



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 03:18 AM UTC

PDB ID : 4WGL / pdb_00004wgl
Title : Crystal structure of a GroEL D83A/R197A double mutant
Authors : Yang, D.; Fei, X.; LaRonde, N.A.; Beckett, D.; Lund, P.A.; Lorimer, G.H.
Deposited on : 2014-09-19
Resolution : 3.13 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

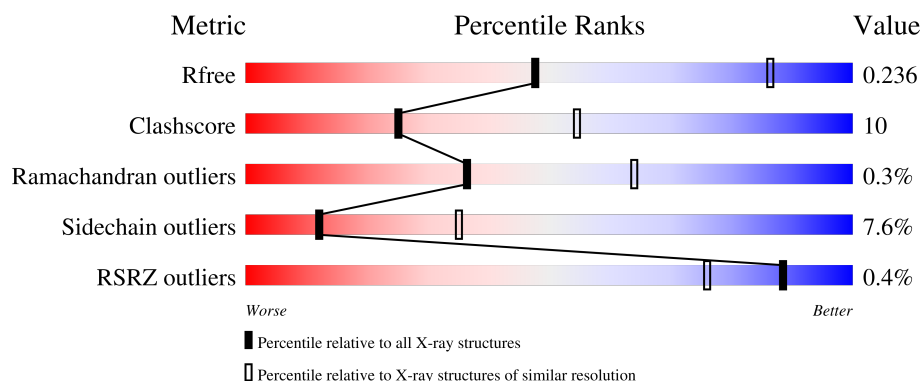
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	 73% 19% . .
1	B	548	 68% 26% . .
1	C	548	 72% 21% . .
1	D	548	 69% 24% . .
1	E	548	 72% 20% . .

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Mol	Chain	Length	Quality of chain
1	F	548	66%27%
1	G	548	70%23%
1	H	548	71%22%
1	I	548	% 69%23%
1	J	548	68%24%
1	K	548	3% 68%24%
1	L	548	71%22%
1	M	548	71%23%
1	N	548	74%19%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53844 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
			3846	2393	662	771	20			
1	B	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	C	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	D	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	E	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	F	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	G	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	H	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	I	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	J	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	K	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	L	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	M	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			
1	N	524	Total	C	N	O	S	0	0	0
			3846	2393	662	771	20			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	ASP	engineered mutation	UNP P0A6F5

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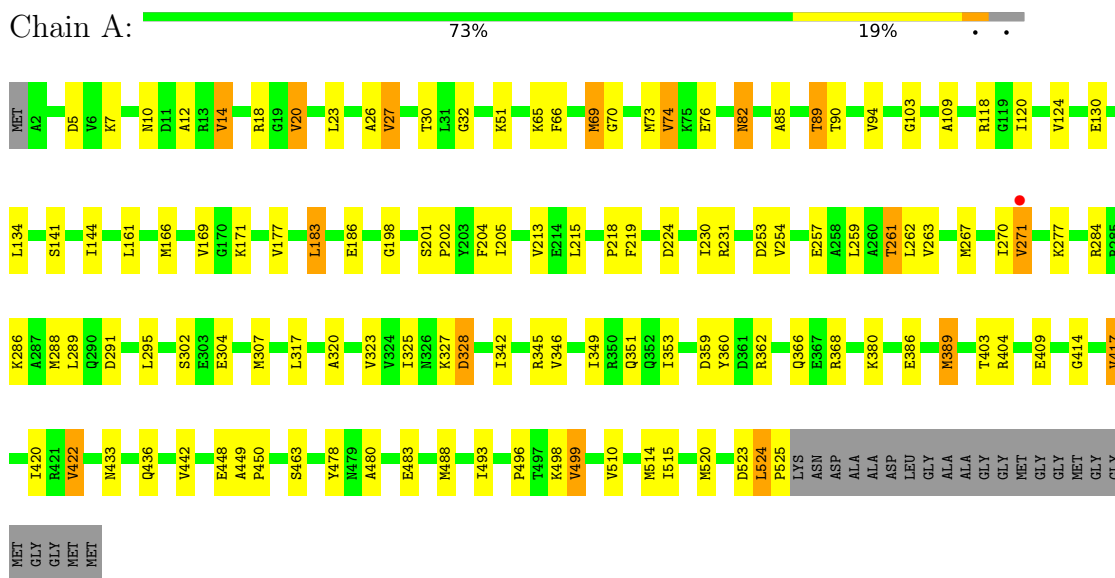
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Chain	Residue	Modelled	Actual	Comment	Reference
A	197	ALA	ARG	engineered mutation	UNP P0A6F5
B	83	ALA	ASP	engineered mutation	UNP P0A6F5
B	197	ALA	ARG	engineered mutation	UNP P0A6F5
C	83	ALA	ASP	engineered mutation	UNP P0A6F5
C	197	ALA	ARG	engineered mutation	UNP P0A6F5
D	83	ALA	ASP	engineered mutation	UNP P0A6F5
D	197	ALA	ARG	engineered mutation	UNP P0A6F5
E	83	ALA	ASP	engineered mutation	UNP P0A6F5
E	197	ALA	ARG	engineered mutation	UNP P0A6F5
F	83	ALA	ASP	engineered mutation	UNP P0A6F5
F	197	ALA	ARG	engineered mutation	UNP P0A6F5
G	83	ALA	ASP	engineered mutation	UNP P0A6F5
G	197	ALA	ARG	engineered mutation	UNP P0A6F5
H	83	ALA	ASP	engineered mutation	UNP P0A6F5
H	197	ALA	ARG	engineered mutation	UNP P0A6F5
I	83	ALA	ASP	engineered mutation	UNP P0A6F5
I	197	ALA	ARG	engineered mutation	UNP P0A6F5
J	83	ALA	ASP	engineered mutation	UNP P0A6F5
J	197	ALA	ARG	engineered mutation	UNP P0A6F5
K	83	ALA	ASP	engineered mutation	UNP P0A6F5
K	197	ALA	ARG	engineered mutation	UNP P0A6F5
L	83	ALA	ASP	engineered mutation	UNP P0A6F5
L	197	ALA	ARG	engineered mutation	UNP P0A6F5
M	83	ALA	ASP	engineered mutation	UNP P0A6F5
M	197	ALA	ARG	engineered mutation	UNP P0A6F5
N	83	ALA	ASP	engineered mutation	UNP P0A6F5
N	197	ALA	ARG	engineered mutation	UNP P0A6F5

