



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:17 PM UTC

PDB ID : 4WSC / pdb_00004wsc
Title : Crystal structure of a GroELK105A mutant
Authors : Lorimer, G.H.; Ye, X.; Fei, X.; Yang, D.; Corsepilus, N.; LaRonde, N.A.
Deposited on : 2014-10-26
Resolution : 3.04 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

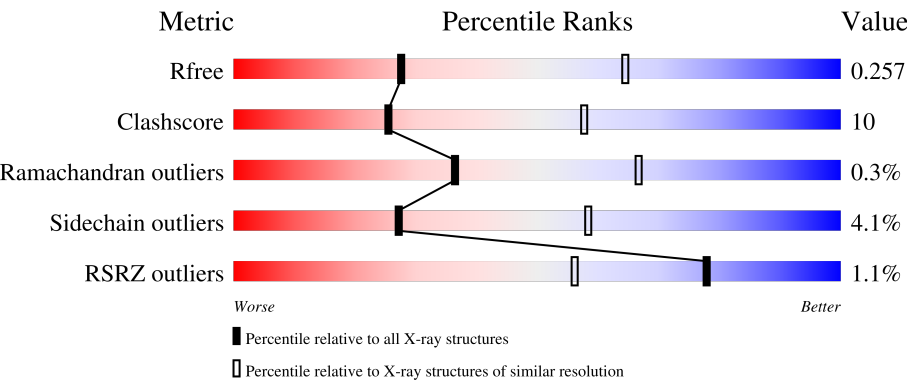
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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}	180053	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	548	2% 71% 22% • •
1	B	548	74% 19% • •
1	C	548	74% 19% • •
1	D	548	• 74% 19% • •
1	E	548	• 72% 20% • •

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Mol	Chain	Length	Quality of chain
1	F	548	70%23%
1	G	548	72%22%
1	H	548	% 71%22%
1	I	548	73%21%
1	J	548	70%24%
1	K	548	73%21%
1	L	548	7% 74%19%
1	M	548	% 70%24%
1	N	548	2% 72%21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53914 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 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3851	2394	664	773	20			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	LYS	engineered mutation	UNP P0A6F5

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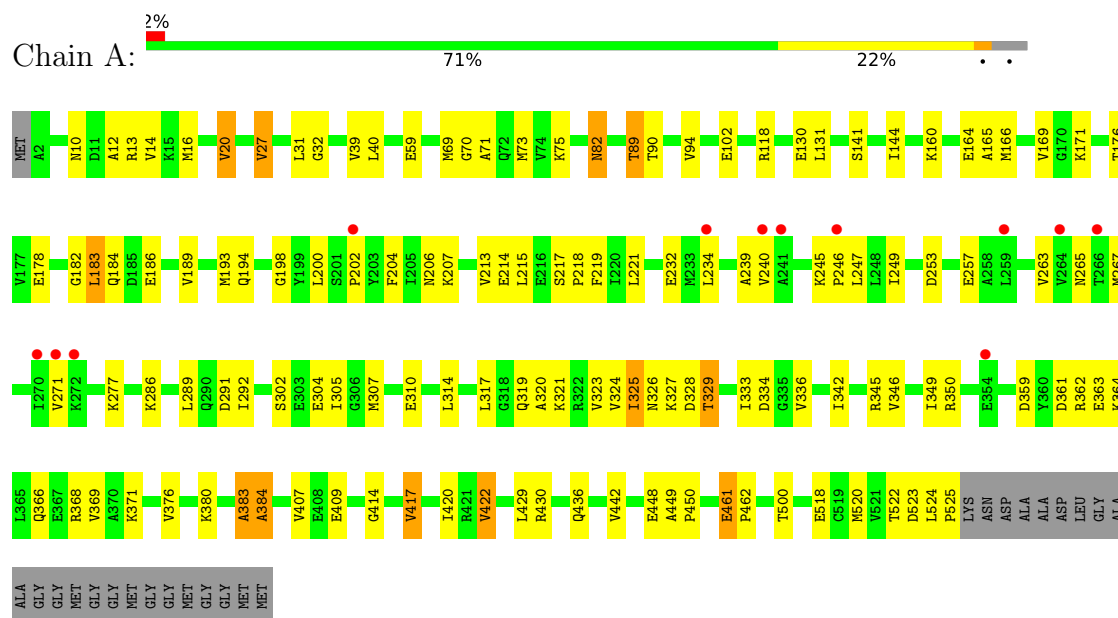
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Chain	Residue	Modelled	Actual	Comment	Reference
B	105	ALA	LYS	engineered mutation	UNP P0A6F5
C	105	ALA	LYS	engineered mutation	UNP P0A6F5
D	105	ALA	LYS	engineered mutation	UNP P0A6F5
E	105	ALA	LYS	engineered mutation	UNP P0A6F5
F	105	ALA	LYS	engineered mutation	UNP P0A6F5
G	105	ALA	LYS	engineered mutation	UNP P0A6F5
H	105	ALA	LYS	engineered mutation	UNP P0A6F5
I	105	ALA	LYS	engineered mutation	UNP P0A6F5
J	105	ALA	LYS	engineered mutation	UNP P0A6F5
K	105	ALA	LYS	engineered mutation	UNP P0A6F5
L	105	ALA	LYS	engineered mutation	UNP P0A6F5
M	105	ALA	LYS	engineered mutation	UNP P0A6F5
N	105	ALA	LYS	engineered mutation	UNP P0A6F5

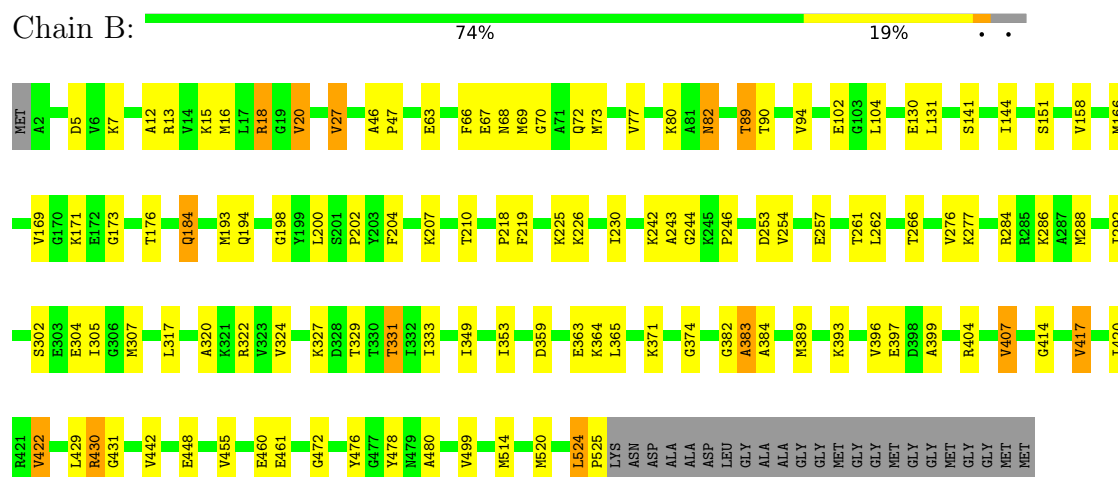
3 Residue-property plots [i](#)

