H:320:ALA:O	2.08	0.54
1:K:23:LEU:CD2	1:K:74:VAL:HG13	2.37	0.53
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: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: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:F:200:LEU:HD21	1:F:277:LYS:HG3	1.89	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: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:B:57:ALA:O	1:B:75:LYS:HE3	2.08	0.53
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.90	0.53
1:L:230:ILE:HD12	1:L:261:THR:HG21	1.90	0.53
1:J:224:ASP:HB3	1:J:302:SER:HB3	1.91	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: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:A:231:ARG:HH12	1:G:242:LYS:HG3	1.74	0.52
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.90	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:M:319:GLN:HB3	1:M:336:VAL:CG2	2.39	0.52
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.91	0.52
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.90	0.52
1:L:80:LYS:HZ3	1:L:80:LYS:CG	2.21	0.52
1:K:404:ARG:HH11	1:K:404:ARG:CG	2.22	0.52
1:A:414:GLY:O	1:A:417:VAL:HG13	2.09	0.52
1:L:158:VAL:HG13	1:L:396:VAL:HG22	1.91	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:H:90:THR:O	1:H:94:VAL:HG13	2.10	0.52
1:H:266:THR:HG22	1:H:273:VAL:H	1.74	0.52
1:J:230:ILE:HD12	1:J:261:THR:HG21	1.90	0.52
1:C:268:ARG:O	1:D:257:GLU:HG3	2.09	0.52
1:A:115:ASP:OD2	5:A:610:HOH:O	2.19	0.52
1:C:272:LYS:NZ	1:D:228:SER:CB	2.73	0.52
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.91	0.52
1:J:37:ASN:ND2	1:J:51:LYS:HE3	2.25	0.52
1:J:458:CYS:SG	1:J:480:ALA:HB1	2.50	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:B:16:MET:O	1:B:20:VAL:HG13	2.09	0.52
1:A:525:PRO:O	1:A:526:LYS:HG2	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: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: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:H:305:ILE:HD12	1:H:307:MET:HE2	1.92	0.51
1:A:272:LYS:NZ	1:B:228:SER:HB2	2.25	0.51
1:H:230:ILE:HD12	1:H:261:THR:HG21	1.93	0.51
1:E:383:ALA:HB3	1:E:389:MET:HB2	1.91	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:M:266:THR:HG22	1:M:271:VAL:O	2.10	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:J:270:ILE:HG22	1:J:271:VAL:HG23	1.92	0.51
1:N:414:GLY:O	1:N:417:VAL:HG13	2.11	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:F:235:PRO:HG3	1:F:310:GLU:HA	1.93	0.51
1:K:57:ALA:O	1:K:75:LYS:HE3	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:B:230:ILE:HD12	1:B:261:THR:HG21	1.91	0.51
1:G:345:ARG:HA	1:G:348:GLN:NE2	2.24	0.51
1:D:132:LYS:CE	5:D:595:HOH:O	2.58	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:H:194:GLN:O	1:H:371:LYS:HE3	2.11	0.50
1:A:489:ILE:HD12	1:A:494:LEU:CD2	2.41	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:F:74:VAL:O	1:F:74:VAL:CG2	2.58	0.50
1:D:37:ASN:ND2	1:D:51:LYS:HE3	2.27	0.50
1:N:230:ILE:HD12	1:N:261:THR:HG21	1.93	0.50
1:C:525:PRO:HD3	5:C:588:HOH:O	2.11	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:I:219:PHE:HB3	1:I:317:LEU:HD23	1.94	0.50
1:F:218:PRO:HD2	1:F:320:ALA:O	2.11	0.50
1:L:514:MET:HE2	1:L:514:MET:CB	2.41	0.50
1:D:345:ARG:HA	1:D:348:GLN:NE2	2.24	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:G:219:PHE:HB3	1:G:317:LEU:HD23	1.94	0.50
1:N:345:ARG:HA	1:N:348:GLN:NE2	2.24	0.50
1:I:70:GLY:HA2	1:I:73:MET:HE3	1.94	0.50
1:A:266:THR:HG22	1:A:273:VAL:H	1.76	0.50
1:M:270:ILE:HG22	1:M:271:VAL:HG23	1.93	0.50
1:K:305:ILE:HD12	1:K:307:MET:HE2	1.94	0.50
1:B:452:ARG:HD3	5:B:594:HOH:O	2.11	0.50
1:K:270:ILE:HG22	1:K:271:VAL:HG23	1.93	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:M:272:LYS:HZ3	1:N:228:SER:HB2	1.77	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:I:176:THR:HG21	1:I:322:ARG:HH12	1.76	0.49
1:D:525:PRO:O	1:D:526:LYS:HG2	2.11	0.49
1:J:525:PRO:O	1:J:526:LYS:HG2	2.11	0.49
1:E:266:THR:HG22	1:E:271:VAL:O	2.12	0.49
1:K:460:GLU:HB3	5:K:586:HOH: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:E:23:LEU:HD22	1:E:74:VAL:HG13	1.93	0.49
1:F:90:THR:O	1:F:94:VAL:HG13	2.13	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: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:L:186:GLU:HB2	1:L:380:LYS:HB2	1.95	0.49
1:F:319:GLN:HB3	1:F:336:VAL:HG21	1.93	0.49
1:L:305:ILE:HD12	1:L:307:MET:HE2	1.94	0.49
1:H:235:PRO:HG3	1:H:310:GLU:HA	1.95	0.49
1:E:366:GLN:O	1:E:369:VAL:HG22	2.13	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:I:325:ILE:HG22	1:I:330:THR:HG23	1.95	0.49
1:N:266:THR:HG22	1:N:271:VAL:O	2.12	0.49
1:K:266:THR:HG22	1:K:271:VAL:O	2.13	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: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:F:151:SER:HB2	1:F:399:ALA:HA	1.96	0.48
1:C:36:ARG:HG3	1:D:518:GLU:HG2	1.95	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:B:151:SER:HB2	1:B:399:ALA:HA	1.96	0.48
1:N:77:VAL:O	1:N:78:ALA:C	2.51	0.48
1:J:345:ARG:HA	1:J:348:GLN:NE2	2.26	0.48
1:I:266:THR:HG22	1:I:273:VAL:H	1.79	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:K:460:GLU:O	1:K:462:PRO:HD3	2.14	0.48
1:I:121:ASP:OD1	5:I:594:HOH:O	2.20	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:E:82:ASN:HB2	1:E:89:THR:HG21	1.95	0.48
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.96	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:M:404:ARG:CG	1:M:404:ARG:HH11	2.26	0.48
1:H:266:THR:HG21	1:H:273:VAL:H	1.78	0.48
1:N:74:VAL:HG22	1:N:74:VAL:O	2.13	0.48
1:B:176:THR:HG22	1:B:177:VAL:H	1.78	0.48
1:I:345:ARG:HA	1:I:348:GLN:NE2	2.26	0.48
1:A:178:GLU:OE2	1:A:322:ARG:HD3	2.13	0.48
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.95	0.48
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.96	0.48
1:N:266:THR:HG22	1:N:273:VAL:H	1.78	0.47
1:I:23:LEU:CD2	1:I:74:VAL:HG13	2.43	0.47
1:M:321:LYS:HB2	1:M:334:ASP:HB3	1.96	0.47
1:J:383:ALA:HB3	1:J:389:MET:HB2	1.95	0.47
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:L:80:LYS:HB2	1:L:80:LYS:CD	2.43	0.47
1:G:90:THR:O	1:G:94:VAL:HG13	2.13	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: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:F:63:GLU:HB2	1:G:524:LEU:CD2	2.45	0.47
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.96	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: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:F:85:ALA:O	1:F:401:HIS:HE1	1.98	0.47
1:E:82:ASN:HB2	1:E:89:THR:CG2	2.45	0.47
1:D:29:VAL:HG11	1:E:518:GLU:HG3	1.97	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:K:345:ARG:HA	1:K:348:GLN:NE2	2.26	0.47
1:H:345:ARG:HA	1:H:348:GLN:NE2	2.29	0.47
1:F:270:ILE:HG22	1:F:271:VAL:HG23	1.95	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:I:221:LEU:HD23	1:I:249:ILE:HD12	1.96	0.47
1:H:479:ASN:OD1	1:H:479:ASN:C	2.53	0.47
1:E:489:ILE:HD12	1:E:494:LEU:HD22	1.97	0.47
1:E:319:GLN:HB3	1:E:336:VAL:CG2	2.44	0.47
1:D:263:VAL:O	1:D:267:MET:HB2	2.14	0.47
1:J:305:ILE:HD12	1:J:307:MET:HE2	1.96	0.47
1:I:319:GLN:HB3	1:I:336:VAL:HG21	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:N:525:PRO:O	1:N:526:LYS:HG2	2.14	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:B:319:GLN:HB3	1:B:336:VAL:HG21	1.97	0.46
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.96	0.46
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.96	0.46
1:N:90:THR:OG1	4:N:1:AGS:S1G	2.63	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:348:GLN:O	1:N:352:GLN:HG2	2.15	0.46
1:I:177:VAL:CG2	1:I:397:GLU:HG3	2.40	0.46
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.97	0.46