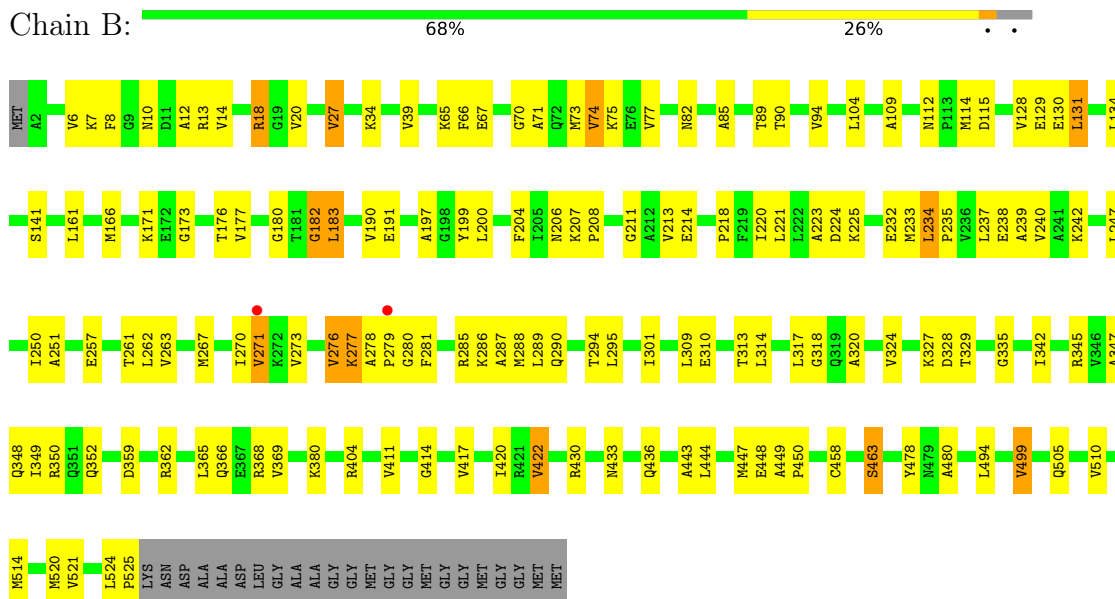
3 Residue-property plots

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

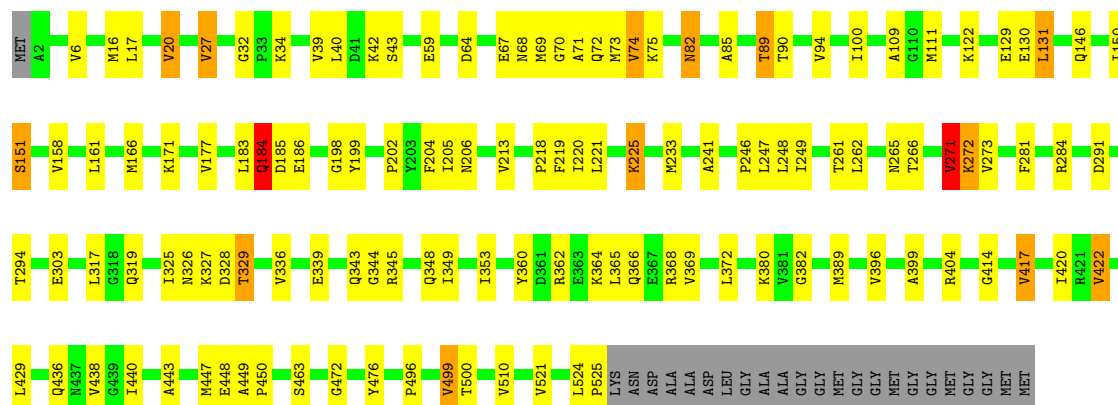


• Molecule 1: 60 kDa chaperonin



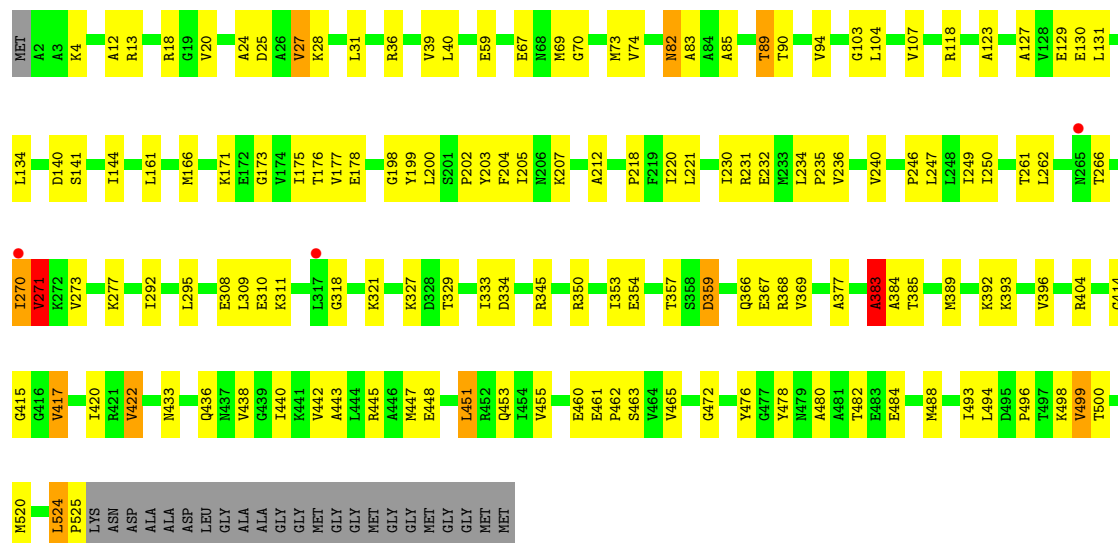
• Molecule 1: 60 kDa chaperonin

Chain C:  72% 21%



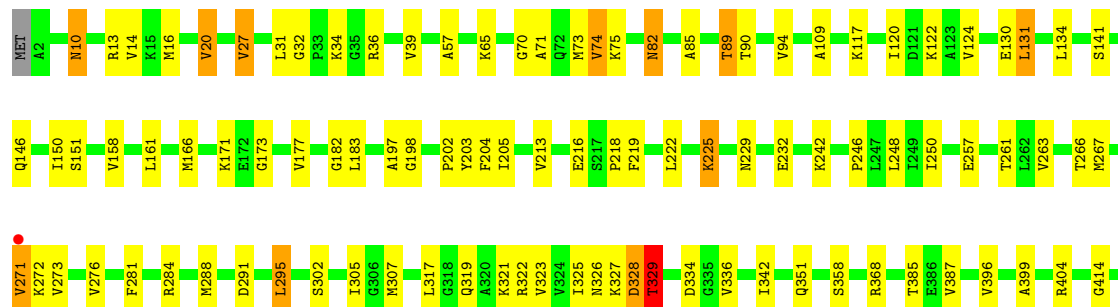
• Molecule 1: 60 kDa chaperonin

Chain D:  69% 24%

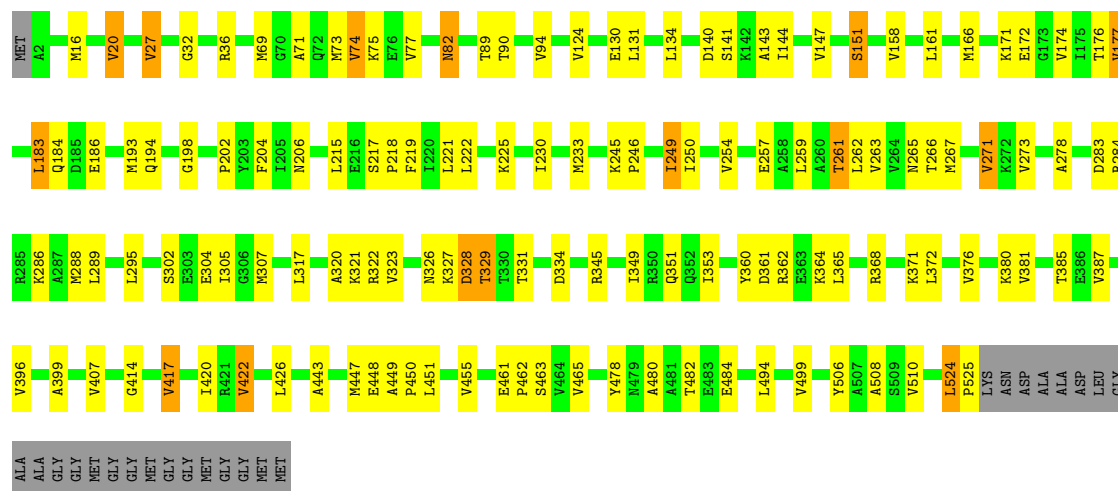


• Molecule 1: 60 kDa chaperonin

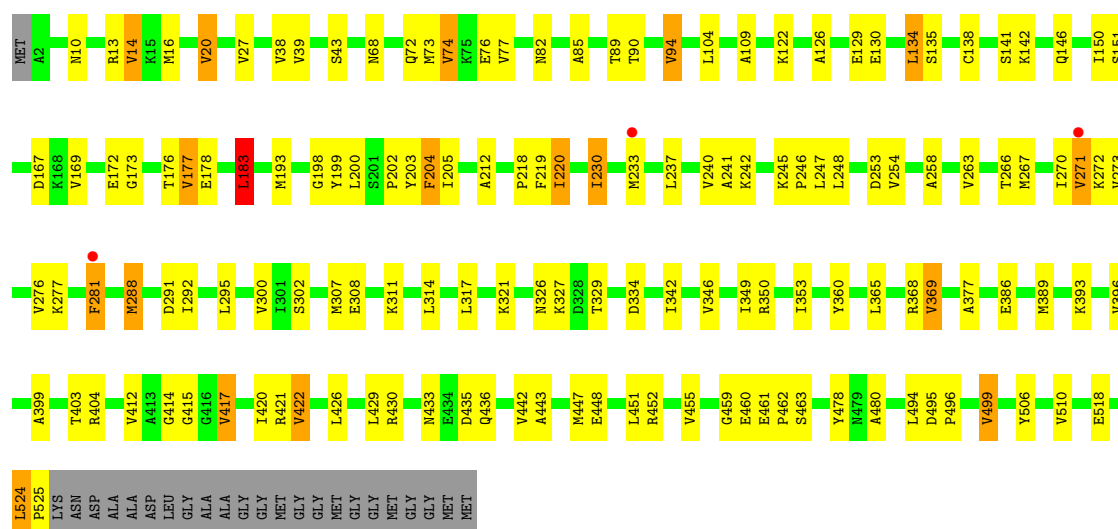
Chain E:  72% 20%



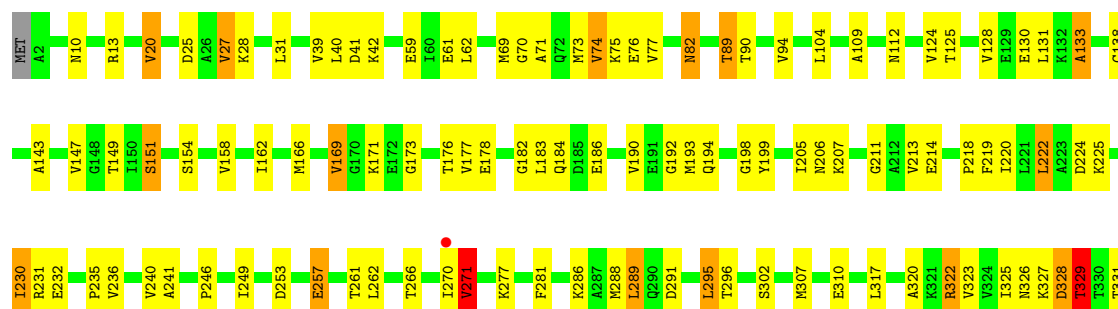


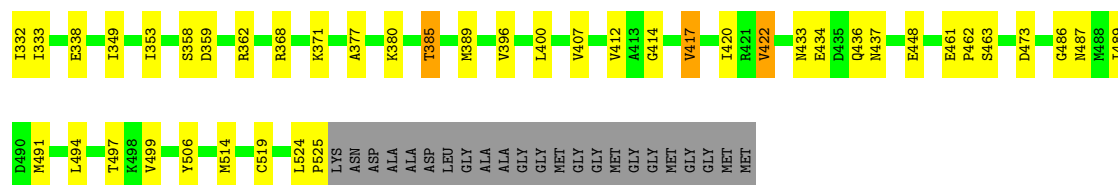


• Molecule 1: 60 kDa chaperonin

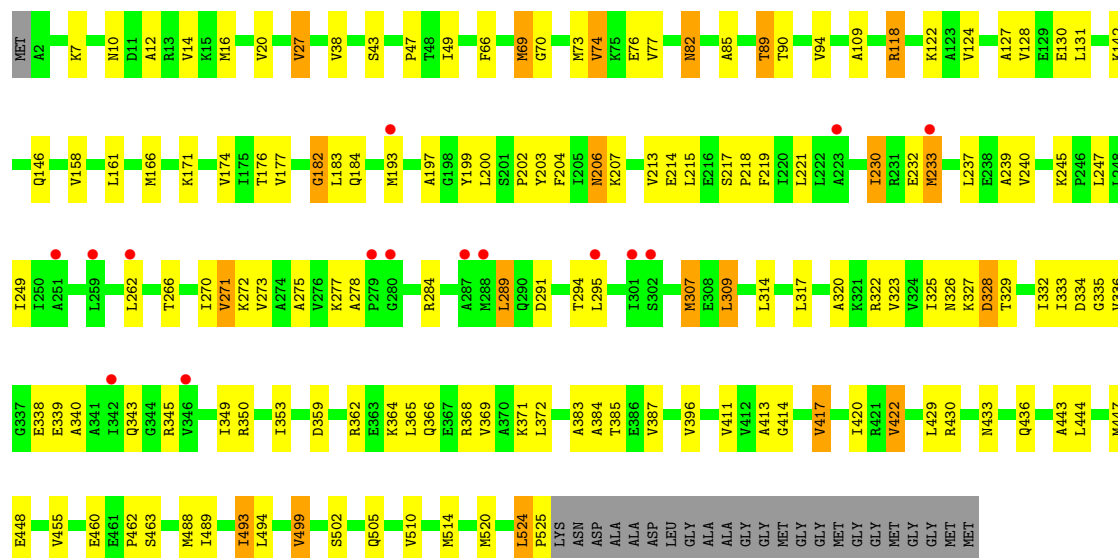


• Molecule 1: 60 kDa chaperonin

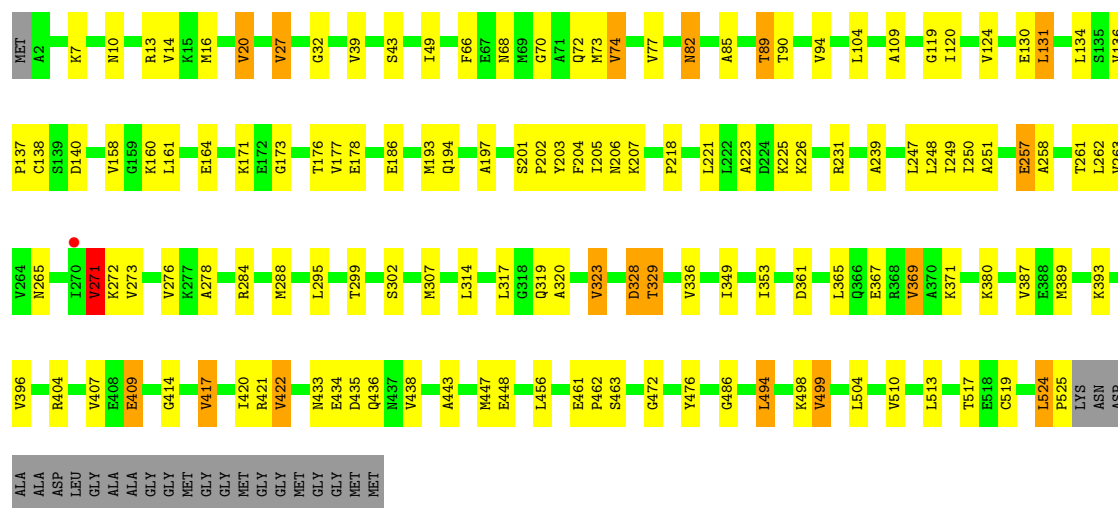




- Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.62Å 259.71Å 280.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.52 – 3.13 123.52 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.6 (123.52-3.13) 99.6 (123.52-3.13)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.166 , 0.233 0.174 , 0.236	Depositor DCC
R_{free} test set	2003 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	53844	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0.59	0/3874	0.94	4/5232 (0.1%)
1	B	0.58	0/3874	0.96	6/5232 (0.1%)
1	C	0.57	0/3874	0.89	2/5232 (0.0%)
1	D	0.59	1/3874 (0.0%)	0.92	4/5232 (0.1%)
1	E	0.57	0/3874	0.93	7/5232 (0.1%)
1	F	0.55	0/3874	0.94	5/5232 (0.1%)
1	G	0.56	0/3874	0.91	6/5232 (0.1%)
1	H	0.61	0/3874	0.95	5/5232 (0.1%)
1	I	0.63	0/3874	0.97	3/5232 (0.1%)
1	J	0.62	0/3874	0.96	6/5232 (0.1%)
1	K	0.58	0/3874	0.93	4/5232 (0.1%)
1	L	0.63	0/3874	0.97	7/5232 (0.1%)
1	M	0.55	0/3874	0.91	3/5232 (0.1%)
1	N	0.59	0/3874	0.94	4/5232 (0.1%)
All	All	0.59	1/54236 (0.0%)	0.94	66/73248 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	J	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	383	ALA	CA-CB	-6.00	1.45	1.54