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

- Molecule 1: 60 kDa chaperonin

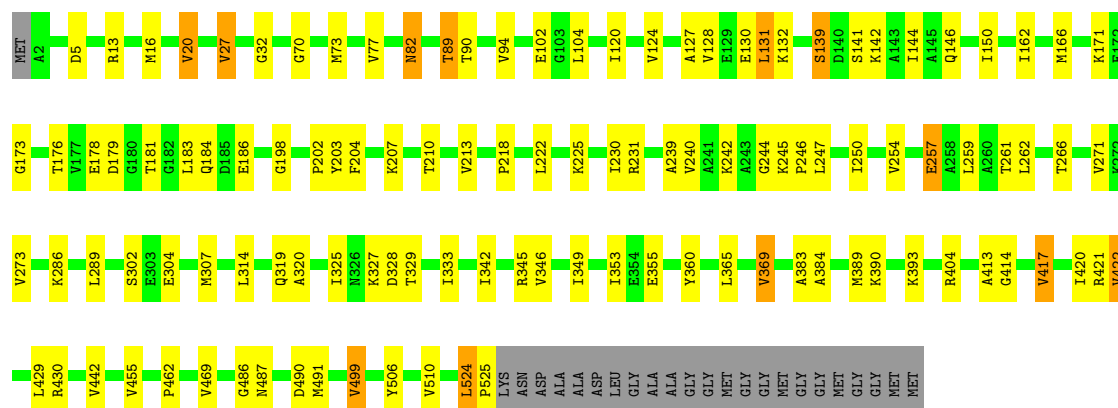


- Molecule 1: 60 kDa chaperonin



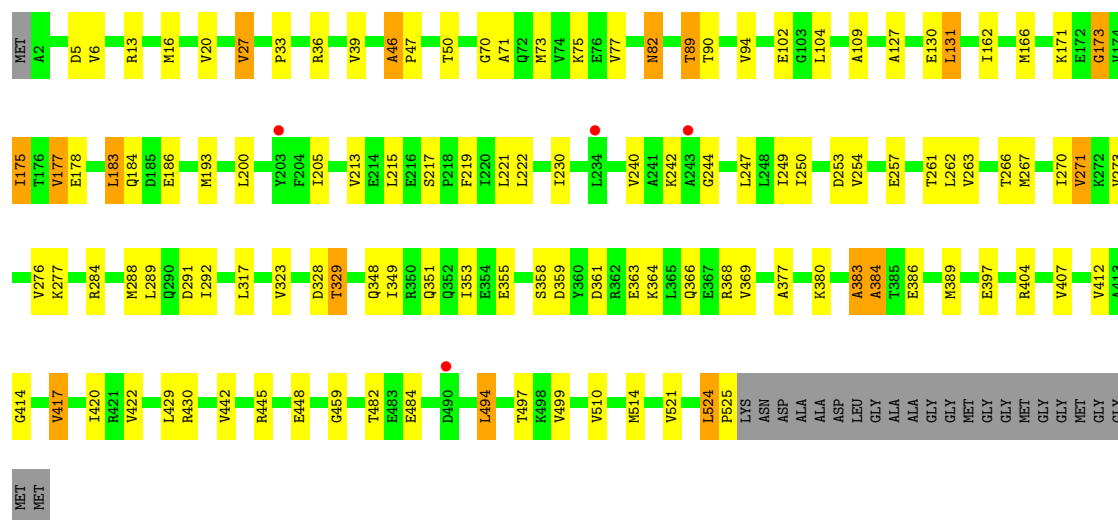
- Molecule 1: 60 kDa chaperonin

Chain C:  74% 19%



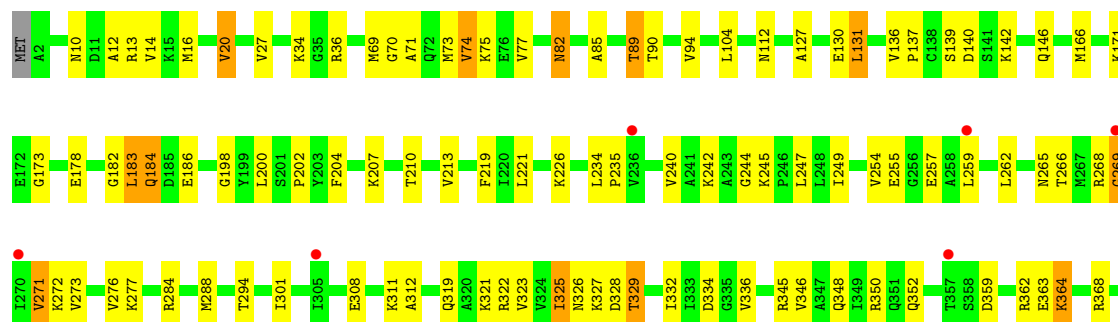
• Molecule 1: 60 kDa chaperonin

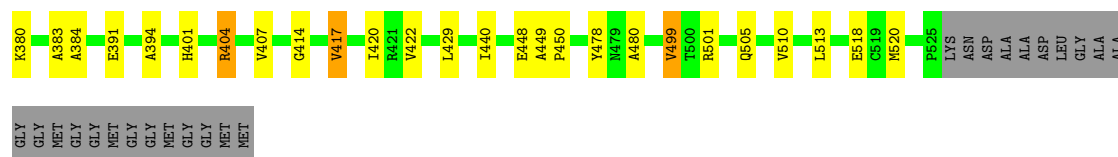
Chain D:  74% 19%



• Molecule 1: 60 kDa chaperonin

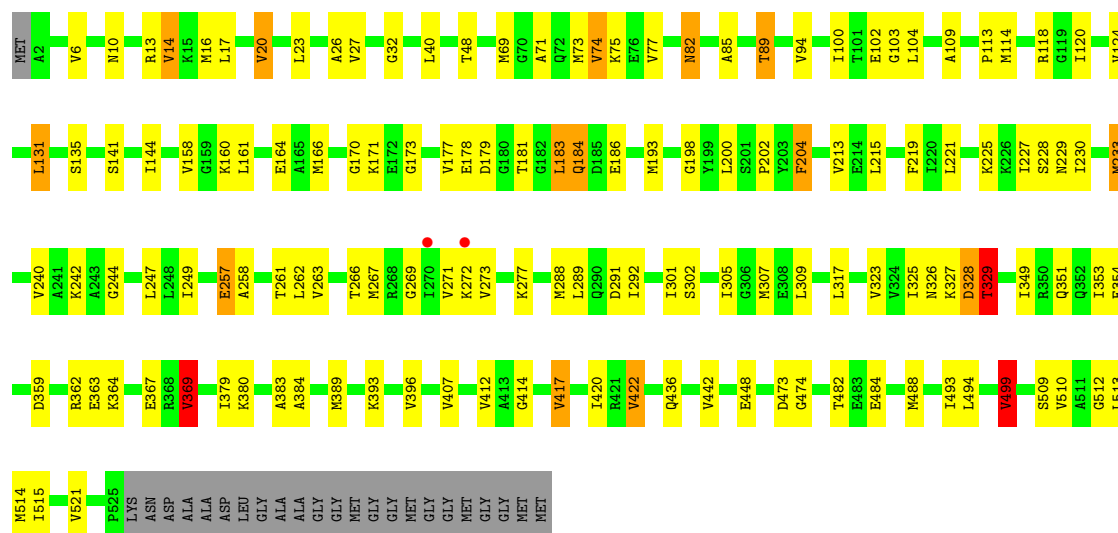
Chain E:  72% 20%





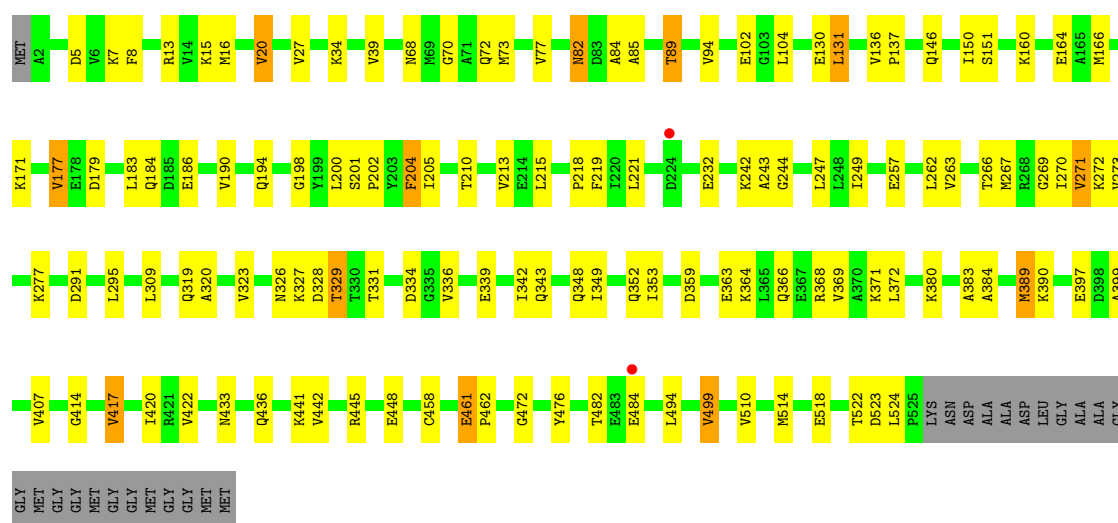
- Molecule 1: 60 kDa chaperonin

Chain F: 70% 23%



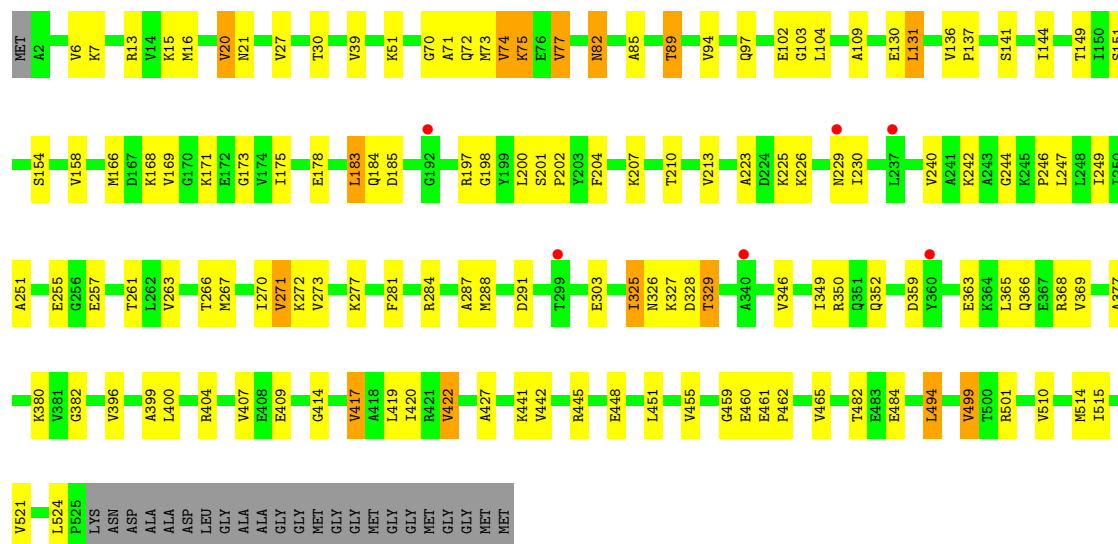
- Molecule 1: 60 kDa chaperonin

Chain G: 72% 22%



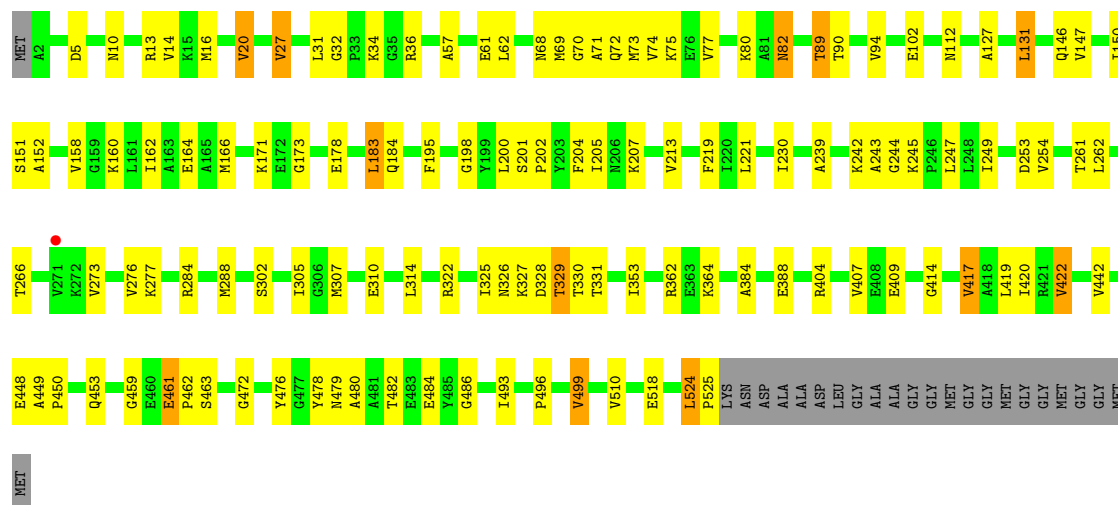
- Molecule 1: 60 kDa chaperonin

Chain H: 71% 22%



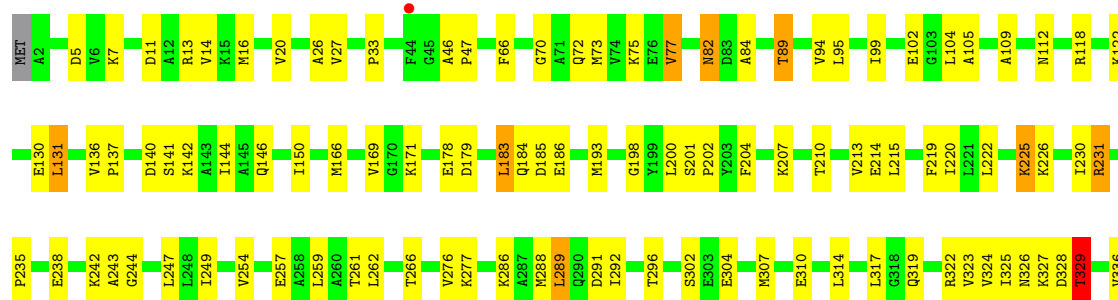
• Molecule 1: 60 kDa chaperonin

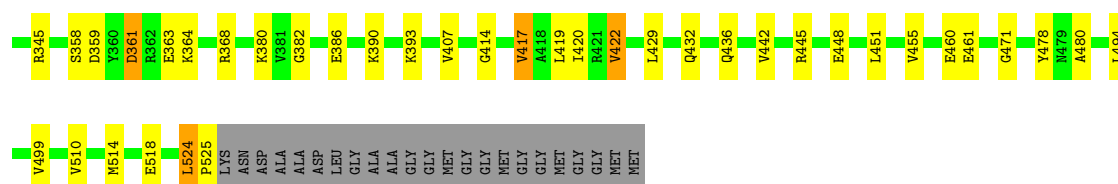
Chain I: 73% 21% . .



• Molecule 1: 60 kDa chaperonin

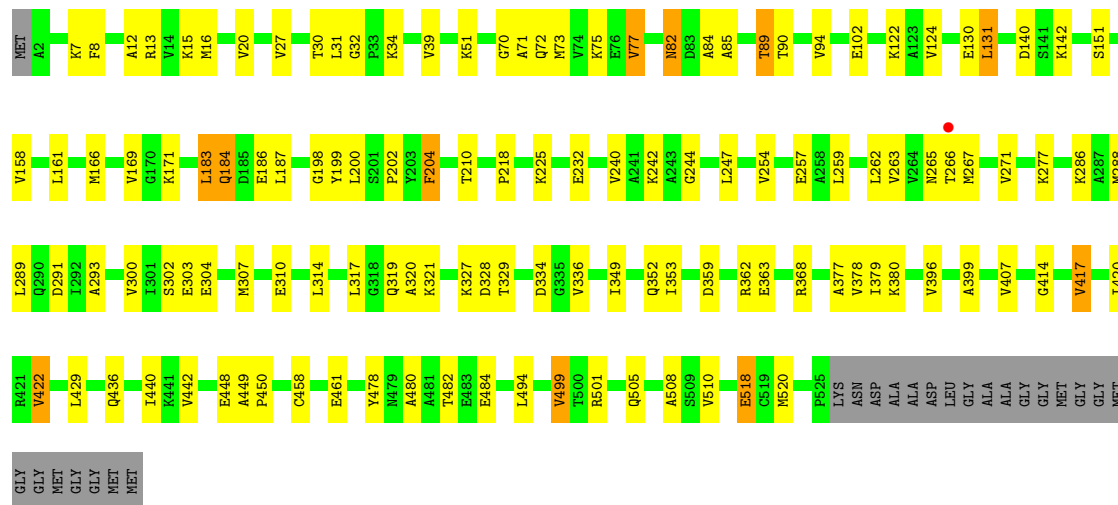
Chain J: 70% 24% . .





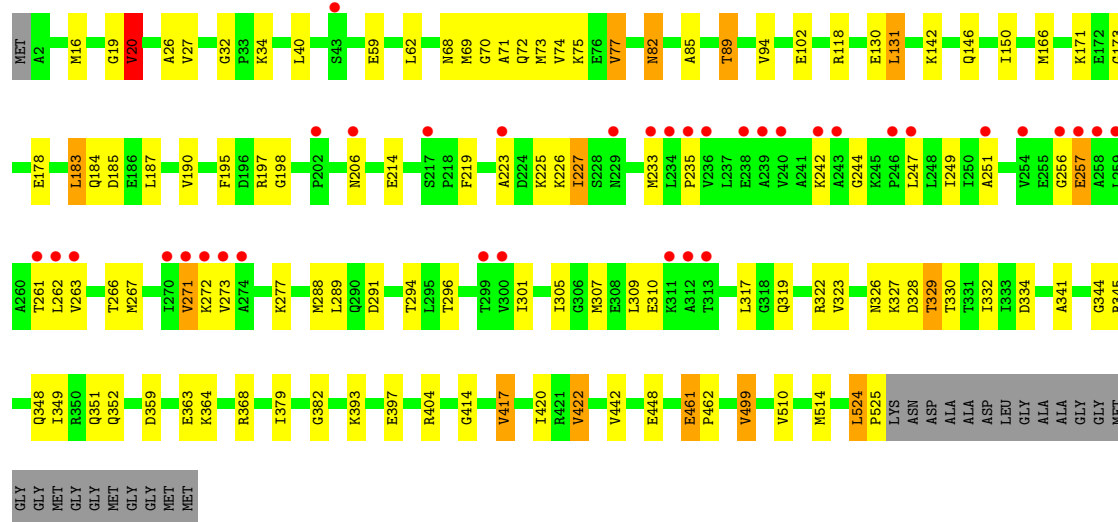
- Molecule 1: 60 kDa chaperonin

Chain K: 73% 21%



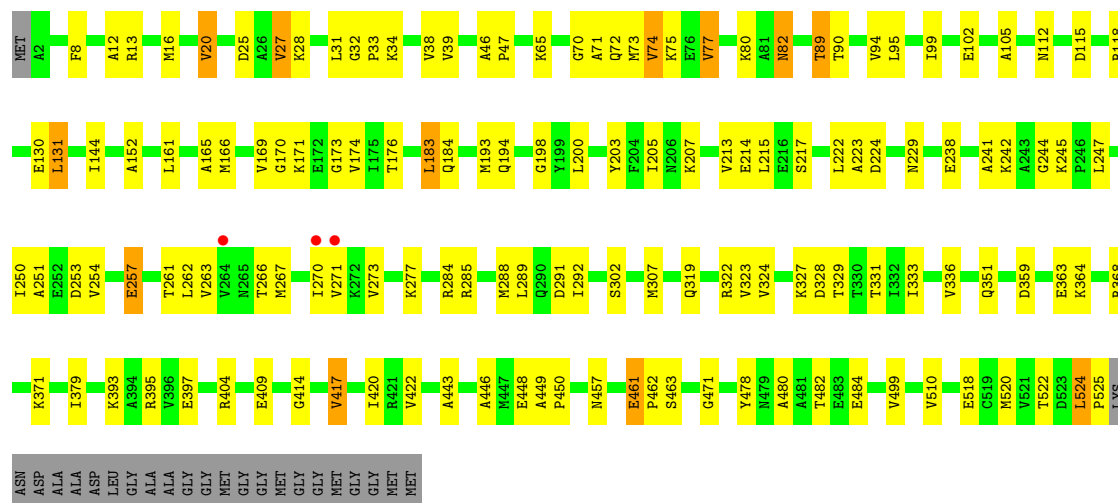
- Molecule 1: 60 kDa chaperonin

Chain L: 7% 74% 19%

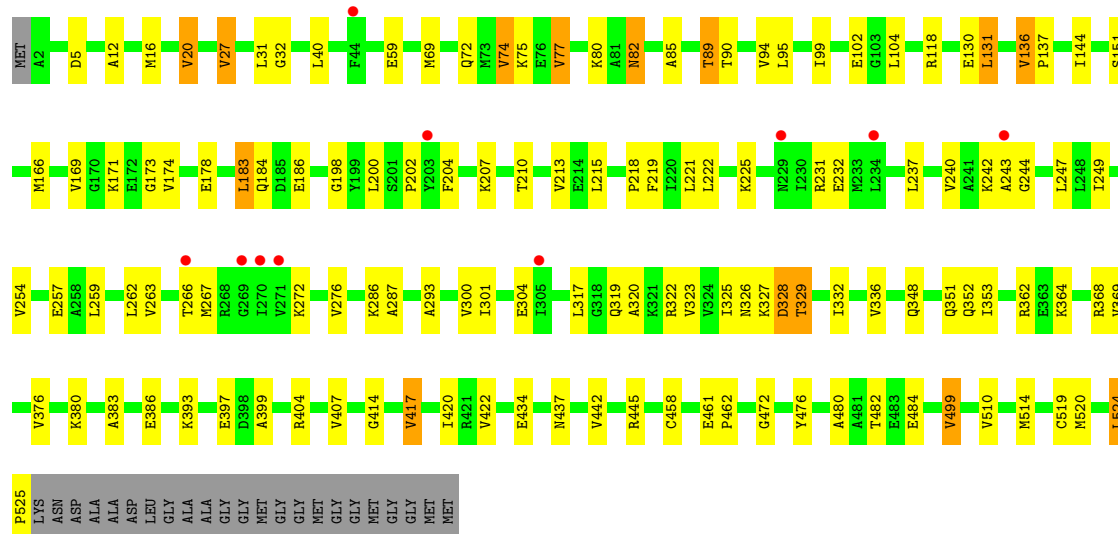
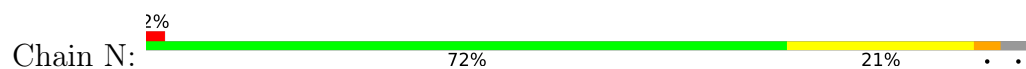


- Molecule 1: 60 kDa chaperonin

Chain M: 70% 24%



• Molecule 1: 60 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	135.64Å 259.39Å 143.31Å 90.00° 105.12° 90.00°	Depositor
Resolution (Å)	80.52 – 3.04 80.52 – 3.04	Depositor EDS
% Data completeness (in resolution range)	98.4 (80.52-3.04) 96.2 (80.52-3.04)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.190 , 0.256 0.194 , 0.257	Depositor DCC
R_{free} test set	2001 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	53914	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.68	0/3879	1.08	14/5239 (0.3%)
1	B	0.70	1/3879 (0.0%)	1.05	8/5239 (0.2%)
1	C	0.72	2/3879 (0.1%)	1.10	6/5239 (0.1%)
1	D	0.69	1/3879 (0.0%)	1.09	11/5239 (0.2%)
1	E	0.63	0/3879	1.06	9/5239 (0.2%)
1	F	0.71	1/3879 (0.0%)	1.08	9/5239 (0.2%)
1	G	0.65	0/3879	1.04	7/5239 (0.1%)
1	H	0.62	0/3879	1.01	4/5239 (0.1%)
1	I	0.66	0/3879	1.04	7/5239 (0.1%)
1	J	0.66	0/3879	1.08	10/5239 (0.2%)
1	K	0.65	0/3879	1.02	9/5239 (0.2%)
1	L	0.62	1/3879 (0.0%)	1.04	10/5239 (0.2%)
1	M	0.63	0/3879	1.03	11/5239 (0.2%)
1	N	0.63	0/3879	1.02	7/5239 (0.1%)
All	All	0.66	6/54306 (0.0%)	1.05	122/73346 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	499	VAL	CA-CB	6.01	1.62	1.54
1	F	499	VAL	CA-CB	5.83	1.62	1.54
1	D	383	ALA	CA-CB	-5.72	1.46	1.54
1	C	139	SER	CA-C	-5.52	1.48	1.52
1	B	383	ALA	CA-CB	-5.42	1.44	1.53
1	L	20	VAL	CA-CB	5.39	1.61	1.54