1:F:389:MET:CE	1:G:281:PHE:CE2	2.97	0.46
1:M:218:PRO:HB3	1:M:246:PRO:HG2	1.97	0.46
1:C:319:GLN:HB3	1:C:336:VAL:CG2	2.45	0.46
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.98	0.46
1:A:124:VAL:HG21	1:A:508:ALA:HB2	1.97	0.46
1:K:235:PRO:HG3	1:K:310:GLU:HA	1.98	0.46
1:G:77:VAL:HG23	1:G:510:VAL:HG21	1.98	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:C:219:PHE:HB3	1:C:317:LEU:HD23	1.95	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:J:193:MET:CE	1:J:292:ILE:HG12	2.46	0.46
1:D:57:ALA:O	1:D:75:LYS:CE	2.63	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:L:102:GLU:HB2	1:L:442:VAL:HG13	1.98	0.46
1:K:319:GLN:HB3	1:K:336:VAL:HG21	1.96	0.46
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.97	0.46
1:K:404:ARG:NH1	1:K:404:ARG:CG	2.79	0.46
1:E:270:ILE:HG22	1:E:271:VAL:HG23	1.97	0.46
1:A:404:ARG:HH11	1:A:404:ARG:CG	2.28	0.46
1:I:179:ASP:OD1	1:I:393:LYS:HE3	2.16	0.46
1:M:360:TYR:CE1	1:M:364:LYS:HE3	2.51	0.46
1:D:34:LYS:HE2	1:E:118:ARG:HH22	1.80	0.46
1:L:221:LEU:HD23	1:L:249:ILE:HD12	1.98	0.46
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.98	0.46
1:J:489:ILE:HD12	1:J:494:LEU:CD2	2.46	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:N:263:VAL:O	1:N:267:MET:HB2	2.16	0.46
1:G:284:ARG:HH12	1:G:364:LYS:NZ	2.14	0.46
1:K:451:LEU:C	1:K:451:LEU:HD23	2.36	0.46
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.97	0.46
1:J:218:PRO:HB3	1:J:246:PRO:HG2	1.97	0.46
1:I:151:SER:HB2	1:I:399:ALA:HA	1.98	0.46
1:H:489:ILE:HD12	1:H:494:LEU:CD2	2.45	0.46
1:B:191:GLU:O	1:B:334:ASP:HA	2.14	0.46
1:M:57:ALA:O	1:M:75:LYS:CE	2.63	0.46
1:I:57:ALA:O	1:I:75:LYS:CE	2.64	0.46
1:E:176:THR:HG21	1:E:322:ARG:HH12	1.81	0.46
1:D:68:ASN:O	1:D:72:GLN:HG2	2.16	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:70:GLY:HA2	1:A:73:MET:HE3	1.98	0.45
1:A:171:LYS:HB2	1:A:407:VAL:HG11	1.98	0.45
1:C:321:LYS:HB2	1:C:334:ASP:HB3	1.97	0.45
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.98	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:449:ALA:N	1:F:450:PRO:CD	2.79	0.45
1:E:193:MET:CE	1:E:292:ILE:HG12	2.47	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:G:284:ARG:HH11	1:G:364:LYS:HD2	1.80	0.45
1:E:463:SER:HB2	5:E:649:HOH:O	2.16	0.45
1:N:351:GLN:HE21	1:N:351:GLN:HB3	1.65	0.45
1:F:386:GLU:O	1:F:390:LYS:HG2	2.16	0.45
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.98	0.45
1:H:35:GLY:O	1:H:51:LYS:HE2	2.16	0.45
1:E:404:ARG:HG2	1:E:404:ARG:HH11	1.82	0.45
1:B:345:ARG:HA	1:B:348:GLN:NE2	2.27	0.45
1:H:63:GLU:OE2	1:I:526:LYS:HE2	2.16	0.45
1:B:263:VAL:O	1:B:267:MET:HB2	2.17	0.45
1:L:80:LYS:HG2	1:L:80:LYS:NZ	2.32	0.45
1:B:90:THR:OG1	4:B:1:AGS:S1G	2.66	0.45
1:H:177:VAL:CG2	1:H:397:GLU:HG3	2.40	0.45
1:L:177:VAL:CG2	1:L:397:GLU:HG3	2.42	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:K:77:VAL:O	1:K:78:ALA:C	2.55	0.45
1:H:263:VAL:O	1:H:267:MET:HB2	2.17	0.45
1:E:218:PRO:HB3	1:E:246:PRO:HG2	1.99	0.45
1:D:57:ALA:O	1:D:75:LYS:HE3	2.16	0.45
1:G:413:ALA:HB3	1:G:417:VAL:HG22	1.99	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:D:221:LEU:HD23	1:D:249:ILE:HD12	1.98	0.45
1:L:224:ASP:HB3	1:L:302:SER:HB3	1.98	0.45
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.98	0.45
1:L:78:ALA:HB1	1:L:89:THR:HB	1.99	0.45
1:J:57:ALA:O	1:J:75:LYS:CE	2.65	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:H:360:TYR:CE1	1:H:364:LYS:HE3	2.52	0.45
1:K:321:LYS:HB2	1:K:334:ASP:HB3	1.98	0.45
1:K:221:LEU:HD23	1:K:249:ILE:HD12	1.98	0.45
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.99	0.45
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.99	0.45
1:D:325:ILE:HD13	1:D:325:ILE:HG23	1.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:413:ALA:CB	1:F:417:VAL:HG22	2.47	0.45
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.97	0.45
1:L:449:ALA:N	1:L:450:PRO:CD	2.79	0.45
1:C:449:ALA:N	1:C:450:PRO:CD	2.79	0.45
1:C:57:ALA:O	1:C:75:LYS:HE3	2.17	0.45
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.98	0.45
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.99	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: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: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:G:200:LEU:HD21	1:G:277:LYS:HG3	1.99	0.44
1:A:386:GLU:O	1:A:390:LYS:HG2	2.16	0.44
1:I:366:GLN:O	1:I:369:VAL:HG22	2.17	0.44
1:G:514:MET:HB3	1:G:514:MET:HE3	1.92	0.44
1:F:221:LEU:HD23	1:F:249:ILE:HD12	1.98	0.44
1:F:266:THR:HG22	1:F:271:VAL:O	2.18	0.44
1:K:218:PRO:HB3	1:K:246:PRO:HG2	1.99	0.44
1:E:449:ALA:N	1:E:450:PRO:CD	2.80	0.44
1:K:186:GLU:HB2	1:K:380:LYS:HB2	2.00	0.44
1:F:236:VAL:O	1:F:240:VAL:HG23	2.17	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: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:C:57:ALA:O	1:C:75:LYS:CE	2.66	0.44
1:J:319:GLN:HB3	1:J:336:VAL:HG21	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:C:383:ALA:HB3	1:C:389:MET:HB2	1.99	0.44
1:J:90:THR:O	1:J:94:VAL:HG13	2.17	0.44
1:I:348:GLN:O	1:I:352:GLN:HG2	2.17	0.44
1:H:224:ASP:HB3	1:H:302:SER:HB3	2.00	0.44
1:K:383:ALA:HB3	1:K:389:MET:HB2	1.98	0.44
1:L:463:SER:HB2	5:L:612:HOH:O	2.17	0.44
1:K:179:ASP:OD1	1:K:393:LYS:HE3	2.18	0.44
1:A:383:ALA:HB3	1:A:389:MET:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:458:CYS:SG	1:I:480:ALA:HB1	2.58	0.44
1:D:404:ARG:NH1	1:D:404:ARG:CG	2.79	0.44
1:D:217:SER:N	1:D:218:PRO:HD3	2.33	0.44
1:H:386:GLU:O	1:H:390:LYS:HG2	2.17	0.44
1:F:36:ARG:HG3	1:G:518:GLU:HG2	1.98	0.44
1:N:236:VAL:O	1:N:240:VAL:HG23	2.17	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:I:186:GLU:HB2	1:I:380:LYS:HB2	1.99	0.44
1:F:524:LEU:O	1:F:526:LYS:N	2.51	0.44
1:J:63:GLU:HB2	1:K:524:LEU:HD21	2.00	0.44
1:N:69:MET:O	1:N:73:MET:HE2	2.17	0.44
1:J:325:ILE:HG22	1:J:330:THR:HG23	2.00	0.44
1:J:404:ARG:CG	1:J:404:ARG:HH11	2.29	0.44
1:J:151:SER:HB2	1:J:399:ALA:HA	1.99	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:I:514:MET:HE3	1:I:514:MET:HB3	1.94	0.44
1:E:369:VAL:HG23	1:E:370:ALA:N	2.33	0.44
1:C:178:GLU:OE2	1:C:322:ARG:HD3	2.18	0.44
1:N:37:ASN:ND2	1:N:51:LYS:HE3	2.33	0.44
1:B:186:GLU:HB2	1:B:380:LYS:HB2	2.00	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: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:L:263:VAL:O	1:L:267:MET:HB2	2.18	0.43
1:J:364:LYS:HA	1:J:364:LYS:HD3	1.84	0.43
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.99	0.43
1:N:319:GLN:HB3	1:N:336:VAL:CG2	2.48	0.43
1:F:263:VAL:O	1:F:267:MET:HB2	2.18	0.43
1:M:158:VAL:HG13	1:M:396:VAL:HG22	1.99	0.43
1:J:263:VAL:O	1:J:267:MET:HB2	2.18	0.43
1:K:524:LEU:O	1:K:526:LYS:N	2.51	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:A:525:PRO:O	1:A:526:LYS:CG	2.65	0.43
1:N:506:TYR:O	1:N:507:ALA:C	2.56	0.43
1:F:369:VAL:HG23	1:F:370:ALA:N	2.33	0.43
1:D:524:LEU:O	1:D:526:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:VAL:O	1:F:151:SER:OG	2.36	0.43
1:E:386:GLU:O	1:E:390:LYS:HG2	2.17	0.43
1:J:235:PRO:HG3	1:J:310:GLU:HA	2.00	0.43
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.76	0.43
1:B:473:ASP:HB2	5:B:599:HOH:O	2.19	0.43
1:L:151:SER:HB2	1:L:399:ALA:HA	2.00	0.43
1:K:144:ILE:HG23	1:K:403:THR:HG21	2.00	0.43
1:L:489:ILE:HD12	1:L:494:LEU:CD2	2.49	0.43
1:F:514:MET:HE3	1:F:514:MET:HB3	1.85	0.43
1:D:284:ARG:HH12	1:D:364:LYS:NZ	2.16	0.43
1:C:23:LEU:O	1:C:23:LEU:HG	2.11	0.43
1:H:218:PRO:HB3	1:H:246:PRO:HG2	2.00	0.43
1:A:118:ARG:HH22	1:G:34:LYS:HE2	1.84	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:514:MET:HB3	1:C:514:MET:HE3	1.93	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:B:221:LEU:HD23	1:B:249:ILE:HD12	2.01	0.43