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	182	GLY	N-CA-C	10.85	125.94	111.72
1	G	32	GLY	CA-C-N	8.47	128.17	119.19
1	G	32	GLY	C-N-CA	8.47	128.17	119.19
1	D	383	ALA	N-CA-C	7.67	124.78	114.12
1	B	204	PHE	N-CA-C	-7.51	103.70	113.17
1	N	207	LYS	CA-C-N	7.20	126.88	119.82
1	N	207	LYS	C-N-CA	7.20	126.88	119.82
1	L	32	GLY	CA-C-N	7.05	126.68	119.56
1	L	32	GLY	C-N-CA	7.05	126.68	119.56
1	H	271	VAL	N-CA-C	6.65	120.68	113.43
1	J	182	GLY	N-CA-C	6.64	122.88	114.25
1	C	32	GLY	CA-C-N	6.62	126.21	119.19
1	C	32	GLY	C-N-CA	6.62	126.21	119.19
1	E	461	GLU	CA-C-N	6.61	126.05	118.85
1	E	461	GLU	C-N-CA	6.61	126.05	118.85
1	H	278	ALA	CA-C-N	6.52	126.47	119.76
1	H	278	ALA	C-N-CA	6.52	126.47	119.76
1	M	207	LYS	CA-C-N	6.48	126.17	119.56
1	M	207	LYS	C-N-CA	6.48	126.17	119.56
1	K	334	ASP	N-CA-C	6.47	119.37	110.24
1	N	409	GLU	N-CA-C	6.17	120.84	112.88
1	A	32	GLY	CA-C-N	6.17	125.89	119.05
1	A	32	GLY	C-N-CA	6.17	125.89	119.05
1	F	204	PHE	N-CA-C	-6.14	105.43	113.17
1	F	32	GLY	CA-C-N	6.03	126.19	119.32
1	F	32	GLY	C-N-CA	6.03	126.19	119.32
1	I	495	ASP	CA-C-N	-5.97	113.38	119.83
1	I	495	ASP	C-N-CA	-5.97	113.38	119.83
1	H	32	GLY	CA-C-N	5.96	125.34	118.85
1	H	32	GLY	C-N-CA	5.96	125.34	118.85
1	E	32	GLY	CA-C-N	5.84	125.38	119.19
1	E	32	GLY	C-N-CA	5.84	125.38	119.19
1	B	277	LYS	CA-C-N	5.78	132.10	121.70
1	B	277	LYS	C-N-CA	5.78	132.10	121.70
1	L	207	LYS	CA-C-N	5.70	125.37	119.56
1	L	207	LYS	C-N-CA	5.70	125.37	119.56
1	K	207	LYS	CA-C-N	5.64	125.34	119.82
1	K	207	LYS	C-N-CA	5.64	125.34	119.82
1	J	133	ALA	CA-C-N	5.63	128.60	120.38
1	J	133	ALA	C-N-CA	5.63	128.60	120.38
1	L	328	ASP	N-CA-C	5.63	120.26	113.17
1	E	328	ASP	N-CA-C	5.54	120.72	113.30
1	I	204	PHE	N-CA-C	-5.38	106.22	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	329	THR	N-CA-C	5.36	117.91	108.75
1	F	269	GLY	N-CA-C	5.32	122.66	115.00
1	L	409	GLU	N-CA-C	5.31	120.41	113.30
1	E	329	THR	N-CA-C	5.30	118.07	109.06
1	M	333	ILE	N-CA-C	5.29	115.48	107.75
1	N	229	ASN	N-CA-C	5.27	117.01	108.26
1	D	207	LYS	CA-C-N	5.25	124.87	119.56
1	D	207	LYS	C-N-CA	5.25	124.87	119.56
1	D	31	LEU	N-CA-C	5.25	116.81	111.14
1	J	329	THR	N-CA-C	5.24	117.97	108.69
1	B	182	GLY	N-CA-C	5.23	122.75	111.04
1	G	46	ALA	CA-C-N	5.23	125.22	119.89
1	G	46	ALA	C-N-CA	5.23	125.22	119.89
1	J	169	VAL	N-CA-C	5.22	117.99	112.83
1	E	325	ILE	N-CA-C	5.20	115.39	108.11
1	B	207	LYS	CA-C-N	5.18	124.84	119.56
1	B	207	LYS	C-N-CA	5.18	124.84	119.56
1	A	169	VAL	N-CA-C	5.13	117.91	112.83
1	A	328	ASP	N-CA-C	5.10	119.60	113.17
1	G	112	ASN	CA-C-N	5.09	125.13	119.32
1	G	112	ASN	C-N-CA	5.09	125.13	119.32
1	J	328	ASP	N-CA-C	5.09	119.58	113.17
1	F	314	LEU	N-CA-C	5.05	117.68	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	383	ALA	Peptide
1	J	31	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	3846	0	3969	64	0
1	B	3846	0	3969	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3846	0	3969	82	0
1	D	3846	0	3969	83	0
1	E	3846	0	3969	70	0
1	F	3846	0	3969	92	0
1	G	3846	0	3969	79	0
1	H	3846	0	3969	77	0
1	I	3846	0	3969	90	0
1	J	3846	0	3969	83	0
1	K	3846	0	3969	95	0
1	L	3846	0	3969	76	0
1	M	3846	0	3969	74	0
1	N	3846	0	3969	60	0
All	All	53844	0	55566	1059	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 (1059) 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:K:232:GLU:HB3	1:K:309:LEU:HD11	1.46	0.95
1:F:241:ALA:HA	1:F:271:VAL:HG11	1.51	0.92
1:L:130:GLU:HB3	1:L:422:VAL:HG22	1.51	0.91
1:E:173:GLY:O	1:E:404:ARG:NH2	2.08	0.86
1:E:524:LEU:HD12	1:E:525:PRO:HD2	1.56	0.85
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.57	0.85
1:I:39:VAL:HG12	1:J:69:MET:HE2	1.59	0.84
1:F:524:LEU:HD12	1:F:525:PRO:HD2	1.60	0.83
1:G:524:LEU:HD12	1:G:525:PRO:HD2	1.61	0.83
1:A:524:LEU:HD12	1:A:525:PRO:HD2	1.59	0.82
1:J:130:GLU:HB3	1:J:422:VAL:HG22	1.61	0.82
1:A:118:ARG:HH12	1:G:34:LYS:HE2	1.46	0.80
1:H:219:PHE:HB3	1:H:317:LEU:HD23	1.64	0.80
1:D:247:LEU:HB3	1:D:273:VAL:HG22	1.63	0.79
1:L:302:SER:H	1:L:307:MET:HE3	1.48	0.79
1:B:359:ASP:OD1	1:B:362:ARG:NH1	2.14	0.79
1:B:247:LEU:HB3	1:B:273:VAL:HG22	1.64	0.79
1:H:130:GLU:HB3	1:H:422:VAL:HG22	1.66	0.78
1:I:241:ALA:HA	1:I:271:VAL:HG21	1.66	0.77
1:I:130:GLU:HB3	1:I:422:VAL:HG22	1.65	0.77
1:D:130:GLU:HB3	1:D:422:VAL:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:524:LEU:HD12	1:L:525:PRO:HD2	1.67	0.77
1:A:302:SER:H	1:A:307:MET:HE3	1.48	0.77
1:F:270:ILE:HG22	1:F:271:VAL:HG22	1.66	0.77
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.66	0.77
1:B:232:GLU:HG2	1:B:309:LEU:HB2	1.68	0.76
1:I:524:LEU:HD12	1:I:525:PRO:HD2	1.68	0.76
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.69	0.75
1:J:524:LEU:HD12	1:J:525:PRO:HD2	1.68	0.75
1:B:6:VAL:HG22	1:B:521:VAL:HG22	1.69	0.74
1:C:183:LEU:O	1:C:184:GLN:NE2	2.19	0.74
1:E:166:MET:HE2	1:E:171:LYS:HA	1.69	0.74
1:C:186:GLU:HB2	1:C:380:LYS:HB2	1.69	0.74
1:M:158:VAL:HG13	1:M:396:VAL:HG22	1.70	0.73
1:A:270:ILE:HG22	1:A:271:VAL:HG23	1.70	0.73
1:H:420:ILE:HG13	1:H:448:GLU:HG2	1.71	0.73
1:K:320:ALA:HA	1:K:335:GLY:HA3	1.72	0.71
1:L:158:VAL:HG13	1:L:396:VAL:HG22	1.72	0.71
1:J:192:GLY:HA2	1:J:295:LEU:HD11	1.72	0.71
1:B:524:LEU:HD12	1:B:525:PRO:HD2	1.72	0.71
1:E:13:ARG:NH2	1:E:518:GLU:OE2	2.23	0.71
1:J:158:VAL:HG13	1:J:396:VAL:HG22	1.72	0.71
1:J:183:LEU:HD23	1:J:184:GLN:HG3	1.73	0.70
1:H:302:SER:H	1:H:307:MET:HE3	1.56	0.70
1:K:353:ILE:HG23	1:K:362:ARG:HG3	1.72	0.70
1:C:271:VAL:H	1:D:231:ARG:NH1	1.89	0.70
1:H:27:VAL:HG13	1:H:90:THR:HG23	1.74	0.70
1:L:173:GLY:O	1:L:404:ARG:NH2	2.24	0.70
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.72	0.70
1:E:216:GLU:OE1	1:F:226:LYS:NZ	2.25	0.69
1:I:420:ILE:HG13	1:I:448:GLU:HG2	1.74	0.69
1:G:151:SER:HB2	1:G:399:ALA:HA	1.75	0.69
1:C:166:MET:HE2	1:C:171:LYS:HA	1.75	0.69
1:F:158:VAL:HG13	1:F:396:VAL:HG22	1.73	0.69
1:G:294:THR:HG21	1:G:345:ARG:HB2	1.75	0.69
1:I:203:TYR:HB3	1:I:267:MET:HE1	1.75	0.69
1:E:130:GLU:HB3	1:E:422:VAL:HG22	1.75	0.69
1:M:130:GLU:HB3	1:M:422:VAL:HG22	1.74	0.69
1:K:524:LEU:HD12	1:K:525:PRO:HD2	1.75	0.69
1:B:166:MET:HE2	1:B:171:LYS:HA	1.75	0.69
1:B:206:ASN:HD22	1:B:214:GLU:H	1.39	0.69
1:M:27:VAL:HG13	1:M:90:THR:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:PRO:HB3	1:D:246:PRO:HG2	1.75	0.68
1:A:27:VAL:HG13	1:A:90:THR:HG23	1.76	0.68
1:G:293:ALA:HB2	1:G:300:VAL:HG23	1.76	0.68
1:K:420:ILE:HG13	1:K:448:GLU:HG2	1.76	0.68
1:D:173:GLY:O	1:D:404:ARG:NH2	2.27	0.68
1:D:230:ILE:HD12	1:D:261:THR:HG21	1.75	0.67
1:D:420:ILE:HG13	1:D:448:GLU:HG2	1.76	0.67
1:F:166:MET:HE2	1:F:171:LYS:HA	1.77	0.67
1:L:27:VAL:HG13	1:L:90:THR:HG23	1.75	0.67
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.77	0.67
1:N:130:GLU:HB3	1:N:422:VAL:HG22	1.75	0.67
1:I:13:ARG:HD2	1:I:104:LEU:HD22	1.77	0.67
1:B:70:GLY:HA2	1:B:73:MET:HE3	1.77	0.66
1:K:323:VAL:HG12	1:K:332:ILE:HG12	1.77	0.66
1:N:420:ILE:HG13	1:N:448:GLU:HG2	1.77	0.66
1:F:420:ILE:HG13	1:F:448:GLU:HG2	1.78	0.66
1:C:130:GLU:HB3	1:C:422:VAL:HG22	1.78	0.65
1:A:70:GLY:HA2	1:A:73:MET:HE3	1.78	0.65
1:J:166:MET:HE2	1:J:171:LYS:HA	1.77	0.65
1:D:166:MET:HE2	1:D:171:LYS:HA	1.79	0.65
1:G:130:GLU:HB3	1:G:422:VAL:HG22	1.78	0.65
1:B:173:GLY:O	1:B:404:ARG:NH2	2.29	0.65
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.79	0.65
1:G:353:ILE:HD13	1:G:366:GLN:HG3	1.77	0.65
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.79	0.65
1:K:278:ALA:HB1	1:K:289:LEU:HD11	1.79	0.65
1:L:13:ARG:HD2	1:L:104:LEU:HD22	1.78	0.64
1:M:38:VAL:HG22	1:N:519:CYS:HB3	1.79	0.64
1:N:218:PRO:HG3	1:N:323:VAL:HG22	1.79	0.64
1:J:489:ILE:HG22	1:J:494:LEU:HD23	1.80	0.64
1:N:353:ILE:HG23	1:N:362:ARG:HG3	1.78	0.64
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.78	0.64
1:G:166:MET:HE1	1:G:407:VAL:HG21	1.78	0.64
1:K:130:GLU:HB3	1:K:422:VAL:HG22	1.80	0.64
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.78	0.64
1:M:166:MET:HE2	1:M:171:LYS:HA	1.80	0.64
1:N:359:ASP:OD1	1:N:362:ARG:NH1	2.30	0.64
1:F:183:LEU:HD12	1:F:383:ALA:HA	1.79	0.64
1:H:158:VAL:HG13	1:H:396:VAL:HG22	1.79	0.64
1:E:70:GLY:HA2	1:E:73:MET:HE3	1.79	0.63
1:D:524:LEU:HD12	1:D:525:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:414:GLY:O	1:E:417:VAL:HG13	1.99	0.63
1:B:294:THR:HG22	1:B:342:ILE:HD13	1.80	0.63
1:C:241:ALA:HB1	1:D:231:ARG:HH22	1.63	0.63
1:F:34:LYS:HD2	1:F:458:CYS:HA	1.79	0.63
1:N:27:VAL:HG13	1:N:90:THR:HG23	1.80	0.63
1:B:278:ALA:HB1	1:B:279:PRO:HD2	1.80	0.63
1:F:151:SER:HB2	1:F:399:ALA:HA	1.80	0.63
1:M:302:SER:H	1:M:307:MET:HE3	1.62	0.63
1:J:359:ASP:OD1	1:J:362:ARG:NH1	2.31	0.63
1:F:6:VAL:HG22	1:F:521:VAL:HG22	1.80	0.62
1:F:122:LYS:HE2	1:F:429:LEU:HD11	1.80	0.62
1:M:186:GLU:HB2	1:M:380:LYS:HB2	1.81	0.62
1:J:70:GLY:HA2	1:J:73:MET:HE3	1.79	0.62
1:K:338:GLU:HG3	1:K:340:ALA:H	1.64	0.62
1:F:314:LEU:HD23	1:F:317:LEU:HD22	1.80	0.62
1:I:433:ASN:HD21	1:I:436:GLN:HG3	1.64	0.62
1:J:186:GLU:HB2	1:J:380:LYS:HB2	1.81	0.62
1:B:220:ILE:N	1:B:318:GLY:O	2.25	0.62
1:I:126:ALA:HB1	1:I:426:LEU:HD22	1.82	0.62
1:N:229:ASN:ND2	1:N:257:GLU:OE1	2.32	0.62
1:B:18:ARG:HG2	1:B:67:GLU:CD	2.25	0.62
1:D:366:GLN:HA	1:D:369:VAL:HG22	1.82	0.62
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.80	0.62
1:C:219:PHE:HB3	1:C:317:LEU:HD23	1.82	0.62
1:H:198:GLY:HA3	1:H:327:LYS:O	1.99	0.62
1:F:12:ALA:HB1	1:F:520:MET:HG3	1.82	0.61
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.82	0.61
1:M:524:LEU:HD12	1:M:525:PRO:HD2	1.82	0.61
1:H:286:LYS:NZ	1:H:304:GLU:OE2	2.32	0.61
1:A:257:GLU:O	1:A:261:THR:OG1	2.16	0.61
1:I:433:ASN:ND2	1:I:436:GLN:HG3	2.16	0.61
1:C:524:LEU:HD12	1:C:525:PRO:HD2	1.83	0.61
1:L:414:GLY:O	1:L:417:VAL:HG13	2.01	0.61
1:A:386:GLU:HA	1:B:281:PHE:HZ	1.66	0.61
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.81	0.61
1:E:321:LYS:HB2	1:E:334:ASP:HB3	1.81	0.61
1:G:219:PHE:HB3	1:G:317:LEU:HD23	1.82	0.61
1:N:257:GLU:O	1:N:261:THR:OG1	2.19	0.61
1:N:10:ASN:O	1:N:14:VAL:HG13	2.01	0.61
1:E:288:MET:HG2	1:E:368:ARG:HD3	1.83	0.60
1:G:27:VAL:HG13	1:G:90:THR:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.36	0.60
1:I:134:LEU:HD11	1:I:421:ARG:HG2	1.84	0.60
1:N:353:ILE:HD13	1:N:366:GLN:HG3	1.82	0.60
1:A:286:LYS:NZ	1:A:304:GLU:OE2	2.32	0.60
1:G:478:TYR:CE2	1:G:480:ALA:HA	2.35	0.60
1:H:222:LEU:HB3	1:H:289:LEU:HD22	1.84	0.60
1:K:488:MET:HE3	1:K:493:ILE:HB	1.83	0.60
1:J:82:ASN:HB2	1:J:89:THR:OG1	2.01	0.60
1:D:83:ALA:HB2	1:D:327:LYS:HD2	1.83	0.60
1:G:414:GLY:O	1:G:417:VAL:HG13	2.01	0.60
1:H:524:LEU:HD12	1:H:525:PRO:HD2	1.82	0.60
1:E:305:ILE:HB	1:E:307:MET:HE2	1.84	0.60
1:B:128:VAL:HG21	1:B:505:GLN:HE21	1.66	0.59
1:F:70:GLY:HA2	1:F:73:MET:HE3	1.82	0.59
1:L:82:ASN:HB2	1:L:89:THR:OG1	2.02	0.59
1:L:284:ARG:NH2	1:L:361:ASP:OD1	2.36	0.59
1:C:271:VAL:H	1:D:231:ARG:HH12	1.50	0.59
1:C:366:GLN:HA	1:C:369:VAL:HG22	1.84	0.59
1:F:414:GLY:O	1:F:417:VAL:HG13	2.03	0.59
1:G:166:MET:HE2	1:G:171:LYS:HA	1.82	0.59
1:J:198:GLY:HA3	1:J:327:LYS:O	2.03	0.59
1:K:291:ASP:OD1	1:K:345:ARG:NE	2.26	0.59
1:M:70:GLY:HA2	1:M:73:MET:HE3	1.84	0.59
1:F:13:ARG:HD2	1:F:104:LEU:HD22	1.85	0.59
1:J:131:LEU:HD13	1:J:422:VAL:HG21	1.84	0.59
1:G:158:VAL:HG13	1:G:396:VAL:HG22	1.84	0.59
1:H:82:ASN:HB2	1:H:89:THR:OG1	2.03	0.59
1:J:241:ALA:HB2	1:J:271:VAL:HG22	1.83	0.59
1:K:213:VAL:HB	1:K:325:ILE:HB	1.85	0.58
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.86	0.58
1:N:301:ILE:HG21	1:N:309:LEU:HD23	1.85	0.58
1:D:232:GLU:HB3	1:D:309:LEU:HB2	1.85	0.58
1:E:302:SER:H	1:E:307:MET:HE3	1.69	0.58
1:B:130:GLU:HB3	1:B:422:VAL:HG22	1.86	0.58
1:G:321:LYS:HB2	1:G:334:ASP:HB3	1.85	0.58
1:D:359:ASP:OD1	1:D:359:ASP:N	2.35	0.58
1:E:257:GLU:O	1:E:261:THR:OG1	2.16	0.58
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.03	0.58
1:K:233:MET:HE2	1:K:262:LEU:HD21	1.86	0.58
1:N:13:ARG:HD2	1:N:104:LEU:HD22	1.85	0.58
1:H:183:LEU:HD22	1:I:360:TYR:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:VAL:HG13	1:E:90:THR:HG23	1.86	0.58
1:K:366:GLN:HA	1:K:369:VAL:HG22	1.86	0.58
1:A:414:GLY:O	1:A:417:VAL:HG13	2.03	0.58
1:F:319:GLN:HB3	1:F:336:VAL:HG21	1.86	0.58
1:H:147:VAL:O	1:H:151:SER:OG	2.22	0.58
1:J:178:GLU:OE1	1:J:322:ARG:NH1	2.36	0.58
1:G:120:ILE:O	1:G:124:VAL:HG23	2.04	0.57
1:M:219:PHE:HE1	1:M:319:GLN:HE21	1.50	0.57
1:A:166:MET:HE2	1:A:171:LYS:HA	1.87	0.57
1:B:250:ILE:HG23	1:B:276:VAL:HG11	1.87	0.57
1:B:270:ILE:HG22	1:B:271:VAL:HG23	1.87	0.57
1:H:328:ASP:OD1	1:H:328:ASP:N	2.38	0.57
1:D:131:LEU:HD21	1:D:500:THR:HG22	1.86	0.57
1:E:225:LYS:NZ	1:E:232:GLU:OE2	2.36	0.57
1:F:266:THR:HB	1:F:272:LYS:HA	1.87	0.57
1:J:291:ASP:OD2	1:J:368:ARG:HD2	2.04	0.57
1:I:430:ARG:HG2	1:I:430:ARG:HH11	1.69	0.57
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.86	0.57
1:D:271:VAL:O	1:D:273:VAL:HG23	2.04	0.57
1:G:124:VAL:HG13	1:G:504:LEU:HG	1.87	0.57
1:H:186:GLU:HB2	1:H:380:LYS:HB2	1.87	0.57
1:K:128:VAL:HG21	1:K:505:GLN:HE21	1.69	0.57
1:B:240:VAL:HG11	1:B:247:LEU:HB2	1.87	0.57
1:K:122:LYS:NZ	1:K:430:ARG:O	2.30	0.57
1:D:178:GLU:HA	1:D:393:LYS:HE2	1.86	0.56
1:E:109:ALA:HB2	1:N:109:ALA:HB2	1.86	0.56
1:E:478:TYR:CE2	1:E:480:ALA:HA	2.40	0.56
1:F:496:PRO:HB2	1:F:499:VAL:HG13	1.86	0.56
1:G:176:THR:HG21	1:G:333:ILE:HD11	1.87	0.56
1:I:219:PHE:HB3	1:I:317:LEU:HD23	1.86	0.56
1:L:39:VAL:HG12	1:M:69:MET:HE2	1.86	0.56
1:C:266:THR:HB	1:C:272:LYS:HA	1.86	0.56
1:C:284:ARG:NH1	1:C:364:LYS:HG3	2.20	0.56
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.87	0.56
1:J:27:VAL:HG13	1:J:90:THR:HG23	1.87	0.56
1:N:291:ASP:OD2	1:N:368:ARG:HD2	2.05	0.56
1:J:13:ARG:HD2	1:J:104:LEU:HD22	1.87	0.56
1:C:183:LEU:HD12	1:C:184:GLN:H	1.71	0.56
1:F:219:PHE:HB3	1:F:317:LEU:HD23	1.88	0.56
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.88	0.56
1:K:70:GLY:HA2	1:K:73:MET:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:198:GLY:HA3	1:M:327:LYS:O	2.05	0.56
1:H:414:GLY:O	1:H:417:VAL:HG13	2.06	0.56
1:J:147:VAL:O	1:J:151:SER:OG	2.23	0.56
1:F:82:ASN:HB2	1:F:89:THR:OG1	2.06	0.56
1:G:124:VAL:O	1:G:128:VAL:HG23	2.05	0.56
1:A:69:MET:HE2	1:G:39:VAL:HG12	1.88	0.55
1:E:198:GLY:HA3	1:E:327:LYS:O	2.06	0.55
1:K:127:ALA:O	1:K:131:LEU:HB2	2.07	0.55
1:N:70:GLY:HA2	1:N:73:MET:HE3	1.88	0.55
1:F:254:VAL:HG12	1:F:259:LEU:HB2	1.88	0.55
1:G:177:VAL:HG21	1:G:397:GLU:HG3	1.87	0.55
1:D:27:VAL:HG13	1:D:90:THR:HG23	1.89	0.55
1:I:218:PRO:HB3	1:I:246:PRO:HG2	1.88	0.55
1:F:198:GLY:HA3	1:F:327:LYS:O	2.06	0.55
1:K:489:ILE:HG23	1:K:494:LEU:HD23	1.88	0.55
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.89	0.55
1:E:219:PHE:HB3	1:E:317:LEU:HD23	1.89	0.55
1:E:501:ARG:NH1	1:E:505:GLN:OE1	2.40	0.55
1:L:134:LEU:HD11	1:L:421:ARG:HG2	1.88	0.55
1:L:247:LEU:HB3	1:L:273:VAL:HG22	1.88	0.55
1:G:433:ASN:ND2	1:G:436:GLN:HG3	2.21	0.55
1:J:224:ASP:OD2	1:J:286:LYS:HG2	2.07	0.55
1:M:269:GLY:HA3	1:N:229:ASN:ND2	2.22	0.55
1:A:130:GLU:HB3	1:A:422:VAL:HG22	1.88	0.55
1:B:250:ILE:HA	1:B:276:VAL:HB	1.89	0.55
1:J:39:VAL:HG12	1:K:69:MET:HE2	1.89	0.55
1:D:18:ARG:HG2	1:D:67:GLU:CD	2.32	0.55
1:N:476:TYR:HA	1:N:486:GLY:O	2.06	0.55
1:A:345:ARG:O	1:A:349:ILE:HG13	2.07	0.54
1:C:184:GLN:O	1:C:382:GLY:HA3	2.08	0.54
1:A:186:GLU:HB2	1:A:380:LYS:HB2	1.89	0.54
1:H:284:ARG:O	1:H:288:MET:HG3	2.08	0.54
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.89	0.54
1:K:291:ASP:OD2	1:K:368:ARG:NH1	2.40	0.54
1:N:128:VAL:HG21	1:N:505:GLN:HE21	1.73	0.54
1:N:222:LEU:HD23	1:N:250:ILE:HB	1.87	0.54
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.07	0.54
1:C:345:ARG:O	1:C:349:ILE:HG13	2.08	0.54
1:F:124:VAL:HG13	1:F:504:LEU:HG	1.89	0.54
1:J:220:ILE:HD12	1:J:296:THR:HG21	1.89	0.54
1:M:433:ASN:ND2	1:M:436:GLN:HG3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:GLU:HB2	1:G:380:LYS:HB2	1.89	0.54
1:H:69:MET:HE2	1:N:39:VAL:HG12	1.90	0.54
1:K:322:ARG:HB3	1:K:333:ILE:HD12	1.88	0.54
1:B:208:PRO:HA	1:B:211:GLY:HA2	1.89	0.54
1:K:74:VAL:HA	1:K:510:VAL:HG21	1.89	0.54
1:L:70:GLY:HA2	1:L:73:MET:HE3	1.88	0.54
1:I:414:GLY:O	1:I:417:VAL:HG13	2.08	0.54
1:J:323:VAL:HG12	1:J:332:ILE:HG12	1.89	0.54
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.90	0.54
1:M:291:ASP:OD2	1:M:368:ARG:HD2	2.07	0.54
1:K:443:ALA:O	1:K:447:MET:HG3	2.07	0.54
1:D:433:ASN:ND2	1:D:436:GLN:HG3	2.23	0.54
1:G:18:ARG:HD2	1:G:67:GLU:OE2	2.08	0.54
1:B:131:LEU:HD13	1:B:422:VAL:HG21	1.90	0.53
1:H:266:THR:HG22	1:H:271:VAL:HG23	1.88	0.53
1:M:305:ILE:HB	1:M:307:MET:HE2	1.91	0.53
1:A:420:ILE:HG13	1:A:448:GLU:HG2	1.90	0.53
1:B:257:GLU:O	1:B:261:THR:OG1	2.15	0.53
1:I:270:ILE:HG22	1:I:271:VAL:HG23	1.89	0.53
1:K:38:VAL:HG22	1:L:519:CYS:HB3	1.89	0.53
1:K:359:ASP:OD1	1:K:362:ARG:NH1	2.39	0.53
1:C:20:VAL:HB	1:C:74:VAL:HG11	1.90	0.53
1:M:414:GLY:O	1:M:417:VAL:HG13	2.07	0.53
1:B:345:ARG:NH1	1:B:348:GLN:OE1	2.42	0.53
1:D:308:GLU:H	1:D:311:LYS:HD3	1.74	0.53
1:H:151:SER:HB2	1:H:399:ALA:HA	1.89	0.53
1:K:218:PRO:HG3	1:K:323:VAL:HG22	1.91	0.53
1:M:253:ASP:OD1	1:M:254:VAL:N	2.41	0.53
1:M:417:VAL:HA	1:M:420:ILE:HG22	1.91	0.53
1:F:302:SER:H	1:F:307:MET:HE3	1.73	0.53
1:K:49:ILE:HD12	1:L:513:LEU:HD13	1.90	0.53
1:A:215:LEU:HB2	1:A:323:VAL:HG22	1.90	0.53
1:B:240:VAL:HG21	1:B:247:LEU:HD22	1.91	0.53
1:D:461:GLU:OE2	1:N:463:SER:HB3	2.09	0.53
1:A:478:TYR:CE2	1:A:480:ALA:HA	2.44	0.53
1:C:198:GLY:HA3	1:C:327:LYS:O	2.08	0.52
1:I:302:SER:H	1:I:307:MET:HE3	1.74	0.52