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	269	GLY	N-CA-C	7.83	126.18	115.30
1	M	169	VAL	N-CA-C	7.42	120.18	112.83
1	N	207	LYS	CA-C-N	7.41	127.12	119.56
1	N	207	LYS	C-N-CA	7.41	127.12	119.56
1	C	32	GLY	CA-C-N	7.37	127.00	119.19
1	C	32	GLY	C-N-CA	7.37	127.00	119.19
1	K	32	GLY	CA-C-N	7.33	126.96	119.19
1	K	32	GLY	C-N-CA	7.33	126.96	119.19
1	E	207	LYS	CA-C-N	7.33	127.04	119.56
1	E	207	LYS	C-N-CA	7.33	127.04	119.56
1	L	461	GLU	CA-C-N	7.08	126.91	119.05
1	L	461	GLU	C-N-CA	7.08	126.91	119.05
1	I	461	GLU	CA-C-N	6.93	126.75	119.05
1	I	461	GLU	C-N-CA	6.93	126.75	119.05
1	C	328	ASP	N-CA-C	6.85	121.80	113.17
1	N	169	VAL	N-CA-C	6.81	119.57	112.83
1	D	383	ALA	N-CA-C	6.78	123.55	114.12
1	N	328	ASP	N-CA-C	6.78	122.38	113.30
1	A	207	LYS	CA-C-N	6.43	126.36	119.28
1	A	207	LYS	C-N-CA	6.43	126.36	119.28
1	D	33	PRO	N-CA-C	-6.42	105.84	113.86
1	J	33	PRO	N-CA-C	-6.41	105.85	113.86
1	M	461	GLU	CA-C-N	6.38	126.14	119.05
1	M	461	GLU	C-N-CA	6.38	126.14	119.05
1	E	265	ASN	N-CA-C	6.34	117.85	111.07
1	E	328	ASP	N-CA-C	6.33	121.79	113.30
1	K	328	ASP	N-CA-C	6.33	121.78	113.30
1	A	184	GLN	N-CA-C	-6.29	97.39	110.80
1	M	31	LEU	N-CA-C	6.08	118.81	111.40
1	A	265	ASN	N-CA-C	6.07	117.57	111.07
1	L	227	ILE	N-CA-C	6.02	116.48	107.51
1	B	169	VAL	N-CA-C	5.99	118.76	112.83
1	J	329	THR	N-CA-C	5.98	119.23	109.06
1	G	84	ALA	N-CA-C	5.97	117.65	111.03
1	C	355	GLU	N-CA-C	5.95	120.54	113.16
1	L	32	GLY	CA-C-N	5.95	125.57	119.56
1	L	32	GLY	C-N-CA	5.95	125.57	119.56
1	J	328	ASP	N-CA-C	5.94	120.66	113.17
1	J	471	GLY	N-CA-C	5.94	121.02	113.24
1	K	84	ALA	N-CA-C	5.91	117.59	111.03
1	F	329	THR	N-CA-C	5.88	119.06	109.24
1	L	256	GLY	N-CA-C	5.86	121.91	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	461	GLU	CA-C-N	5.83	125.52	119.05
1	J	461	GLU	C-N-CA	5.83	125.52	119.05
1	F	233	MET	N-CA-C	5.83	119.57	112.23
1	B	461	GLU	CA-C-N	5.79	125.47	119.05
1	B	461	GLU	C-N-CA	5.79	125.47	119.05
1	F	173	GLY	N-CA-C	5.73	119.87	112.54
1	M	471	GLY	N-CA-C	5.71	120.72	113.24
1	A	383	ALA	N-CA-C	5.70	122.66	114.39
1	J	207	LYS	CA-C-N	5.63	125.47	119.28
1	J	207	LYS	C-N-CA	5.63	125.47	119.28
1	J	169	VAL	N-CA-C	5.62	118.40	112.83
1	L	249	ILE	N-CA-C	5.59	116.16	107.99
1	F	32	GLY	CA-C-N	5.58	125.11	119.19
1	F	32	GLY	C-N-CA	5.58	125.11	119.19
1	F	328	ASP	N-CA-C	5.56	120.75	113.30
1	D	175	ILE	N-CA-C	5.55	116.11	108.12
1	A	182	GLY	N-CA-C	5.54	126.32	113.18
1	E	268	ARG	N-CA-C	-5.53	106.20	113.17
1	D	217	SER	CA-C-N	-5.52	114.90	120.31
1	D	217	SER	C-N-CA	-5.52	114.90	120.31
1	M	333	ILE	N-CA-C	5.51	115.80	107.75
1	M	207	LYS	CA-C-N	5.51	125.34	119.28
1	M	207	LYS	C-N-CA	5.51	125.34	119.28
1	A	325	ILE	N-CA-C	5.50	115.79	107.75
1	L	19	GLY	N-CA-C	5.48	118.86	112.50
1	K	204	PHE	N-CA-C	-5.48	106.10	112.89
1	D	46	ALA	CA-C-N	5.47	125.77	119.92
1	D	46	ALA	C-N-CA	5.47	125.77	119.92
1	D	329	THR	N-CA-C	5.45	118.32	109.06
1	B	374	GLY	N-CA-C	5.45	119.26	112.73
1	M	409	GLU	N-CA-C	5.44	120.02	113.17
1	H	325	ILE	N-CA-C	5.43	115.81	107.77
1	C	207	LYS	CA-C-N	5.43	125.10	119.56
1	C	207	LYS	C-N-CA	5.43	125.10	119.56
1	L	233	MET	N-CA-C	5.43	119.07	112.23
1	F	204	PHE	N-CA-C	-5.42	106.16	112.89
1	I	409	GLU	N-CA-C	5.42	120.57	113.30
1	A	461	GLU	CA-C-N	5.42	125.07	119.05
1	A	461	GLU	C-N-CA	5.42	125.07	119.05
1	A	234	LEU	N-CA-C	5.41	120.28	113.25
1	E	184	GLN	N-CA-C	-5.39	99.33	110.80
1	F	512	GLY	N-CA-C	-5.38	106.26	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	461	GLU	CA-C-N	5.38	125.02	119.05
1	K	461	GLU	C-N-CA	5.38	125.02	119.05
1	A	32	GLY	CA-C-N	5.36	124.97	119.56
1	A	32	GLY	C-N-CA	5.36	124.97	119.56
1	F	369	VAL	CB-CA-C	-5.33	104.86	112.22
1	A	328	ASP	N-CA-C	5.31	120.41	113.30
1	D	328	ASP	N-CA-C	5.30	119.85	113.17
1	M	33	PRO	N-CA-C	-5.29	107.25	113.86
1	J	84	ALA	N-CA-C	5.28	116.89	111.03
1	D	50	THR	N-CA-C	5.25	117.24	108.99
1	B	207	LYS	CA-C-N	5.23	124.89	119.56
1	B	207	LYS	C-N-CA	5.23	124.89	119.56
1	G	461	GLU	CA-C-N	5.21	124.83	119.05
1	G	461	GLU	C-N-CA	5.21	124.83	119.05
1	E	182	GLY	N-CA-C	-5.20	104.17	111.09
1	H	207	LYS	CA-C-N	5.20	126.34	119.84
1	H	207	LYS	C-N-CA	5.20	126.34	119.84
1	B	430	ARG	N-CA-C	5.20	117.58	109.52
1	G	518	GLU	N-CA-C	5.20	119.77	113.38
1	G	494	LEU	N-CA-C	5.17	116.70	108.79
1	N	32	GLY	CA-C-N	5.16	124.66	119.19
1	N	32	GLY	C-N-CA	5.16	124.66	119.19
1	A	409	GLU	N-CA-C	5.15	120.20	113.30
1	N	136	VAL	N-CA-C	5.14	113.49	107.89
1	K	265	ASN	N-CA-C	5.12	116.86	111.28
1	G	204	PHE	N-CA-C	-5.09	106.57	112.89
1	D	173	GLY	N-CA-C	5.08	117.92	112.33
1	I	207	LYS	CA-C-N	5.07	125.35	119.47
1	I	207	LYS	C-N-CA	5.07	125.35	119.47
1	M	328	ASP	N-CA-C	5.05	119.54	113.17
1	G	328	ASP	N-CA-C	5.04	119.53	113.17
1	I	328	ASP	N-CA-C	5.03	119.50	113.17
1	B	431	GLY	N-CA-C	5.02	118.81	112.79
1	L	328	ASP	N-CA-C	5.02	119.49	113.17
1	H	328	ASP	N-CA-C	5.01	119.49	113.17
1	K	518	GLU	N-CA-C	5.01	119.55	113.38
1	I	32	GLY	N-CA-C	5.01	118.01	112.00
1	E	325	ILE	N-CA-C	5.00	115.17	107.77