1:H:366:GLN:O	1:H:369:VAL:HG22	2.18	0.43
1:B:193:MET:HE1	1:B:292:ILE:HG12	2.00	0.43
1:F:351:GLN:HB3	1:F:351:GLN:HE21	1.64	0.43
1:J:351:GLN:HE21	1:J:351:GLN:HB3	1.66	0.43
1:M:178:GLU:HG2	1:M:322:ARG:NH1	2.33	0.43
1:L:266:THR:HG22	1:L:271:VAL:O	2.18	0.43
1:D:325:ILE:HG21	1:D:325:ILE:HD12	1.64	0.43
1:C:191:GLU:O	1:C:334:ASP:HA	2.18	0.43
1:B:224:ASP:HB3	1:B:302:SER:HB3	1.99	0.43
1:K:364:LYS:HD3	1:K:364:LYS:HA	1.83	0.43
1:H:351:GLN:HB3	1:H:351:GLN:HE21	1.68	0.43
1:M:404:ARG:CG	1:M:404:ARG:NH1	2.82	0.43
1:B:82:ASN:HB2	1:B:89:THR:CG2	2.49	0.43
1:K:366:GLN:O	1:K:369:VAL:HG22	2.19	0.43
1:I:224:ASP:HB3	1:I:302:SER:HB3	2.01	0.43
1:H:458:CYS:SG	1:H:480:ALA:HB1	2.58	0.43
1:H:158:VAL:HG13	1:H:396:VAL:HG22	2.00	0.43
1:A:186:GLU:HB2	1:A:380:LYS:HB2	2.01	0.43
1:C:284:ARG:HH11	1:C:364:LYS:HD2	1.84	0.43
1:J:186:GLU:HB2	1:J:380:LYS:HB2	2.01	0.43
1:L:39:VAL:HG12	1:M:69:MET:CE	2.49	0.43
1:A:466:ALA:O	1:A:470:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:VAL:O	1:E:240:VAL:HG23	2.19	0.43
1:G:325:ILE:HD13	1:G:325:ILE:HG23	1.78	0.42
1:K:63:GLU:OE2	1:L:526:LYS:HE2	2.18	0.42
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.49	0.42
1:F:366:GLN:O	1:F:369:VAL:HG22	2.18	0.42
1:K:284:ARG:HH11	1:K:364:LYS:HD2	1.84	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:A:364:LYS:HD3	1:A:364:LYS:HA	1.85	0.42
1:F:177:VAL:CG2	1:F:397:GLU:HG3	2.43	0.42
1:L:345:ARG:HA	1:L:348:GLN:NE2	2.34	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:J:389:MET:HE3	1:K:281:PHE:CD2	2.54	0.42
1:N:284:ARG:HH11	1:N:364:LYS:HD2	1.84	0.42
1:B:193:MET:CE	1:B:292:ILE:HG12	2.49	0.42
1:H:219:PHE:HB3	1:H:317:LEU:HD23	2.00	0.42
1:N:179:ASP:OD1	1:N:393:LYS:HE3	2.19	0.42
1:N:240:VAL:HG11	1:N:247:LEU:HB2	2.01	0.42
1:M:186:GLU:HB2	1:M:380:LYS:HB2	2.01	0.42
1:B:514:MET:HE3	1:B:514:MET:HB3	1.71	0.42
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.32	0.42
1:F:413:ALA:HB3	1:F:417:VAL:HG22	2.00	0.42
1:F:319:GLN:HB3	1:F:336:VAL:CG2	2.50	0.42
1:J:360:TYR:CE1	1:J:364:LYS:HE3	2.54	0.42
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.01	0.42
1:K:37:ASN:ND2	1:K:51:LYS:HE3	2.34	0.42
1:E:135:SER:HB3	5:E:618:HOH:O	2.18	0.42
1:C:263:VAL:O	1:C:267:MET:HB2	2.19	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:A:263:VAL:O	1:A:267:MET:HB2	2.18	0.42
1:J:288:MET:HG2	1:J:368:ARG:HD3	2.02	0.42
1:G:18:ARG:CZ	5:G:595:HOH:O	2.66	0.42
1:J:217:SER:N	1:J:218:PRO:HD3	2.35	0.42
1:F:389:MET:CE	1:G:281:PHE:HE2	2.33	0.42
1:I:218:PRO:HB3	1:I:246:PRO:HG2	2.01	0.42
1:F:109:ALA:HB2	1:H:109:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:ILE:HD12	1:C:494:LEU:CD2	2.49	0.42
1:F:466:ALA:O	1:F:470:LYS:HG3	2.20	0.42
1:F:158:VAL:HG13	1:F:396:VAL:HG22	2.01	0.42
1:B:386:GLU:O	1:B:390:LYS:HG2	2.19	0.42
1:N:57:ALA:O	1:N:75:LYS:CE	2.68	0.42
1:C:63:GLU:HB2	1:D:524:LEU:HD21	2.01	0.42
1:N:404:ARG:HH11	1:N:404:ARG:CG	2.32	0.42
1:E:171:LYS:HB2	1:E:407:VAL:HG11	2.02	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:B:153:ASN:O	1:B:154:SER:HB2	2.20	0.42
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.49	0.42
1:H:118:ARG:HG3	5:H:587:HOH:O	2.18	0.42
1:F:348:GLN:O	1:F:352:GLN:HG2	2.20	0.42
1:G:489:ILE:HD12	1:G:494:LEU:HD21	2.01	0.42
1:H:413:ALA:HB3	1:H:417:VAL:HG22	2.01	0.42
1:C:272:LYS:NZ	1:D:228:SER:HB3	2.35	0.42
1:H:305:ILE:O	1:H:305:ILE:HG22	2.20	0.42
1:J:489:ILE:HD12	1:J:494:LEU:HD22	2.00	0.42
1:E:351:GLN:HB3	1:E:351:GLN:HE21	1.66	0.42
1:H:514:MET:HB3	1:H:514:MET:HE3	1.80	0.42
1:G:118:ARG:HE	1:G:118:ARG:HB2	1.78	0.42
1:M:325:ILE:HG22	1:M:330:THR:HG23	2.01	0.42
1:L:218:PRO:HB3	1:L:246:PRO:HG2	2.00	0.42
1:I:414:GLY:O	1:I:417:VAL:HG13	2.20	0.42
1:I:158:VAL:HG13	1:I:396:VAL:HG22	2.01	0.42
1:L:171:LYS:HB2	1:L:407:VAL:HG11	2.02	0.42
1:D:65:LYS:HG2	5:D:646:HOH:O	2.19	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:E:421:ARG:HD3	1:E:421:ARG:HH11	1.60	0.42
1:H:270:ILE:HG22	1:H:271:VAL:HG23	2.02	0.42
1:E:118:ARG:HB2	1:E:118:ARG:HE	1.80	0.42
1:H:383:ALA:HB3	1:H:389:MET:HB2	2.01	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:L:288:MET:HG2	1:L:368:ARG:HD3	2.02	0.41
1:N:489:ILE:HD12	1:N:494:LEU:HD22	2.00	0.41
1:K:319:GLN:HB3	1:K:336:VAL:CG2	2.50	0.41
1:H:284:ARG:HH11	1:H:364:LYS:HD2	1.85	0.41
1:A:236:VAL:O	1:A:240:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:502:SER:O	1:N:503:ALA:C	2.59	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:H:18:ARG:NE	5:H:584:HOH:O	2.32	0.41
1:A:37:ASN:ND2	1:A:51:LYS:HE3	2.35	0.41
1:M:409:GLU:OE1	5:M:578:HOH:O	2.22	0.41
1:F:321:LYS:HB2	1:F:334:ASP:HB3	2.02	0.41
1:M:23:LEU:CD2	1:M:74:VAL:HG13	2.49	0.41
1:H:69:MET:O	1:H:73:MET:HG3	2.20	0.41
1:F:305:ILE:HG22	1:F:305:ILE:O	2.20	0.41
1:F:218:PRO:HB3	1:F:246:PRO:HG2	2.03	0.41
1:N:224:ASP:HB3	1:N:302:SER:HB3	2.02	0.41
1:M:263:VAL:O	1:M:267:MET:HB2	2.20	0.41
1:M:179:ASP:OD1	1:M:393:LYS:HE3	2.20	0.41
1:B:27:VAL:HG12	1:B:90:THR:HG23	2.02	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:C:118:ARG:HE	1:C:118:ARG:HB2	1.79	0.41
1:A:319:GLN:HB3	1:A:336:VAL:HG21	2.02	0.41
1:N:219:PHE:HB3	1:N:317:LEU:HD23	2.02	0.41
1:A:351:GLN:HB3	1:A:351:GLN:HE21	1.65	0.41
4:I:1:AGS:O3B	4:I:1:AGS:S1G	2.59	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
1:M:360:TYR:CZ	1:M:364:LYS:HE3	2.55	0.41
1:B:219:PHE:HB3	1:B:317:LEU:HD23	2.02	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:D:419:LEU:HD23	1:D:419:LEU:HA	1.82	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:C:524:LEU:O	1:C:526:LYS:N	2.53	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:N:366:GLN:O	1:N:369:VAL:HG22	2.21	0.41
1:M:345:ARG:HA	1:M:348:GLN:NE2	2.32	0.41
1:G:266:THR:HG21	1:G:273:VAL:H	1.86	0.41
1:M:305:ILE:O	1:M:305:ILE:HG22	2.21	0.41
1:K:219:PHE:O	1:K:247:LEU:HD12	2.20	0.41
1:B:37:ASN:ND2	5:B:628:HOH:O	2.47	0.41
1:L:419:LEU:HD23	1:L:419:LEU:HA	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:419:LEU:HD23	1:N:419:LEU:HA	1.91	0.41
1:L:236:VAL:O	1:L:240:VAL:HG23	2.21	0.41
4:J:1:AGS:S1G	4:J:1:AGS:O3G	2.57	0.41
1:K:177:VAL:CG2	1:K:397:GLU:HG3	2.44	0.41
1:I:235:PRO:CG	1:I:310:GLU:HA	2.51	0.41
1:G:319:GLN:HB3	1:G:336:VAL:CG2	2.50	0.41
1:J:73:MET:O	1:J:76:GLU:HB2	2.20	0.41
1:C:90:THR:O	1:C:94:VAL:HG13	2.21	0.41
1:M:57:ALA:O	1:M:75:LYS:HE2	2.21	0.41
1:N:221:LEU:HD23	1:N:249:ILE:HD12	2.02	0.41
1:A:158:VAL:HG13	1:A:396:VAL:HG22	2.02	0.41
1:J:78:ALA:HB1	1:J:89:THR:HB	2.03	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:N:112:ASN:HA	1:N:113:PRO:HD3	1.96	0.41
1:D:39:VAL:HG23	1:E:517:THR:CG2	2.51	0.41
1:B:426:LEU:HA	1:B:426:LEU:HD23	1.82	0.41
1:E:16:MET:O	1:E:20:VAL:HG13	2.21	0.41
1:K:348:GLN:O	1:K:352:GLN:HG2	2.20	0.41
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.33	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:C:224:ASP:HB3	1:C:302:SER:HB3	2.03	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: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:E:39:VAL:HG12	1:F:69:MET:CE	2.51	0.41
1:I:263:VAL:O	1:I:267:MET:HB2	2.21	0.41
1:L:364:LYS:HA	1:L:364:LYS:HD3	1.73	0.41
1:K:325:ILE:HG22	1:K:330:THR:HG23	2.02	0.41
1:D:302:SER:H	1:D:307:MET:CE	2.34	0.41
1:N:197:ARG:HD2	1:N:277:LYS:HB2	2.03	0.41
1:C:176:THR:HG21	1:C:322:ARG:HH12	1.86	0.41
1:D:463:SER:HB2	5:D:644:HOH:O	2.20	0.41
1:D:386:GLU:O	1:D:390:LYS:HG2	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:D:124:VAL:HG21	1:D:508:ALA:HB2	2.03	0.41
1:D:319:GLN:HB3	1:D:336:VAL:HG21	2.02	0.41