1:B:263:VAL:O	1:B:267:MET:HB2	2.10	0.52
1:F:131:LEU:HD21	1:F:500:THR:HG22	1.91	0.52
1:H:263:VAL:O	1:H:267:MET:HB2	2.10	0.52
1:J:270:ILE:HG22	1:J:271:VAL:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:VAL:O	1:E:267:MET:HB2	2.10	0.52
1:K:16:MET:SD	1:K:73:MET:HE1	2.48	0.52
1:L:221:LEU:HB3	1:L:249:ILE:HD13	1.92	0.52
1:B:280:GLY:O	1:B:285:ARG:HB2	2.09	0.52
1:E:463:SER:HB3	1:M:461:GLU:OE2	2.09	0.52
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.92	0.52
1:I:365:LEU:O	1:I:369:VAL:HG22	2.10	0.52
1:B:213:VAL:O	1:B:324:VAL:HA	2.09	0.52
1:C:109:ALA:HB2	1:I:109:ALA:HB2	1.90	0.52
1:F:247:LEU:HB3	1:F:273:VAL:HG22	1.91	0.52
1:H:321:LYS:HB2	1:H:334:ASP:HB3	1.90	0.52
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.91	0.52
1:C:34:LYS:HD3	1:D:118:ARG:HH22	1.75	0.52
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.90	0.52
1:C:262:LEU:O	1:C:266:THR:HG23	2.09	0.52
1:L:434:GLU:O	1:L:438:VAL:HG23	2.09	0.52
1:N:254:VAL:HG12	1:N:259:LEU:HB2	1.92	0.52
1:A:20:VAL:HB	1:A:74:VAL:HG11	1.92	0.52
1:D:24:ALA:O	1:D:28:LYS:HG2	2.10	0.52
1:D:262:LEU:O	1:D:266:THR:HG23	2.09	0.52
1:B:349:ILE:HA	1:B:352:GLN:HB2	1.92	0.52
1:E:266:THR:HG21	1:E:273:VAL:HB	1.92	0.52
1:H:221:LEU:HD22	1:H:233:MET:HE1	1.91	0.52
1:J:213:VAL:HB	1:J:325:ILE:HB	1.91	0.52
1:G:23:LEU:HD23	1:G:74:VAL:HG22	1.92	0.52
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.91	0.52
1:I:77:VAL:HG12	1:I:506:TYR:HB3	1.91	0.52
1:B:224:ASP:HB2	1:B:286:LYS:NZ	2.25	0.51
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.92	0.51
1:I:281:PHE:H	1:I:281:PHE:HD2	1.58	0.51
1:L:206:ASN:HD22	1:L:272:LYS:HE3	1.74	0.51
1:C:39:VAL:HG12	1:D:69:MET:HE2	1.91	0.51
1:H:262:LEU:O	1:H:266:THR:HG23	2.10	0.51
1:B:27:VAL:HG13	1:B:90:THR:HG23	1.91	0.51
1:D:205:ILE:HG23	1:D:212:ALA:O	2.11	0.51
1:G:12:ALA:HB1	1:G:520:MET:HG3	1.92	0.51
1:I:459:GLY:HA3	1:J:112:ASN:HD22	1.74	0.51
1:N:240:VAL:HG12	1:N:271:VAL:HG11	1.92	0.51
1:B:278:ALA:HB1	1:B:279:PRO:CD	2.40	0.51
1:I:415:GLY:O	1:I:451:LEU:HD23	2.10	0.51
1:J:433:ASN:ND2	1:J:436:GLN:HG3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:262:LEU:O	1:K:266:THR:HG23	2.10	0.51
1:G:68:ASN:O	1:G:72:GLN:HG2	2.10	0.51
1:G:501:ARG:NH1	1:G:505:GLN:OE1	2.44	0.51
1:H:230:ILE:HD12	1:H:261:THR:HB	1.92	0.51
1:J:257:GLU:O	1:J:261:THR:OG1	2.19	0.51
1:K:232:GLU:CD	1:K:309:LEU:HD21	2.36	0.51
1:N:158:VAL:HG13	1:N:396:VAL:HG22	1.91	0.51
1:J:225:LYS:NZ	1:J:232:GLU:OE2	2.42	0.51
1:K:47:PRO:HG2	1:L:73:MET:HG3	1.92	0.51
1:M:213:VAL:O	1:M:324:VAL:HA	2.11	0.51
1:M:215:LEU:HB2	1:M:323:VAL:HG22	1.92	0.51
1:N:271:VAL:HG12	1:N:272:LYS:H	1.76	0.51
1:N:455:VAL:HG11	1:N:462:PRO:HA	1.92	0.51
1:B:365:LEU:O	1:B:368:ARG:HG2	2.11	0.51
1:E:447:MET:HE2	1:E:504:LEU:HD21	1.92	0.51
1:F:342:ILE:O	1:F:346:VAL:HG23	2.11	0.51
1:K:249:ILE:HB	1:K:275:ALA:HA	1.91	0.51
1:L:433:ASN:ND2	1:L:436:GLN:HG3	2.26	0.51
1:D:414:GLY:N	1:D:494:LEU:HA	2.26	0.51
1:H:183:LEU:HD13	1:I:360:TYR:CD1	2.46	0.51
1:I:326:ASN:HB2	1:I:329:THR:HB	1.93	0.51
1:K:240:VAL:HG11	1:K:247:LEU:HB2	1.93	0.51
1:D:438:VAL:O	1:D:442:VAL:HG23	2.10	0.51
1:C:291:ASP:OD2	1:C:368:ARG:HD2	2.11	0.51
1:B:206:ASN:HD22	1:B:214:GLU:N	2.08	0.50
1:D:198:GLY:HA3	1:D:327:LYS:O	2.11	0.50
1:D:414:GLY:O	1:D:417:VAL:HG13	2.11	0.50
1:F:266:THR:HG21	1:F:273:VAL:H	1.76	0.50
1:I:178:GLU:HA	1:I:393:LYS:HE2	1.93	0.50
1:K:206:ASN:ND2	1:K:214:GLU:O	2.44	0.50
1:K:433:ASN:ND2	1:K:436:GLN:HG3	2.26	0.50
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.41	0.50
1:H:171:LYS:HB3	1:H:407:VAL:HG11	1.93	0.50
1:B:347:ALA:HA	1:B:350:ARG:HG2	1.92	0.50
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.92	0.50
1:G:213:VAL:HB	1:G:325:ILE:HB	1.93	0.50
1:G:488:MET:HE3	1:G:493:ILE:HB	1.93	0.50
1:I:247:LEU:HB3	1:I:273:VAL:HG22	1.92	0.50
1:A:14:VAL:O	1:A:18:ARG:HG3	2.10	0.50
1:F:184:GLN:H	1:F:382:GLY:HA3	1.76	0.50
1:H:326:ASN:HB2	1:H:329:THR:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:460:GLU:O	1:K:462:PRO:HD3	2.11	0.50
1:L:49:ILE:HD12	1:M:513:LEU:HD13	1.93	0.50
1:L:206:ASN:ND2	1:L:272:LYS:HE3	2.26	0.50
1:I:10:ASN:O	1:I:14:VAL:HG13	2.11	0.50
1:J:218:PRO:HD2	1:J:320:ALA:O	2.11	0.50
1:D:240:VAL:HG12	1:D:271:VAL:HG12	1.93	0.50
1:G:263:VAL:O	1:G:267:MET:HB2	2.11	0.50
1:J:326:ASN:HB2	1:J:329:THR:H	1.77	0.50
1:L:7:LYS:HD2	1:L:66:PHE:CE2	2.47	0.50
1:L:443:ALA:O	1:L:447:MET:HG3	2.12	0.50
1:E:16:MET:O	1:E:20:VAL:HG13	2.12	0.50
1:E:151:SER:HB2	1:E:399:ALA:HA	1.93	0.50
1:H:177:VAL:HG11	1:H:396:VAL:HG12	1.92	0.50
1:J:40:LEU:HD13	1:J:59:GLU:HG3	1.94	0.50
1:L:248:LEU:HD22	1:L:323:VAL:HG21	1.93	0.50
1:C:271:VAL:O	1:C:273:VAL:HG23	2.12	0.50
1:D:232:GLU:HA	1:D:310:GLU:HG3	1.94	0.50
1:J:218:PRO:HG3	1:J:323:VAL:HG22	1.93	0.50
1:G:291:ASP:OD2	1:G:368:ARG:HD2	2.12	0.50
1:I:266:THR:HB	1:I:272:LYS:HD2	1.94	0.50
1:K:193:MET:HB2	1:K:372:LEU:HD13	1.93	0.50
1:M:321:LYS:HB2	1:M:334:ASP:HB3	1.93	0.50
1:M:433:ASN:HD21	1:M:436:GLN:HG3	1.76	0.50
1:D:414:GLY:H	1:D:494:LEU:HA	1.77	0.49
1:F:433:ASN:ND2	1:F:436:GLN:HG3	2.26	0.49
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.93	0.49
1:D:478:TYR:CE2	1:D:480:ALA:HA	2.48	0.49
1:G:153:ASN:ND2	1:G:153:ASN:O	2.45	0.49
1:L:203:TYR:HD2	1:L:263:VAL:HG13	1.77	0.49
1:D:270:ILE:HG22	1:D:271:VAL:HG22	1.94	0.49
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.42	0.49
1:F:221:LEU:HD11	1:F:301:ILE:HD12	1.94	0.49
1:G:266:THR:HG21	1:G:273:VAL:HB	1.94	0.49
1:L:247:LEU:HD21	1:L:249:ILE:HD11	1.93	0.49
1:A:7:LYS:HG3	1:A:66:PHE:CZ	2.47	0.49
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.95	0.49
1:F:71:ALA:O	1:F:75:LYS:HB2	2.13	0.49
1:F:205:ILE:HG23	1:F:212:ALA:O	2.12	0.49
1:A:198:GLY:HA3	1:A:327:LYS:O	2.12	0.49
1:I:230:ILE:HB	1:I:258:ALA:HA	1.93	0.49
1:M:269:GLY:HA3	1:N:229:ASN:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ALA:HB2	1:J:109:ALA:HB2	1.93	0.49
1:J:218:PRO:HB3	1:J:246:PRO:HG2	1.94	0.49
1:N:131:LEU:HD13	1:N:422:VAL:HG21	1.95	0.49
1:B:295:LEU:HA	1:B:342:ILE:HD11	1.95	0.49
1:J:434:GLU:O	1:J:437:ASN:HB2	2.13	0.49
1:J:487:ASN:O	1:J:491:MET:HG3	2.13	0.49
1:L:194:GLN:O	1:L:371:LYS:HE3	2.12	0.49
1:C:472:GLY:HA3	1:C:476:TYR:CD2	2.47	0.49
1:D:12:ALA:HB1	1:D:520:MET:HG3	1.94	0.49
1:E:34:LYS:HD2	1:E:458:CYS:HA	1.95	0.49
1:I:386:GLU:HA	1:J:281:PHE:HE2	1.78	0.49
1:M:271:VAL:HG12	1:M:272:LYS:H	1.77	0.49
1:A:263:VAL:O	1:A:267:MET:HB2	2.13	0.49
1:D:389:MET:HE2	1:E:281:PHE:CD2	2.48	0.49
1:I:233:MET:SD	1:I:237:LEU:HD12	2.52	0.49
1:N:263:VAL:O	1:N:267:MET:HB2	2.13	0.49
1:A:359:ASP:OD1	1:A:362:ARG:NH1	2.45	0.49
1:B:478:TYR:CE2	1:B:480:ALA:HA	2.47	0.49
1:G:82:ASN:HB2	1:G:89:THR:OG1	2.13	0.49
1:A:26:ALA:HA	1:B:8:PHE:HE1	1.77	0.48
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.43	0.48
1:D:70:GLY:HA2	1:D:73:MET:HE3	1.95	0.48
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.13	0.48
1:I:20:VAL:HB	1:I:74:VAL:HG11	1.95	0.48
1:J:149:THR:HG22	1:J:154:SER:HA	1.95	0.48
1:J:166:MET:HE1	1:J:407:VAL:HG21	1.94	0.48
1:M:16:MET:O	1:M:20:VAL:HG13	2.12	0.48
1:A:109:ALA:HB2	1:K:109:ALA:HB2	1.94	0.48
1:B:183:LEU:O	1:B:183:LEU:HG	2.13	0.48
1:B:218:PRO:HD2	1:B:320:ALA:O	2.13	0.48
1:F:128:VAL:HG21	1:F:505:GLN:HE21	1.79	0.48
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.95	0.48
1:C:436:GLN:O	1:C:440:ILE:HG13	2.14	0.48
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.43	0.48
1:I:135:SER:HA	1:I:412:VAL:HG12	1.96	0.48
1:J:193:MET:HG2	1:J:371:LYS:HB3	1.95	0.48
1:B:233:MET:SD	1:B:309:LEU:HD13	2.53	0.48
1:K:206:ASN:OD1	1:K:214:GLU:N	2.35	0.48
1:K:414:GLY:O	1:K:417:VAL:HG13	2.13	0.48
1:M:310:GLU:OE1	1:M:310:GLU:N	2.42	0.48
1:J:486:GLY:C	1:J:491:MET:HE2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:LYS:O	1:K:146:GLN:HG3	2.14	0.48
1:M:193:MET:HG3	1:M:371:LYS:HB3	1.93	0.48
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.96	0.48
1:E:202:PRO:O	1:E:203:TYR:HB2	2.14	0.48
1:I:38:VAL:HG22	1:J:519:CYS:HB3	1.95	0.48
1:I:177:VAL:HG11	1:I:396:VAL:HG12	1.96	0.48
1:I:240:VAL:HG21	1:I:247:LEU:HD13	1.96	0.48
1:L:124:VAL:HG13	1:L:504:LEU:HG	1.96	0.48
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.95	0.48
1:B:74:VAL:HA	1:B:510:VAL:HG21	1.96	0.48
1:E:295:LEU:HA	1:E:342:ILE:HD11	1.95	0.48
1:G:417:VAL:HA	1:G:420:ILE:HG22	1.94	0.48
1:I:68:ASN:O	1:I:72:GLN:HG2	2.14	0.48
1:M:213:VAL:HB	1:M:325:ILE:HB	1.95	0.48
1:C:146:GLN:O	1:C:150:ILE:HG13	2.14	0.48
1:C:353:ILE:HG23	1:C:362:ARG:HG3	1.96	0.48
1:D:266:THR:CG2	1:D:273:VAL:H	2.27	0.48
1:D:392:LYS:O	1:D:396:VAL:HG23	2.14	0.48
1:H:259:LEU:O	1:H:263:VAL:HG23	2.13	0.48
1:I:150:ILE:HD12	1:I:494:LEU:HD21	1.96	0.48
1:I:198:GLY:HA3	1:I:327:LYS:O	2.14	0.48
1:M:345:ARG:HH21	1:M:368:ARG:HH12	1.62	0.48
1:A:120:ILE:O	1:A:124:VAL:HG23	2.14	0.47
1:A:496:PRO:HB2	1:A:499:VAL:HG13	1.95	0.47
1:B:444:LEU:HD23	1:B:447:MET:HE3	1.95	0.47
1:C:326:ASN:HB2	1:C:329:THR:HB	1.95	0.47
1:E:426:LEU:HD22	1:E:429:LEU:HD22	1.95	0.47
1:G:235:PRO:HG3	1:G:310:GLU:HA	1.95	0.47
1:N:496:PRO:O	1:N:499:VAL:HG13	2.14	0.47
1:B:320:ALA:HA	1:B:335:GLY:HA2	1.97	0.47
1:F:111:MET:SD	1:F:438:VAL:HG11	2.54	0.47
1:F:221:LEU:HB3	1:F:249:ILE:HD13	1.96	0.47
1:H:172:GLU:H	1:H:172:GLU:CD	2.22	0.47
1:H:257:GLU:O	1:H:261:THR:OG1	2.32	0.47
1:K:383:ALA:O	1:K:384:ALA:HB3	2.14	0.47
1:N:68:ASN:O	1:N:72:GLN:HG2	2.14	0.47
1:C:199:TYR:CZ	1:C:327:LYS:HA	2.49	0.47
1:G:247:LEU:HB3	1:G:273:VAL:HG22	1.95	0.47
1:H:218:PRO:HD2	1:H:320:ALA:O	2.14	0.47
1:K:411:VAL:HG21	1:K:494:LEU:HD22	1.96	0.47
1:B:180:GLY:HA2	1:B:380:LYS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:VAL:HG22	1:C:521:VAL:HG22	1.95	0.47
1:C:266:THR:HG22	1:C:271:VAL:O	2.14	0.47
1:E:465:VAL:O	1:E:469:VAL:HG23	2.13	0.47
1:F:222:LEU:HD23	1:F:250:ILE:HB	1.96	0.47
1:G:183:LEU:HG	1:G:184:GLN:H	1.79	0.47
1:K:7:LYS:HG3	1:K:66:PHE:CZ	2.49	0.47
1:K:27:VAL:HG13	1:K:90:THR:HG23	1.95	0.47
1:M:124:VAL:O	1:M:128:VAL:HG23	2.14	0.47
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.97	0.47
1:E:414:GLY:H	1:E:494:LEU:HA	1.80	0.47
1:B:183:LEU:HD22	1:C:360:TYR:CD2	2.50	0.47
1:B:206:ASN:ND2	1:B:214:GLU:O	2.47	0.47
1:C:131:LEU:HD13	1:C:422:VAL:HG21	1.97	0.47
1:I:263:VAL:O	1:I:267:MET:HB2	2.14	0.47
1:I:342:ILE:O	1:I:346:VAL:HG23	2.14	0.47
1:I:448:GLU:O	1:I:452:ARG:HD2	2.14	0.47
1:N:82:ASN:HB2	1:N:89:THR:OG1	2.15	0.47
1:A:342:ILE:O	1:A:346:VAL:HG23	2.14	0.47
1:B:39:VAL:HG12	1:C:69:MET:HE2	1.96	0.47
1:C:68:ASN:O	1:C:72:GLN:HG2	2.15	0.47
1:D:250:ILE:HD13	1:D:292:ILE:HD13	1.97	0.47
1:E:20:VAL:HB	1:E:74:VAL:HG11	1.96	0.47
1:E:117:LYS:HD3	1:E:516:THR:HG21	1.95	0.47
1:E:229:ASN:ND2	1:E:257:GLU:OE1	2.32	0.47
1:F:117:LYS:HD3	1:F:516:THR:HG21	1.97	0.47
1:F:236:VAL:O	1:F:240:VAL:HG23	2.14	0.47
1:H:305:ILE:HB	1:H:307:MET:HE2	1.97	0.47
1:I:430:ARG:HG2	1:I:430:ARG:NH1	2.30	0.47
1:J:353:ILE:HG23	1:J:362:ARG:HG3	1.97	0.47
1:L:476:TYR:HA	1:L:486:GLY:O	2.14	0.47
1:F:218:PRO:HG3	1:F:323:VAL:HG22	1.96	0.47
1:I:321:LYS:HB2	1:I:334:ASP:HB3	1.97	0.47
1:J:171:LYS:HB3	1:J:407:VAL:HG11	1.97	0.47
1:K:327:LYS:HG3	1:K:328:ASP:H	1.79	0.47
1:A:118:ARG:NH1	1:G:34:LYS:HE2	2.24	0.47
1:H:221:LEU:HD23	1:H:249:ILE:HG23	1.97	0.47
1:K:326:ASN:N	1:K:329:THR:O	2.42	0.47
1:C:353:ILE:HD13	1:C:366:GLN:HG3	1.97	0.47
1:F:349:ILE:O	1:F:353:ILE:HG13	2.15	0.47
1:I:142:LYS:O	1:I:146:GLN:HG3	2.15	0.47
1:K:118:ARG:HA	1:K:118:ARG:HD2	1.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:385:THR:HG22	1:K:387:VAL:H	1.80	0.47
1:L:171:LYS:HB3	1:L:407:VAL:HG11	1.97	0.47
1:L:349:ILE:O	1:L:353:ILE:HG13	2.15	0.47
1:C:82:ASN:OD1	1:C:89:THR:HB	2.15	0.46
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.97	0.46
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.67	0.46
1:D:496:PRO:O	1:D:499:VAL:HG13	2.15	0.46
1:E:414:GLY:N	1:E:494:LEU:HA	2.30	0.46
1:F:20:VAL:HB	1:F:74:VAL:HG11	1.97	0.46
1:F:184:GLN:O	1:F:382:GLY:N	2.45	0.46
1:H:345:ARG:O	1:H:349:ILE:HG13	2.16	0.46
1:I:241:ALA:CA	1:I:271:VAL:HG21	2.41	0.46
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.98	0.46
1:E:122:LYS:NZ	1:E:430:ARG:O	2.40	0.46
1:E:420:ILE:HG13	1:E:448:GLU:HG2	1.96	0.46
1:I:193:MET:HE1	1:I:292:ILE:HG12	1.96	0.46
1:J:169:VAL:HG23	1:J:173:GLY:HA3	1.96	0.46
1:J:302:SER:H	1:J:307:MET:HE3	1.80	0.46
1:K:339:GLU:O	1:K:343:GLN:HB2	2.15	0.46
1:L:225:LYS:HG2	1:L:226:LYS:O	2.15	0.46
1:L:271:VAL:O	1:L:273:VAL:HG23	2.14	0.46
1:M:182:GLY:O	1:M:183:LEU:HG	2.15	0.46
1:B:12:ALA:HB1	1:B:520:MET:HG3	1.95	0.46
1:D:202:PRO:C	1:D:204:PHE:H	2.23	0.46
1:F:173:GLY:O	1:F:404:ARG:NH2	2.48	0.46
1:G:109:ALA:HB2	1:L:109:ALA:HB2	1.96	0.46
1:G:127:ALA:O	1:G:131:LEU:HB2	2.14	0.46
1:J:25:ASP:OD1	1:J:28:LYS:HE2	2.15	0.46
1:J:385:THR:O	1:J:389:MET:HB2	2.15	0.46
1:K:217:SER:HA	1:K:320:ALA:O	2.16	0.46
1:A:218:PRO:HD2	1:A:320:ALA:O	2.15	0.46
1:C:122:LYS:HE2	1:C:429:LEU:HD11	1.96	0.46
1:E:319:GLN:HB3	1:E:336:VAL:HG21	1.97	0.46
1:H:183:LEU:O	1:H:184:GLN:NE2	2.49	0.46
1:I:349:ILE:O	1:I:353:ILE:HG13	2.15	0.46
1:G:251:ALA:O	1:G:278:ALA:N	2.46	0.46
1:G:319:GLN:HG3	1:G:336:VAL:HG21	1.97	0.46
1:K:230:ILE:HA	1:K:233:MET:HG3	1.97	0.46
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.98	0.46
1:H:194:GLN:HB2	1:H:331:THR:HG23	1.97	0.46
1:H:289:LEU:HD23	1:H:289:LEU:HA	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:162:ILE:HG12	1:J:400:LEU:HD13	1.97	0.46
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.98	0.46
1:L:349:ILE:CG2	1:L:369:VAL:HG13	2.46	0.46
1:A:360:TYR:CD2	1:G:183:LEU:HD22	2.51	0.46
1:C:74:VAL:HA	1:C:510:VAL:HG21	1.98	0.46
1:D:82:ASN:HB2	1:D:89:THR:OG1	2.16	0.46
1:D:140:ASP:OD1	1:D:140:ASP:N	2.49	0.46
1:F:461:GLU:HA	1:F:462:PRO:HD3	1.85	0.46
1:I:202:PRO:C	1:I:204:PHE:H	2.22	0.46
1:A:74:VAL:HA	1:A:510:VAL:HG21	1.97	0.46
1:B:13:ARG:HD3	1:B:104:LEU:HD22	1.98	0.46
1:B:232:GLU:HG3	1:B:310:GLU:CD	2.41	0.46
1:I:183:LEU:HD13	1:I:183:LEU:O	2.16	0.46
1:M:284:ARG:O	1:M:288:MET:HG3	2.16	0.46
1:N:262:LEU:O	1:N:266:THR:HG23	2.16	0.46
1:D:127:ALA:O	1:D:131:LEU:HB2	2.16	0.46
1:E:146:GLN:O	1:E:150:ILE:HG13	2.15	0.46
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.97	0.46
1:J:262:LEU:O	1:J:266:THR:HG23	2.16	0.46
1:K:230:ILE:HG12	1:K:233:MET:HB2	1.97	0.46
1:L:20:VAL:HB	1:L:74:VAL:HG11	1.98	0.46
1:M:221:LEU:HD22	1:M:233:MET:HE1	1.97	0.46
1:N:447:MET:HE2	1:N:504:LEU:HD21	1.98	0.46
1:G:193:MET:HE3	1:G:195:PHE:HB3	1.97	0.45
1:H:222:LEU:HD23	1:H:250:ILE:HB	1.98	0.45
1:H:455:VAL:HG11	1:H:462:PRO:HA	1.98	0.45
1:K:294:THR:HG21	1:K:345:ARG:HB3	1.97	0.45
1:L:131:LEU:HD13	1:L:422:VAL:HG21	1.97	0.45
1:F:218:PRO:HD2	1:F:320:ALA:O	2.16	0.45
1:I:199:TYR:CZ	1:I:327:LYS:HA	2.50	0.45
1:I:200:LEU:HG	1:I:276:VAL:HA	1.99	0.45
1:M:168:LYS:HG3	1:M:187:LEU:HD21	1.97	0.45
1:A:23:LEU:HD23	1:A:74:VAL:HG22	1.98	0.45
1:C:221:LEU:HB3	1:C:249:ILE:HD13	1.97	0.45
1:G:20:VAL:HB	1:G:74:VAL:HG11	1.98	0.45
1:K:10:ASN:O	1:K:14:VAL:HG13	2.17	0.45
1:L:420:ILE:HG13	1:L:448:GLU:HG2	1.97	0.45
1:C:344:GLY:O	1:C:348:GLN:HG3	2.17	0.45
1:H:193:MET:HE2	1:H:371:LYS:HB3	1.98	0.45
1:L:16:MET:SD	1:L:73:MET:HE1	2.57	0.45
1:M:478:TYR:CE2	1:M:480:ALA:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.97	0.45
1:F:232:GLU:HB3	1:F:309:LEU:HB2	1.97	0.45
1:G:56:VAL:O	1:G:60:ILE:HG12	2.17	0.45
1:J:414:GLY:N	1:J:494:LEU:HA	2.31	0.45
1:N:7:LYS:HG3	1:N:66:PHE:CZ	2.51	0.45
1:N:205:ILE:HG23	1:N:212:ALA:O	2.17	0.45
1:B:463:SER:HB3	1:I:461:GLU:OE2	2.17	0.45
1:H:265:ASN:HB3	1:H:271:VAL:HG22	1.99	0.45
1:H:443:ALA:O	1:H:447:MET:HG3	2.16	0.45
1:M:482:THR:O	1:M:484:GLU:HG2	2.16	0.45
1:N:465:VAL:O	1:N:469:VAL:HG23	2.16	0.45
1:A:488:MET:HE3	1:A:493:ILE:HB	1.98	0.45
1:D:85:ALA:HB2	1:D:498:LYS:HG2	1.98	0.45
1:D:220:ILE:N	1:D:318:GLY:O	2.41	0.45
1:E:10:ASN:O	1:E:14:VAL:HG13	2.16	0.45
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.99	0.45
1:J:253:ASP:OD2	1:J:277:LYS:HE2	2.16	0.45
1:N:458:CYS:SG	1:N:480:ALA:HB1	2.56	0.45
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.99	0.45
1:A:433:ASN:HD21	1:A:436:GLN:HG3	1.82	0.45
1:B:34:LYS:HG3	1:B:458:CYS:SG	2.56	0.45
1:B:182:GLY:HA2	1:C:281:PHE:CE2	2.51	0.45
1:C:70:GLY:HA2	1:C:73:MET:HE3	1.98	0.45
1:C:233:MET:HE2	1:C:262:LEU:HD11	1.99	0.45
1:E:288:MET:HE2	1:E:288:MET:HB3	1.85	0.45
1:F:42:LYS:HE2	1:F:42:LYS:HB3	1.66	0.45
1:G:37:ASN:OD1	1:G:51:LYS:HE3	2.17	0.45
1:G:345:ARG:NH1	1:G:348:GLN:OE1	2.48	0.45
1:H:254:VAL:HG12	1:H:259:LEU:HB2	1.97	0.45
1:I:291:ASP:OD2	1:I:368:ARG:HD2	2.17	0.45
1:M:200:LEU:HG	1:M:275:ALA:O	2.17	0.45
1:N:266:THR:HG21	1:N:273:VAL:H	1.81	0.45
1:B:287:ALA:O	1:B:368:ARG:NH2	2.50	0.45
1:F:65:LYS:HB2	1:F:522:THR:HG21	1.99	0.45
1:F:271:VAL:O	1:F:273:VAL:HG23	2.16	0.45
1:H:266:THR:CG2	1:H:273:VAL:H	2.30	0.45
1:J:71:ALA:O	1:J:75:LYS:HB2	2.16	0.45
1:L:250:ILE:HG22	1:L:278:ALA:HB2	1.99	0.45
1:L:261:THR:O	1:L:265:ASN:HB2	2.17	0.45
1:L:389:MET:HE3	1:L:389:MET:HB3	1.89	0.45
1:L:414:GLY:N	1:L:494:LEU:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:MET:HE3	1:A:488:MET:HB3	1.79	0.45
1:B:191:GLU:HB3	1:B:295:LEU:HD11	1.99	0.45
1:C:17:LEU:HD13	1:C:100:ILE:HG22	1.99	0.45
1:H:202:PRO:C	1:H:204:PHE:H	2.25	0.45
1:H:414:GLY:H	1:H:494:LEU:HA	1.82	0.45
1:N:478:TYR:CE2	1:N:480:ALA:HA	2.52	0.45
1:A:219:PHE:HB3	1:A:317:LEU:HD23	1.99	0.44
1:C:16:MET:SD	1:C:73:MET:HE1	2.57	0.44
1:C:151:SER:HB2	1:C:399:ALA:HA	1.98	0.44