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	183	LEU	Peptide

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	3851	0	3968	77	0
1	B	3851	0	3968	69	0
1	C	3851	0	3968	70	0
1	D	3851	0	3968	74	0
1	E	3851	0	3968	81	0
1	F	3851	0	3968	87	0
1	G	3851	0	3968	72	0
1	H	3851	0	3968	83	0
1	I	3851	0	3968	78	0
1	J	3851	0	3968	89	0
1	K	3851	0	3968	71	0
1	L	3851	0	3968	68	0
1	M	3851	0	3968	85	0
1	N	3851	0	3968	82	0
All	All	53914	0	55552	1048	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (1048) 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:34:LYS:HE2	1:M:118:ARG:HH22	1.31	0.95
1:M:173:GLY:O	1:M:404:ARG:NH2	2.07	0.87
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.56	0.85
1:A:183:LEU:HG	1:A:384:ALA:HB2	1.60	0.83
1:N:524:LEU:HD12	1:N:525:PRO:HD2	1.61	0.82
1:K:183:LEU:HD22	1:K:184:GLN:H	1.42	0.82
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.59	0.82
1:N:225:LYS:NZ	1:N:232:GLU:OE1	2.12	0.81
1:E:186:GLU:HB2	1:E:380:LYS:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:269:GLY:HA2	1:F:272:LYS:HE3	1.64	0.79
1:I:524:LEU:HD12	1:I:525:PRO:HD2	1.64	0.78
1:C:130:GLU:HB3	1:C:422:VAL:HG22	1.66	0.78
1:H:173:GLY:O	1:H:404:ARG:NH2	2.17	0.78
1:K:166:MET:HE2	1:K:171:LYS:HA	1.65	0.78
1:F:351:GLN:HA	1:F:354:GLU:HG2	1.65	0.78
1:G:166:MET:HE2	1:G:171:LYS:HA	1.64	0.77
1:M:241:ALA:HB1	1:N:231:ARG:HH12	1.50	0.77
1:B:302:SER:H	1:B:307:MET:HE3	1.50	0.77
1:H:13:ARG:HD2	1:H:104:LEU:HD22	1.66	0.77
1:F:166:MET:HE2	1:F:171:LYS:HA	1.67	0.76
1:I:34:LYS:HE2	1:J:118:ARG:HH22	1.48	0.76
1:A:166:MET:HE2	1:A:171:LYS:HA	1.67	0.75
1:M:241:ALA:HB1	1:N:231:ARG:NH1	2.01	0.75
1:G:171:LYS:HB3	1:G:407:VAL:HG11	1.67	0.75
1:G:179:ASP:HA	1:G:389:MET:HE1	1.69	0.74
1:L:166:MET:HE2	1:L:171:LYS:HA	1.70	0.74
1:J:302:SER:H	1:J:307:MET:HE3	1.53	0.74
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.70	0.73
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.68	0.73
1:A:239:ALA:HB1	1:A:314:LEU:HG	1.71	0.73
1:M:34:LYS:HE2	1:N:118:ARG:HH22	1.54	0.73
1:M:200:LEU:HD21	1:M:277:LYS:HG3	1.68	0.73
1:G:319:GLN:HB3	1:G:336:VAL:HG21	1.71	0.72
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.72	0.72
1:I:183:LEU:HD22	1:I:184:GLN:H	1.54	0.72
1:I:82:ASN:HB2	1:I:89:THR:OG1	1.89	0.72
1:J:171:LYS:HB3	1:J:407:VAL:HG11	1.73	0.71
1:J:524:LEU:HD12	1:J:525:PRO:HD2	1.73	0.70
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.74	0.69
1:E:166:MET:HE1	1:E:407:VAL:HG21	1.73	0.69
1:B:173:GLY:O	1:B:404:ARG:NH2	2.25	0.69
1:B:286:LYS:NZ	1:B:304:GLU:OE2	2.25	0.69
1:H:185:ASP:OD1	1:H:382:GLY:N	2.25	0.69
1:E:13:ARG:NH2	1:E:518:GLU:OE2	2.26	0.69
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.74	0.69
1:C:82:ASN:HB2	1:C:89:THR:OG1	1.93	0.68
1:M:417:VAL:HA	1:M:420:ILE:HG22	1.75	0.68
1:I:166:MET:HE1	1:I:407:VAL:HG21	1.74	0.68
1:N:166:MET:HE2	1:N:171:LYS:HA	1.74	0.68
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.74	0.68
1:I:131:LEU:HD13	1:I:422:VAL:HG21	1.75	0.68
1:J:82:ASN:HB2	1:J:89:THR:OG1	1.93	0.68
1:G:131:LEU:HD13	1:G:422:VAL:HG21	1.76	0.67
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.76	0.67
1:D:173:GLY:O	1:D:404:ARG:NH2	2.26	0.67
1:F:158:VAL:HG13	1:F:396:VAL:HG22	1.75	0.67
1:F:186:GLU:HB2	1:F:380:LYS:HB2	1.75	0.67
1:M:70:GLY:HA2	1:M:73:MET:HE3	1.75	0.67
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.76	0.67
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.76	0.67
1:B:198:GLY:HA3	1:B:327:LYS:O	1.94	0.67
1:G:82:ASN:HB2	1:G:89:THR:OG1	1.95	0.67
1:G:166:MET:HE1	1:G:407:VAL:HG21	1.76	0.67
1:B:166:MET:HE2	1:B:171:LYS:HA	1.77	0.67
1:C:5:ASP:HB2	1:C:524:LEU:HD13	1.75	0.67
1:D:70:GLY:HA2	1:D:73:MET:HE3	1.76	0.67
1:B:305:ILE:HD11	1:B:307:MET:HE2	1.77	0.67
1:L:393:LYS:NZ	1:L:397:GLU:OE1	2.28	0.67
1:C:139:SER:O	1:C:171:LYS:NZ	2.26	0.66
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.78	0.66
1:I:13:ARG:NH1	1:I:518:GLU:OE2	2.29	0.66
1:M:16:MET:SD	1:M:73:MET:HE1	2.35	0.66
1:C:27:VAL:HG13	1:C:90:THR:HG23	1.77	0.66
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.76	0.66
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.77	0.66
1:C:166:MET:HE2	1:C:171:LYS:HA	1.77	0.65
1:F:131:LEU:HD13	1:F:422:VAL:HG21	1.78	0.65
1:H:70:GLY:HA2	1:H:73:MET:HE3	1.78	0.65
1:K:293:ALA:HB2	1:K:300:VAL:HG23	1.79	0.65
1:F:183:LEU:HB2	1:F:384:ALA:HB2	1.79	0.65
1:H:166:MET:HE1	1:H:407:VAL:HG21	1.79	0.65
1:N:5:ASP:HB2	1:N:524:LEU:HD13	1.79	0.65
1:F:193:MET:HE1	1:F:292:ILE:HG12	1.78	0.65
1:J:16:MET:SD	1:J:73:MET:HE1	2.37	0.65
1:E:171:LYS:HB3	1:E:407:VAL:HG11	1.80	0.64
1:A:193:MET:HE1	1:A:292:ILE:HG12	1.79	0.64
1:I:414:GLY:O	1:I:417:VAL:HG13	1.97	0.64
1:N:72:GLN:HE22	1:N:75:LYS:HE2	1.62	0.64
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.79	0.64
1:N:198:GLY:HA3	1:N:327:LYS:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASN:HB2	1:A:329:THR:H	1.63	0.64
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.80	0.64
1:H:197:ARG:NH2	1:N:386:GLU:OE1	2.31	0.64
1:M:25:ASP:HA	1:M:28:LYS:HE2	1.80	0.64
1:J:183:LEU:HD22	1:J:184:GLN:H	1.63	0.64
1:C:524:LEU:HD12	1:C:525:PRO:HD2	1.80	0.64
1:B:524:LEU:HD12	1:B:525:PRO:HD2	1.79	0.63
1:H:82:ASN:HB2	1:H:89:THR:OG1	1.98	0.63
1:L:524:LEU:HD12	1:L:525:PRO:HD2	1.80	0.63
1:B:262:LEU:O	1:B:266:THR:HG23	1.97	0.63
1:E:173:GLY:O	1:E:404:ARG:NH2	2.27	0.63
1:J:286:LYS:NZ	1:J:304:GLU:OE2	2.32	0.63
1:K:183:LEU:HD22	1:K:184:GLN:N	2.13	0.63
1:L:173:GLY:O	1:L:404:ARG:NH2	2.31	0.63
1:A:13:ARG:NH2	1:A:518:GLU:OE2	2.32	0.63
1:A:198:GLY:HA3	1:A:327:LYS:O	1.98	0.63
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.81	0.63
1:M:262:LEU:O	1:M:266:THR:HG23	1.99	0.63
1:E:166:MET:HE2	1:E:171:LYS:HA	1.79	0.63
1:C:128:VAL:HG12	1:C:132:LYS:HE3	1.79	0.62
1:J:102:GLU:OE1	1:J:445:ARG:NH1	2.31	0.62
1:B:82:ASN:HB2	1:B:89:THR:OG1	1.99	0.62
1:F:359:ASP:O	1:F:363:GLU:HG3	1.99	0.62
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.81	0.62
1:M:13:ARG:NH1	1:M:518:GLU:OE2	2.32	0.62
1:E:308:GLU:HB2	1:E:311:LYS:HG3	1.81	0.62
1:F:473:ASP:OD1	1:F:474:GLY:N	2.32	0.62
1:I:5:ASP:HB2	1:I:524:LEU:HD13	1.80	0.62
1:N:130:GLU:HB3	1:N:422:VAL:HG22	1.81	0.62
1:A:183:LEU:HB2	1:A:384:ALA:N	2.14	0.62
1:E:198:GLY:HA3	1:E:327:LYS:O	1.98	0.62
1:F:242:LYS:C	1:F:244:GLY:H	2.07	0.62
1:G:359:ASP:O	1:G:363:GLU:HG3	2.00	0.62
1:B:27:VAL:HG13	1:B:90:THR:HG23	1.82	0.62
1:E:247:LEU:HB3	1:E:273:VAL:HG22	1.82	0.61
1:M:393:LYS:NZ	1:M:397:GLU:OE1	2.33	0.61
1:D:420:ILE:HG13	1:D:448:GLU:HG2	1.81	0.61
1:G:326:ASN:HB2	1:G:329:THR:H	1.65	0.61
1:N:166:MET:HE1	1:N:407:VAL:HG21	1.82	0.61
1:E:82:ASN:HB2	1:E:89:THR:OG1	1.99	0.61
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ASP:OD2	1:A:368:ARG:HD2	1.99	0.61
1:I:302:SER:H	1:I:307:MET:HE3	1.65	0.61
1:F:305:ILE:HD12	1:F:307:MET:HE2	1.81	0.61
1:I:247:LEU:HB3	1:I:273:VAL:HG22	1.82	0.61
1:I:262:LEU:O	1:I:266:THR:HG23	2.00	0.61
1:K:420:ILE:HG13	1:K:448:GLU:HG2	1.83	0.61
1:F:262:LEU:O	1:F:266:THR:HG23	2.01	0.61
1:N:102:GLU:HB3	1:N:442:VAL:HG22	1.83	0.61
1:E:284:ARG:HH11	1:E:364:LYS:HG3	1.64	0.61
1:L:130:GLU:HB3	1:L:422:VAL:HG22	1.82	0.61
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.83	0.60
1:G:7:LYS:HE3	1:G:15:LYS:HE3	1.83	0.60
1:M:176:THR:HG21	1:M:322:ARG:HH12	1.66	0.60
1:A:16:MET:O	1:A:20:VAL:HG13	2.01	0.60
1:B:193:MET:HE1	1:B:292:ILE:HG12	1.82	0.60
1:L:16:MET:SD	1:L:73:MET:HE1	2.42	0.60
1:M:193:MET:HE1	1:M:292:ILE:HG12	1.84	0.60
1:L:131:LEU:HD13	1:L:422:VAL:HG21	1.84	0.60
1:N:326:ASN:HB2	1:N:329:THR:H	1.66	0.60
1:B:171:LYS:HB3	1:B:407:VAL:HG11	1.83	0.60
1:D:263:VAL:O	1:D:267:MET:HB2	2.01	0.60
1:K:291:ASP:OD2	1:K:368:ARG:HD2	2.02	0.60
1:L:344:GLY:O	1:L:348:GLN:HG3	2.02	0.60
1:E:254:VAL:HG12	1:E:259:LEU:HB2	1.84	0.59
1:H:359:ASP:O	1:H:363:GLU:HG2	2.03	0.59
1:B:218:PRO:HB3	1:B:246:PRO:HG2	1.85	0.59
1:B:414:GLY:O	1:B:417:VAL:HG13	2.01	0.59
1:G:414:GLY:O	1:G:417:VAL:HG13	2.03	0.59
1:K:183:LEU:O	1:K:184:GLN:HB2	2.01	0.59
1:B:242:LYS:C	1:B:244:GLY:H	2.10	0.59
1:I:183:LEU:HD22	1:I:184:GLN:N	2.18	0.59
1:L:62:LEU:N	1:L:68:ASN:OD1	2.22	0.59
1:A:359:ASP:O	1:A:363:GLU:HG3	2.03	0.59
1:K:39:VAL:HG12	1:L:69:MET:HE2	1.84	0.59
1:C:286:LYS:NZ	1:C:304:GLU:OE2	2.31	0.59
1:E:13:ARG:HD3	1:E:104:LEU:HD22	1.85	0.59
1:I:420:ILE:HG13	1:I:448:GLU:HG2	1.83	0.59
1:D:177:VAL:HG21	1:D:397:GLU:HG3	1.84	0.59
1:H:198:GLY:HA3	1:H:327:LYS:O	2.03	0.59
1:H:459:GLY:HA3	1:I:112:ASN:ND2	2.18	0.59
1:L:198:GLY:HA3	1:L:327:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:ARG:HD3	1:E:364:LYS:HE2	1.83	0.58
1:I:16:MET:SD	1:I:73:MET:HE1	2.43	0.58
1:J:72:GLN:HE22	1:J:75:LYS:HE2	1.68	0.58
1:D:222:LEU:HD23	1:D:250:ILE:HB	1.84	0.58
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.85	0.58
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.84	0.58
1:A:417:VAL:HA	1:A:420:ILE:HG22	1.85	0.58
1:B:284:ARG:NH1	1:B:364:LYS:HD2	2.18	0.58
1:D:82:ASN:HB2	1:D:89:THR:OG1	2.03	0.58
1:D:242:LYS:C	1:D:244:GLY:H	2.11	0.58
1:F:181:THR:OG1	1:F:186:GLU:OE1	2.21	0.58
1:A:40:LEU:HD13	1:A:59:GLU:HG3	1.86	0.58
1:A:302:SER:H	1:A:307:MET:HE3	1.68	0.58
1:A:16:MET:SD	1:A:73:MET:HE1	2.43	0.58
1:G:215:LEU:HB2	1:G:323:VAL:HG22	1.85	0.58
1:E:226:LYS:HD3	1:E:255:GLU:OE2	2.04	0.58
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.86	0.58
1:M:82:ASN:HB2	1:M:89:THR:OG1	2.04	0.58
1:C:198:GLY:HA3	1:C:327:LYS:O	2.03	0.58
1:C:349:ILE:O	1:C:353:ILE:HG13	2.04	0.58
1:F:488:MET:HE3	1:F:493:ILE:HB	1.84	0.58
1:H:144:ILE:HD13	1:H:166:MET:SD	2.44	0.58
1:J:72:GLN:NE2	1:J:75:LYS:HE2	2.19	0.58
1:J:166:MET:HE2	1:J:171:LYS:HA	1.84	0.58
1:L:257:GLU:O	1:L:261:THR:OG1	2.18	0.58
1:K:140:ASP:OD2	1:K:142:LYS:HB3	2.04	0.58
1:M:524:LEU:HD12	1:M:525:PRO:HD2	1.86	0.58
1:G:242:LYS:C	1:G:244:GLY:H	2.11	0.57
1:H:482:THR:O	1:H:484:GLU:HG2	2.04	0.57
1:H:130:GLU:HB3	1:H:422:VAL:HG22	1.86	0.57
1:L:82:ASN:HB2	1:L:89:THR:OG1	2.03	0.57
1:E:213:VAL:HB	1:E:325:ILE:HB	1.86	0.57
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.86	0.57
1:H:183:LEU:HD22	1:H:184:GLN:H	1.69	0.57
1:I:198:GLY:HA3	1:I:327:LYS:O	2.05	0.57
1:A:240:VAL:HG21	1:A:247:LEU:HD22	1.86	0.57
1:G:221:LEU:HD23	1:G:249:ILE:HD12	1.87	0.57
1:B:359:ASP:O	1:B:363:GLU:HG3	2.04	0.57
1:C:302:SER:H	1:C:307:MET:HE3	1.70	0.57
1:J:122:LYS:HG2	1:J:429:LEU:HD21	1.87	0.57
1:L:183:LEU:HD22	1:L:184:GLN:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:482:THR:O	1:M:484:GLU:HG2	2.05	0.57
1:G:270:ILE:HG22	1:G:271:VAL:HG23	1.87	0.57
1:H:201:SER:OG	1:H:202:PRO:O	2.23	0.57
1:K:82:ASN:HB2	1:K:89:THR:OG1	2.05	0.57
1:D:221:LEU:HB3	1:D:249:ILE:HD13	1.87	0.57
1:N:414:GLY:O	1:N:417:VAL:HG13	2.05	0.57
1:A:118:ARG:HE	1:A:436:GLN:NE2	2.03	0.56
1:D:166:MET:HE2	1:D:171:LYS:HA	1.86	0.56
1:J:386:GLU:O	1:J:390:LYS:HG2	2.04	0.56
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.86	0.56
1:L:183:LEU:O	1:L:184:GLN:HB2	2.05	0.56
1:A:10:ASN:O	1:A:14:VAL:HG13	2.05	0.56
1:F:302:SER:H	1:F:307:MET:HE3	1.69	0.56
1:G:194:GLN:O	1:G:371:LYS:HE3	2.05	0.56
1:H:247:LEU:HB3	1:H:273:VAL:HG22	1.86	0.56
1:I:173:GLY:O	1:I:404:ARG:NH2	2.38	0.56
1:H:420:ILE:HG13	1:H:448:GLU:HG2	1.88	0.56
1:L:16:MET:HB3	1:L:514:MET:HE3	1.88	0.56
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.86	0.56
1:I:16:MET:O	1:I:20:VAL:HG13	2.05	0.56
1:K:70:GLY:HA2	1:K:73:MET:HE3	1.88	0.56
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.88	0.56
1:D:102:GLU:OE1	1:D:445:ARG:NH1	2.39	0.56
1:K:501:ARG:NH1	1:K:505:GLN:OE1	2.39	0.56
1:F:227:ILE:HD13	1:F:233:MET:HE3	1.87	0.56
1:H:246:PRO:HB3	1:H:272:LYS:HG3	1.87	0.56
1:I:202:PRO:C	1:I:204:PHE:H	2.14	0.56
1:K:72:GLN:HE22	1:K:75:LYS:HE2	1.69	0.56
1:K:199:TYR:CZ	1:K:327:LYS:HA	2.41	0.56
1:L:262:LEU:O	1:L:266:THR:HG23	2.06	0.55
1:M:198:GLY:HA3	1:M:327:LYS:O	2.05	0.55
1:D:127:ALA:O	1:D:131:LEU:HB2	2.06	0.55
1:D:270:ILE:HG22	1:D:271:VAL:HG23	1.88	0.55
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.06	0.55
1:J:201:SER:OG	1:J:202:PRO:O	2.23	0.55
1:K:262:LEU:O	1:K:266:THR:HG23	2.05	0.55
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.86	0.55
1:N:31:LEU:HD13	1:N:90:THR:HG21	1.87	0.55
1:N:72:GLN:NE2	1:N:75:LYS:HE2	2.21	0.55
1:C:141:SER:HA	1:C:144:ILE:HD12	1.88	0.55
1:F:420:ILE:HG13	1:F:448:GLU:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:183:LEU:O	1:I:184:GLN:HB2	2.07	0.55
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.88	0.55
1:K:242:LYS:C	1:K:244:GLY:H	2.13	0.55
1:N:262:LEU:O	1:N:266:THR:HG23	2.07	0.55
1:L:71:ALA:O	1:L:75:LYS:HB2	2.05	0.55
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.87	0.55
1:I:68:ASN:O	1:I:72:GLN:HG2	2.06	0.55
1:I:70:GLY:HA2	1:I:73:MET:HE3	1.88	0.55
1:L:272:LYS:NZ	1:M:229:ASN:OD1	2.38	0.55
1:K:13:ARG:NH1	1:K:518:GLU:OE2	2.39	0.55
1:N:319:GLN:HB3	1:N:336:VAL:HG21	1.89	0.55
1:J:198:GLY:HA3	1:J:327:LYS:O	2.06	0.55
1:F:257:GLU:O	1:F:261:THR:OG1	2.20	0.55
1:F:266:THR:CG2	1:F:273:VAL:H	2.20	0.55
1:F:414:GLY:O	1:F:417:VAL:HG13	2.07	0.55
1:H:414:GLY:O	1:H:417:VAL:HG13	2.07	0.55
1:H:102:GLU:HB3	1:H:442:VAL:HG22	1.88	0.54
1:D:39:VAL:HG12	1:E:69:MET:HE2	1.89	0.54
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.89	0.54
1:K:131:LEU:HD13	1:K:422:VAL:HG21	1.88	0.54
1:K:478:TYR:CE2	1:K:480:ALA:HA	2.42	0.54
1:A:183:LEU:HB2	1:A:384:ALA:H	1.73	0.54
1:C:242:LYS:C	1:C:244:GLY:H	2.14	0.54
1:E:323:VAL:HG22	1:E:332:ILE:HG12	1.88	0.54
1:F:349:ILE:O	1:F:353:ILE:HG13	2.07	0.54
1:G:198:GLY:HA3	1:G:327:LYS:O	2.07	0.54
1:K:254:VAL:HG12	1:K:259:LEU:HB2	1.89	0.54
1:B:130:GLU:HB3	1:B:422:VAL:HG22	1.89	0.54
1:D:186:GLU:HB2	1:D:380:LYS:HB2	1.88	0.54
1:G:420:ILE:HG13	1:G:448:GLU:HG2	1.89	0.54
1:I:71:ALA:O	1:I:75:LYS:HB2	2.07	0.54
1:L:195:PHE:CE2	1:L:330:THR:HB	2.43	0.54
1:L:359:ASP:O	1:L:363:GLU:HG2	2.08	0.54
1:N:242:LYS:C	1:N:244:GLY:H	2.15	0.54
1:C:254:VAL:HG12	1:C:259:LEU:HB2	1.90	0.54
1:H:158:VAL:HG13	1:H:396:VAL:HG22	1.89	0.54
1:K:7:LYS:HE3	1:K:15:LYS:HE3	1.90	0.54
1:A:429:LEU:O	1:A:430:ARG:NH1	2.36	0.54
1:E:326:ASN:HB2	1:E:329:THR:H	1.73	0.54
1:K:319:GLN:HB3	1:K:336:VAL:HG21	1.90	0.54
1:N:82:ASN:HB2	1:N:89:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:254:VAL:HG12	1:N:259:LEU:HB2	1.89	0.54
1:A:141:SER:HA	1:A:144:ILE:HB	1.90	0.53
1:A:166:MET:HE1	1:A:407:VAL:HG21	1.90	0.53
1:D:524:LEU:HD12	1:D:525:PRO:HD2	1.89	0.53
1:D:193:MET:HE1	1:D:292:ILE:HG12	1.90	0.53
1:G:70:GLY:HA2	1:G:73:MET:HE3	1.90	0.53
1:B:176:THR:HG21	1:B:322:ARG:HH12	1.74	0.53
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.38	0.53
1:F:102:GLU:HB3	1:F:442:VAL:HG22	1.90	0.53
1:M:73:MET:O	1:M:77:VAL:HG13	2.09	0.53
1:D:171:LYS:HB3	1:D:407:VAL:HG11	1.90	0.53
1:I:242:LYS:C	1:I:244:GLY:H	2.17	0.53
1:K:359:ASP:O	1:K:363:GLU:HG2	2.08	0.53
1:L:349:ILE:HA	1:L:352:GLN:HG3	1.89	0.53
1:N:353:ILE:HG23	1:N:362:ARG:HG3	1.90	0.53
1:N:393:LYS:NZ	1:N:397:GLU:OE1	2.42	0.53
1:B:158:VAL:HG13	1:B:396:VAL:HG22	1.89	0.53
1:L:301:ILE:HD12	1:L:309:LEU:HD23	1.90	0.53
1:A:130:GLU:HB3	1:A:422:VAL:HG22	1.90	0.53
1:F:258:ALA:O	1:F:262:LEU:HG	2.09	0.53
1:H:226:LYS:HD3	1:H:255:GLU:OE2	2.09	0.53
1:F:326:ASN:HB2	1:F:329:THR:H	1.73	0.53
1:J:219:PHE:O	1:J:247:LEU:HD12	2.09	0.53
1:C:239:ALA:HB1	1:C:314:LEU:HG	1.91	0.52
1:G:16:MET:O	1:G:20:VAL:HG13	2.09	0.52
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.91	0.52
1:L:235:PRO:HG3	1:L:310:GLU:HA	1.90	0.52
1:M:222:LEU:HD23	1:M:250:ILE:HB	1.91	0.52
1:D:183:LEU:HB2	1:D:384:ALA:HB2	1.91	0.52
1:E:414:GLY:O	1:E:417:VAL:HG13	2.08	0.52
1:J:13:ARG:HD3	1:J:104:LEU:HD22	1.91	0.52
1:I:326:ASN:HB2	1:I:329:THR:H	1.74	0.52
1:L:417:VAL:HA	1:L:420:ILE:HG22	1.91	0.52
1:D:6:VAL:HG22	1:D:521:VAL:HG22	1.90	0.52
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.91	0.52
1:E:130:GLU:HB3	1:E:422:VAL:HG22	1.91	0.52
1:H:72:GLN:HE22	1:H:75:LYS:HE2	1.74	0.52
1:K:34:LYS:HE2	1:L:118:ARG:HH22	1.74	0.52
1:L:40:LEU:HD13	1:L:59:GLU:HG3	1.92	0.52
1:A:194:GLN:O	1:A:371:LYS:HE3	2.09	0.52
1:A:414:GLY:O	1:A:417:VAL:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:345:ARG:O	1:L:348:GLN:HB2	2.09	0.52
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.91	0.52
1:H:16:MET:SD	1:H:73:MET:HE1	2.50	0.52