1:K:16:MET:O	1:K:20:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:GLN:O	1:C:369:VAL:HG22	2.21	0.41
1:A:348:GLN:O	1:A:352:GLN:HG2	2.22	0.40
1:D:266:THR:HG22	1:D:271:VAL:O	2.21	0.40
1:M:364:LYS:HA	1:M:364:LYS:HD3	1.86	0.40
1:K:191:GLU:O	1:K:334:ASP:HA	2.22	0.40
1:C:193:MET:HE1	1:C:292:ILE:HG12	2.01	0.40
1:B:236:VAL:O	1:B:240:VAL:HG23	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:M:16:MET:O	1:M:20:VAL:HG13	2.21	0.40
1:A:231:ARG:NH1	1:G:242:LYS:CG	2.83	0.40
1:F:178:GLU:HG2	1:F:322:ARG:NH1	2.36	0.40
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.61	0.40
1:E:360:TYR:CE1	1:E:364:LYS:HE3	2.56	0.40
1:G:66:PHE:CZ	1:G:522:THR:HG22	2.57	0.40
1:N:466:ALA:O	1:N:470:LYS:HG3	2.21	0.40
1:N:325:ILE:HG22	1:N:330:THR:HG23	2.02	0.40
1:J:57:ALA:O	1:J:75:LYS:HE3	2.20	0.40
1:A:284:ARG:HH11	1:A:364:LYS:HD2	1.87	0.40
1:M:124:VAL:HG21	1:M:508:ALA:CB	2.51	0.40
1:L:348:GLN:O	1:L:352:GLN:HG2	2.21	0.40
1:H:404:ARG:CG	1:H:404:ARG:NH1	2.83	0.40
1:M:176:THR:HG22	1:M:177:VAL:N	2.36	0.40
1:I:63:GLU:HB2	1:J:524:LEU:HD21	2.04	0.40
1:M:57:ALA:O	1:M:75:LYS:HE3	2.20	0.40
1:C:360:TYR:CE1	1:C:364:LYS:HE3	2.56	0.40
1:K:419:LEU:HD23	1:K:419:LEU:HA	1.94	0.40
1:D:114:MET:CG	1:D:114:MET:CE	2.99	0.40
1:M:63:GLU:HB2	1:N:524:LEU:CD2	2.52	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:M:369:VAL:HG23	1:M:370:ALA:N	2.36	0.40
1:C:221:LEU:HD23	1:C:249:ILE:HD12	2.03	0.40
1:J:321:LYS:HB2	1:J:334:ASP:HB3	2.03	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%)	39	33
1	B	523/525 (100%)	506 (97%)	15 (3%)	2 (0%)	39	33
1	C	523/525 (100%)	505 (97%)	16 (3%)	2 (0%)	39	33
1	D	523/525 (100%)	509 (97%)	13 (2%)	1 (0%)	52	48
1	E	523/525 (100%)	507 (97%)	14 (3%)	2 (0%)	39	33
1	F	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	39	33
1	G	523/525 (100%)	511 (98%)	10 (2%)	2 (0%)	39	33
1	H	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	39	33
1	I	523/525 (100%)	511 (98%)	10 (2%)	2 (0%)	39	33
1	J	523/525 (100%)	509 (97%)	12 (2%)	2 (0%)	39	33
1	K	523/525 (100%)	505 (97%)	15 (3%)	3 (1%)	30	22
1	L	523/525 (100%)	508 (97%)	13 (2%)	2 (0%)	39	33
1	M	523/525 (100%)	512 (98%)	9 (2%)	2 (0%)	39	33
1	N	523/525 (100%)	503 (96%)	18 (3%)	2 (0%)	39	33
All	All	7322/7350 (100%)	7111 (97%)	183 (2%)	28 (0%)	39	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%)	29	23
1	B	404/405 (100%)	379 (94%)	25 (6%)	23	16
1	C	404/405 (100%)	381 (94%)	23 (6%)	25	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	404/405 (100%)	383 (95%)	21 (5%)	29	23
1	E	404/405 (100%)	382 (95%)	22 (5%)	27	21
1	F	404/405 (100%)	385 (95%)	19 (5%)	32	27
1	G	404/405 (100%)	381 (94%)	23 (6%)	25	19
1	H	404/405 (100%)	382 (95%)	22 (5%)	27	21
1	I	404/405 (100%)	387 (96%)	17 (4%)	36	31
1	J	404/405 (100%)	383 (95%)	21 (5%)	29	23
1	K	404/405 (100%)	384 (95%)	20 (5%)	30	24
1	L	404/405 (100%)	382 (95%)	22 (5%)	27	21
1	M	404/405 (100%)	384 (95%)	20 (5%)	30	24
1	N	404/405 (100%)	381 (94%)	23 (6%)	25	19
All	All	5656/5670 (100%)	5357 (95%)	299 (5%)	28	22

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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	24,33,33	4.11	5 (20%)	28,52,52	3.35	9 (32%)
4	AGS	B	1	3,2	24,33,33	4.23	4 (16%)	28,52,52	2.81	8 (28%)
4	AGS	C	1	3,2	24,33,33	4.32	4 (16%)	28,52,52	3.57	5 (17%)
4	AGS	D	561	3,2	24,33,33	4.75	7 (29%)	28,52,52	2.07	9 (32%)
4	AGS	E	1	3,2	24,33,33	4.84	5 (20%)	28,52,52	2.91	10 (35%)
4	AGS	F	1	3,2	24,33,33	4.37	4 (16%)	28,52,52	2.27	8 (28%)
4	AGS	G	1	3,2	24,33,33	4.99	6 (25%)	28,52,52	2.76	11 (39%)
4	AGS	H	1	3,2	24,33,33	4.40	6 (25%)	28,52,52	2.74	9 (32%)
4	AGS	I	1	3,2	24,33,33	4.45	4 (16%)	28,52,52	2.48	9 (32%)
4	AGS	J	1	3,2	24,33,33	4.17	3 (12%)	28,52,52	2.47	8 (28%)
4	AGS	K	1	3,2	24,33,33	4.43	6 (25%)	28,52,52	2.46	6 (21%)
4	AGS	L	1	3,2	24,33,33	4.49	5 (20%)	28,52,52	3.77	7 (25%)
4	AGS	M	1	3,2	24,33,33	4.30	4 (16%)	28,52,52	3.77	5 (17%)
4	AGS	N	1	3,2	24,33,33	4.82	5 (20%)	28,52,52	3.20	11 (39%)

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	-	0/15/38/38	0/3/3/3
4	AGS	B	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	C	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	D	561	3,2	-	0/15/38/38	0/3/3/3
4	AGS	E	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	F	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	G	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	H	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	I	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	J	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	K	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	L	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	M	1	3,2	-	0/15/38/38	0/3/3/3
4	AGS	N	1	3,2	-	0/15/38/38	0/3/3/3

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	AGS	PG-S1G	-23.10	1.45	1.90
4	E	1	AGS	PG-S1G	-22.39	1.47	1.90
4	N	1	AGS	PG-S1G	-22.37	1.47	1.90
4	D	561	AGS	PG-S1G	-21.48	1.48	1.90
4	L	1	AGS	PG-S1G	-21.03	1.49	1.90
4	I	1	AGS	PG-S1G	-20.62	1.50	1.90
4	F	1	AGS	PG-S1G	-20.36	1.51	1.90
4	C	1	AGS	PG-S1G	-20.34	1.51	1.90
4	H	1	AGS	PG-S1G	-20.33	1.51	1.90
4	K	1	AGS	PG-S1G	-20.25	1.51	1.90
4	M	1	AGS	PG-S1G	-20.20	1.51	1.90
4	B	1	AGS	PG-S1G	-19.78	1.52	1.90
4	J	1	AGS	PG-S1G	-19.67	1.52	1.90
4	A	1	AGS	PG-S1G	-19.07	1.53	1.90
4	N	1	AGS	O4'-C1'	-4.69	1.35	1.41
4	E	1	AGS	PA-O1A	-4.04	1.36	1.51
4	F	1	AGS	PA-O1A	-3.47	1.38	1.51
4	F	1	AGS	O3'-C3'	-3.30	1.35	1.43
4	G	1	AGS	PA-O1A	-3.08	1.39	1.51
4	K	1	AGS	PB-O1B	-3.00	1.40	1.51
4	L	1	AGS	PA-O1A	-2.93	1.40	1.51
4	A	1	AGS	O4'-C1'	-2.92	1.37	1.41
4	I	1	AGS	O4'-C4'	-2.71	1.38	1.45
4	B	1	AGS	O4'-C1'	-2.71	1.37	1.41
4	N	1	AGS	PA-O1A	-2.68	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	AGS	PA-O1A	-2.56	1.41	1.51
4	G	1	AGS	O3'-C3'	-2.45	1.37	1.43
4	H	1	AGS	O4'-C1'	-2.44	1.38	1.41
4	E	1	AGS	PB-O1B	-2.44	1.42	1.51
4	H	1	AGS	O2'-C2'	-2.41	1.37	1.43
4	D	561	AGS	PA-O1A	-2.36	1.42	1.51
4	M	1	AGS	O2'-C2'	-2.25	1.37	1.43
4	C	1	AGS	PA-O1A	-2.21	1.43	1.51
4	D	561	AGS	O4'-C1'	-2.20	1.38	1.41
4	H	1	AGS	C4-N3	-2.15	1.32	1.35
4	J	1	AGS	O4'-C4'	-2.14	1.40	1.45
4	H	1	AGS	PB-O1B	-2.09	1.43	1.51
4	A	1	AGS	PA-O1A	-2.07	1.43	1.51
4	L	1	AGS	C5-C4	-2.07	1.35	1.40
4	K	1	AGS	O2'-C2'	-2.05	1.38	1.43
4	K	1	AGS	C2-N1	2.00	1.37	1.33
4	L	1	AGS	C2-N3	2.02	1.35	1.32
4	E	1	AGS	C5-N7	2.05	1.46	1.39
4	M	1	AGS	C8-N7	2.06	1.38	1.34
4	G	1	AGS	O4'-C1'	2.15	1.43	1.41
4	F	1	AGS	C2-N3	2.22	1.36	1.32
4	A	1	AGS	C8-N7	2.23	1.38	1.34
4	N	1	AGS	C2-N1	2.24	1.38	1.33
4	C	1	AGS	C2-N1	2.33	1.38	1.33
4	J	1	AGS	C2-N3	2.48	1.36	1.32
4	I	1	AGS	PA-O2A	2.51	1.65	1.54
4	D	561	AGS	PG-O2G	2.55	1.64	1.55
4	G	1	AGS	C2-N1	2.72	1.39	1.33
4	L	1	AGS	C2-N1	2.75	1.39	1.33
4	B	1	AGS	C2-N3	2.81	1.37	1.32
4	C	1	AGS	C2-N3	3.04	1.37	1.32
4	H	1	AGS	C2-N3	3.06	1.37	1.32
4	M	1	AGS	C2-N3	3.12	1.37	1.32
4	I	1	AGS	C2-N3	3.41	1.38	1.32
4	D	561	AGS	C2-N1	3.42	1.40	1.33
4	K	1	AGS	C2-N3	3.47	1.38	1.32
4	A	1	AGS	C2-N3	3.73	1.38	1.32
4	N	1	AGS	C2-N3	3.77	1.38	1.32
4	K	1	AGS	O4'-C1'	4.24	1.46	1.41
4	G	1	AGS	C2-N3	4.25	1.39	1.32
4	D	561	AGS	C2-N3	4.34	1.39	1.32
4	E	1	AGS	C2-N3	4.41	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	561	AGS	C4-N3	4.79	1.42	1.35

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	1	AGS	N3-C2-N1	-18.39	114.81	128.89
4	L	1	AGS	N3-C2-N1	-17.31	115.64	128.89
4	C	1	AGS	N3-C2-N1	-17.14	115.77	128.89
4	A	1	AGS	N3-C2-N1	-14.84	117.53	128.89
4	N	1	AGS	N3-C2-N1	-11.94	119.75	128.89
4	E	1	AGS	N3-C2-N1	-11.06	120.43	128.89
4	B	1	AGS	N3-C2-N1	-11.02	120.46	128.89
4	G	1	AGS	N3-C2-N1	-10.17	121.11	128.89