1:E:36:ARG:NH1	1:F:113:PRO:HG2	2.32	0.44
1:E:71:ALA:O	1:E:75:LYS:HB2	2.17	0.44
1:E:183:LEU:HD22	1:F:360:TYR:CD2	2.52	0.44
1:F:213:VAL:O	1:F:324:VAL:HA	2.17	0.44
1:G:71:ALA:O	1:G:75:LYS:HB2	2.17	0.44
1:G:122:LYS:NZ	1:G:430:ARG:O	2.43	0.44
1:G:202:PRO:O	1:G:203:TYR:HB2	2.17	0.44
1:I:122:LYS:HE2	1:I:429:LEU:HD11	1.99	0.44
1:K:199:TYR:CE2	1:K:327:LYS:HA	2.51	0.44
1:N:16:MET:O	1:N:20:VAL:HG13	2.16	0.44
1:C:284:ARG:HH11	1:C:364:LYS:HG3	1.82	0.44
1:F:514:MET:HE3	1:F:514:MET:HB3	1.82	0.44
1:H:36:ARG:HG3	1:I:518:GLU:HG3	1.98	0.44
1:L:160:LYS:NZ	1:L:164:GLU:OE2	2.30	0.44
1:L:218:PRO:HD2	1:L:320:ALA:O	2.18	0.44
1:M:234:LEU:HD23	1:M:237:LEU:HD12	1.99	0.44
1:N:433:ASN:ND2	1:N:436:GLN:HG3	2.32	0.44
1:C:372:LEU:HD12	1:C:372:LEU:HA	1.85	0.44
1:C:496:PRO:HB2	1:C:499:VAL:HG13	1.99	0.44
1:D:13:ARG:HD2	1:D:104:LEU:HD22	2.00	0.44
1:E:248:LEU:HD22	1:E:323:VAL:HG11	1.99	0.44
1:F:193:MET:HG3	1:F:371:LYS:HB3	1.99	0.44
1:H:478:TYR:CE2	1:H:480:ALA:HA	2.53	0.44
1:M:461:GLU:HA	1:M:462:PRO:HD3	1.82	0.44
1:C:59:GLU:O	1:D:4:LYS:HG3	2.16	0.44
1:C:205:ILE:HD12	1:C:205:ILE:H	1.82	0.44
1:K:122:LYS:HE2	1:K:429:LEU:HD11	1.99	0.44
1:L:239:ALA:HB1	1:L:314:LEU:HG	1.99	0.44
1:B:233:MET:HE3	1:B:233:MET:HB3	1.84	0.44
1:D:321:LYS:HD2	1:D:334:ASP:OD2	2.18	0.44
1:F:353:ILE:HG23	1:F:362:ARG:HG3	1.98	0.44
1:G:322:ARG:HB3	1:G:333:ILE:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:77:VAL:HG21	1:I:510:VAL:HB	2.00	0.44
1:I:496:PRO:HB2	1:I:499:VAL:HG13	1.99	0.44
1:K:124:VAL:O	1:K:128:VAL:HG23	2.18	0.44
1:M:178:GLU:HA	1:M:393:LYS:HE2	2.00	0.44
1:A:409:GLU:OE2	1:A:498:LYS:HG3	2.18	0.44
1:B:221:LEU:HD11	1:B:301:ILE:HD12	1.98	0.44
1:D:488:MET:HE3	1:D:493:ILE:HB	2.00	0.44
1:I:478:TYR:CE2	1:I:480:ALA:HA	2.52	0.44
1:K:197:ALA:HB1	1:K:277:LYS:HB2	1.99	0.44
1:M:323:VAL:HG12	1:M:332:ILE:HG12	1.99	0.44
1:D:389:MET:HE3	1:D:389:MET:HB3	1.87	0.44
1:G:112:ASN:HA	1:G:113:PRO:HD3	1.85	0.44
1:G:215:LEU:HB2	1:G:323:VAL:CG2	2.47	0.44
1:G:271:VAL:O	1:G:273:VAL:HG23	2.18	0.44
1:H:69:MET:O	1:H:73:MET:HG3	2.18	0.44
1:I:219:PHE:CE2	1:I:245:LYS:HD2	2.52	0.44
1:K:183:LEU:O	1:K:183:LEU:HG	2.18	0.44
1:A:5:ASP:HB2	1:A:524:LEU:HD13	1.98	0.44
1:B:13:ARG:CD	1:B:104:LEU:HD22	2.47	0.44
1:B:313:THR:O	1:B:317:LEU:HD13	2.17	0.44
1:E:57:ALA:O	1:E:75:LYS:HE3	2.18	0.44
1:F:284:ARG:NH1	1:F:364:LYS:HD2	2.33	0.44
1:F:345:ARG:O	1:F:349:ILE:HG13	2.18	0.44
1:I:281:PHE:N	1:I:281:PHE:CD2	2.86	0.44
1:I:346:VAL:HG13	1:I:369:VAL:HG12	1.98	0.44
1:K:166:MET:HE2	1:K:171:LYS:HA	1.98	0.44
1:K:284:ARG:CZ	1:K:364:LYS:HD2	2.48	0.44
1:L:119:GLY:HA3	1:L:436:GLN:O	2.18	0.44
1:A:144:ILE:HG23	1:A:403:THR:CG2	2.48	0.44
1:B:433:ASN:ND2	1:B:436:GLN:HG3	2.33	0.44
1:D:472:GLY:HA3	1:D:476:TYR:CD2	2.53	0.44
1:E:31:LEU:HD12	1:E:31:LEU:HA	1.83	0.44
1:E:461:GLU:OE2	1:M:463:SER:HB3	2.18	0.44
1:H:364:LYS:HA	1:H:364:LYS:HD3	1.64	0.44
1:J:143:ALA:O	1:J:147:VAL:HG23	2.18	0.44
1:A:231:ARG:NH2	1:G:242:LYS:HG3	2.33	0.43
1:C:389:MET:HE3	1:C:389:MET:HB3	1.97	0.43
1:E:120:ILE:O	1:E:124:VAL:HG23	2.17	0.43
1:F:230:ILE:HD12	1:F:261:THR:HB	2.00	0.43
1:G:420:ILE:HG13	1:G:448:GLU:HG2	2.00	0.43
1:H:166:MET:HE2	1:H:171:LYS:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:451:LEU:HD21	1:H:465:VAL:HG12	2.00	0.43
1:I:173:GLY:O	1:I:404:ARG:NH2	2.49	0.43
1:J:414:GLY:O	1:J:417:VAL:HG13	2.18	0.43
1:C:213:VAL:HB	1:C:325:ILE:HB	1.99	0.43
1:C:294:THR:HG21	1:C:345:ARG:HB2	2.00	0.43
1:C:414:GLY:O	1:C:417:VAL:HG13	2.17	0.43
1:F:120:ILE:O	1:F:124:VAL:HG23	2.18	0.43
1:F:449:ALA:HB3	1:F:450:PRO:HD3	2.00	0.43
1:G:223:ALA:O	1:G:251:ALA:HA	2.18	0.43
1:L:13:ARG:HA	1:L:16:MET:HE3	2.00	0.43
1:L:186:GLU:HB2	1:L:380:LYS:HB2	1.99	0.43
1:A:389:MET:HE3	1:A:389:MET:HB3	1.96	0.43
1:C:16:MET:O	1:C:20:VAL:HG13	2.18	0.43
1:D:103:GLY:O	1:D:107:VAL:HG23	2.18	0.43
1:F:262:LEU:O	1:F:266:THR:HG23	2.18	0.43
1:H:16:MET:O	1:H:20:VAL:HG13	2.19	0.43
1:H:131:LEU:HD13	1:H:422:VAL:HG21	2.01	0.43
1:H:360:TYR:CZ	1:N:183:LEU:HD13	2.53	0.43
1:J:461:GLU:HA	1:J:462:PRO:HD3	1.75	0.43
1:F:291:ASP:OD2	1:F:368:ARG:HD2	2.18	0.43
1:F:443:ALA:O	1:F:447:MET:HG3	2.18	0.43
1:K:206:ASN:CG	1:K:214:GLU:H	2.24	0.43
1:L:193:MET:HG2	1:L:371:LYS:HB3	2.00	0.43
1:N:166:MET:HE2	1:N:171:LYS:HA	2.00	0.43
1:D:36:ARG:HG3	1:E:518:GLU:HG3	2.00	0.43
1:D:141:SER:HA	1:D:144:ILE:HB	2.01	0.43
1:K:237:LEU:O	1:K:271:VAL:HG11	2.19	0.43
1:L:77:VAL:HG21	1:L:510:VAL:HB	2.00	0.43
1:L:178:GLU:HA	1:L:393:LYS:HE2	2.01	0.43
1:L:218:PRO:HG3	1:L:323:VAL:HG13	2.01	0.43
1:L:472:GLY:HA3	1:L:476:TYR:CD2	2.53	0.43
1:M:202:PRO:C	1:M:204:PHE:H	2.24	0.43
1:M:301:ILE:HG21	1:M:309:LEU:HD23	2.00	0.43
1:N:414:GLY:H	1:N:494:LEU:HA	1.84	0.43
1:C:42:LYS:HB3	1:C:42:LYS:HE2	1.71	0.43
1:F:74:VAL:HA	1:F:510:VAL:HG21	2.00	0.43
1:F:417:VAL:HA	1:F:420:ILE:HG22	2.00	0.43
1:H:361:ASP:O	1:H:365:LEU:HG	2.19	0.43
1:I:288:MET:O	1:I:291:ASP:HB2	2.18	0.43
1:J:417:VAL:HA	1:J:420:ILE:HG22	2.00	0.43
1:A:65:LYS:NZ	1:A:523:ASP:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:VAL:HB	1:A:325:ILE:HB	2.00	0.43
1:B:112:ASN:HB3	1:B:115:ASP:HB2	2.01	0.43
1:D:202:PRO:O	1:D:203:TYR:HB2	2.19	0.43
1:F:359:ASP:OD1	1:F:362:ARG:NH1	2.52	0.43
1:G:70:GLY:HA2	1:G:73:MET:HE3	2.01	0.43
1:H:124:VAL:HG21	1:H:508:ALA:HB2	2.01	0.43
1:I:220:ILE:HG23	1:I:248:LEU:HD23	2.00	0.43
1:J:20:VAL:HB	1:J:74:VAL:HG11	2.01	0.43
1:M:465:VAL:O	1:M:469:VAL:HG23	2.18	0.43
1:C:202:PRO:C	1:C:204:PHE:H	2.27	0.43
1:F:36:ARG:HG3	1:G:518:GLU:HG3	2.01	0.43
1:G:31:LEU:HD23	1:G:453:GLN:HB3	2.00	0.43
1:H:218:PRO:HB3	1:H:246:PRO:HG2	2.01	0.43
1:I:90:THR:O	1:I:94:VAL:HG13	2.18	0.43
1:J:124:VAL:O	1:J:128:VAL:HG23	2.19	0.43
1:K:200:LEU:HD12	1:K:275:ALA:HB1	2.00	0.43
1:A:144:ILE:HG23	1:A:403:THR:HG21	2.01	0.43
1:F:180:GLY:HA2	1:F:380:LYS:HB3	2.00	0.43
1:F:181:THR:O	1:G:282:GLY:HA3	2.18	0.43
1:F:225:LYS:HB2	1:F:225:LYS:HE3	1.76	0.43
1:G:177:VAL:HG11	1:G:396:VAL:HG12	2.01	0.43
1:M:314:LEU:HD23	1:M:314:LEU:HA	1.87	0.43
1:N:524:LEU:HD12	1:N:525:PRO:HD2	2.00	0.43
1:A:417:VAL:HA	1:A:420:ILE:HG22	2.00	0.43
1:E:182:GLY:HA2	1:F:281:PHE:CE2	2.53	0.43
1:E:222:LEU:HD23	1:E:250:ILE:HB	2.01	0.43
1:E:326:ASN:HB2	1:E:329:THR:H	1.83	0.43
1:G:218:PRO:HD2	1:G:320:ALA:O	2.19	0.43
1:G:266:THR:HG22	1:G:271:VAL:O	2.18	0.43
1:K:314:LEU:HD23	1:K:314:LEU:HA	1.84	0.43
1:L:134:LEU:HD23	1:L:134:LEU:HA	1.86	0.43
1:C:247:LEU:HB3	1:C:273:VAL:HG22	2.00	0.42
1:F:288:MET:HG2	1:F:368:ARG:HD3	2.01	0.42
1:G:173:GLY:O	1:G:404:ARG:NH2	2.51	0.42
1:J:61:GLU:C	1:J:62:LEU:HD23	2.44	0.42
1:J:230:ILE:HD12	1:J:261:THR:HB	1.99	0.42
1:L:10:ASN:O	1:L:14:VAL:HG13	2.19	0.42
1:B:449:ALA:HB3	1:B:450:PRO:HD3	2.02	0.42
1:C:71:ALA:O	1:C:75:LYS:HB2	2.20	0.42
1:D:123:ALA:HB2	1:D:440:ILE:HG23	2.00	0.42
1:I:433:ASN:OD1	1:I:435:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:350:ARG:HH21	1:K:369:VAL:HG23	1.84	0.42
1:N:13:ARG:CD	1:N:104:LEU:HD22	2.49	0.42
1:N:302:SER:H	1:N:307:MET:HE3	1.83	0.42
1:A:449:ALA:HB3	1:A:450:PRO:HD3	2.00	0.42
1:B:114:MET:HE3	1:B:114:MET:HB3	1.86	0.42
1:B:223:ALA:O	1:B:251:ALA:HA	2.19	0.42
1:B:234:LEU:HA	1:B:237:LEU:HB2	2.01	0.42
1:C:64:ASP:HB3	1:C:67:GLU:HB2	2.01	0.42
1:D:345:ARG:HH21	1:D:368:ARG:HH12	1.68	0.42
1:K:233:MET:HE3	1:K:233:MET:HB3	1.79	0.42
1:L:202:PRO:O	1:L:205:ILE:HG13	2.20	0.42
1:M:426:LEU:HA	1:M:426:LEU:HD23	1.75	0.42
1:A:30:THR:HB	1:A:51:LYS:O	2.19	0.42
1:A:202:PRO:C	1:A:204:PHE:H	2.28	0.42
1:B:349:ILE:HD13	1:B:368:ARG:NE	2.34	0.42
1:C:131:LEU:HD21	1:C:500:THR:HG22	2.01	0.42
1:C:443:ALA:O	1:C:447:MET:HG3	2.18	0.42
1:D:455:VAL:HG13	1:D:460:GLU:HB2	2.00	0.42
1:I:242:LYS:HG2	1:J:231:ARG:NH2	2.34	0.42
1:K:270:ILE:HB	1:L:231:ARG:NH1	2.33	0.42
1:A:12:ALA:HB1	1:A:520:MET:HG3	2.00	0.42
1:C:345:ARG:HH21	1:C:368:ARG:HH12	1.67	0.42
1:J:207:LYS:HE3	1:J:214:GLU:OE1	2.19	0.42
1:K:204:PHE:O	1:K:213:VAL:HG13	2.19	0.42
1:N:149:THR:HG23	1:N:155:ASP:C	2.45	0.42
1:A:85:ALA:HB1	1:A:499:VAL:HG12	2.02	0.42
1:B:366:GLN:HA	1:B:369:VAL:HG22	2.02	0.42
1:D:455:VAL:HG21	1:D:465:VAL:HG11	2.01	0.42
1:L:223:ALA:O	1:L:251:ALA:HA	2.20	0.42
1:L:257:GLU:O	1:L:261:THR:OG1	2.28	0.42
1:L:258:ALA:O	1:L:262:LEU:HG	2.20	0.42
1:M:140:ASP:OD1	1:M:140:ASP:N	2.53	0.42
1:M:239:ALA:O	1:M:242:LYS:HB3	2.20	0.42
1:M:472:GLY:HA3	1:M:476:TYR:CD2	2.54	0.42
1:A:82:ASN:HB2	1:A:89:THR:OG1	2.20	0.42
1:A:224:ASP:OD2	1:A:286:LYS:HG2	2.19	0.42
1:B:71:ALA:O	1:B:75:LYS:HB2	2.19	0.42
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.91	0.42
1:E:197:ALA:HB1	1:E:276:VAL:HB	2.02	0.42
1:F:68:ASN:O	1:F:72:GLN:HG2	2.20	0.42
1:F:69:MET:O	1:F:73:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:ALA:HB1	1:I:426:LEU:CD2	2.48	0.42
1:I:205:ILE:HG23	1:I:212:ALA:O	2.20	0.42
1:L:68:ASN:O	1:L:72:GLN:HG2	2.20	0.42
1:C:184:GLN:HG2	1:C:185:ASP:N	2.35	0.42
1:F:444:LEU:HD23	1:F:444:LEU:HA	1.83	0.42
1:H:77:VAL:HG12	1:H:506:TYR:HB3	2.01	0.42
1:I:16:MET:SD	1:I:73:MET:HE1	2.60	0.42
1:I:253:ASP:CG	1:I:277:LYS:HE2	2.45	0.42
1:I:349:ILE:HB	1:I:369:VAL:HG13	2.00	0.42
1:J:412:VAL:HG13	1:J:497:THR:OG1	2.19	0.42
1:L:197:ALA:HB1	1:L:276:VAL:HB	2.01	0.42
1:M:82:ASN:HB2	1:M:89:THR:OG1	2.20	0.42
1:M:420:ILE:HG13	1:M:448:GLU:HG2	2.01	0.42
1:N:24:ALA:O	1:N:28:LYS:HG2	2.20	0.42
1:N:221:LEU:HD23	1:N:249:ILE:HD12	2.01	0.42
1:N:514:MET:HE2	1:N:514:MET:HB3	1.75	0.42
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.79	0.42
1:B:7:LYS:HG3	1:B:66:PHE:CZ	2.55	0.42
1:B:225:LYS:HE3	1:B:225:LYS:HB2	1.81	0.42
1:B:279:PRO:HG2	1:B:285:ARG:HA	2.02	0.42
1:D:266:THR:HG21	1:D:273:VAL:H	1.85	0.42
1:H:174:VAL:HB	1:H:376:VAL:HG22	2.02	0.42
1:I:455:VAL:HG13	1:I:460:GLU:HB2	2.02	0.42
1:C:339:GLU:O	1:C:343:GLN:HG2	2.20	0.42
1:D:383:ALA:HB2	1:D:389:MET:HA	2.02	0.42
1:F:140:ASP:OD2	1:F:142:LYS:HB3	2.20	0.42
1:M:263:VAL:O	1:M:267:MET:HB2	2.20	0.42
1:A:10:ASN:O	1:A:14:VAL:HG13	2.20	0.41
1:A:284:ARG:O	1:A:288:MET:HG3	2.20	0.41
1:A:433:ASN:ND2	1:A:436:GLN:HG3	2.35	0.41
1:C:151:SER:HB2	1:C:399:ALA:CB	2.50	0.41
1:H:193:MET:HE1	1:H:372:LEU:HD13	2.02	0.41
1:H:461:GLU:HA	1:H:462:PRO:HD3	1.84	0.41
1:I:267:MET:HB2	1:I:267:MET:HE2	1.80	0.41
1:J:207:LYS:O	1:J:211:GLY:N	2.53	0.41
1:K:193:MET:HG3	1:K:371:LYS:HB3	2.02	0.41
1:N:288:MET:HG2	1:N:368:ARG:HD3	2.02	0.41
1:C:111:MET:SD	1:C:438:VAL:HG21	2.60	0.41
1:D:461:GLU:HA	1:D:462:PRO:HD3	1.85	0.41
1:F:235:PRO:HG3	1:F:310:GLU:HA	2.02	0.41
1:F:263:VAL:O	1:F:267:MET:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:169:VAL:HG11	1:I:377:ALA:HB2	2.02	0.41
1:J:176:THR:HG21	1:J:333:ILE:HD13	2.01	0.41
1:J:389:MET:HE3	1:J:389:MET:HB3	1.96	0.41
1:K:414:GLY:N	1:K:494:LEU:HA	2.35	0.41
1:L:365:LEU:O	1:L:369:VAL:HG22	2.19	0.41
1:N:414:GLY:N	1:N:494:LEU:HA	2.34	0.41
1:B:197:ALA:HB1	1:B:277:LYS:HB2	2.01	0.41
1:B:234:LEU:N	1:B:235:PRO:HD2	2.35	0.41
1:E:202:PRO:C	1:E:204:PHE:H	2.28	0.41
1:G:160:LYS:O	1:G:164:GLU:HG3	2.20	0.41
1:B:520:MET:HE2	1:B:520:MET:HB3	1.87	0.41
1:C:319:GLN:HB3	1:C:336:VAL:HG21	2.02	0.41
1:C:349:ILE:O	1:C:353:ILE:HG13	2.20	0.41
1:D:383:ALA:O	1:D:384:ALA:HB3	2.20	0.41
1:F:478:TYR:CE2	1:F:480:ALA:HA	2.55	0.41
1:G:13:ARG:HA	1:G:16:MET:HE3	2.03	0.41
1:H:143:ALA:O	1:H:147:VAL:HG23	2.20	0.41
1:K:221:LEU:HB2	1:K:247:LEU:HD11	2.03	0.41
1:L:433:ASN:OD1	1:L:435:ASP:HB2	2.21	0.41
1:M:7:LYS:HD2	1:M:66:PHE:CE2	2.55	0.41
1:B:414:GLY:N	1:B:494:LEU:HA	2.35	0.41
1:E:513:LEU:HD23	1:E:513:LEU:HA	1.89	0.41
1:F:361:ASP:O	1:F:365:LEU:HG	2.20	0.41
1:H:288:MET:HG2	1:H:368:ARG:HD3	2.01	0.41
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.49	0.41
1:K:12:ALA:HB1	1:K:520:MET:HG3	2.02	0.41
1:K:230:ILE:HA	1:K:233:MET:CG	2.51	0.41
1:K:307:MET:HB2	1:K:307:MET:HE3	1.63	0.41
1:K:365:LEU:CD2	1:K:368:ARG:HH21	2.33	0.41
1:L:225:LYS:HG2	1:L:226:LYS:N	2.34	0.41
1:A:103:GLY:HA3	1:A:515:ILE:HD11	2.02	0.41
1:C:225:LYS:HE2	1:C:303:GLU:CD	2.46	0.41
1:D:200:LEU:HD23	1:D:200:LEU:HA	1.82	0.41
1:G:366:GLN:HA	1:G:369:VAL:HG22	2.03	0.41
1:I:241:ALA:HA	1:I:271:VAL:CG2	2.44	0.41
1:K:266:THR:HG22	1:K:273:VAL:H	1.85	0.41
1:K:413:ALA:CB	1:K:417:VAL:HG22	2.50	0.41
1:M:262:LEU:HD23	1:M:262:LEU:HA	1.85	0.41
1:M:472:GLY:HA3	1:M:476:TYR:HD2	1.85	0.41
1:A:253:ASP:CG	1:A:277:LYS:HE2	2.46	0.41
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:ALA:O	1:H:75:LYS:HB2	2.21	0.41
1:H:353:ILE:HG23	1:H:362:ARG:HG3	2.02	0.41
1:H:482:THR:OG1	1:H:484:GLU:HG2	2.19	0.41
1:I:16:MET:O	1:I:20:VAL:HG13	2.20	0.41
1:K:291:ASP:OD2	1:K:368:ARG:HD2	2.19	0.41
1:K:294:THR:HG21	1:K:345:ARG:CB	2.51	0.41
1:L:201:SER:HB3	1:L:204:PHE:CE2	2.56	0.41
1:L:409:GLU:OE2	1:L:498:LYS:HG3	2.21	0.41
1:M:30:THR:HB	1:M:51:LYS:O	2.21	0.41
1:B:430:ARG:HG2	1:B:430:ARG:HH11	1.85	0.41
1:G:391:GLU:CD	1:G:395:ARG:HE	2.28	0.41
1:K:239:ALA:O	1:K:314:LEU:HD21	2.20	0.41
1:D:28:LYS:HD2	1:D:453:GLN:CD	2.45	0.41
1:D:199:TYR:OH	1:D:327:LYS:HG2	2.20	0.41
1:D:234:LEU:N	1:D:235:PRO:HD2	2.35	0.41
1:D:443:ALA:O	1:D:447:MET:HG3	2.20	0.41
1:E:82:ASN:HB2	1:E:89:THR:OG1	2.21	0.41
1:F:141:SER:HA	1:F:144:ILE:HB	2.03	0.41
1:G:16:MET:SD	1:G:73:MET:HE1	2.61	0.41
1:I:151:SER:HB2	1:I:399:ALA:HA	2.02	0.41
1:I:459:GLY:HA3	1:J:112:ASN:ND2	2.36	0.41
1:J:77:VAL:HG12	1:J:506:TYR:HB3	2.02	0.41
1:J:169:VAL:CG1	1:J:377:ALA:HB2	2.51	0.41
1:K:82:ASN:HB2	1:K:89:THR:OG1	2.21	0.41
1:K:270:ILE:HB	1:L:231:ARG:CZ	2.51	0.41
1:M:385:THR:HG22	1:M:387:VAL:H	1.86	0.41
1:B:288:MET:HG3	1:B:368:ARG:NE	2.36	0.41
1:E:13:ARG:HH11	1:E:13:ARG:HD2	1.73	0.41
1:E:85:ALA:HB1	1:E:499:VAL:HG12	2.02	0.41
1:F:247:LEU:HD21	1:F:249:ILE:HD11	2.02	0.41
1:G:122:LYS:HE2	1:G:429:LEU:HD11	2.03	0.41
1:G:142:LYS:O	1:G:146:GLN:HG3	2.21	0.41
1:H:426:LEU:HD23	1:H:426:LEU:HA	1.87	0.41
1:K:182:GLY:C	1:K:184:GLN:H	2.29	0.41
1:K:202:PRO:O	1:K:203:TYR:HB2	2.21	0.41
1:L:461:GLU:HA	1:L:462:PRO:HD3	1.95	0.41
1:M:12:ALA:HB1	1:M:520:MET:HG3	2.03	0.41
1:M:455:VAL:HG11	1:M:462:PRO:HA	2.03	0.41
1:N:120:ILE:O	1:N:124:VAL:HG23	2.20	0.41
1:A:201:SER:OG	1:A:202:PRO:O	2.31	0.40
1:D:524:LEU:HD12	1:D:524:LEU:HA	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:VAL:HB	1:H:74:VAL:HG11	2.02	0.40
1:I:253:ASP:OD1	1:I:254:VAL:N	2.54	0.40
1:J:130:GLU:O	1:J:133:ALA:HB3	2.22	0.40
1:J:349:ILE:O	1:J:353:ILE:HG13	2.21	0.40
1:M:199:TYR:CZ	1:M:327:LYS:HA	2.56	0.40
1:N:218:PRO:HB3	1:N:246:PRO:HG2	2.03	0.40
1:A:353:ILE:HD13	1:A:366:GLN:HG3	2.02	0.40
1:C:220:ILE:HG23	1:C:248:LEU:HD23	2.02	0.40
1:G:455:VAL:HG21	1:G:465:VAL:HG11	2.03	0.40
1:J:199:TYR:CE2	1:J:205:ILE:HD11	2.56	0.40
1:J:222:LEU:HB3	1:J:289:LEU:HD22	2.03	0.40
1:K:444:LEU:HA	1:K:447:MET:HE3	2.01	0.40
1:L:319:GLN:O	1:L:336:VAL:HG23	2.21	0.40
1:M:144:ILE:HD13	1:M:166:MET:SD	2.61	0.40
1:M:288:MET:O	1:M:291:ASP:HB2	2.20	0.40
1:B:10:ASN:O	1:B:14:VAL:HG13	2.21	0.40
1:B:77:VAL:HG21	1:B:510:VAL:HB	2.03	0.40
1:B:238:GLU:O	1:B:242:LYS:HG3	2.21	0.40
1:B:239:ALA:HB1	1:B:314:LEU:HG	2.02	0.40
1:D:175:ILE:HG12	1:D:377:ALA:HB3	2.03	0.40
1:D:350:ARG:HG3	1:D:353:ILE:HD12	2.03	0.40
1:D:415:GLY:O	1:D:451:LEU:HD12	2.21	0.40
1:D:482:THR:O	1:D:484:GLU:HG2	2.21	0.40
1:E:421:ARG:HH11	1:E:421:ARG:HD3	1.76	0.40
1:H:140:ASP:OD1	1:H:140:ASP:N	2.54	0.40
1:H:217:SER:O	1:H:245:LYS:HD3	2.21	0.40
1:J:41:ASP:O	1:J:42:LYS:HD3	2.21	0.40
1:J:194:GLN:O	1:J:371:LYS:HE3	2.22	0.40
1:M:23:LEU:HD23	1:M:74:VAL:HG22	2.02	0.40
1:M:69:MET:O	1:M:73:MET:HG3	2.21	0.40
1:C:365:LEU:O	1:C:369:VAL:HG13	2.22	0.40
1:D:221:LEU:HD23	1:D:249:ILE:HD12	2.03	0.40
1:F:276:VAL:HG11	1:F:330:THR:OG1	2.21	0.40
1:F:287:ALA:HB1	1:F:368:ARG:NH1	2.35	0.40
1:K:128:VAL:HG21	1:K:505:GLN:NE2	2.35	0.40
1:K:349:ILE:HG23	1:K:365:LEU:HD22	2.03	0.40
1:L:120:ILE:O	1:L:124:VAL:HG23	2.21	0.40
1:L:136:VAL:HA	1:L:137:PRO:HD3	1.90	0.40
1:M:80:LYS:HA	1:M:83:ALA:HB3	2.04	0.40
1:M:221:LEU:HB3	1:M:249:ILE:HD13	2.04	0.40
1:M:234:LEU:N	1:M:235:PRO:HD2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ALA:HB1	1:B:499:VAL:HG12	2.03	0.40
1:B:443:ALA:O	1:B:447:MET:HG3	2.21	0.40
1:C:261:THR:O	1:C:265:ASN:HB2	2.22	0.40
1:D:451:LEU:HD21	1:D:465:VAL:HG12	2.03	0.40
1:E:218:PRO:HB3	1:E:246:PRO:HG2	2.04	0.40
1:F:39:VAL:HG12	1:G:69:MET:HE2	2.03	0.40
1:F:131:LEU:HD13	1:F:422:VAL:HG21	2.02	0.40
1:H:225:LYS:HB2	1:H:225:LYS:HE3	1.83	0.40
1:I:308:GLU:HB2	1:I:311:LYS:HG2	2.04	0.40
1:I:443:ALA:O	1:I:447:MET:HG3	2.21	0.40
1:I:461:GLU:HA	1:I:462:PRO:HD3	1.93	0.40
1:J:236:VAL:O	1:J:240:VAL:HG23	2.22	0.40
1:J:420:ILE:HG13	1:J:448:GLU:HG2	2.02	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%)	512 (98%)	8 (2%)	2 (0%)	30	59
1	B	522/548 (95%)	510 (98%)	10 (2%)	2 (0%)	30	59
1	C	522/548 (95%)	510 (98%)	10 (2%)	2 (0%)	30	59
1	D	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	43	70
1	E	522/548 (95%)	510 (98%)	10 (2%)	2 (0%)	30	59
1	F	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	43	70
1	G	522/548 (95%)	512 (98%)	9 (2%)	1 (0%)	43	70
1	H	522/548 (95%)	514 (98%)	8 (2%)	0	100	100
1	I	522/548 (95%)	507 (97%)	13 (2%)	2 (0%)	30	59
1	J	522/548 (95%)	514 (98%)	7 (1%)	1 (0%)	43	70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	522/548 (95%)	506 (97%)	14 (3%)	2 (0%)	30	59
1	L	522/548 (95%)	511 (98%)	10 (2%)	1 (0%)	43	70
1	M	522/548 (95%)	507 (97%)	14 (3%)	1 (0%)	43	70
1	N	522/548 (95%)	513 (98%)	8 (2%)	1 (0%)	43	70
All	All	7308/7672 (95%)	7148 (98%)	141 (2%)	19 (0%)	36	64