1:I:36:ARG:HG3	1:J:518:GLU:HG3	1.92	0.52
1:M:65:LYS:HE3	1:M:522:THR:OG1	2.10	0.52
1:M:359:ASP:O	1:M:363:GLU:HG2	2.10	0.52
1:N:173:GLY:O	1:N:404:ARG:NH2	2.43	0.52
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.92	0.52
1:D:291:ASP:OD2	1:D:368:ARG:HD2	2.10	0.52
1:J:200:LEU:HG	1:J:276:VAL:HA	1.91	0.52
1:M:131:LEU:HD13	1:M:422:VAL:HG21	1.92	0.52
1:A:232:GLU:HA	1:A:310:GLU:CD	2.34	0.52
1:C:240:VAL:HG11	1:C:247:LEU:HB2	1.91	0.52
1:F:198:GLY:HA3	1:F:327:LYS:O	2.09	0.52
1:E:16:MET:O	1:E:20:VAL:HG13	2.10	0.51
1:E:271:VAL:O	1:E:273:VAL:HG23	2.09	0.51
1:L:16:MET:HB3	1:L:514:MET:CE	2.40	0.51
1:L:414:GLY:O	1:L:417:VAL:HG13	2.11	0.51
1:A:219:PHE:O	1:A:247:LEU:HA	2.10	0.51
1:K:314:LEU:HD23	1:K:317:LEU:HD22	1.92	0.51
1:B:194:GLN:O	1:B:371:LYS:HE3	2.10	0.51
1:D:16:MET:SD	1:D:73:MET:HE1	2.50	0.51
1:F:166:MET:HE1	1:F:407:VAL:HG21	1.93	0.51
1:M:16:MET:O	1:M:20:VAL:HG13	2.11	0.51
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.40	0.51
1:A:71:ALA:O	1:A:75:LYS:HB2	2.11	0.51
1:B:176:THR:HG21	1:B:333:ILE:HD13	1.92	0.51
1:F:17:LEU:HD13	1:F:100:ILE:HG22	1.92	0.51
1:H:131:LEU:HD13	1:H:422:VAL:HG21	1.91	0.51
1:F:215:LEU:HB2	1:F:323:VAL:HG22	1.93	0.51
1:I:160:LYS:O	1:I:164:GLU:HG3	2.11	0.51
1:J:183:LEU:HD22	1:J:184:GLN:N	2.26	0.51
1:K:130:GLU:HB3	1:K:422:VAL:HG22	1.93	0.51
1:N:151:SER:HB2	1:N:399:ALA:HA	1.91	0.51
1:B:5:ASP:HB2	1:B:524:LEU:HD13	1.92	0.51
1:N:247:LEU:HD21	1:N:249:ILE:HD11	1.92	0.51
1:D:178:GLU:HG3	1:D:380:LYS:HG2	1.93	0.51
1:J:359:ASP:O	1:J:363:GLU:HG2	2.11	0.51
1:A:218:PRO:O	1:A:319:GLN:HG3	2.11	0.51
1:D:219:PHE:HB3	1:D:317:LEU:HD23	1.92	0.51
1:E:221:LEU:HD23	1:E:249:ILE:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:SER:HA	1:F:412:VAL:HG12	1.93	0.51
1:M:71:ALA:O	1:M:75:LYS:HB2	2.11	0.51
1:F:225:LYS:HD3	1:F:309:LEU:HD11	1.93	0.50
1:G:151:SER:HB2	1:G:399:ALA:HA	1.92	0.50
1:G:160:LYS:O	1:G:164:GLU:HG3	2.10	0.50
1:J:131:LEU:HD13	1:J:422:VAL:HG21	1.92	0.50
1:L:263:VAL:O	1:L:267:MET:HB2	2.11	0.50
1:M:420:ILE:HG13	1:M:448:GLU:HG2	1.93	0.50
1:D:383:ALA:HB3	1:D:389:MET:HB2	1.93	0.50
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.93	0.50
1:F:109:ALA:HB2	1:H:109:ALA:HB2	1.91	0.50
1:G:319:GLN:HB3	1:G:336:VAL:CG2	2.39	0.50
1:M:130:GLU:HB3	1:M:422:VAL:HG22	1.94	0.50
1:M:291:ASP:OD2	1:M:368:ARG:HD2	2.10	0.50
1:C:262:LEU:O	1:C:266:THR:HG23	2.12	0.50
1:G:5:ASP:HB2	1:G:524:LEU:HD23	1.92	0.50
1:L:183:LEU:HD22	1:L:184:GLN:N	2.26	0.50
1:E:242:LYS:C	1:E:244:GLY:H	2.19	0.50
1:G:34:LYS:HD2	1:G:458:CYS:HA	1.94	0.50
1:H:455:VAL:HG13	1:H:460:GLU:HB2	1.91	0.50
1:J:296:THR:HB	1:J:319:GLN:H	1.76	0.50
1:K:225:LYS:HE2	1:K:303:GLU:HG3	1.93	0.50
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.93	0.50
1:A:213:VAL:O	1:A:324:VAL:HA	2.11	0.50
1:F:230:ILE:HG22	1:F:257:GLU:OE2	2.12	0.50
1:H:74:VAL:HA	1:H:510:VAL:HG21	1.93	0.50
1:H:409:GLU:CD	1:H:501:ARG:HH21	2.20	0.50
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.93	0.50
1:M:253:ASP:OD1	1:M:254:VAL:N	2.44	0.50
1:D:162:ILE:O	1:D:166:MET:HG3	2.11	0.50
1:F:71:ALA:O	1:F:75:LYS:HB2	2.12	0.50
1:F:141:SER:HA	1:F:144:ILE:HB	1.93	0.50
1:H:6:VAL:HG22	1:H:521:VAL:HG22	1.94	0.50
1:I:417:VAL:HA	1:I:420:ILE:HG22	1.93	0.50
1:A:321:LYS:HB2	1:A:334:ASP:HB3	1.94	0.50
1:F:161:LEU:HD22	1:F:379:ILE:HG23	1.94	0.50
1:K:414:GLY:N	1:K:494:LEU:HA	2.26	0.50
1:E:359:ASP:OD1	1:E:362:ARG:NH1	2.45	0.50
1:I:219:PHE:CE2	1:I:245:LYS:HB2	2.47	0.50
1:D:71:ALA:O	1:D:75:LYS:HB2	2.12	0.49
1:E:348:GLN:O	1:E:352:GLN:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:GLU:HB2	1:C:442:VAL:HG13	1.93	0.49
1:C:257:GLU:O	1:C:261:THR:OG1	2.27	0.49
1:E:36:ARG:NH1	1:F:113:PRO:HG2	2.27	0.49
1:I:305:ILE:HD12	1:I:307:MET:HE2	1.94	0.49
1:L:305:ILE:HD12	1:L:307:MET:HE2	1.93	0.49
1:C:222:LEU:HD23	1:C:250:ILE:HB	1.94	0.49
1:I:102:GLU:HB3	1:I:442:VAL:HG22	1.94	0.49
1:M:242:LYS:C	1:M:244:GLY:H	2.20	0.49
1:N:222:LEU:HD13	1:N:293:ALA:HA	1.95	0.49
1:F:266:THR:HG22	1:F:273:VAL:H	1.76	0.49
1:H:326:ASN:HB2	1:H:329:THR:H	1.78	0.49
1:I:266:THR:HG21	1:I:273:VAL:O	2.13	0.49
1:J:102:GLU:HB3	1:J:442:VAL:HG22	1.95	0.49
1:D:459:GLY:HA3	1:E:112:ASN:ND2	2.27	0.49
1:G:202:PRO:C	1:G:204:PHE:H	2.21	0.49
1:G:242:LYS:O	1:G:244:GLY:N	2.45	0.49
1:J:254:VAL:HG12	1:J:259:LEU:HB2	1.94	0.49
1:K:200:LEU:HD21	1:K:277:LYS:HG3	1.94	0.49
1:J:140:ASP:OD1	1:J:140:ASP:N	2.46	0.49
1:M:302:SER:H	1:M:307:MET:HE3	1.77	0.49
1:A:218:PRO:HB3	1:A:246:PRO:HG2	1.95	0.49
1:B:383:ALA:O	1:B:384:ALA:HB3	2.12	0.49
1:D:414:GLY:H	1:D:494:LEU:HA	1.78	0.49
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.42	0.49
1:J:7:LYS:HE2	1:J:66:PHE:CE2	2.48	0.49
1:K:263:VAL:O	1:K:267:MET:HB2	2.12	0.49
1:B:63:GLU:HB2	1:C:524:LEU:HD21	1.94	0.49
1:C:16:MET:O	1:C:20:VAL:HG13	2.11	0.49
1:D:130:GLU:HB3	1:D:422:VAL:HG22	1.95	0.49
1:I:353:ILE:HG23	1:I:362:ARG:HG3	1.95	0.49
1:K:198:GLY:HA3	1:K:327:LYS:O	2.12	0.49
1:K:414:GLY:H	1:K:494:LEU:HA	1.78	0.49
1:M:414:GLY:O	1:M:417:VAL:HG13	2.13	0.49
1:A:286:LYS:NZ	1:A:304:GLU:OE2	2.29	0.49
1:A:346:VAL:O	1:A:350:ARG:HB2	2.13	0.49
1:D:366:GLN:HA	1:D:369:VAL:HG22	1.94	0.49
1:D:414:GLY:O	1:D:417:VAL:HG13	2.13	0.49
1:F:266:THR:HG21	1:F:273:VAL:O	2.13	0.49
1:E:142:LYS:HE2	1:E:146:GLN:OE1	2.12	0.48
1:E:321:LYS:HB2	1:E:334:ASP:HB3	1.95	0.48
1:F:103:GLY:HA3	1:F:515:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:TYR:CE2	1:B:480:ALA:HA	2.48	0.48
1:D:284:ARG:O	1:D:288:MET:HG3	2.13	0.48
1:E:266:THR:HG21	1:E:273:VAL:O	2.13	0.48
1:G:522:THR:OG1	1:G:523:ASP:N	2.44	0.48
1:J:144:ILE:HD11	1:J:171:LYS:HE2	1.93	0.48
1:K:12:ALA:HB1	1:K:520:MET:HG3	1.95	0.48
1:K:34:LYS:HG3	1:K:458:CYS:HA	1.94	0.48
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.94	0.48
1:E:501:ARG:NH1	1:E:505:GLN:OE1	2.46	0.48
1:H:16:MET:O	1:H:20:VAL:HG13	2.13	0.48
1:J:345:ARG:HH21	1:J:368:ARG:HH12	1.61	0.48
1:K:414:GLY:O	1:K:417:VAL:HG13	2.13	0.48
1:D:13:ARG:HD2	1:D:104:LEU:HD22	1.94	0.48
1:G:232:GLU:OE1	1:G:309:LEU:HD12	2.13	0.48
1:G:266:THR:CG2	1:G:273:VAL:H	2.26	0.48
1:H:103:GLY:HA3	1:H:515:ILE:HD11	1.95	0.48
1:J:185:ASP:OD1	1:J:382:GLY:N	2.41	0.48
1:K:359:ASP:OD1	1:K:362:ARG:NH1	2.46	0.48
1:B:151:SER:HB2	1:B:399:ALA:HA	1.95	0.48
1:H:284:ARG:O	1:H:288:MET:HG3	2.12	0.48
1:K:30:THR:HB	1:K:51:LYS:O	2.14	0.48
1:I:162:ILE:O	1:I:166:MET:HG3	2.13	0.48
1:I:178:GLU:HG2	1:I:322:ARG:NH1	2.28	0.48
1:K:482:THR:O	1:K:484:GLU:HG2	2.13	0.48
1:N:183:LEU:HD22	1:N:184:GLN:N	2.29	0.48
1:D:5:ASP:HB2	1:D:524:LEU:CD1	2.43	0.48
1:H:229:ASN:HD21	1:N:272:LYS:HZ2	1.62	0.48
1:J:358:SER:HB3	1:J:361:ASP:CG	2.38	0.48
1:L:34:LYS:HE2	1:M:118:ARG:NH2	2.14	0.48
1:M:183:LEU:HD22	1:M:184:GLN:N	2.28	0.48
1:M:217:SER:O	1:M:245:LYS:HD3	2.13	0.48
1:C:124:VAL:O	1:C:128:VAL:HG23	2.13	0.48
1:F:263:VAL:O	1:F:267:MET:HB2	2.14	0.48
1:H:202:PRO:C	1:H:204:PHE:H	2.22	0.48
1:H:230:ILE:HD12	1:H:261:THR:HB	1.96	0.48
1:A:213:VAL:HB	1:A:325:ILE:HB	1.94	0.48
1:E:247:LEU:O	1:E:273:VAL:HG13	2.13	0.48
1:G:68:ASN:O	1:G:72:GLN:HG2	2.13	0.48
1:I:239:ALA:HB1	1:I:314:LEU:HG	1.96	0.48
1:J:238:GLU:O	1:J:242:LYS:HD3	2.14	0.48
1:N:40:LEU:HD13	1:N:59:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:GLU:HB3	1:G:442:VAL:HG22	1.96	0.47
1:J:95:LEU:O	1:J:99:ILE:HG13	2.13	0.47
1:D:253:ASP:OD1	1:D:254:VAL:N	2.47	0.47
1:H:149:THR:HG22	1:H:154:SER:HA	1.96	0.47
1:N:131:LEU:HD13	1:N:422:VAL:HG21	1.96	0.47
1:N:348:GLN:O	1:N:352:GLN:HG3	2.14	0.47
1:N:16:MET:O	1:N:20:VAL:HG13	2.14	0.47
1:B:68:ASN:O	1:B:72:GLN:HG2	2.15	0.47
1:E:34:LYS:HB3	1:F:114:MET:HG3	1.96	0.47
1:F:359:ASP:OD1	1:F:362:ARG:NH1	2.47	0.47
1:H:71:ALA:O	1:H:75:LYS:HB2	2.15	0.47
1:I:242:LYS:HA	1:J:231:ARG:HH11	1.78	0.47
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.96	0.47
1:M:284:ARG:O	1:M:288:MET:HG3	2.15	0.47
1:C:178:GLU:HA	1:C:393:LYS:HE2	1.96	0.47
1:D:351:GLN:O	1:D:355:GLU:HG3	2.15	0.47
1:F:23:LEU:HD23	1:F:74:VAL:HG22	1.95	0.47
1:G:482:THR:O	1:G:484:GLU:HG2	2.13	0.47
1:J:202:PRO:C	1:J:204:PHE:H	2.22	0.47
1:J:478:TYR:CE2	1:J:480:ALA:HA	2.49	0.47
1:N:183:LEU:O	1:N:184:GLN:HB2	2.15	0.47
1:F:16:MET:HB3	1:F:514:MET:HE3	1.96	0.47
1:F:171:LYS:HB3	1:F:407:VAL:HG11	1.95	0.47
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.96	0.47
1:G:364:LYS:HD3	1:G:364:LYS:HA	1.70	0.47
1:J:262:LEU:O	1:J:266:THR:HG23	2.14	0.47
1:M:20:VAL:HB	1:M:74:VAL:HG11	1.96	0.47
1:A:253:ASP:CG	1:A:277:LYS:HE2	2.40	0.47
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.97	0.47
1:C:342:ILE:O	1:C:346:VAL:HG23	2.15	0.47
1:D:414:GLY:N	1:D:494:LEU:HA	2.30	0.47
1:F:225:LYS:HD3	1:F:309:LEU:CD1	2.45	0.47
1:G:349:ILE:O	1:G:353:ILE:HG13	2.14	0.47
1:I:284:ARG:O	1:I:288:MET:HG3	2.15	0.47
1:K:202:PRO:C	1:K:204:PHE:H	2.23	0.47
1:B:141:SER:HA	1:B:144:ILE:HB	1.97	0.47
1:B:202:PRO:C	1:B:204:PHE:H	2.23	0.47
1:E:321:LYS:HD2	1:E:334:ASP:OD2	2.14	0.47
1:G:366:GLN:HA	1:G:369:VAL:HG22	1.97	0.47
1:E:200:LEU:HG	1:E:276:VAL:HA	1.96	0.47
1:G:472:GLY:HA3	1:G:476:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:ASN:HD21	1:N:272:LYS:NZ	2.13	0.47
1:H:242:LYS:C	1:H:244:GLY:H	2.23	0.47
1:H:281:PHE:HZ	1:N:383:ALA:O	1.98	0.47
1:J:319:GLN:HB3	1:J:336:VAL:HG21	1.98	0.47
1:L:291:ASP:OD2	1:L:368:ARG:HD2	2.15	0.47
1:M:214:GLU:CD	1:M:322:ARG:HH21	2.23	0.47
1:C:218:PRO:HD2	1:C:320:ALA:O	2.15	0.46
1:C:413:ALA:HB1	1:C:417:VAL:HG22	1.97	0.46
1:E:139:SER:O	1:E:171:LYS:NZ	2.44	0.46
1:F:240:VAL:HG11	1:F:247:LEU:HB2	1.97	0.46
1:H:287:ALA:HB1	1:H:368:ARG:NH1	2.30	0.46
1:I:57:ALA:O	1:I:75:LYS:HD2	2.16	0.46
1:N:213:VAL:HB	1:N:325:ILE:HB	1.97	0.46
1:C:345:ARG:O	1:C:349:ILE:HG13	2.15	0.46
1:H:270:ILE:HG13	1:H:271:VAL:HG23	1.97	0.46
1:L:142:LYS:O	1:L:146:GLN:HG3	2.16	0.46
1:C:413:ALA:CB	1:C:417:VAL:HG22	2.45	0.46
1:D:77:VAL:HG21	1:D:510:VAL:HB	1.97	0.46
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.96	0.46
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.97	0.46
1:I:384:ALA:HB3	1:I:388:GLU:OE1	2.15	0.46
1:F:10:ASN:O	1:F:14:VAL:HG13	2.15	0.46
1:I:205:ILE:HA	1:I:213:VAL:HG22	1.97	0.46
1:J:183:LEU:O	1:J:184:GLN:HB2	2.15	0.46
1:L:242:LYS:C	1:L:244:GLY:H	2.22	0.46
1:M:203:TYR:H	1:M:205:ILE:HD12	1.79	0.46
1:N:16:MET:HB3	1:N:514:MET:HE3	1.97	0.46
1:C:70:GLY:HA2	1:C:73:MET:HE3	1.97	0.46
1:C:142:LYS:O	1:C:146:GLN:HG3	2.15	0.46
1:J:179:ASP:OD1	1:J:393:LYS:HE3	2.16	0.46
1:J:414:GLY:N	1:J:494:LEU:HA	2.31	0.46
1:N:417:VAL:O	1:N:420:ILE:HG22	2.16	0.46
1:N:482:THR:O	1:N:484:GLU:HG2	2.16	0.46
1:H:102:GLU:OE1	1:H:445:ARG:NH1	2.48	0.46
1:J:5:ASP:HB2	1:J:524:LEU:HD13	1.97	0.46
1:J:213:VAL:HB	1:J:325:ILE:HB	1.97	0.46
1:J:242:LYS:C	1:J:244:GLY:H	2.23	0.46
1:K:16:MET:SD	1:K:73:MET:HE1	2.55	0.46
1:B:455:VAL:HG13	1:B:460:GLU:HB2	1.97	0.46
1:C:77:VAL:HG12	1:C:506:TYR:HB3	1.97	0.46
1:C:266:THR:HG21	1:C:273:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:225:LYS:HD3	1:J:226:LYS:O	2.16	0.46
1:M:72:GLN:HE22	1:M:75:LYS:HE2	1.81	0.46
1:M:161:LEU:HD22	1:M:379:ILE:HG23	1.97	0.46
1:M:166:MET:O	1:M:170:GLY:N	2.47	0.46
1:M:224:ASP:OD1	1:M:285:ARG:NH1	2.46	0.46
1:A:102:GLU:HB3	1:A:442:VAL:HG22	1.98	0.46
1:A:218:PRO:HD2	1:A:320:ALA:O	2.16	0.46
1:B:200:LEU:HG	1:B:276:VAL:HA	1.98	0.46
1:D:364:LYS:HA	1:D:364:LYS:HD3	1.69	0.46
1:G:433:ASN:ND2	1:G:436:GLN:HG3	2.31	0.46
1:N:364:LYS:HD3	1:N:364:LYS:HA	1.73	0.46
1:A:202:PRO:C	1:A:204:PHE:H	2.24	0.46
1:B:349:ILE:O	1:B:353:ILE:HG13	2.16	0.46
1:B:429:LEU:O	1:B:430:ARG:NH1	2.46	0.46
1:E:202:PRO:C	1:E:204:PHE:H	2.24	0.46
1:I:200:LEU:HG	1:I:276:VAL:HA	1.98	0.46
1:K:122:LYS:HE2	1:K:429:LEU:HD11	1.97	0.46
1:K:288:MET:O	1:K:291:ASP:HB2	2.15	0.46
1:M:183:LEU:HD22	1:M:184:GLN:H	1.81	0.46
1:A:178:GLU:HG3	1:A:380:LYS:HG2	1.98	0.46
1:C:383:ALA:O	1:C:384:ALA:HB3	2.16	0.46
1:D:221:LEU:HD23	1:D:249:ILE:HD12	1.97	0.46
1:H:288:MET:O	1:H:291:ASP:HB2	2.16	0.46
1:J:7:LYS:HG3	1:J:66:PHE:CZ	2.51	0.46
1:N:200:LEU:HG	1:N:276:VAL:HA	1.98	0.46
1:B:288:MET:O	1:B:292:ILE:HG13	2.16	0.45
1:C:486:GLY:C	1:C:491:MET:HE2	2.41	0.45
1:E:345:ARG:HH21	1:E:368:ARG:HH12	1.64	0.45
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.46	0.45
1:L:178:GLU:HG2	1:L:322:ARG:NH1	2.31	0.45
1:B:218:PRO:HD2	1:B:320:ALA:O	2.17	0.45
1:F:230:ILE:HB	1:F:258:ALA:HA	1.98	0.45
1:H:349:ILE:HA	1:H:352:GLN:HG3	1.98	0.45
1:I:213:VAL:HB	1:I:325:ILE:HB	1.98	0.45
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.97	0.45
1:M:152:ALA:O	1:M:395:ARG:HD2	2.17	0.45
1:D:359:ASP:O	1:D:363:GLU:HG3	2.17	0.45
1:H:247:LEU:HD21	1:H:249:ILE:HD11	1.98	0.45
1:J:314:LEU:HD23	1:J:317:LEU:HD22	1.97	0.45
1:K:286:LYS:NZ	1:K:304:GLU:OE2	2.49	0.45
1:M:183:LEU:O	1:M:184:GLN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:HB	1:A:307:MET:HE2	1.97	0.45
1:E:178:GLU:OE2	1:E:322:ARG:HD3	2.15	0.45
1:N:31:LEU:HD12	1:N:31:LEU:HA	1.72	0.45
1:A:319:GLN:O	1:A:336:VAL:HG23	2.17	0.45
1:C:421:ARG:NH2	1:C:469:VAL:O	2.43	0.45
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.98	0.45
1:D:240:VAL:HG11	1:D:247:LEU:HB2	1.98	0.45
1:D:429:LEU:O	1:D:430:ARG:NH1	2.45	0.45
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.98	0.45
1:E:183:LEU:HB2	1:E:384:ALA:HB2	1.98	0.45
1:F:118:ARG:HD2	1:F:436:GLN:NE2	2.32	0.45
1:F:233:MET:CE	1:F:309:LEU:HD13	2.46	0.45
1:A:82:ASN:HB2	1:A:89:THR:OG1	2.16	0.45
1:C:245:LYS:NZ	1:C:319:GLN:OE1	2.46	0.45
1:C:383:ALA:CB	1:C:389:MET:HB2	2.47	0.45
1:H:151:SER:HB2	1:H:399:ALA:HA	1.97	0.45
1:H:225:LYS:HE2	1:H:303:GLU:OE2	2.16	0.45
1:L:223:ALA:O	1:L:251:ALA:HA	2.17	0.45
1:F:414:GLY:N	1:F:494:LEU:HA	2.31	0.45
1:G:190:VAL:HB	1:G:334:ASP:OD1	2.17	0.45
1:G:441:LYS:O	1:G:445:ARG:HB2	2.17	0.45
1:I:310:GLU:OE1	1:I:310:GLU:N	2.47	0.45
1:L:223:ALA:HB2	1:L:309:LEU:HD21	1.98	0.45
1:A:217:SER:HA	1:A:320:ALA:O	2.17	0.45
1:B:384:ALA:HA	1:C:360:TYR:OH	2.17	0.45
1:C:202:PRO:C	1:C:204:PHE:H	2.25	0.45
1:H:77:VAL:CG2	1:H:510:VAL:HB	2.47	0.45
1:H:183:LEU:HD22	1:H:184:GLN:N	2.32	0.45
1:M:319:GLN:HB3	1:M:336:VAL:HG21	1.98	0.45
1:N:12:ALA:HB1	1:N:520:MET:HG3	1.98	0.45
1:N:221:LEU:HD11	1:N:301:ILE:HD12	1.98	0.45
1:B:176:THR:CG2	1:B:322:ARG:HH12	2.29	0.45
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.83	0.45
1:F:179:ASP:OD1	1:F:393:LYS:HE3	2.17	0.45
1:F:233:MET:HE1	1:F:309:LEU:HD13	1.98	0.45
1:G:77:VAL:HG21	1:G:510:VAL:HB	1.98	0.45
1:M:77:VAL:O	1:M:80:LYS:HB2	2.17	0.45
1:B:102:GLU:HB3	1:B:442:VAL:HG22	1.99	0.45
1:C:176:THR:HG21	1:C:333:ILE:HD13	1.98	0.45
1:E:240:VAL:HG21	1:E:247:LEU:HD22	1.98	0.45
1:E:284:ARG:O	1:E:288:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:ASP:OD2	1:G:368:ARG:HD2	2.17	0.45
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.99	0.45
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.99	0.45
1:B:242:LYS:C	1:B:244:GLY:N	2.75	0.44
1:F:230:ILE:HD12	1:F:261:THR:HB	1.99	0.44
1:H:213:VAL:HB	1:H:325:ILE:HB	1.99	0.44
1:L:364:LYS:HD3	1:L:364:LYS:HA	1.67	0.44
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.99	0.44
1:B:417:VAL:HA	1:B:420:ILE:HG22	1.97	0.44
1:C:127:ALA:O	1:C:131:LEU:HB2	2.16	0.44
1:E:136:VAL:HA	1:E:137:PRO:HD3	1.88	0.44
1:E:269:GLY:O	1:F:229:ASN:ND2	2.51	0.44
1:E:383:ALA:O	1:E:384:ALA:HB3	2.18	0.44
1:F:69:MET:O	1:F:73:MET:HG3	2.17	0.44
1:G:269:GLY:HA2	1:G:272:LYS:HE3	2.00	0.44
1:I:201:SER:OG	1:I:202:PRO:O	2.26	0.44
1:J:414:GLY:O	1:J:417:VAL:HG13	2.17	0.44
1:K:151:SER:HB2	1:K:399:ALA:HA	1.99	0.44
1:M:12:ALA:HB1	1:M:520:MET:HG3	1.99	0.44
1:N:183:LEU:HD22	1:N:184:GLN:H	1.82	0.44
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.65	0.44
1:B:16:MET:O	1:B:20:VAL:HG13	2.16	0.44
1:B:230:ILE:HD12	1:B:261:THR:HB	1.99	0.44
1:B:242:LYS:HG3	1:C:231:ARG:CZ	2.47	0.44
1:F:213:VAL:HB	1:F:325:ILE:HB	1.99	0.44
1:G:77:VAL:HG11	1:G:510:VAL:HB	1.99	0.44
1:K:218:PRO:HD2	1:K:320:ALA:O	2.18	0.44
1:N:218:PRO:HD2	1:N:320:ALA:O	2.17	0.44
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.78	0.44
1:C:120:ILE:O	1:C:124:VAL:HG23	2.18	0.44
1:D:200:LEU:HG	1:D:276:VAL:HA	1.99	0.44
1:H:30:THR:HB	1:H:51:LYS:O	2.18	0.44
1:I:77:VAL:O	1:I:80:LYS:HB2	2.18	0.44
1:A:359:ASP:OD1	1:A:362:ARG:NH1	2.51	0.44
1:E:10:ASN:O	1:E:14:VAL:HG13	2.17	0.44
1:G:514:MET:HE2	1:G:514:MET:HB3	1.74	0.44
1:H:72:GLN:NE2	1:H:75:LYS:HE2	2.33	0.44