4	J	1	AGS	N3-C2-N1	-9.79	121.40	128.89
4	H	1	AGS	N3-C2-N1	-9.64	121.51	128.89
4	I	1	AGS	N3-C2-N1	-9.30	121.77	128.89
4	K	1	AGS	N3-C2-N1	-9.06	121.96	128.89
4	F	1	AGS	N3-C2-N1	-8.08	122.70	128.89
4	D	561	AGS	N3-C2-N1	-7.21	123.37	128.89
4	E	1	AGS	C2'-C1'-N9	-5.54	105.83	114.29
4	G	1	AGS	C1'-N9-C4	-5.31	118.93	126.94
4	N	1	AGS	C1'-N9-C4	-5.28	118.98	126.94
4	L	1	AGS	C1'-N9-C4	-5.25	119.02	126.94
4	B	1	AGS	C2'-C1'-N9	-5.20	106.35	114.29
4	H	1	AGS	O5'-PA-O1A	-5.02	90.15	109.62
4	N	1	AGS	O5'-PA-O1A	-5.00	90.20	109.62
4	N	1	AGS	C4-C5-N7	-4.76	105.10	109.48
4	I	1	AGS	C1'-N9-C4	-4.68	119.88	126.94
4	A	1	AGS	O3'-C3'-C4'	-4.61	97.21	111.05
4	M	1	AGS	C1'-N9-C4	-4.51	120.14	126.94
4	F	1	AGS	C2'-C1'-N9	-4.48	107.44	114.29
4	B	1	AGS	C1'-N9-C4	-4.17	120.65	126.94
4	E	1	AGS	C1'-N9-C4	-4.14	120.69	126.94
4	A	1	AGS	C1'-N9-C4	-4.02	120.88	126.94
4	J	1	AGS	C4-C5-N7	-3.98	105.82	109.48
4	G	1	AGS	C2'-C1'-N9	-3.88	108.37	114.29
4	B	1	AGS	C4'-O4'-C1'	-3.72	105.63	109.72
4	K	1	AGS	PB-O3B-PG	-3.66	120.39	132.67
4	H	1	AGS	C1'-N9-C4	-3.64	121.46	126.94
4	K	1	AGS	PA-O3A-PB	-3.55	122.75	132.73
4	F	1	AGS	C5'-C4'-C3'	-3.48	101.38	115.21
4	D	561	AGS	O5'-PA-O1A	-3.40	96.44	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	AGS	PB-O3B-PG	-3.34	121.47	132.67
4	D	561	AGS	C1'-N9-C4	-3.21	122.09	126.94
4	N	1	AGS	PB-O3B-PG	-3.21	121.90	132.67
4	N	1	AGS	C5'-C4'-C3'	-3.16	102.68	115.21
4	L	1	AGS	O3'-C3'-C4'	-3.10	101.75	111.05
4	C	1	AGS	C2'-C1'-N9	-3.05	109.63	114.29
4	F	1	AGS	C1'-N9-C4	-3.01	122.41	126.94
4	E	1	AGS	C5'-C4'-C3'	-2.88	103.79	115.21
4	M	1	AGS	N6-C6-N1	-2.85	113.08	119.20
4	J	1	AGS	C2'-C1'-N9	-2.79	110.03	114.29
4	H	1	AGS	C4'-O4'-C1'	-2.76	106.69	109.72
4	E	1	AGS	O2B-PB-O3A	-2.76	92.59	105.09
4	G	1	AGS	C4'-O4'-C1'	-2.75	106.69	109.72
4	L	1	AGS	C2'-C1'-N9	-2.71	110.16	114.29
4	I	1	AGS	PB-O3B-PG	-2.70	123.63	132.67
4	G	1	AGS	PB-O3B-PG	-2.65	123.77	132.67
4	D	561	AGS	C5'-C4'-C3'	-2.64	104.75	115.21
4	E	1	AGS	PB-O3B-PG	-2.62	123.90	132.67
4	F	1	AGS	C4-C5-N7	-2.53	107.15	109.48
4	A	1	AGS	O5'-PA-O1A	-2.53	99.82	109.62
4	I	1	AGS	C5'-C4'-C3'	-2.52	105.22	115.21
4	N	1	AGS	C2'-C1'-N9	-2.50	110.47	114.29
4	L	1	AGS	C5'-C4'-C3'	-2.49	105.34	115.21
4	C	1	AGS	C5'-C4'-C3'	-2.47	105.39	115.21
4	A	1	AGS	O2B-PB-O3A	-2.47	93.88	105.09
4	B	1	AGS	C5'-C4'-C3'	-2.45	105.49	115.21
4	D	561	AGS	PA-O3A-PB	-2.42	125.92	132.73
4	G	1	AGS	C4-C5-N7	-2.38	107.29	109.48
4	I	1	AGS	C2'-C1'-N9	-2.31	110.76	114.29
4	J	1	AGS	N6-C6-N1	-2.30	114.26	119.20
4	E	1	AGS	O4'-C4'-C3'	-2.28	100.55	105.15
4	J	1	AGS	PA-O3A-PB	-2.18	126.62	132.73
4	N	1	AGS	C4'-O4'-C1'	-2.17	107.34	109.72
4	A	1	AGS	N6-C6-N1	-2.16	114.58	119.20
4	F	1	AGS	C4'-O4'-C1'	-2.15	107.35	109.72
4	M	1	AGS	O5'-PA-O1A	-2.14	101.29	109.62
4	F	1	AGS	O3'-C3'-C4'	-2.14	104.64	111.05
4	I	1	AGS	C4-C5-N7	-2.13	107.52	109.48
4	D	561	AGS	O3'-C3'-C4'	-2.13	104.67	111.05
4	G	1	AGS	N6-C6-N1	-2.13	114.64	119.20
4	A	1	AGS	PB-O3B-PG	-2.09	125.67	132.67
4	D	561	AGS	PB-O3B-PG	-2.08	125.70	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1	AGS	C4'-O4'-C1'	-2.07	107.44	109.72
4	G	1	AGS	O3'-C3'-C4'	-2.05	104.89	111.05
4	G	1	AGS	O5'-PA-O1A	-2.01	101.82	109.62
4	J	1	AGS	O2B-PB-O3A	2.01	114.23	105.09
4	E	1	AGS	C2'-C3'-C4'	2.03	106.79	102.61
4	H	1	AGS	O3G-PG-O3B	2.04	114.35	105.09
4	B	1	AGS	O4'-C4'-C3'	2.07	109.32	105.15
4	A	1	AGS	O2B-PB-O3B	2.09	114.56	105.09
4	K	1	AGS	O2A-PA-O5'	2.11	119.12	108.46
4	F	1	AGS	O3A-PA-O5'	2.14	108.61	102.94
4	G	1	AGS	O2B-PB-O3A	2.17	114.96	105.09
4	M	1	AGS	O3A-PA-O5'	2.18	108.71	102.94
4	E	1	AGS	O3G-PG-O3B	2.23	115.23	105.09
4	N	1	AGS	O2A-PA-O1A	2.24	124.67	112.53
4	B	1	AGS	O4'-C1'-N9	2.26	112.82	108.10
4	H	1	AGS	O4'-C1'-N9	2.29	112.89	108.10
4	K	1	AGS	O2G-PG-O3B	2.32	115.60	105.09
4	D	561	AGS	O4'-C1'-N9	2.32	112.96	108.10
4	I	1	AGS	O2B-PB-O3A	2.33	115.67	105.09
4	G	1	AGS	O3A-PA-O5'	2.39	109.28	102.94
4	D	561	AGS	O2B-PB-O1B	2.41	125.59	112.53
4	B	1	AGS	O3A-PA-O5'	2.42	109.36	102.94
4	N	1	AGS	O2B-PB-O3A	2.44	116.18	105.09
4	C	1	AGS	C2-N1-C6	2.57	123.36	118.77
4	J	1	AGS	O4'-C1'-N9	2.66	113.67	108.10
4	A	1	AGS	O4'-C1'-N9	2.70	113.74	108.10
4	E	1	AGS	O2A-PA-O5'	2.75	122.31	108.46
4	I	1	AGS	O3A-PA-O5'	3.07	111.09	102.94
4	N	1	AGS	O3A-PA-O5'	3.18	111.38	102.94
4	J	1	AGS	O3A-PA-O5'	3.34	111.80	102.94
4	I	1	AGS	O4'-C1'-N9	3.47	115.37	108.10
4	H	1	AGS	O3A-PA-O5'	3.50	112.21	102.94
4	H	1	AGS	O2B-PB-O3A	3.71	121.94	105.09
4	C	1	AGS	O4'-C1'-N9	3.98	116.42	108.10
4	L	1	AGS	O4'-C1'-N9	4.40	117.31	108.10
4	K	1	AGS	O4'-C1'-N9	5.28	119.15	108.10

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%)	0.76	67 (12%) 5 5	10, 14, 16, 20	0
1	B	525/525 (100%)	1.42	126 (24%) 1 1	10, 14, 16, 20	0
1	C	525/525 (100%)	1.22	117 (22%) 1 1	10, 14, 16, 20	0
1	D	525/525 (100%)	0.58	30 (5%) 27 29	10, 14, 16, 20	0
1	E	525/525 (100%)	1.11	92 (17%) 2 2	9, 14, 16, 20	0
1	F	525/525 (100%)	1.37	129 (24%) 1 1	10, 14, 16, 20	0
1	G	525/525 (100%)	0.72	42 (8%) 15 16	10, 14, 16, 20	0
1	H	525/525 (100%)	0.73	56 (10%) 8 8	9, 14, 16, 20	0
1	I	525/525 (100%)	1.07	93 (17%) 2 2	9, 14, 16, 20	0
1	J	525/525 (100%)	1.00	83 (15%) 3 3	10, 14, 16, 20	0
1	K	525/525 (100%)	1.49	148 (28%) 1 1	10, 14, 16, 20	0
1	L	525/525 (100%)	0.96	91 (17%) 2 2	10, 14, 16, 20	0
1	M	525/525 (100%)	1.46	140 (26%) 1 1	10, 14, 16, 20	0
1	N	525/525 (100%)	0.75	56 (10%) 8 8	10, 14, 16, 20	0
All	All	7350/7350 (100%)	1.05	1270 (17%) 2 2	9, 14, 16, 20	0

All (1270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	270	ILE	13.7
1	F	240	VAL	12.4
1	K	269	GLY	12.1
1	C	349	ILE	11.6
1	B	353	ILE	11.4
1	B	349	ILE	11.1
1	F	233	MET	11.1
1	F	353	ILE	10.9

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Mol	Chain	Res	Type	RSRZ
1	K	305	ILE	10.9
1	M	267	MET	10.7
1	K	349	ILE	10.7
1	M	356	ALA	10.3
1	F	349	ILE	10.0
1	K	271	VAL	9.9
1	M	223	ALA	9.8
1	K	270	ILE	9.8
1	F	309	LEU	9.7
1	I	270	ILE	9.7
1	E	353	ILE	9.7
1	B	233	MET	9.6
1	J	271	VAL	9.6
1	K	309	LEU	9.6
1	K	231	ARG	9.6
1	M	309	LEU	9.5
1	B	264	VAL	9.5
1	F	314	LEU	9.4
1	E	356	ALA	9.3
1	J	356	ALA	9.3
1	M	353	ILE	9.2
1	K	230	ILE	9.1
1	C	356	ALA	9.1
1	K	260	ALA	9.0
1	E	234	LEU	9.0
1	E	271	VAL	9.0
1	F	357	THR	8.8
1	J	269	GLY	8.6
1	K	236	VAL	8.6
1	M	221	LEU	8.6
1	B	257	GLU	8.5
1	C	353	ILE	8.4
1	F	219	PHE	8.4
1	M	271	VAL	8.3
1	B	240	VAL	8.3
1	F	268	ARG	8.3
1	J	270	ILE	8.1
1	I	305	ILE	8.1
1	M	263	VAL	8.1
1	M	357	THR	8.0
1	B	258	ALA	8.0
1	K	233	MET	7.9

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Mol	Chain	Res	Type	RSRZ
1	K	265	ASN	7.9
1	K	259	LEU	7.9
1	L	264	VAL	7.8
1	M	237	LEU	7.8
1	F	242	LYS	7.7
1	J	349	ILE	7.7
1	M	264	VAL	7.7
1	B	356	ALA	7.6
1	B	281	PHE	7.6
1	B	301	ILE	7.6
1	F	270	ILE	7.5
1	F	237	LEU	7.5
1	J	44	PHE	7.5
1	J	357	THR	7.5
1	N	263	VAL	7.5
1	N	349	ILE	7.5
1	M	306	GLY	7.4
1	M	349	ILE	7.4
1	M	268	ARG	7.4
1	K	335	GLY	7.3
1	M	203	TYR	7.3
1	M	233	MET	7.3
1	L	231	ARG	7.3
1	K	268	ARG	7.3
1	K	360	TYR	7.3
1	K	203	TYR	7.2
1	B	270	ILE	7.2
1	K	237	LEU	7.2
1	C	270	ILE	7.1
1	L	266	THR	7.1
1	K	267	MET	7.1
1	B	268	ARG	7.0
1	B	357	THR	7.0
1	B	271	VAL	7.0
1	H	270	ILE	7.0
1	C	271	VAL	6.9
1	A	353	ILE	6.9
1	L	234	LEU	6.9
1	L	270	ILE	6.9
1	L	230	ILE	6.9
1	I	268	ARG	6.9
1	M	244	GLY	6.9

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Mol	Chain	Res	Type	RSRZ
1	E	305	ILE	6.9
1	J	233	MET	6.8
1	M	240	VAL	6.8
1	I	356	ALA	6.8
1	B	365	LEU	6.8
1	E	230	ILE	6.8
1	E	233	MET	6.8
1	E	223	ALA	6.8
1	F	260	ALA	6.8
1	F	230	ILE	6.8
1	E	349	ILE	6.7
1	C	44	PHE	6.7
1	K	219	PHE	6.7