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	271	VAL
1	J	271	VAL
1	M	271	VAL
1	N	271	VAL
1	A	183	LEU
1	K	336	VAL
1	L	271	VAL
1	E	225	LYS
1	F	271	VAL
1	I	183	LEU
1	B	183	LEU
1	C	184	GLN
1	D	271	VAL
1	C	271	VAL
1	G	271	VAL
1	B	271	VAL
1	K	271	VAL
1	A	271	VAL
1	I	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	402/413 (97%)	371 (92%)	31 (8%)	12	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	402/413 (97%)	374 (93%)	28 (7%)	14	37
1	C	402/413 (97%)	378 (94%)	24 (6%)	17	43
1	D	402/413 (97%)	372 (92%)	30 (8%)	12	36
1	E	402/413 (97%)	372 (92%)	30 (8%)	12	36
1	F	402/413 (97%)	373 (93%)	29 (7%)	13	37
1	G	402/413 (97%)	379 (94%)	23 (6%)	18	45
1	H	402/413 (97%)	372 (92%)	30 (8%)	12	36
1	I	402/413 (97%)	368 (92%)	34 (8%)	10	31
1	J	402/413 (97%)	367 (91%)	35 (9%)	9	30
1	K	402/413 (97%)	369 (92%)	33 (8%)	10	32
1	L	402/413 (97%)	369 (92%)	33 (8%)	10	32
1	M	402/413 (97%)	370 (92%)	32 (8%)	11	33
1	N	402/413 (97%)	367 (91%)	35 (9%)	9	30
All	All	5628/5782 (97%)	5201 (92%)	427 (8%)	12	35