1:H:223:ALA:O	1:H:251:ALA:HA	2.18	0.44
1:J:77:VAL:CG2	1:J:510:VAL:HB	2.46	0.44
1:K:85:ALA:HB1	1:K:499:VAL:HG12	2.00	0.44
1:M:364:LYS:HA	1:M:364:LYS:HD3	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:O	1:A:164:GLU:HG3	2.18	0.44
1:B:305:ILE:CD1	1:B:307:MET:HE2	2.45	0.44
1:C:455:VAL:HG11	1:C:462:PRO:HA	2.00	0.44
1:D:183:LEU:HG	1:D:384:ALA:HB2	2.00	0.44
1:E:140:ASP:OD2	1:E:142:LYS:HB3	2.18	0.44
1:G:389:MET:HG3	1:G:390:LYS:N	2.33	0.44
1:H:427:ALA:O	1:H:441:LYS:NZ	2.50	0.44
1:H:514:MET:HE2	1:H:514:MET:HB3	1.73	0.44
1:J:247:LEU:HD21	1:J:249:ILE:HD11	1.99	0.44
1:L:266:THR:CG2	1:L:273:VAL:H	2.30	0.44
1:L:461:GLU:HA	1:L:462:PRO:HD3	1.68	0.44
1:M:194:GLN:O	1:M:371:LYS:HE3	2.18	0.44
1:N:219:PHE:HB3	1:N:317:LEU:HD23	1.98	0.44
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.83	0.44
1:A:263:VAL:O	1:A:267:MET:HB2	2.18	0.44
1:A:420:ILE:HG13	1:A:448:GLU:HG2	1.99	0.44
1:B:393:LYS:NZ	1:B:397:GLU:OE1	2.51	0.44
1:D:417:VAL:O	1:D:420:ILE:HG22	2.18	0.44
1:H:419:LEU:HD23	1:H:419:LEU:HA	1.87	0.44
1:I:10:ASN:O	1:I:14:VAL:HG13	2.18	0.44
1:L:296:THR:HB	1:L:319:GLN:H	1.83	0.44
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.99	0.44
1:A:342:ILE:O	1:A:346:VAL:HG23	2.18	0.44
1:F:202:PRO:C	1:F:204:PHE:H	2.26	0.44
1:K:161:LEU:HD22	1:K:379:ILE:HG23	1.99	0.44
1:L:326:ASN:HB2	1:L:329:THR:H	1.83	0.44
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.99	0.44
1:N:144:ILE:HD11	1:N:171:LYS:HE2	2.00	0.44
1:N:434:GLU:O	1:N:437:ASN:HB2	2.17	0.44
1:C:146:GLN:O	1:C:150:ILE:HG13	2.18	0.44
1:D:171:LYS:HD3	1:D:407:VAL:HG13	2.00	0.44
1:F:364:LYS:O	1:F:367:GLU:HB2	2.18	0.44
1:G:263:VAL:O	1:G:267:MET:HB2	2.18	0.44
1:H:7:LYS:HE3	1:H:15:LYS:HE3	1.99	0.44
1:H:169:VAL:HG11	1:H:377:ALA:HB2	1.99	0.44
1:L:247:LEU:HB3	1:L:273:VAL:HG22	2.00	0.44
1:L:266:THR:HG21	1:L:273:VAL:H	1.83	0.44
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.48	0.44
1:M:95:LEU:O	1:M:99:ILE:HG13	2.17	0.44
1:N:102:GLU:OE1	1:N:445:ARG:NH1	2.50	0.44
1:A:39:VAL:HG12	1:B:69:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLU:HB3	1:D:442:VAL:HG22	1.99	0.43
1:F:77:VAL:HG21	1:F:510:VAL:HB	2.00	0.43
1:I:27:VAL:HG13	1:I:90:THR:HG23	2.00	0.43
1:J:102:GLU:O	1:J:105:ALA:HB3	2.17	0.43
1:J:288:MET:O	1:J:291:ASP:HB2	2.18	0.43
1:M:213:VAL:O	1:M:324:VAL:HA	2.18	0.43
1:A:69:MET:HE2	1:G:39:VAL:HG12	2.00	0.43
1:D:36:ARG:HG3	1:E:518:GLU:HG3	2.00	0.43
1:D:358:SER:HB3	1:D:361:ASP:CG	2.43	0.43
1:E:71:ALA:O	1:E:75:LYS:HB2	2.18	0.43
1:E:301:ILE:HD13	1:E:312:ALA:HB2	2.00	0.43
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.99	0.43
1:G:219:PHE:O	1:G:247:LEU:HD12	2.18	0.43
1:G:417:VAL:HA	1:G:420:ILE:HG22	2.00	0.43
1:J:122:LYS:HE2	1:J:429:LEU:HD11	2.00	0.43
1:K:72:GLN:NE2	1:K:75:LYS:HE2	2.33	0.43
1:L:16:MET:O	1:L:20:VAL:HG13	2.18	0.43
1:M:174:VAL:HG21	1:M:194:GLN:HB3	1.98	0.43
1:D:230:ILE:HD12	1:D:261:THR:HB	2.01	0.43
1:D:514:MET:HE2	1:D:514:MET:HB3	1.52	0.43
1:E:359:ASP:O	1:E:363:GLU:HG3	2.18	0.43
1:I:31:LEU:HD23	1:I:453:GLN:HB3	2.01	0.43
1:I:195:PHE:CE2	1:I:330:THR:HB	2.53	0.43
1:I:230:ILE:HD12	1:I:261:THR:HB	1.99	0.43
1:M:144:ILE:HD11	1:M:171:LYS:HE2	2.00	0.43
1:M:215:LEU:HB2	1:M:323:VAL:HG22	2.00	0.43
1:M:266:THR:HG21	1:M:273:VAL:O	2.18	0.43
1:C:183:LEU:HD12	1:C:383:ALA:O	2.18	0.43
1:D:417:VAL:HA	1:D:420:ILE:HG22	2.01	0.43
1:G:218:PRO:HD2	1:G:320:ALA:O	2.19	0.43
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.99	0.43
1:K:169:VAL:HG13	1:K:377:ALA:HB2	2.01	0.43
1:N:174:VAL:HB	1:N:376:VAL:HG22	2.00	0.43
1:B:472:GLY:HA3	1:B:476:TYR:CD2	2.53	0.43
1:E:346:VAL:O	1:E:350:ARG:HB2	2.19	0.43
1:I:166:MET:HE2	1:I:171:LYS:HA	2.01	0.43
1:J:178:GLU:HG2	1:J:322:ARG:NH1	2.34	0.43
1:J:451:LEU:C	1:J:451:LEU:HD23	2.43	0.43
1:M:166:MET:HE2	1:M:171:LYS:HA	1.99	0.43
1:B:349:ILE:HG23	1:B:365:LEU:HD22	1.99	0.43
1:E:478:TYR:CE2	1:E:480:ALA:HA	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:77:VAL:O	1:N:80:LYS:HB2	2.18	0.43
1:C:183:LEU:HB2	1:C:384:ALA:HB2	2.01	0.43
1:K:102:GLU:HB3	1:K:442:VAL:HG22	2.01	0.43
1:L:288:MET:O	1:L:291:ASP:HB2	2.18	0.43
1:M:72:GLN:NE2	1:M:75:LYS:HE2	2.33	0.43
1:N:237:LEU:HD23	1:N:237:LEU:HA	1.84	0.43
1:A:345:ARG:O	1:A:349:ILE:HG13	2.19	0.43
1:B:219:PHE:HB3	1:B:317:LEU:HD23	2.01	0.43
1:D:200:LEU:HD21	1:D:277:LYS:HG3	2.01	0.43
1:F:6:VAL:HG22	1:F:521:VAL:HG13	1.99	0.43
1:G:339:GLU:O	1:G:343:GLN:HB2	2.19	0.43
1:L:185:ASP:OD1	1:L:382:GLY:N	2.47	0.43
1:L:197:ARG:HD2	1:L:277:LYS:HB2	2.01	0.43
1:A:176:THR:HG21	1:A:333:ILE:HD13	2.00	0.43
1:B:7:LYS:HE3	1:B:15:LYS:HE3	2.01	0.43
1:B:225:LYS:HG2	1:B:226:LYS:O	2.19	0.43
1:C:417:VAL:HA	1:C:420:ILE:HG22	2.00	0.43
1:E:417:VAL:HA	1:E:420:ILE:HG22	2.01	0.43
1:F:120:ILE:O	1:F:124:VAL:HG23	2.18	0.43
1:F:215:LEU:HB2	1:F:323:VAL:CG2	2.49	0.43
1:H:365:LEU:O	1:H:369:VAL:HG22	2.19	0.43
1:J:193:MET:HE1	1:J:292:ILE:HG12	2.01	0.43
1:K:140:ASP:OD1	1:K:140:ASP:N	2.52	0.43
1:K:349:ILE:O	1:K:352:GLN:HB2	2.19	0.43
1:C:16:MET:SD	1:C:73:MET:HE1	2.59	0.43
1:I:459:GLY:HA3	1:J:112:ASN:ND2	2.34	0.43
1:I:476:TYR:HA	1:I:486:GLY:O	2.19	0.43
1:J:215:LEU:O	1:J:322:ARG:HA	2.19	0.43
1:L:68:ASN:O	1:L:72:GLN:HG2	2.18	0.43
1:M:112:ASN:HB3	1:M:115:ASP:HB2	2.00	0.43
1:M:176:THR:CG2	1:M:322:ARG:HH12	2.28	0.43
1:N:458:CYS:SG	1:N:480:ALA:HB1	2.59	0.43
1:A:524:LEU:HD23	1:A:525:PRO:HD2	2.01	0.42
1:B:18:ARG:HD2	1:B:67:GLU:OE2	2.19	0.42
1:D:349:ILE:O	1:D:353:ILE:HG13	2.18	0.42
1:F:178:GLU:HG3	1:F:380:LYS:HG2	2.00	0.42
1:H:461:GLU:HA	1:H:462:PRO:HD3	1.83	0.42
1:K:458:CYS:SG	1:K:480:ALA:HB1	2.59	0.42
1:L:206:ASN:ND2	1:L:214:GLU:O	2.48	0.42
1:M:165:ALA:HB2	1:M:379:ILE:HD11	2.01	0.42
1:N:20:VAL:HB	1:N:74:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ALA:HA	1:B:47:PRO:HD3	1.88	0.42
1:C:13:ARG:HD2	1:C:104:LEU:HD22	2.00	0.42
1:H:166:MET:HE2	1:H:171:LYS:HA	2.01	0.42
1:J:420:ILE:HG13	1:J:448:GLU:HG2	2.01	0.42
1:M:39:VAL:HG12	1:N:69:MET:HE2	2.01	0.42
1:M:263:VAL:O	1:M:267:MET:HB2	2.18	0.42
1:M:478:TYR:CE2	1:M:480:ALA:HA	2.53	0.42
1:N:104:LEU:HD23	1:N:104:LEU:HA	1.79	0.42
1:N:286:LYS:NZ	1:N:304:GLU:OE2	2.52	0.42
1:C:131:LEU:HD13	1:C:422:VAL:HG21	2.00	0.42
1:F:16:MET:O	1:F:20:VAL:HG13	2.20	0.42
1:G:372:LEU:HD12	1:G:372:LEU:HA	1.87	0.42
1:I:478:TYR:CE2	1:I:480:ALA:HA	2.54	0.42
1:J:364:LYS:HA	1:J:364:LYS:HD3	1.81	0.42
1:L:271:VAL:O	1:L:273:VAL:HG23	2.19	0.42
1:M:32:GLY:H	1:M:457:ASN:HD22	1.67	0.42
1:A:219:PHE:CE2	1:A:245:LYS:HD2	2.54	0.42
1:A:366:GLN:HA	1:A:369:VAL:HG22	2.02	0.42
1:F:221:LEU:HD11	1:F:301:ILE:HD12	2.00	0.42
1:G:348:GLN:O	1:G:352:GLN:HG3	2.19	0.42
1:I:326:ASN:HB2	1:I:329:THR:N	2.35	0.42
1:I:479:ASN:CG	1:I:493:ILE:HD11	2.45	0.42
1:G:295:LEU:HD22	1:G:342:ILE:HD13	2.01	0.42
1:J:136:VAL:HA	1:J:137:PRO:HD3	1.92	0.42
1:J:288:MET:O	1:J:292:ILE:HG13	2.20	0.42
1:L:26:ALA:HA	1:M:8:PHE:HE1	1.84	0.42
1:L:187:LEU:HD13	1:L:379:ILE:HG12	2.01	0.42
1:L:190:VAL:HB	1:L:334:ASP:OD1	2.20	0.42
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.79	0.42
1:C:225:LYS:HE3	1:C:225:LYS:HB2	1.86	0.42
1:E:429:LEU:HG	1:E:440:ILE:HD13	2.02	0.42
1:G:461:GLU:HA	1:G:462:PRO:HD3	1.88	0.42
1:H:363:GLU:O	1:H:366:GLN:HB2	2.20	0.42
1:I:127:ALA:O	1:I:131:LEU:HB2	2.19	0.42
1:M:102:GLU:O	1:M:105:ALA:HB3	2.19	0.42
1:N:202:PRO:C	1:N:204:PHE:H	2.26	0.42
1:B:7:LYS:HE2	1:B:66:PHE:CE2	2.54	0.42
1:D:271:VAL:O	1:D:273:VAL:HG23	2.20	0.42
1:D:482:THR:O	1:D:484:GLU:HG2	2.20	0.42
1:E:449:ALA:HB3	1:E:450:PRO:HD3	2.01	0.42
1:F:160:LYS:O	1:F:164:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:321:LYS:HD2	1:K:334:ASP:OD2	2.20	0.42
1:K:449:ALA:HB3	1:K:450:PRO:HD3	2.01	0.42
1:M:266:THR:HG22	1:M:271:VAL:O	2.19	0.42
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.49	0.42
1:D:348:GLN:O	1:D:351:GLN:HB3	2.20	0.42
1:E:404:ARG:HH11	1:E:404:ARG:HG2	1.85	0.42
1:F:166:MET:O	1:F:170:GLY:N	2.52	0.42
1:H:141:SER:HA	1:H:144:ILE:HB	2.01	0.42
1:H:266:THR:HG21	1:H:273:VAL:O	2.20	0.42
1:I:146:GLN:O	1:I:150:ILE:HG13	2.20	0.42
1:I:221:LEU:HD23	1:I:249:ILE:HD12	2.02	0.42
1:I:479:ASN:ND2	1:I:493:ILE:HD11	2.34	0.42
1:J:26:ALA:HA	1:K:8:PHE:HE1	1.84	0.42
1:L:146:GLN:O	1:L:150:ILE:HG13	2.20	0.42
1:L:294:THR:HG23	1:L:341:ALA:HB1	2.02	0.42
1:M:257:GLU:O	1:M:261:THR:OG1	2.27	0.42
1:B:77:VAL:O	1:B:80:LYS:HB2	2.20	0.42
1:B:184:GLN:H	1:B:382:GLY:HA3	1.84	0.42
1:E:74:VAL:HA	1:E:510:VAL:HG21	2.01	0.42
1:E:266:THR:CG2	1:E:273:VAL:H	2.33	0.42
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.50	0.42
1:J:222:LEU:HD22	1:J:289:LEU:HD23	2.02	0.42
1:K:71:ALA:O	1:K:75:LYS:HB2	2.20	0.42
1:K:166:MET:HE1	1:K:407:VAL:HG21	2.01	0.42
1:K:187:LEU:HA	1:K:378:VAL:O	2.19	0.42
1:K:242:LYS:C	1:K:244:GLY:N	2.78	0.42
1:L:420:ILE:HG13	1:L:448:GLU:HG2	2.01	0.42
1:N:16:MET:HB3	1:N:514:MET:CE	2.49	0.42
1:N:263:VAL:O	1:N:267:MET:HB2	2.20	0.42
1:C:202:PRO:O	1:C:203:TYR:HB2	2.20	0.42
1:C:230:ILE:HD12	1:C:261:THR:HB	2.02	0.42
1:C:487:ASN:HB3	1:C:490:ASP:HB2	2.01	0.42
1:D:412:VAL:HG13	1:D:497:THR:OG1	2.19	0.42
1:D:524:LEU:HD12	1:D:524:LEU:HA	1.73	0.42
1:E:266:THR:HB	1:E:272:LYS:HA	2.02	0.42
1:G:130:GLU:HB3	1:G:422:VAL:HG22	2.02	0.42
1:H:441:LYS:O	1:H:445:ARG:HB2	2.19	0.42
1:H:451:LEU:HD21	1:H:465:VAL:HG12	2.02	0.42
1:M:38:VAL:HG22	1:N:519:CYS:HB3	2.02	0.42
1:N:215:LEU:HB2	1:N:323:VAL:HG22	2.01	0.42
1:N:222:LEU:CD1	1:N:293:ALA:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ALA:O	1:E:131:LEU:HB2	2.20	0.41
1:E:219:PHE:CE2	1:E:245:LYS:HD2	2.55	0.41
1:E:247:LEU:HD21	1:E:249:ILE:HD11	2.00	0.41
1:G:205:ILE:HA	1:G:213:VAL:HG22	2.02	0.41
1:G:383:ALA:O	1:G:384:ALA:HB3	2.20	0.41
1:H:175:ILE:HB	1:H:400:LEU:HD21	2.02	0.41
1:J:235:PRO:HG3	1:J:310:GLU:HA	2.01	0.41
1:N:218:PRO:O	1:N:319:GLN:HG3	2.20	0.41
1:A:165:ALA:O	1:A:169:VAL:HG22	2.20	0.41
1:D:46:ALA:HA	1:D:47:PRO:HD3	1.86	0.41
1:E:77:VAL:HG21	1:E:510:VAL:HB	2.03	0.41
1:F:26:ALA:HA	1:G:8:PHE:HE1	1.84	0.41
1:H:21:ASN:HA	1:H:97:GLN:HE21	1.86	0.41
1:H:271:VAL:O	1:H:273:VAL:HG23	2.21	0.41
1:K:232:GLU:HA	1:K:310:GLU:HG3	2.02	0.41
1:M:238:GLU:O	1:M:241:ALA:HB3	2.20	0.41
1:N:240:VAL:HG11	1:N:247:LEU:HB2	2.03	0.41
1:A:186:GLU:HB2	1:A:380:LYS:HB2	2.01	0.41
1:C:162:ILE:O	1:C:166:MET:HG3	2.20	0.41
1:C:213:VAL:HB	1:C:325:ILE:HB	2.01	0.41
1:D:166:MET:HE1	1:D:407:VAL:HG21	2.02	0.41
1:D:175:ILE:HG12	1:D:377:ALA:HB3	2.02	0.41
1:F:221:LEU:HB3	1:F:249:ILE:HD13	2.02	0.41
1:I:461:GLU:HA	1:I:462:PRO:HD3	1.74	0.41
1:J:146:GLN:O	1:J:150:ILE:HG13	2.20	0.41
1:A:102:GLU:HB2	1:A:442:VAL:HG13	2.02	0.41
1:A:206:ASN:OD1	1:A:214:GLU:N	2.51	0.41
1:A:361:ASP:OD1	1:A:361:ASP:N	2.51	0.41
1:D:288:MET:O	1:D:291:ASP:HB2	2.20	0.41
1:D:353:ILE:HD13	1:D:366:GLN:HG3	2.02	0.41
1:G:266:THR:HG21	1:G:273:VAL:O	2.20	0.41
1:H:263:VAL:O	1:H:267:MET:HB2	2.21	0.41
1:H:346:VAL:O	1:H:350:ARG:HB2	2.20	0.41
1:I:253:ASP:OD1	1:I:254:VAL:N	2.53	0.41
1:J:11:ASP:O	1:J:14:VAL:HG22	2.20	0.41
1:J:141:SER:HA	1:J:144:ILE:HB	2.01	0.41
1:L:102:GLU:HB2	1:L:442:VAL:HG13	2.03	0.41
1:M:46:ALA:HA	1:M:47:PRO:HD3	1.89	0.41
1:N:287:ALA:HB1	1:N:368:ARG:CZ	2.50	0.41
1:A:522:THR:OG1	1:A:523:ASP:N	2.53	0.41
1:B:383:ALA:CB	1:B:389:MET:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:LYS:O	1:J:146:GLN:HG3	2.21	0.41
1:B:514:MET:HE2	1:B:514:MET:HB3	1.77	0.41
1:E:12:ALA:HB1	1:E:520:MET:HG3	2.02	0.41
1:F:349:ILE:CG2	1:F:369:VAL:HG13	2.49	0.41
1:J:46:ALA:HA	1:J:47:PRO:HD3	1.88	0.41
1:M:223:ALA:O	1:M:251:ALA:HA	2.20	0.41
1:N:293:ALA:HB2	1:N:300:VAL:HG23	2.01	0.41
1:A:364:LYS:HD3	1:A:364:LYS:HA	1.77	0.41
1:E:262:LEU:O	1:E:266:THR:HG23	2.21	0.41
1:F:288:MET:O	1:F:291:ASP:HB2	2.21	0.41
1:I:152:ALA:HB2	1:I:158:VAL:HG11	2.02	0.41
1:I:266:THR:CG2	1:I:273:VAL:H	2.34	0.41
1:I:364:LYS:HA	1:I:364:LYS:HD3	1.68	0.41
1:I:496:PRO:HB2	1:I:499:VAL:HG13	2.02	0.41
1:N:323:VAL:HG12	1:N:332:ILE:HG12	2.03	0.41
1:N:472:GLY:HA3	1:N:476:TYR:CD2	2.55	0.41
1:D:383:ALA:O	1:D:384:ALA:HB3	2.21	0.41
1:E:391:GLU:O	1:E:394:ALA:HB3	2.21	0.41
1:G:136:VAL:HA	1:G:137:PRO:HD3	1.91	0.41
1:J:130:GLU:HB3	1:J:422:VAL:HG22	2.03	0.41
1:M:288:MET:HG2	1:M:368:ARG:HD3	2.03	0.41
1:N:319:GLN:HB3	1:N:336:VAL:CG2	2.51	0.41
1:A:383:ALA:O	1:A:384:ALA:HB3	2.21	0.41
1:B:12:ALA:HB1	1:B:520:MET:SD	2.60	0.41
1:C:365:LEU:O	1:C:369:VAL:HG22	2.21	0.41
1:C:429:LEU:O	1:C:430:ARG:NH1	2.51	0.41
1:D:205:ILE:HA	1:D:213:VAL:HG22	2.03	0.41
1:D:242:LYS:C	1:D:244:GLY:N	2.76	0.41
1:G:85:ALA:HB1	1:G:499:VAL:HG12	2.03	0.41
1:H:178:GLU:HB2	1:H:380:LYS:HG2	2.02	0.41
1:J:432:GLN:HB2	1:J:436:GLN:NE2	2.36	0.41
1:K:31:LEU:HD13	1:K:90:THR:HG21	2.03	0.41
1:M:34:LYS:HE2	1:N:118:ARG:NH2	2.29	0.41
1:A:12:ALA:HB1	1:A:520:MET:HG3	2.02	0.41
1:A:461:GLU:HA	1:A:462:PRO:HD3	1.81	0.41
1:B:324:VAL:O	1:B:331:THR:HG23	2.21	0.41
1:C:218:PRO:HB3	1:C:246:PRO:HG2	2.02	0.41
1:C:383:ALA:HB3	1:C:389:MET:HB2	2.02	0.41
1:D:109:ALA:HB2	1:J:109:ALA:HB2	2.01	0.41
1:F:383:ALA:HB2	1:F:389:MET:HA	2.03	0.41
1:G:146:GLN:O	1:G:150:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:201:SER:OG	1:G:202:PRO:O	2.27	0.41
1:H:103:GLY:HA3	1:H:515:ILE:CD1	2.52	0.41
1:K:240:VAL:HG11	1:K:247:LEU:HB2	2.03	0.41
1:A:27:VAL:HG12	1:A:90:THR:HG23	2.02	0.40
1:C:179:ASP:OD2	1:C:390:LYS:NZ	2.47	0.40
1:C:319:GLN:HE21	1:C:319:GLN:HB2	1.65	0.40
1:F:228:SER:O	1:F:257:GLU:HB3	2.21	0.40
1:F:482:THR:O	1:F:484:GLU:HG2	2.20	0.40
1:G:16:MET:SD	1:G:73:MET:HE1	2.61	0.40
1:J:419:LEU:HD23	1:J:419:LEU:HA	1.93	0.40
1:K:353:ILE:HG23	1:K:362:ARG:HG3	2.03	0.40
1:L:323:VAL:HG12	1:L:332:ILE:HA	2.04	0.40
1:N:136:VAL:HA	1:N:137:PRO:HD3	1.89	0.40
1:N:461:GLU:HA	1:N:462:PRO:HD3	1.82	0.40
1:A:189:VAL:HA	1:A:376:VAL:O	2.21	0.40
1:C:414:GLY:O	1:C:417:VAL:HG13	2.21	0.40
1:E:234:LEU:N	1:E:235:PRO:HD2	2.36	0.40
1:E:513:LEU:HD23	1:E:513:LEU:HA	1.90	0.40
1:F:509:SER:O	1:F:513:LEU:HG	2.22	0.40
1:I:61:GLU:C	1:I:62:LEU:HD23	2.46	0.40
1:I:147:VAL:O	1:I:151:SER:OG	2.30	0.40
1:I:419:LEU:HA	1:I:419:LEU:HD23	1.75	0.40
1:I:472:GLY:HA3	1:I:476:TYR:CD2	2.56	0.40
1:J:455:VAL:HG13	1:J:460:GLU:HB2	2.03	0.40
1:M:461:GLU:HA	1:M:462:PRO:HD3	1.76	0.40
1:C:173:GLY:O	1:C:404:ARG:NH2	2.54	0.40
1:C:181:THR:OG1	1:C:186:GLU:OE1	2.27	0.40
1:E:171:LYS:O	1:E:404:ARG:NH1	2.54	0.40
1:E:269:GLY:HA3	1:F:229:ASN:HD21	1.86	0.40
1:E:319:GLN:HB3	1:E:336:VAL:HG21	2.04	0.40
1:F:383:ALA:O	1:F:384:ALA:HB3	2.21	0.40
1:H:39:VAL:HG12	1:I:69:MET:HE2	2.03	0.40
1:H:136:VAL:HA	1:H:137:PRO:HD3	1.95	0.40
1:H:240:VAL:HG21	1:H:247:LEU:HD22	2.04	0.40
1:H:414:GLY:H	1:H:494:LEU:HA	1.86	0.40
1:J:102:GLU:HB2	1:J:442:VAL:HG13	2.02	0.40
1:M:443:ALA:O	1:M:446:ALA:HB3	2.21	0.40
1:N:27:VAL:HG12	1:N:90:THR:HG23	2.03	0.40
1:B:253:ASP:OD1	1:B:254:VAL:N	2.51	0.40
1:D:262:LEU:O	1:D:266:THR:HG23	2.22	0.40
1:F:183:LEU:HD22	1:F:184:GLN:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:16:MET:HB3	1:J:514:MET:HE3	2.04	0.40
1:J:214:GLU:HG3	1:J:324:VAL:HG22	2.04	0.40
1:J:326:ASN:HB2	1:J:329:THR:HB	2.03	0.40
1:K:436:GLN:O	1:K:440:ILE:HG13	2.21	0.40
1:N:95:LEU:O	1:N:99:ILE:HG13	2.22	0.40
1:F:40:LEU:HB2	1:F:48:THR:HB	2.04	0.40
1:G:262:LEU:O	1:G:266:THR:HG23	2.21	0.40
1:G:441:LYS:HA	1:G:441:LYS:HD3	1.95	0.40
1:I:482:THR:O	1:I:484:GLU:HG2	2.21	0.40
1:J:230:ILE:HD12	1:J:261:THR:HB	2.04	0.40
1:J:231:ARG:HH21	1:J:231:ARG:HD2	1.78	0.40
1:K:302:SER:H	1:K:307:MET:HE3	1.87	0.40
1:L:225:LYS:HG2	1:L:226:LYS:N	2.37	0.40
1:N:178:GLU:HG2	1:N:322:ARG:NH1	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	522/548 (95%)	509 (98%)	11 (2%)	2 (0%)	30	61
1	B	522/548 (95%)	508 (97%)	12 (2%)	2 (0%)	30	61
1	C	522/548 (95%)	507 (97%)	14 (3%)	1 (0%)	43	73
1	D	522/548 (95%)	507 (97%)	11 (2%)	4 (1%)	16	46
1	E	522/548 (95%)	509 (98%)	11 (2%)	2 (0%)	30	61
1	F	522/548 (95%)	507 (97%)	13 (2%)	2 (0%)	30	61
1	G	522/548 (95%)	512 (98%)	7 (1%)	3 (1%)	21	53
1	H	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	43	73
1	I	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	43	73
1	K	522/548 (95%)	513 (98%)	8 (2%)	1 (0%)	43	73
1	L	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	43	73
1	M	522/548 (95%)	511 (98%)	11 (2%)	0	100	100
1	N	522/548 (95%)	510 (98%)	11 (2%)	1 (0%)	43	73
All	All	7308/7672 (95%)	7137 (98%)	149 (2%)	22 (0%)	36	67