1	J	266	THR	6.6
1	K	264	VAL	6.6
1	L	309	LEU	6.6
1	M	314	LEU	6.6
1	K	234	LEU	6.6
1	A	263	VAL	6.6
1	E	309	LEU	6.6
1	K	356	ALA	6.6
1	E	272	LYS	6.6
1	B	234	LEU	6.6
1	F	360	TYR	6.5
1	F	317	LEU	6.5
1	C	268	ARG	6.5
1	G	230	ILE	6.5
1	K	353	ILE	6.5
1	F	346	VAL	6.4
1	F	356	ALA	6.4
1	M	186	GLU	6.4
1	I	264	VAL	6.4
1	I	267	MET	6.3
1	C	266	THR	6.2
1	B	259	LEU	6.2
1	L	271	VAL	6.2
1	B	355	GLU	6.2
1	I	230	ILE	6.2
1	F	267	MET	6.2
1	B	77	VAL	6.2
1	K	188	ASP	6.2
1	M	238	GLU	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	203	TYR	6.2
1	J	305	ILE	6.2
1	M	204	PHE	6.2
1	B	314	LEU	6.1
1	C	360	TYR	6.1
1	F	272	LYS	6.1
1	C	292	ILE	6.0
1	K	357	THR	6.0
1	A	356	ALA	6.0
1	M	358	SER	6.0
1	C	362	ARG	6.0
1	F	222	LEU	6.0
1	N	231	ARG	6.0
1	B	44	PHE	6.0
1	B	230	ILE	6.0
1	M	260	ALA	6.0
1	I	349	ILE	6.0
1	M	305	ILE	6.0
1	F	44	PHE	5.9
1	E	357	THR	5.9
1	L	268	ARG	5.9
1	M	266	THR	5.9
1	M	273	VAL	5.9
1	J	264	VAL	5.9
1	I	265	ASN	5.9
1	F	263	VAL	5.8
1	K	228	SER	5.8
1	B	351	GLN	5.8
1	E	270	ILE	5.8
1	J	309	LEU	5.8
1	F	342	ILE	5.8
1	C	351	GLN	5.8
1	I	44	PHE	5.8
1	M	320	ALA	5.8
1	H	309	LEU	5.8
1	I	351	GLN	5.8
1	J	526	LYS	5.8
1	F	264	VAL	5.7
1	J	353	ILE	5.7
1	B	286	LYS	5.7
1	M	351	GLN	5.7
1	F	244	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	M	336	VAL	5.7
1	F	231	ARG	5.7
1	M	340	ALA	5.6
1	K	232	GLU	5.6
1	K	351	GLN	5.6
1	B	304	GLU	5.6
1	M	300	VAL	5.6
1	M	230	ILE	5.6
1	C	263	VAL	5.6
1	J	229	ASN	5.6
1	B	266	THR	5.6
1	K	256	GLY	5.6
1	G	264	VAL	5.6
1	K	276	VAL	5.5
1	B	307	MET	5.5
1	C	365	LEU	5.5
1	H	234	LEU	5.5
1	E	268	ARG	5.5
1	K	369	VAL	5.5
1	E	301	ILE	5.5
1	J	268	ARG	5.5
1	H	233	MET	5.5
1	E	269	GLY	5.5
1	I	240	VAL	5.4
1	K	306	GLY	5.4
1	G	267	MET	5.4
1	I	353	ILE	5.4
1	B	526	LYS	5.4
1	C	259	LEU	5.4
1	I	266	THR	5.4
1	B	223	ALA	5.4
1	I	271	VAL	5.4
1	B	354	GLU	5.4
1	M	365	LEU	5.4
1	B	227	ILE	5.4
1	J	358	SER	5.3
1	F	269	GLY	5.3
1	L	267	MET	5.3
1	D	271	VAL	5.3
1	K	340	ALA	5.3
1	C	242	LYS	5.3
1	H	266	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	J	263	VAL	5.3
1	C	237	LEU	5.3
1	J	237	LEU	5.3
1	G	268	ARG	5.3
1	N	270	ILE	5.2
1	B	229	ASN	5.2
1	I	360	TYR	5.2
1	B	260	ALA	5.2
1	I	234	LEU	5.2
1	I	526	LYS	5.2
1	C	295	LEU	5.2
1	K	227	ILE	5.2
1	M	317	LEU	5.2
1	C	233	MET	5.1
1	I	233	MET	5.1
1	C	244	GLY	5.1
1	H	353	ILE	5.1
1	N	230	ILE	5.1
1	H	44	PHE	5.1
1	M	272	LYS	5.1
1	F	271	VAL	5.1
1	G	269	GLY	5.1
1	M	259	LEU	5.1
1	I	203	TYR	5.1
1	M	251	ALA	5.1
1	J	204	PHE	5.1
1	N	281	PHE	5.1
1	C	369	VAL	5.1
1	I	355	GLU	5.1
1	J	231	ARG	5.0
1	I	352	GLN	5.0
1	K	341	ALA	5.0
1	C	273	VAL	5.0
1	F	203	TYR	5.0
1	M	218	PRO	5.0
1	L	305	ILE	5.0
1	F	255	GLU	5.0
1	J	360	TYR	5.0
1	J	351	GLN	5.0
1	M	235	PRO	5.0
1	B	309	LEU	4.9
1	K	365	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	K	302	SER	4.9
1	A	284	ARG	4.9
1	E	263	VAL	4.9
1	F	236	VAL	4.9
1	M	236	VAL	4.9
1	I	363	GLU	4.9
1	C	333	ILE	4.9
1	G	44	PHE	4.9
1	F	256	GLY	4.9
1	H	264	VAL	4.9
1	E	354	GLU	4.9
1	C	181	THR	4.9
1	M	335	GLY	4.9
1	J	367	GLU	4.9
1	A	305	ILE	4.9
1	K	358	SER	4.9
1	B	251	ALA	4.9
1	H	265	ASN	4.9
1	M	219	PHE	4.8
1	C	340	ALA	4.8
1	K	304	GLU	4.8
1	J	248	LEU	4.8
1	M	183	LEU	4.8
1	M	262	LEU	4.8
1	H	297	GLY	4.8
1	B	293	ALA	4.8
1	F	241	ALA	4.8
1	K	272	LYS	4.8
1	L	269	GLY	4.8
1	K	275	ALA	4.8
1	E	44	PHE	4.8
1	D	264	VAL	4.7
1	F	204	PHE	4.7
1	A	44	PHE	4.7
1	I	336	VAL	4.7
1	A	358	SER	4.7
1	M	159	GLY	4.7
1	E	240	VAL	4.7
1	F	259	LEU	4.7
1	B	206	ASN	4.7
1	M	265	ASN	4.7
1	F	355	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	H	242	LYS	4.7
1	I	269	GLY	4.7
1	M	44	PHE	4.7
1	L	224	ASP	4.7
1	K	160	LYS	4.7
1	K	205	ILE	4.7
1	K	44	PHE	4.7
1	M	216	GLU	4.7
1	C	357	THR	4.6
1	A	361	ASP	4.6
1	K	224	ASP	4.6
1	K	281	PHE	4.6
1	M	526	LYS	4.6
1	E	295	LEU	4.6
1	B	265	ASN	4.6
1	F	266	THR	4.6
1	L	233	MET	4.6
1	B	372	LEU	4.6
1	M	222	LEU	4.6
1	C	240	VAL	4.6
1	A	357	THR	4.5
1	C	350	ARG	4.5
1	A	271	VAL	4.5
1	C	355	GLU	4.5
1	F	181	THR	4.5
1	I	237	LEU	4.5
1	E	231	ARG	4.5
1	M	301	ILE	4.5
1	F	261	THR	4.5
1	K	181	THR	4.5
1	N	309	LEU	4.5
1	B	363	GLU	4.5
1	K	249	ILE	4.5
1	F	221	LEU	4.5
1	B	263	VAL	4.5
1	C	256	GLY	4.5
1	H	263	VAL	4.5
1	D	268	ARG	4.5
1	B	272	LYS	4.5
1	D	270	ILE	4.5
1	F	249	ILE	4.5
1	F	358	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	273	VAL	4.5
1	B	244	GLY	4.5
1	F	234	LEU	4.4
1	I	309	LEU	4.4
1	G	229	ASN	4.4
1	E	355	GLU	4.4
1	B	295	LEU	4.4
1	C	347	ALA	4.4
1	M	187	LEU	4.4
1	C	264	VAL	4.4
1	B	302	SER	4.4
1	K	191	GLU	4.4
1	L	237	LEU	4.4
1	M	220	ILE	4.4
1	C	249	ILE	4.4
1	J	342	ILE	4.4
1	I	211	GLY	4.4
1	B	236	VAL	4.4
1	E	351	GLN	4.4
1	E	267	MET	4.4
1	K	204	PHE	4.4
1	I	184	GLN	4.3
1	D	526	LYS	4.3
1	M	160	LYS	4.3
1	H	268	ARG	4.3
1	J	317	LEU	4.3
1	K	273	VAL	4.3
1	E	526	LYS	4.3
1	A	257	GLU	4.3
1	M	248	LEU	4.3
1	K	250	ILE	4.3
1	F	351	GLN	4.3
1	K	301	ILE	4.3
1	H	356	ALA	4.3
1	E	242	LYS	4.2
1	E	264	VAL	4.2
1	I	263	VAL	4.2
1	K	350	ARG	4.2
1	F	337	GLY	4.2
1	L	306	GLY	4.2
1	H	357	THR	4.2
1	B	237	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	346	VAL	4.2
1	L	227	ILE	4.2
1	N	264	VAL	4.2
1	I	357	THR	4.2
1	B	303	GLU	4.2
1	C	204	PHE	4.2
1	G	257	GLU	4.2
1	F	225	LYS	4.2
1	B	269	GLY	4.2
1	C	358	SER	4.2
1	L	228	SER	4.2
1	C	230	ILE	4.1
1	L	336	VAL	4.1
1	I	272	LYS	4.1
1	M	249	ILE	4.1
1	B	209	GLU	4.1
1	B	204	PHE	4.1
1	I	260	ALA	4.1
1	J	265	ASN	4.1
1	E	247	LEU	4.1
1	L	311	LYS	4.1
1	L	203	TYR	4.1
1	M	355	GLU	4.1
1	M	363	GLU	4.1
1	M	350	ARG	4.1
1	C	274	ALA	4.1
1	M	347	ALA	4.1
1	E	273	VAL	4.1
1	F	227	ILE	4.1
1	E	307	MET	4.1
1	B	242	LYS	4.1
1	M	360	TYR	4.1
1	I	310	GLU	4.1
1	K	261	THR	4.1
1	G	259	LEU	4.1
1	J	262	LEU	4.1
1	J	281	PHE	4.1
1	K	248	LEU	4.1
1	C	526	LYS	4.0
1	K	355	GLU	4.0
1	K	247	LEU	4.0
1	E	358	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	K	307	MET	4.0
1	K	266	THR	4.0
1	B	289	LEU	4.0
1	M	250	ILE	4.0
1	H	526	LYS	4.0
1	N	44	PHE	4.0
1	F	389	MET	4.0
1	K	240	VAL	4.0
1	B	305	ILE	4.0
1	D	230	ILE	4.0
1	M	333	ILE	4.0
1	F	186	GLU	4.0
1	H	355	GLU	4.0
1	K	257	GLU	4.0
1	A	187	LEU	4.0
1	D	269	GLY	4.0
1	B	249	ILE	4.0
1	K	342	ILE	4.0
1	C	346	VAL	3.9
1	M	202	PRO	3.9
1	J	257	GLU	3.9
1	B	231	ARG	3.9
1	F	180	GLY	3.9
1	J	256	GLY	3.9
1	F	365	LEU	3.9
1	G	258	ALA	3.9
1	F	354	GLU	3.9
1	M	181	THR	3.9
1	B	224	ASP	3.9
1	F	273	VAL	3.9
1	K	263	VAL	3.9
1	K	345	ARG	3.9
1	B	342	ILE	3.9
1	H	305	ILE	3.9
1	H	351	GLN	3.9
1	C	304	GLU	3.9
1	K	362	ARG	3.9
1	G	266	THR	3.9
1	M	168	LYS	3.9
1	B	284	ARG	3.9
1	A	355	GLU	3.8
1	K	202	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	L	249	ILE	3.8
1	E	256	GLY	3.8
1	F	363	GLU	3.8
1	B	134	LEU	3.8
1	E	229	ASN	3.8
1	C	272	LYS	3.8
1	B	282	GLY	3.8
1	M	241	ALA	3.8
1	M	342	ILE	3.8
1	B	262	LEU	3.8
1	E	219	PHE	3.8
1	N	283	ASP	3.8
1	C	286	LYS	3.8
1	L	526	LYS	3.8
1	D	44	PHE	3.8
1	M	310	GLU	3.8
1	F	229	ASN	3.7
1	H	243	ALA	3.7
1	I	358	SER	3.7
1	A	349	ILE	3.7
1	K	183	LEU	3.7
1	A	268	ARG	3.7
1	F	347	ALA	3.7
1	A	209	GLU	3.7
1	A	351	GLN	3.7
1	D	266	THR	3.7
1	M	254	VAL	3.7
1	F	319	GLN	3.7
1	L	356	ALA	3.7
1	I	231	ARG	3.7
1	I	256	GLY	3.7
1	N	354	GLU	3.7
1	J	223	ALA	3.7
1	F	214	GLU	3.7
1	J	228	SER	3.6
1	E	236	VAL	3.6
1	E	266	THR	3.6
1	N	266	THR	3.6
1	F	251	ALA	3.6
1	H	360	TYR	3.6
1	I	183	LEU	3.6
1	L	258	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	238	GLU	3.6
1	J	267	MET	3.6
1	M	346	VAL	3.6
1	J	365	LEU	3.6
1	K	312	ALA	3.6
1	A	264	VAL	3.6
1	E	136	VAL	3.6
1	N	240	VAL	3.6
1	B	335	GLY	3.6
1	K	347	ALA	3.6
1	E	360	TYR	3.6
1	A	266	THR	3.6
1	C	261	THR	3.6
1	J	361	ASP	3.6
1	K	310	GLU	3.6
1	C	161	LEU	3.6
1	C	265	ASN	3.6
1	B	350	ARG	3.6
1	N	350	ARG	3.6
1	J	260	ALA	3.6
1	A	265	ASN	3.6