All (427) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	20	VAL
1	A	27	VAL
1	A	69	MET
1	A	74	VAL
1	A	76	GLU
1	A	82	ASN
1	A	89	THR
1	A	94	VAL
1	A	134	LEU
1	A	141	SER
1	A	161	LEU
1	A	177	VAL
1	A	183	LEU
1	A	205	ILE
1	A	230	ILE
1	A	261	THR
1	A	289	LEU
1	A	295	LEU

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Mol	Chain	Res	Type
1	A	328	ASP
1	A	351	GLN
1	A	389	MET
1	A	404	ARG
1	A	417	VAL
1	A	422	VAL
1	A	442	VAL
1	A	463	SER
1	A	483	GLU
1	A	499	VAL
1	A	514	MET
1	A	524	LEU
1	B	18	ARG
1	B	20	VAL
1	B	27	VAL
1	B	65	LYS
1	B	74	VAL
1	B	82	ASN
1	B	89	THR
1	B	94	VAL
1	B	129	GLU
1	B	131	LEU
1	B	134	LEU
1	B	141	SER
1	B	161	LEU
1	B	176	THR
1	B	177	VAL
1	B	190	VAL
1	B	234	LEU
1	B	276	VAL
1	B	289	LEU
1	B	290	GLN
1	B	328	ASP
1	B	329	THR
1	B	411	VAL
1	B	417	VAL
1	B	422	VAL
1	B	463	SER
1	B	499	VAL
1	B	514	MET
1	C	20	VAL
1	C	27	VAL