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	184	GLN
1	B	184	GLN
1	D	184	GLN
1	F	184	GLN
1	G	243	ALA
1	B	243	ALA
1	E	184	GLN
1	G	184	GLN
1	D	386	GLU
1	I	243	ALA
1	J	243	ALA
1	K	184	GLN
1	N	243	ALA
1	A	384	ALA
1	D	384	ALA
1	A	271	VAL
1	L	271	VAL
1	F	271	VAL
1	G	271	VAL
1	D	271	VAL
1	E	271	VAL
1	H	271	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/414 (97%)	391 (97%)	12 (3%)	36	66
1	B	403/414 (97%)	387 (96%)	16 (4%)	28	59
1	C	403/414 (97%)	387 (96%)	16 (4%)	28	59
1	D	403/414 (97%)	388 (96%)	15 (4%)	30	61
1	E	403/414 (97%)	388 (96%)	15 (4%)	30	61
1	F	403/414 (97%)	385 (96%)	18 (4%)	24	56
1	G	403/414 (97%)	388 (96%)	15 (4%)	30	61
1	H	403/414 (97%)	384 (95%)	19 (5%)	23	55
1	I	403/414 (97%)	388 (96%)	15 (4%)	30	61
1	J	403/414 (97%)	384 (95%)	19 (5%)	23	55
1	K	403/414 (97%)	387 (96%)	16 (4%)	28	59
1	L	403/414 (97%)	385 (96%)	18 (4%)	24	56
1	M	403/414 (97%)	384 (95%)	19 (5%)	23	55
1	N	403/414 (97%)	385 (96%)	18 (4%)	24	56
All	All	5642/5796 (97%)	5411 (96%)	231 (4%)	27	58