1	A	183	LEU	3.5
1	G	271	VAL	3.5
1	K	371	LYS	3.5
1	C	222	LEU	3.5
1	F	305	ILE	3.5
1	H	230	ILE	3.5
1	M	304	GLU	3.5
1	C	223	ALA	3.5
1	K	152	ALA	3.5
1	N	351	GLN	3.5
1	C	221	LEU	3.5
1	K	317	LEU	3.5
1	E	342	ILE	3.5
1	G	311	LYS	3.5
1	F	384	ALA	3.5
1	L	44	PHE	3.5
1	L	307	MET	3.5
1	A	363	GLU	3.5
1	B	183	LEU	3.5
1	G	231	ARG	3.5
1	L	272	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	314	LEU	3.5
1	C	301	ILE	3.5
1	I	354	GLU	3.5
1	J	333	ILE	3.5
1	B	298	GLY	3.5
1	M	269	GLY	3.5
1	C	215	LEU	3.4
1	G	181	THR	3.4
1	E	265	ASN	3.4
1	F	290	GLN	3.4
1	E	312	ALA	3.4
1	C	372	LEU	3.4
1	C	337	GLY	3.4
1	G	306	GLY	3.4
1	K	354	GLU	3.4
1	L	353	ILE	3.4
1	N	526	LYS	3.4
1	F	352	GLN	3.4
1	M	299	THR	3.4
1	C	309	LEU	3.4
1	E	222	LEU	3.4
1	E	250	ILE	3.4
1	D	281	PHE	3.4
1	I	204	PHE	3.4
1	M	224	ASP	3.4
1	C	267	MET	3.4
1	B	317	LEU	3.4
1	I	258	ALA	3.4
1	K	223	ALA	3.4
1	M	295	LEU	3.4
1	M	384	ALA	3.4
1	K	229	ASN	3.4
1	E	292	ILE	3.4
1	F	306	GLY	3.4
1	C	336	VAL	3.3
1	E	345	ARG	3.3
1	H	358	SER	3.3
1	B	221	LEU	3.3
1	K	221	LEU	3.3
1	K	262	LEU	3.3
1	M	388	GLU	3.3
1	J	230	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	H	313	THR	3.3
1	F	178	GLU	3.3
1	I	242	LYS	3.3
1	L	259	LEU	3.3
1	L	317	LEU	3.3
1	K	322	ARG	3.3
1	H	257	GLU	3.3
1	L	310	GLU	3.3
1	F	369	VAL	3.3
1	F	215	LEU	3.3
1	C	363	GLU	3.3
1	M	242	LYS	3.3
1	J	261	THR	3.3
1	F	315	GLU	3.3
1	F	335	GLY	3.3
1	K	311	LYS	3.3
1	B	215	LEU	3.3
1	A	339	GLU	3.3
1	E	304	GLU	3.3
1	M	195	PHE	3.3
1	F	372	LEU	3.3
1	L	183	LEU	3.3
1	F	232	GLU	3.3
1	K	255	GLU	3.3
1	K	331	THR	3.3
1	M	322	ARG	3.3
1	A	270	ILE	3.2
1	E	384	ALA	3.2
1	N	356	ALA	3.2
1	L	314	LEU	3.2
1	E	188	ASP	3.2
1	C	260	ALA	3.2
1	E	300	VAL	3.2
1	M	389	MET	3.2
1	I	365	LEU	3.2
1	B	297	GLY	3.2
1	C	191	GLU	3.2
1	C	315	GLU	3.2
1	N	265	ASN	3.2
1	F	362	ARG	3.2
1	N	353	ILE	3.2
1	E	255	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	164	GLU	3.2
1	D	267	MET	3.2
1	K	299	THR	3.2
1	B	222	LEU	3.2
1	L	222	LEU	3.2
1	M	372	LEU	3.2
1	A	304	GLU	3.2
1	C	243	ALA	3.2
1	F	228	SER	3.2
1	F	343	GLN	3.2
1	B	202	PRO	3.2
1	L	244	GLY	3.2
1	A	346	VAL	3.2
1	G	262	LEU	3.2
1	F	265	ASN	3.2
1	L	265	ASN	3.2
1	A	335	GLY	3.2
1	E	317	LEU	3.2
1	F	161	LEU	3.2
1	J	219	PHE	3.2
1	K	235	PRO	3.1
1	F	526	LYS	3.1
1	F	361	ASP	3.1
1	K	334	ASP	3.1
1	C	300	VAL	3.1
1	L	236	VAL	3.1
1	G	228	SER	3.1
1	I	215	LEU	3.1
1	A	260	ALA	3.1
1	F	297	GLY	3.1
1	J	220	ILE	3.1
1	C	354	GLU	3.1
1	J	363	GLU	3.1
1	I	259	LEU	3.1
1	L	202	PRO	3.1
1	L	185	ASP	3.1
1	M	344	GLY	3.1
1	J	354	GLU	3.1
1	D	284	ARG	3.1
1	C	342	ILE	3.1
1	L	238	GLU	3.1
1	M	290	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	259	LEU	3.1
1	D	262	LEU	3.1
1	M	142	LYS	3.1
1	K	209	GLU	3.1
1	E	224	ASP	3.1
1	E	284	ARG	3.1
1	F	239	ALA	3.0
1	F	275	ALA	3.0
1	G	136	VAL	3.0
1	N	267	MET	3.0
1	C	284	ARG	3.0
1	I	202	PRO	3.0
1	J	232	GLU	3.0
1	N	304	GLU	3.0
1	B	360	TYR	3.0
1	E	203	TYR	3.0
1	C	217	SER	3.0
1	F	336	VAL	3.0
1	M	234	LEU	3.0
1	F	224	ASP	3.0
1	K	253	ASP	3.0
1	G	525	PRO	3.0
1	E	249	ILE	3.0
1	F	250	ILE	3.0
1	A	223	ALA	3.0
1	F	340	ALA	3.0
1	L	275	ALA	3.0
1	I	361	ASP	3.0
1	L	283	ASP	3.0
1	A	354	GLU	3.0
1	M	286	LYS	3.0
1	B	358	SER	3.0
1	D	325	ILE	3.0
1	I	325	ILE	3.0
1	N	228	SER	3.0
1	B	300	VAL	3.0
1	H	300	VAL	3.0
1	N	317	LEU	3.0
1	M	334	ASP	3.0
1	B	228	SER	3.0
1	E	383	ALA	3.0
1	N	358	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	333	ILE	3.0
1	C	322	ARG	3.0
1	M	339	GLU	3.0
1	J	242	LYS	3.0
1	C	216	GLU	2.9
1	C	232	GLU	2.9
1	E	220	ILE	2.9
1	G	325	ILE	2.9
1	K	283	ASP	2.9
1	F	295	LEU	2.9
1	M	229	ASN	2.9
1	A	231	ARG	2.9
1	J	362	ARG	2.9
1	F	258	ALA	2.9
1	G	383	ALA	2.9
1	N	260	ALA	2.9
1	M	188	ASP	2.9
1	B	248	LEU	2.9
1	E	257	GLU	2.9
1	L	346	VAL	2.9
1	M	366	GLN	2.9
1	K	292	ILE	2.9
1	C	231	ARG	2.9
1	G	265	ASN	2.9
1	F	292	ILE	2.9
1	B	252	GLU	2.9
1	I	257	GLU	2.9
1	M	217	SER	2.9
1	J	366	GLN	2.9
1	N	256	GLY	2.9
1	C	325	ILE	2.9
1	J	250	ILE	2.9
1	K	243	ALA	2.9
1	C	203	TYR	2.9
1	M	255	GLU	2.9
1	M	180	GLY	2.8
1	B	292	ILE	2.8
1	D	305	ILE	2.8
1	J	301	ILE	2.8
1	K	363	GLU	2.8
1	E	346	VAL	2.8
1	K	241	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	316	ASP	2.8
1	H	284	ARG	2.8
1	N	268	ARG	2.8
1	M	307	MET	2.8
1	J	221	LEU	2.8
1	L	262	LEU	2.8
1	M	215	LEU	2.8
1	A	242	LYS	2.8
1	I	245	LYS	2.8
1	M	231	ARG	2.8
1	F	245	LYS	2.8
1	B	133	ALA	2.8
1	J	243	ALA	2.8
1	N	363	GLU	2.8
1	A	261	THR	2.8
1	L	240	VAL	2.8
1	K	288	MET	2.8
1	F	235	PRO	2.8
1	I	302	SER	2.8
1	A	342	ILE	2.8
1	B	205	ILE	2.8
1	G	305	ILE	2.8
1	H	361	ASP	2.8
1	I	364	LYS	2.8
1	A	273	VAL	2.8
1	L	281	PHE	2.8
1	M	281	PHE	2.8
1	K	139	SER	2.8
1	C	334	ASP	2.8
1	M	343	GLN	2.8
1	B	255	GLU	2.8
1	H	304	GLU	2.8
1	L	308	GLU	2.8
1	E	237	LEU	2.8
1	J	381	VAL	2.8
1	M	369	VAL	2.8
1	M	376	VAL	2.8
1	J	288	MET	2.7
1	N	204	PHE	2.7
1	I	229	ASN	2.7
1	C	373	ALA	2.7
1	J	345	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	239	ALA	2.7
1	M	261	THR	2.7
1	A	262	LEU	2.7
1	A	301	ILE	2.7
1	C	250	ILE	2.7
1	N	161	LEU	2.7
1	B	136	VAL	2.7
1	B	235	PRO	2.7
1	G	310	GLU	2.7
1	N	284	ARG	2.7
1	K	274	ALA	2.7
1	A	214	GLU	2.7
1	I	372	LEU	2.7
1	H	267	MET	2.7
1	F	350	ARG	2.7
1	J	284	ARG	2.7
1	A	526	LYS	2.7
1	G	272	LYS	2.7
1	G	526	LYS	2.7
1	F	157	THR	2.7
1	G	281	PHE	2.7
1	N	362	ARG	2.7
1	E	365	LEU	2.7
1	E	306	GLY	2.7
1	C	341	ALA	2.7
1	H	261	THR	2.7
1	C	281	PHE	2.7
1	I	228	SER	2.7
1	B	388	GLU	2.7
1	K	308	GLU	2.7
1	I	451	LEU	2.7
1	J	280	GLY	2.7
1	C	184	GLN	2.7
1	E	184	GLN	2.7
1	L	348	GLN	2.7
1	B	368	ARG	2.7
1	E	359	ASP	2.7
1	K	242	LYS	2.7
1	C	367	GLU	2.7
1	J	355	GLU	2.7
1	I	525	PRO	2.7
1	C	180	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	256	GLY	2.7
1	A	184	GLN	2.6
1	L	146	GLN	2.6
1	F	321	LYS	2.6
1	N	369	VAL	2.6
1	K	320	ALA	2.6
1	M	157	THR	2.6
1	A	360	TYR	2.6
1	A	182	GLY	2.6
1	A	288	MET	2.6
1	H	198	GLY	2.6
1	E	456	LEU	2.6
1	G	270	ILE	2.6
1	K	381	VAL	2.6
1	J	239	ALA	2.6
1	F	160	LYS	2.6
1	K	366	GLN	2.6
1	M	226	LYS	2.6
1	C	269	GLY	2.6
1	E	361	ASP	2.6
1	F	316	ASP	2.6
1	J	224	ASP	2.6
1	F	281	PHE	2.6
1	H	229	ASN	2.6
1	C	205	ILE	2.6
1	L	351	GLN	2.6
1	E	258	ALA	2.6
1	E	347	ALA	2.6
1	F	300	VAL	2.6
1	F	303	GLU	2.6
1	I	340	ALA	2.6
1	M	315	GLU	2.6
1	G	138	CYS	2.6
1	H	286	LYS	2.6
1	K	526	LYS	2.6
1	I	232	GLU	2.6
1	H	259	LEU	2.6
1	L	284	ARG	2.6
1	G	261	THR	2.6
1	I	235	PRO	2.6
1	H	269	GLY	2.6
1	I	341	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	260	ALA	2.6
1	M	332	ILE	2.6
1	B	346	VAL	2.6
1	I	236	VAL	2.6
1	M	323	VAL	2.6
1	N	273	VAL	2.6
1	F	304	GLU	2.6
1	H	363	GLU	2.6
1	A	188	ASP	2.6
1	K	361	ASP	2.6
1	J	302	SER	2.6
1	I	244	GLY	2.6
1	F	301	ILE	2.6
1	K	325	ILE	2.6
1	K	376	VAL	2.6
1	L	213	VAL	2.6
1	A	350	ARG	2.6
1	L	285	ARG	2.6
1	M	284	ARG	2.6
1	F	155	ASP	2.6
1	A	281	PHE	2.5
1	I	391	GLU	2.5
1	E	215	LEU	2.5
1	F	183	LEU	2.5
1	K	384	ALA	2.5
1	M	258	ALA	2.5
1	A	276	VAL	2.5
1	L	273	VAL	2.5
1	L	300	VAL	2.5
1	B	367	GLU	2.5
1	L	315	GLU	2.5
1	N	280	GLY	2.5
1	G	204	PHE	2.5
1	J	340	ALA	2.5
1	C	168	LYS	2.5
1	M	324	VAL	2.5
1	C	348	GLN	2.5
1	D	184	GLN	2.5
1	I	362	ARG	2.5
1	A	181	THR	2.5
1	C	248	LEU	2.5
1	N	365	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	352	GLN	2.5
1	F	378	VAL	2.5
1	G	323	VAL	2.5
1	I	284	ARG	2.5
1	L	349	ILE	2.5
1	M	213	VAL	2.5
1	M	345	ARG	2.5
1	C	160	LYS	2.5
1	B	238	GLU	2.5
1	C	210	THR	2.5
1	F	312	ALA	2.5
1	L	219	PHE	2.5
1	C	290	GLN	2.5
1	E	372	LEU	2.5
1	I	222	LEU	2.5
1	K	215	LEU	2.5
1	B	130	GLU	2.5
1	M	156	GLU	2.5
1	M	298	GLY	2.5
1	I	177	VAL	2.5
1	B	348	GLN	2.5
1	A	362	ARG	2.5
1	C	258	ALA	2.5
1	F	284	ARG	2.5
1	L	229	ASN	2.5
1	B	211	GLY	2.5
1	K	192	GLY	2.5
1	I	348	GLN	2.5