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Mol	Chain	Res	Type
1	C	43	SER
1	C	74	VAL
1	C	82	ASN
1	C	89	THR
1	C	94	VAL
1	C	129	GLU
1	C	131	LEU
1	C	151	SER
1	C	161	LEU
1	C	177	VAL
1	C	184	GLN
1	C	206	ASN
1	C	225	LYS
1	C	271	VAL
1	C	272	LYS
1	C	328	ASP
1	C	329	THR
1	C	404	ARG
1	C	417	VAL
1	C	422	VAL
1	C	463	SER
1	C	499	VAL
1	D	20	VAL
1	D	27	VAL
1	D	39	VAL
1	D	74	VAL
1	D	82	ASN
1	D	89	THR
1	D	94	VAL
1	D	129	GLU
1	D	134	LEU
1	D	161	LEU
1	D	176	THR
1	D	177	VAL
1	D	236	VAL
1	D	270	ILE
1	D	271	VAL
1	D	295	LEU
1	D	329	THR
1	D	333	ILE
1	D	354	GLU
1	D	357	THR

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Mol	Chain	Res	Type
1	D	359	ASP
1	D	367	GLU
1	D	385	THR
1	D	417	VAL
1	D	422	VAL
1	D	445	ARG
1	D	451	LEU
1	D	463	SER
1	D	499	VAL
1	D	524	LEU
1	E	10	ASN
1	E	20	VAL
1	E	27	VAL
1	E	39	VAL
1	E	65	LYS
1	E	74	VAL
1	E	82	ASN
1	E	89	THR
1	E	94	VAL
1	E	131	LEU
1	E	134	LEU
1	E	141	SER
1	E	161	LEU
1	E	177	VAL
1	E	242	LYS
1	E	271	VAL
1	E	272	LYS
1	E	284	ARG
1	E	295	LEU
1	E	322	ARG
1	E	328	ASP
1	E	329	THR
1	E	351	GLN
1	E	358	SER
1	E	385	THR
1	E	387	VAL
1	E	417	VAL
1	E	422	VAL
1	E	463	SER
1	E	499	VAL
1	F	20	VAL
1	F	27	VAL

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Mol	Chain	Res	Type
1	F	43	SER
1	F	65	LYS
1	F	74	VAL
1	F	75	LYS
1	F	82	ASN
1	F	89	THR
1	F	94	VAL
1	F	129	GLU
1	F	134	LEU
1	F	151	SER
1	F	172	GLU
1	F	176	THR
1	F	181	THR
1	F	183	LEU
1	F	204	PHE
1	F	289	LEU
1	F	328	ASP
1	F	329	THR
1	F	407	VAL
1	F	411	VAL
1	F	417	VAL
1	F	456	LEU
1	F	463	SER
1	F	494	LEU
1	F	499	VAL
1	F	514	MET
1	F	524	LEU
1	G	20	VAL
1	G	27	VAL
1	G	43	SER
1	G	69	MET
1	G	74	VAL
1	G	82	ASN
1	G	89	THR
1	G	94	VAL
1	G	134	LEU
1	G	161	LEU
1	G	176	THR
1	G	190	VAL
1	G	271	VAL
1	G	295	LEU
1	G	328	ASP

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Mol	Chain	Res	Type
1	G	329	THR
1	G	331	THR
1	G	404	ARG
1	G	417	VAL
1	G	422	VAL
1	G	463	SER
1	G	494	LEU
1	G	499	VAL
1	H	20	VAL
1	H	27	VAL
1	H	74	VAL
1	H	82	ASN
1	H	94	VAL
1	H	134	LEU
1	H	141	SER
1	H	144	ILE
1	H	151	SER
1	H	161	LEU
1	H	176	THR
1	H	177	VAL
1	H	183	LEU
1	H	206	ASN
1	H	249	ILE
1	H	261	THR
1	H	283	ASP
1	H	295	LEU
1	H	322	ARG
1	H	328	ASP
1	H	329	THR
1	H	351	GLN
1	H	381	VAL
1	H	385	THR
1	H	387	VAL
1	H	417	VAL
1	H	422	VAL
1	H	463	SER
1	H	499	VAL
1	H	524	LEU
1	I	14	VAL
1	I	20	VAL
1	I	43	SER
1	I	74	VAL

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Mol	Chain	Res	Type
1	I	76	GLU
1	I	82	ASN
1	I	89	THR
1	I	94	VAL
1	I	129	GLU
1	I	134	LEU
1	I	138	CYS
1	I	141	SER
1	I	167	ASP
1	I	172	GLU
1	I	176	THR
1	I	177	VAL
1	I	183	LEU
1	I	220	ILE
1	I	230	ILE
1	I	281	PHE
1	I	288	MET
1	I	295	LEU
1	I	300	VAL
1	I	314	LEU
1	I	350	ARG
1	I	369	VAL
1	I	389	MET
1	I	403	THR
1	I	417	VAL
1	I	422	VAL
1	I	442	VAL
1	I	463	SER
1	I	499	VAL
1	I	524	LEU
1	J	10	ASN
1	J	20	VAL
1	J	27	VAL
1	J	74	VAL
1	J	76	GLU
1	J	82	ASN
1	J	89	THR
1	J	94	VAL
1	J	125	THR
1	J	138	CYS
1	J	151	SER
1	J	177	VAL

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Mol	Chain	Res	Type
1	J	190	VAL
1	J	206	ASN
1	J	222	LEU
1	J	230	ILE
1	J	249	ILE
1	J	257	GLU
1	J	271	VAL
1	J	288	MET
1	J	289	LEU
1	J	295	LEU
1	J	322	ARG
1	J	328	ASP
1	J	329	THR
1	J	331	THR
1	J	338	GLU
1	J	358	SER
1	J	385	THR
1	J	417	VAL
1	J	422	VAL
1	J	463	SER
1	J	473	ASP
1	J	499	VAL
1	J	514	MET
1	K	20	VAL
1	K	27	VAL
1	K	43	SER
1	K	69	MET
1	K	74	VAL
1	K	76	GLU
1	K	82	ASN
1	K	89	THR
1	K	94	VAL
1	K	118	ARG
1	K	161	LEU
1	K	174	VAL
1	K	176	THR
1	K	177	VAL
1	K	206	ASN
1	K	215	LEU
1	K	230	ILE
1	K	233	MET
1	K	245	LYS

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Mol	Chain	Res	Type
1	K	272	LYS
1	K	289	LEU
1	K	295	LEU
1	K	307	MET
1	K	309	LEU
1	K	328	ASP
1	K	417	VAL
1	K	422	VAL
1	K	463	SER
1	K	493	ILE
1	K	499	VAL
1	K	502	SER
1	K	514	MET
1	K	524	LEU
1	L	20	VAL
1	L	27	VAL
1	L	43	SER
1	L	74	VAL
1	L	82	ASN
1	L	89	THR
1	L	94	VAL
1	L	131	LEU
1	L	138	CYS
1	L	140	ASP
1	L	161	LEU
1	L	176	THR
1	L	177	VAL
1	L	257	GLU
1	L	271	VAL
1	L	288	MET
1	L	295	LEU
1	L	299	THR
1	L	317	LEU
1	L	323	VAL
1	L	328	ASP
1	L	329	THR
1	L	367	GLU
1	L	369	VAL
1	L	387	VAL
1	L	417	VAL
1	L	422	VAL
1	L	456	LEU

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Mol	Chain	Res	Type
1	L	463	SER
1	L	494	LEU
1	L	499	VAL
1	L	517	THR
1	L	524	LEU
1	M	10	ASN
1	M	14	VAL
1	M	20	VAL
1	M	27	VAL
1	M	43	SER
1	M	69	MET
1	M	74	VAL
1	M	76	GLU
1	M	82	ASN
1	M	89	THR
1	M	94	VAL
1	M	129	GLU
1	M	134	LEU
1	M	141	SER
1	M	161	LEU
1	M	172	GLU
1	M	177	VAL
1	M	190	VAL
1	M	216	GLU
1	M	271	VAL
1	M	295	LEU
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	404	ARG
1	M	407	VAL
1	M	417	VAL
1	M	422	VAL
1	M	463	SER
1	M	494	LEU
1	M	499	VAL
1	M	524	LEU
1	N	14	VAL
1	N	20	VAL
1	N	27	VAL
1	N	43	SER
1	N	48	THR

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Mol	Chain	Res	Type
1	N	74	VAL
1	N	76	GLU
1	N	82	ASN
1	N	89	THR
1	N	94	VAL
1	N	118	ARG
1	N	131	LEU
1	N	134	LEU
1	N	154	SER
1	N	161	LEU
1	N	176	THR
1	N	183	LEU
1	N	190	VAL
1	N	203	TYR
1	N	206	ASN
1	N	210	THR
1	N	261	THR
1	N	266	THR
1	N	267	MET
1	N	271	VAL
1	N	295	LEU
1	N	328	ASP
1	N	329	THR
1	N	331	THR
1	N	385	THR
1	N	417	VAL
1	N	422	VAL
1	N	463	SER
1	N	494	LEU
1	N	499	VAL

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	326	ASN
1	A	352	GLN
1	A	433	ASN
1	B	206	ASN
1	B	432	GLN
1	C	194	GLN
1	D	10	ASN
1	D	37	ASN

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Mol	Chain	Res	Type
1	D	352	GLN
1	D	457	ASN
1	E	37	ASN
1	F	352	GLN
1	H	97	GLN
1	H	153	ASN
1	H	290	GLN
1	H	326	ASN
1	H	352	GLN
1	H	366	GLN
1	I	97	GLN
1	I	229	ASN
1	J	37	ASN
1	J	146	GLN
1	J	184	GLN
1	J	487	ASN
1	K	37	ASN
1	K	153	ASN
1	K	184	GLN
1	K	194	GLN
1	K	475	ASN
1	L	97	GLN
1	L	290	GLN
1	L	352	GLN
1	M	352	GLN
1	M	433	ASN
1	N	153	ASN
1	N	229	ASN
1	N	343	GLN
1	N	352	GLN
1	N	432	GLN

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 [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%)	-0.65	1 (0%) 91 83	22, 60, 120, 174	0
1	B	524/548 (95%)	-0.45	2 (0%) 88 76	24, 65, 207, 301	0
1	C	524/548 (95%)	-0.51	0 100 100	25, 70, 166, 204	0
1	D	524/548 (95%)	-0.47	3 (0%) 85 70	28, 73, 161, 232	0
1	E	524/548 (95%)	-0.59	1 (0%) 91 83	28, 69, 136, 190	0
1	F	524/548 (95%)	-0.57	0 100 100	31, 77, 135, 190	0
1	G	524/548 (95%)	-0.49	2 (0%) 88 76	27, 80, 167, 208	0
1	H	524/548 (95%)	-0.64	0 100 100	25, 63, 118, 168	0
1	I	524/548 (95%)	-0.62	3 (0%) 85 70	21, 54, 146, 227	0
1	J	524/548 (95%)	-0.63	1 (0%) 91 83	18, 63, 134, 189	0
1	K	524/548 (95%)	-0.25	15 (2%) 53 32	22, 66, 239, 292	0
1	L	524/548 (95%)	-0.65	1 (0%) 91 83	25, 58, 125, 177	0
1	M	524/548 (95%)	-0.44	2 (0%) 88 76	28, 77, 172, 233	0
1	N	524/548 (95%)	-0.55	1 (0%) 91 83	22, 64, 152, 206	0
All	All	7336/7672 (95%)	-0.54	32 (0%) 88 76	18, 66, 167, 301	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	233	MET	3.8
1	K	342	ILE	3.8
1	K	193	MET	3.8
1	G	301	ILE	3.6
1	K	288	MET	3.1
1	D	317	LEU	3.0
1	K	251	ALA	3.0
1	K	295	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	K	223	ALA	2.8
1	K	346	VAL	2.8
1	M	193	MET	2.8
1	I	271	VAL	2.8
1	I	281	PHE	2.8
1	B	279	PRO	2.8
1	M	183	LEU	2.7
1	D	265	ASN	2.7
1	K	279	PRO	2.6
1	E	271	VAL	2.4
1	K	280	GLY	2.4
1	I	233	MET	2.3
1	L	270	ILE	2.3
1	J	270	ILE	2.3
1	K	259	LEU	2.3
1	D	270	ILE	2.2
1	N	270	ILE	2.1
1	K	302	SER	2.1
1	K	262	LEU	2.1
1	B	271	VAL	2.1
1	K	287	ALA	2.1
1	K	301	ILE	2.0
1	A	271	VAL	2.0
1	G	262	LEU	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 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.