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	27	VAL
1	A	82	ASN
1	A	89	THR
1	A	94	VAL
1	A	183	LEU
1	A	257	GLU
1	A	289	LEU
1	A	329	THR
1	A	417	VAL
1	A	422	VAL
1	A	500	THR
1	B	18	ARG
1	B	20	VAL
1	B	27	VAL
1	B	82	ASN
1	B	89	THR

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Mol	Chain	Res	Type
1	B	94	VAL
1	B	131	LEU
1	B	210	THR
1	B	257	GLU
1	B	329	THR
1	B	331	THR
1	B	407	VAL
1	B	417	VAL
1	B	422	VAL
1	B	499	VAL
1	B	524	LEU
1	C	20	VAL
1	C	27	VAL
1	C	82	ASN
1	C	89	THR
1	C	94	VAL
1	C	131	LEU
1	C	210	THR
1	C	257	GLU
1	C	271	VAL
1	C	289	LEU
1	C	329	THR
1	C	369	VAL
1	C	417	VAL
1	C	422	VAL
1	C	499	VAL
1	C	524	LEU
1	D	20	VAL
1	D	27	VAL
1	D	82	ASN
1	D	89	THR
1	D	94	VAL
1	D	131	LEU
1	D	177	VAL
1	D	183	LEU
1	D	257	GLU
1	D	289	LEU
1	D	329	THR
1	D	417	VAL
1	D	494	LEU
1	D	499	VAL
1	D	524	LEU

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Mol	Chain	Res	Type
1	E	20	VAL
1	E	74	VAL
1	E	82	ASN
1	E	89	THR
1	E	94	VAL
1	E	131	LEU
1	E	210	THR
1	E	257	GLU
1	E	294	THR
1	E	329	THR
1	E	364	LYS
1	E	401	HIS
1	E	404	ARG
1	E	417	VAL
1	E	499	VAL
1	F	14	VAL
1	F	20	VAL
1	F	27	VAL
1	F	74	VAL
1	F	82	ASN
1	F	89	THR
1	F	94	VAL
1	F	131	LEU
1	F	177	VAL
1	F	183	LEU
1	F	257	GLU
1	F	289	LEU
1	F	328	ASP
1	F	329	THR
1	F	369	VAL
1	F	417	VAL
1	F	422	VAL
1	F	499	VAL
1	G	20	VAL
1	G	27	VAL
1	G	82	ASN
1	G	89	THR
1	G	94	VAL
1	G	131	LEU
1	G	177	VAL
1	G	183	LEU
1	G	210	THR

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Mol	Chain	Res	Type
1	G	257	GLU
1	G	329	THR
1	G	331	THR
1	G	389	MET
1	G	417	VAL
1	G	499	VAL
1	H	20	VAL
1	H	27	VAL
1	H	74	VAL
1	H	75	LYS
1	H	77	VAL
1	H	82	ASN
1	H	89	THR
1	H	94	VAL
1	H	131	LEU
1	H	168	LYS
1	H	183	LEU
1	H	210	THR
1	H	257	GLU
1	H	329	THR
1	H	417	VAL
1	H	422	VAL
1	H	494	LEU
1	H	499	VAL
1	H	524	LEU
1	I	20	VAL
1	I	27	VAL
1	I	74	VAL
1	I	82	ASN
1	I	89	THR
1	I	94	VAL
1	I	131	LEU
1	I	183	LEU
1	I	329	THR
1	I	331	THR
1	I	417	VAL
1	I	422	VAL
1	I	463	SER
1	I	499	VAL
1	I	524	LEU
1	J	20	VAL
1	J	27	VAL

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Mol	Chain	Res	Type
1	J	77	VAL
1	J	82	ASN
1	J	89	THR
1	J	94	VAL
1	J	131	LEU
1	J	183	LEU
1	J	210	THR
1	J	225	LYS
1	J	231	ARG
1	J	257	GLU
1	J	289	LEU
1	J	329	THR
1	J	361	ASP
1	J	417	VAL
1	J	422	VAL
1	J	499	VAL
1	J	524	LEU
1	K	20	VAL
1	K	27	VAL
1	K	77	VAL
1	K	82	ASN
1	K	89	THR
1	K	94	VAL
1	K	131	LEU
1	K	183	LEU
1	K	210	THR
1	K	257	GLU
1	K	271	VAL
1	K	289	LEU
1	K	329	THR
1	K	417	VAL
1	K	422	VAL
1	K	499	VAL
1	L	20	VAL
1	L	27	VAL
1	L	74	VAL
1	L	77	VAL
1	L	82	ASN
1	L	89	THR
1	L	94	VAL
1	L	131	LEU
1	L	183	LEU

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Mol	Chain	Res	Type
1	L	227	ILE
1	L	257	GLU
1	L	289	LEU
1	L	329	THR
1	L	351	GLN
1	L	417	VAL
1	L	422	VAL
1	L	499	VAL
1	L	524	LEU
1	M	20	VAL
1	M	27	VAL
1	M	74	VAL
1	M	77	VAL
1	M	82	ASN
1	M	89	THR
1	M	94	VAL
1	M	131	LEU
1	M	183	LEU
1	M	257	GLU
1	M	270	ILE
1	M	289	LEU
1	M	329	THR
1	M	331	THR
1	M	351	GLN
1	M	417	VAL
1	M	463	SER
1	M	499	VAL
1	M	524	LEU
1	N	20	VAL
1	N	27	VAL
1	N	74	VAL
1	N	77	VAL
1	N	82	ASN
1	N	89	THR
1	N	94	VAL
1	N	131	LEU
1	N	183	LEU
1	N	210	THR
1	N	257	GLU
1	N	328	ASP
1	N	329	THR
1	N	351	GLN

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Mol	Chain	Res	Type
1	N	369	VAL
1	N	417	VAL
1	N	499	VAL
1	N	524	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	319	GLN
1	A	352	GLN
1	A	475	ASN
1	B	319	GLN
1	B	352	GLN
1	B	436	GLN
1	B	453	GLN
1	C	82	ASN
1	C	194	GLN
1	D	82	ASN
1	E	401	HIS
1	E	453	GLN
1	F	229	ASN
1	F	352	GLN
1	F	433	ASN
1	F	453	GLN
1	G	37	ASN
1	G	146	GLN
1	G	194	GLN
1	G	290	GLN
1	G	352	GLN
1	H	10	ASN
1	H	97	GLN
1	H	194	GLN
1	H	229	ASN
1	H	433	ASN
1	I	146	GLN
1	I	229	ASN
1	I	475	ASN
1	J	194	GLN
1	J	229	ASN
1	J	352	GLN
1	K	194	GLN

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Mol	Chain	Res	Type
1	K	229	ASN
1	L	153	ASN
1	M	97	GLN
1	M	475	ASN
1	N	229	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	524/548 (95%)	-0.15	12 (2%) 61 37	13, 42, 126, 158	0
1	B	524/548 (95%)	-0.47	0 100 100	14, 36, 75, 112	0
1	C	524/548 (95%)	-0.61	0 100 100	12, 32, 65, 93	0
1	D	524/548 (95%)	-0.33	4 (0%) 82 63	11, 44, 93, 130	0
1	E	524/548 (95%)	-0.06	6 (1%) 78 56	18, 54, 125, 155	0
1	F	524/548 (95%)	-0.38	2 (0%) 88 76	15, 40, 94, 137	0
1	G	524/548 (95%)	-0.34	2 (0%) 88 76	19, 47, 86, 111	0
1	H	524/548 (95%)	-0.17	6 (1%) 78 56	18, 52, 105, 144	0
1	I	524/548 (95%)	-0.34	1 (0%) 91 83	14, 42, 83, 108	0
1	J	524/548 (95%)	-0.36	1 (0%) 91 83	18, 45, 77, 101	0
1	K	524/548 (95%)	-0.35	1 (0%) 91 83	18, 46, 86, 111	0
1	L	524/548 (95%)	0.12	36 (6%) 23 11	17, 57, 153, 189	0
1	M	524/548 (95%)	-0.27	3 (0%) 85 69	18, 49, 99, 120	0
1	N	524/548 (95%)	-0.16	10 (1%) 66 42	17, 55, 106, 140	0
All	All	7336/7672 (95%)	-0.28	84 (1%) 78 56	11, 44, 104, 189	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	240	VAL	4.2
1	L	233	MET	3.3
1	A	272	LYS	3.3
1	L	234	LEU	3.2
1	A	240	VAL	3.2
1	L	271	VAL	3.2
1	N	266	THR	3.1
1	L	257	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	270	ILE	3.1
1	L	246	PRO	3.0
1	L	313	THR	3.0
1	L	261	THR	3.0
1	E	270	ILE	3.0
1	M	270	ILE	3.0
1	F	272	LYS	3.0
1	N	44	PHE	3.0
1	A	354	GLU	2.9
1	N	271	VAL	2.9
1	A	202	PRO	2.9
1	A	270	ILE	2.8
1	E	269	GLY	2.8
1	H	229	ASN	2.8
1	L	202	PRO	2.8
1	N	243	ALA	2.7
1	L	256	GLY	2.7
1	E	357	THR	2.7
1	L	299	THR	2.7
1	I	271	VAL	2.7
1	L	229	ASN	2.7
1	N	270	ILE	2.6
1	L	247	LEU	2.6
1	M	271	VAL	2.6
1	F	270	ILE	2.6
1	A	234	LEU	2.6
1	L	262	LEU	2.6
1	L	274	ALA	2.6
1	A	241	ALA	2.6
1	L	273	VAL	2.6
1	L	239	ALA	2.6
1	N	234	LEU	2.5
1	L	312	ALA	2.5
1	E	305	ILE	2.5
1	L	251	ALA	2.4
1	H	340	ALA	2.4
1	K	266	THR	2.4
1	A	271	VAL	2.4
1	L	43	SER	2.4
1	L	242	LYS	2.4
1	L	311	LYS	2.4
1	N	269	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	206	ASN	2.3
1	G	224	ASP	2.3
1	L	236	VAL	2.3
1	L	243	ALA	2.3
1	L	263	VAL	2.3
1	L	258	ALA	2.3
1	L	217	SER	2.3
1	L	300	VAL	2.3
1	L	238	GLU	2.2
1	H	299	THR	2.2
1	M	264	VAL	2.2
1	N	305	ILE	2.2
1	A	259	LEU	2.2
1	L	223	ALA	2.2
1	L	254	VAL	2.2
1	G	484	GLU	2.2
1	D	490	ASP	2.2
1	D	234	LEU	2.2
1	L	259	LEU	2.2
1	N	229	ASN	2.2
1	H	360	TYR	2.1
1	A	246	PRO	2.1
1	A	264	VAL	2.1
1	E	259	LEU	2.1
1	A	266	THR	2.1
1	D	203	TYR	2.1
1	H	237	LEU	2.1
1	J	44	PHE	2.0
1	L	235	PRO	2.0
1	E	236	VAL	2.0
1	D	243	ALA	2.0
1	N	203	TYR	2.0
1	H	192	GLY	2.0
1	L	272	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.