1	B	261	THR	2.5
1	K	168	LYS	2.5
1	M	311	LYS	2.5
1	D	258	ALA	2.4
1	B	361	ASP	2.4
1	F	359	ASP	2.4
1	C	247	LEU	2.4
1	C	317	LEU	2.4
1	L	248	LEU	2.4
1	A	388	GLU	2.4
1	B	191	GLU	2.4
1	B	390	LYS	2.4
1	H	343	GLN	2.4
1	J	364	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	308	GLU	2.4
1	A	240	VAL	2.4
1	G	407	VAL	2.4
1	A	267	MET	2.4
1	B	188	ASP	2.4
1	B	241	ALA	2.4
1	K	201	SER	2.4
1	C	245	LYS	2.4
1	E	352	GLN	2.4
1	J	352	GLN	2.4
1	K	352	GLN	2.4
1	N	184	GLN	2.4
1	A	203	TYR	2.4
1	I	317	LEU	2.4
1	K	134	LEU	2.4
1	J	359	ASP	2.4
1	M	185	ASP	2.4
1	B	239	ALA	2.4
1	C	257	GLU	2.4
1	E	232	GLU	2.4
1	H	260	ALA	2.4
1	I	304	GLU	2.4
1	K	344	GLY	2.4
1	N	186	GLU	2.4
1	F	366	GLN	2.4
1	H	525	PRO	2.4
1	B	187	LEU	2.4
1	B	219	PHE	2.4
1	D	203	TYR	2.4
1	I	238	GLU	2.4
1	L	304	GLU	2.4
1	L	184	GLN	2.4
1	G	263	VAL	2.4
1	K	300	VAL	2.4
1	L	190	VAL	2.4
1	M	387	VAL	2.4
1	K	287	ALA	2.4
1	E	338	GLU	2.4
1	N	242	LYS	2.4
1	C	319	GLN	2.4
1	F	262	LEU	2.4
1	G	219	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	318	GLY	2.4
1	K	374	GLY	2.4
1	C	212	ALA	2.4
1	I	301	ILE	2.4
1	K	208	PRO	2.4
1	B	311	LYS	2.4
1	D	257	GLU	2.4
1	F	257	GLU	2.4
1	M	325	ILE	2.4
1	F	388	GLU	2.4
1	E	340	ALA	2.3
1	L	274	ALA	2.3
1	B	254	VAL	2.3
1	L	381	VAL	2.3
1	N	499	VAL	2.3
1	F	333	ILE	2.3
1	I	350	ARG	2.3
1	K	220	ILE	2.3
1	N	305	ILE	2.3
1	B	180	GLY	2.3
1	F	313	THR	2.3
1	F	287	ALA	2.3
1	F	348	GLN	2.3
1	H	350	ARG	2.3
1	I	384	ALA	2.3
1	N	347	ALA	2.3
1	C	254	VAL	2.3
1	J	369	VAL	2.3
1	K	315	GLU	2.3
1	A	224	ASP	2.3
1	A	237	LEU	2.3
1	E	289	LEU	2.3
1	C	219	PHE	2.3
1	L	391	GLU	2.3
1	G	236	VAL	2.3
1	I	369	VAL	2.3
1	E	333	ILE	2.3
1	I	154	SER	2.3
1	I	159	GLY	2.3
1	L	337	GLY	2.3
1	C	366	GLN	2.3
1	B	267	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	288	MET	2.3
1	H	321	LYS	2.3
1	K	258	ALA	2.3
1	J	203	TYR	2.3
1	E	337	GLY	2.3
1	E	214	GLU	2.3
1	F	338	GLU	2.3
1	N	391	GLU	2.3
1	C	332	ILE	2.3
1	I	286	LYS	2.3
1	B	497	THR	2.3
1	L	261	THR	2.3
1	F	248	LEU	2.3
1	H	372	LEU	2.3
1	J	383	ALA	2.3
1	F	367	GLU	2.3
1	M	191	GLU	2.3
1	M	302	SER	2.3
1	H	240	VAL	2.3
1	J	236	VAL	2.3
1	J	336	VAL	2.3
1	A	205	ILE	2.3
1	K	185	ASP	2.3
1	A	384	ALA	2.3
1	C	293	ALA	2.3
1	D	234	LEU	2.3
1	G	234	LEU	2.3
1	B	374	GLY	2.2
1	E	193	MET	2.2
1	F	254	VAL	2.2
1	K	252	GLU	2.2
1	K	336	VAL	2.2
1	N	254	VAL	2.2
1	N	257	GLU	2.2
1	M	364	LYS	2.2
1	B	344	GLY	2.2
1	I	239	ALA	2.2
1	M	297	GLY	2.2
1	C	289	LEU	2.2
1	G	314	LEU	2.2
1	J	234	LEU	2.2
1	L	204	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	345	ARG	2.2
1	M	319	GLN	2.2
1	J	334	ASP	2.2
1	F	276	VAL	2.2
1	E	363	GLU	2.2
1	J	287	ALA	2.2
1	K	214	GLU	2.2
1	K	251	ALA	2.2
1	C	311	LYS	2.2
1	K	286	LYS	2.2
1	L	225	LYS	2.2
1	H	237	LEU	2.2
1	L	247	LEU	2.2
1	N	259	LEU	2.2
1	A	136	VAL	2.2
1	D	363	GLU	2.2
1	H	323	VAL	2.2
1	L	355	GLU	2.2
1	A	311	LYS	2.2
1	F	382	GLY	2.2
1	J	154	SER	2.2
1	M	337	GLY	2.2
1	D	301	ILE	2.2
1	F	449	ALA	2.2
1	K	348	GLN	2.2
1	E	248	LEU	2.2
1	G	137	PRO	2.2
1	K	367	GLU	2.2
1	K	386	GLU	2.2
1	L	363	GLU	2.2
1	E	344	GLY	2.2
1	E	174	VAL	2.2
1	E	387	VAL	2.2
1	C	361	ASP	2.2
1	H	332	ILE	2.2
1	M	341	ALA	2.2
1	N	301	ILE	2.2
1	C	209	GLU	2.2
1	D	229	ASN	2.2
1	J	304	GLU	2.2
1	E	235	PRO	2.2
1	A	400	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	288	MET	2.2
1	B	184	GLN	2.2
1	F	299	THR	2.2
1	H	395	ARG	2.2
1	A	256	GLY	2.2
1	B	324	VAL	2.2
1	B	387	VAL	2.2
1	C	381	VAL	2.2
1	L	369	VAL	2.2
1	C	275	ALA	2.2
1	J	212	ALA	2.2
1	N	258	ALA	2.2
1	A	366	GLN	2.1
1	D	233	MET	2.1
1	K	368	ARG	2.1
1	M	362	ARG	2.1
1	I	248	LEU	2.1
1	N	262	LEU	2.1
1	E	374	GLY	2.1
1	F	385	THR	2.1
1	H	302	SER	2.1
1	J	244	GLY	2.1
1	K	298	GLY	2.1
1	K	382	GLY	2.1
1	I	499	VAL	2.1
1	J	275	ALA	2.1
1	L	455	VAL	2.1
1	L	186	GLU	2.1
1	L	303	GLU	2.1
1	K	359	ASP	2.1
1	F	311	LYS	2.1
1	L	302	SER	2.1
1	B	131	LEU	2.1
1	C	234	LEU	2.1
1	H	161	LEU	2.1
1	L	221	LEU	2.1
1	B	290	GLN	2.1
1	K	284	ARG	2.1
1	B	214	GLU	2.1
1	L	246	PRO	2.1
1	C	188	ASP	2.1
1	K	321	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	226	LYS	2.1
1	G	233	MET	2.1
1	H	338	GLU	2.1
1	L	232	GLU	2.1
1	K	245	LYS	2.1
1	A	341	ALA	2.1
1	B	274	ALA	2.1
1	M	274	ALA	2.1
1	C	193	MET	2.1
1	C	378	VAL	2.1
1	H	346	VAL	2.1
1	I	387	VAL	2.1
1	C	164	GLU	2.1
1	J	184	GLN	2.1
1	J	294	THR	2.1
1	M	338	GLU	2.1
1	I	161	LEU	2.1
1	C	525	PRO	2.1
1	B	347	ALA	2.1
1	A	244	GLY	2.1
1	E	244	GLY	2.1
1	K	216	GLU	2.1
1	L	256	GLY	2.1
1	I	324	VAL	2.1
1	I	346	VAL	2.1
1	G	220	ILE	2.1
1	C	451	LEU	2.1
1	K	222	LEU	2.1
1	L	200	LEU	2.1
1	N	237	LEU	2.1
1	B	310	GLU	2.1
1	I	388	GLU	2.1
1	K	401	HIS	2.1
1	L	235	PRO	2.1
1	F	159	GLY	2.1
1	N	311	LYS	2.1
1	D	411	VAL	2.1
1	H	273	VAL	2.1
1	K	136	VAL	2.1
1	B	186	GLU	2.0
1	L	172	GLU	2.0
1	N	355	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	220	ILE	2.0
1	H	325	ILE	2.0
1	I	227	ILE	2.0
1	C	352	GLN	2.0
1	N	525	PRO	2.0
1	D	183	LEU	2.0
1	D	237	LEU	2.0
1	I	295	LEU	2.0
1	M	382	GLY	2.0
1	A	253	ASP	2.0
1	B	283	ASP	2.0
1	C	174	VAL	2.0
1	D	236	VAL	2.0
1	D	323	VAL	2.0
1	E	464	VAL	2.0
1	N	77	VAL	2.0
1	N	360	TYR	2.0
1	B	256	GLY	2.0
1	B	379	ILE	2.0
1	K	280	GLY	2.0
1	A	295	LEU	2.0
1	D	314	LEU	2.0
1	I	247	LEU	2.0
1	J	200	LEU	2.0
1	E	216	GLU	2.0
1	I	359	ASP	2.0
1	K	364	LYS	2.0
1	I	90	THR	2.0
1	K	157	THR	2.0
1	L	313	THR	2.0
1	M	184	GLN	2.0
1	H	271	VAL	2.0
1	J	177	VAL	2.0
1	F	279	PRO	2.0
1	C	214	GLU	2.0
1	E	339	GLU	2.0
1	F	216	GLU	2.0
1	K	211	GLY	2.0
1	K	303	GLU	2.0
1	M	257	GLU	2.0
1	M	361	ASP	2.0
1	C	364	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	L	321	LYS	2.0
1	N	325	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	0.99	0.35	4.12	29,29,29,29	0
4	AGS	D	561	31/31	0.95	0.15	0.20	2,11,18,21	0
4	AGS	K	1	31/31	0.95	0.14	0.17	6,14,21,24	0
4	AGS	M	1	31/31	0.95	0.13	-0.10	5,12,18,21	0
4	AGS	A	1	31/31	0.97	0.13	-0.10	4,11,16,20	0
3	K	M	560	1/1	1.00	0.12	-0.18	14,14,14,14	0
4	AGS	C	1	31/31	0.96	0.14	-0.19	8,13,19,20	0
3	K	D	560	1/1	0.98	0.14	-0.29	16,16,16,16	0
4	AGS	G	1	31/31	0.96	0.14	-0.33	4,9,16,16	0
4	AGS	E	1	31/31	0.96	0.12	-0.36	2,11,19,20	0
4	AGS	L	1	31/31	0.94	0.13	-0.37	2,8,11,18	0
4	AGS	I	1	31/31	0.96	0.14	-0.47	5,12,16,20	0
4	AGS	N	1	31/31	0.96	0.12	-0.52	4,10,17,19	0
3	K	H	560	1/1	0.98	0.12	-0.57	15,15,15,15	0
4	AGS	F	1	31/31	0.96	0.13	-0.64	2,11,22,23	0
3	K	E	527	1/1	0.98	0.14	-0.91	31,31,31,31	0
4	AGS	H	1	31/31	0.96	0.12	-0.96	3,9,15,17	0
4	AGS	B	1	31/31	0.97	0.11	-1.20	8,13,21,24	0
3	K	L	560	1/1	0.99	0.12	-1.23	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	AGS	J	1	31/31	0.96	0.10	-1.30	2,7,14,15	0
3	K	I	560	1/1	0.99	0.14	-1.37	11,11,11,11	0
3	K	N	560	1/1	0.97	0.10	-1.56	11,11,11,11	0
3	K	B	560	1/1	0.97	0.12	-1.60	13,13,13,13	0
3	K	J	560	1/1	0.98	0.11	-1.66	11,11,11,11	0
3	K	G	560	1/1	0.98	0.13	-1.97	16,16,16,16	0
3	K	A	560	1/1	0.99	0.09	-2.37	13,13,13,13	0
3	K	F	560	1/1	0.99	0.09	-2.53	13,13,13,13	0
3	K	E	560	1/1	0.99	0.10	-2.76	11,11,11,11	0
3	K	K	560	1/1	0.99	0.09	-2.82	11,11,11,11	0
3	K	C	560	1/1	0.99	0.08	-3.20	19,19,19,19	0
2	MG	J	550	1/1	0.97	0.12	-	8,8,8,8	0
2	MG	L	550	1/1	0.88	0.12	-	9,9,9,9	0
2	MG	G	550	1/1	0.95	0.15	-	9,9,9,9	0
2	MG	I	550	1/1	0.96	0.15	-	9,9,9,9	0
2	MG	D	550	1/1	0.97	0.09	-	10,10,10,10	0
2	MG	E	550	1/1	0.98	0.08	-	6,6,6,6	0
2	MG	H	550	1/1	0.96	0.13	-	4,4,4,4	0
2	MG	F	550	1/1	0.96	0.15	-	7,7,7,7	0
2	MG	C	550	1/1	0.96	0.10	-	9,9,9,9	0
2	MG	B	550	1/1	0.92	0.12	-	8,8,8,8	0
2	MG	A	550	1/1	0.97	0.14	-	7,7,7,7	0
2	MG	N	550	1/1	0.90	0.14	-	7,7,7,7	0
2	MG	M	550	1/1	0.97	0.16	-	7,7,7,7	0
2	MG	K	550	1/1	0.96	0.08	-	7,7,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.