Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 04:29 am BST

PDB ID	:	4HEL
Title	:	Crystal structure analysis of apo-GroEL structure
Authors	:	Saxena, A.K.; Meena, S.R.
Deposited on	:	2012-10-04
Resolution	:	3.20 Å(reported)

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

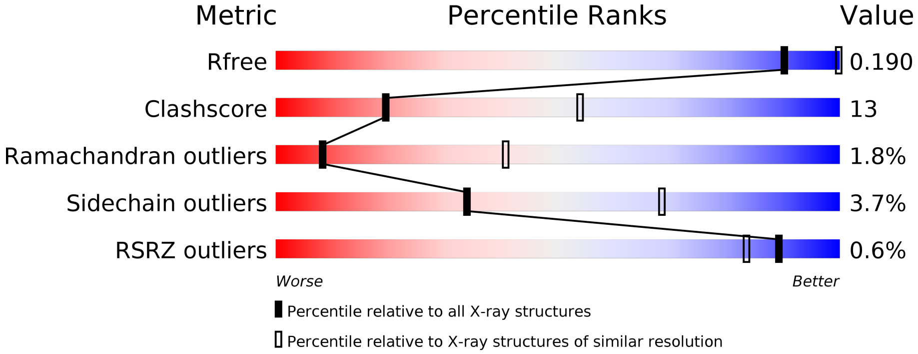
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

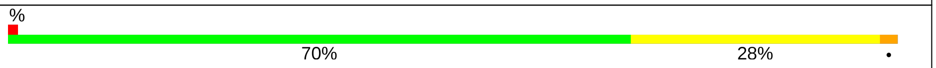
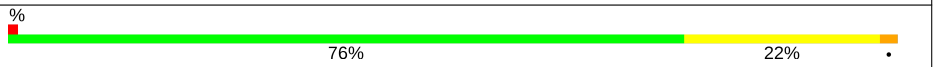
The reported resolution of this entry is 3.20 Å.

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	525	
1	B	525	
1	C	525	
1	D	525	
1	E	525	
1	F	525	

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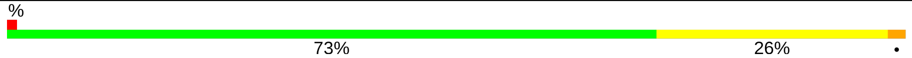
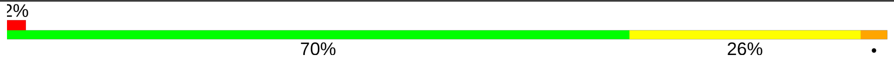
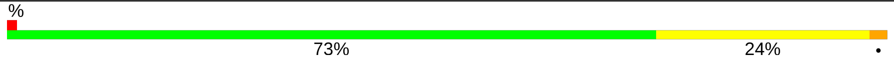
Mol	Chain	Length	Quality of chain
1	G	525	
1	H	525	
1	I	525	
1	J	525	
1	K	525	
1	L	525	
1	M	525	
1	N	525	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 54997 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 4.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	B	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	C	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	D	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	E	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	F	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	G	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	H	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	I	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	J	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	K	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	L	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	M	525	Total C N O S 3864 2403 667 774 20	0	0	0
1	N	525	Total C N O S 3864 2403 667 774 20	0	0	0

- Molecule 2 is water.

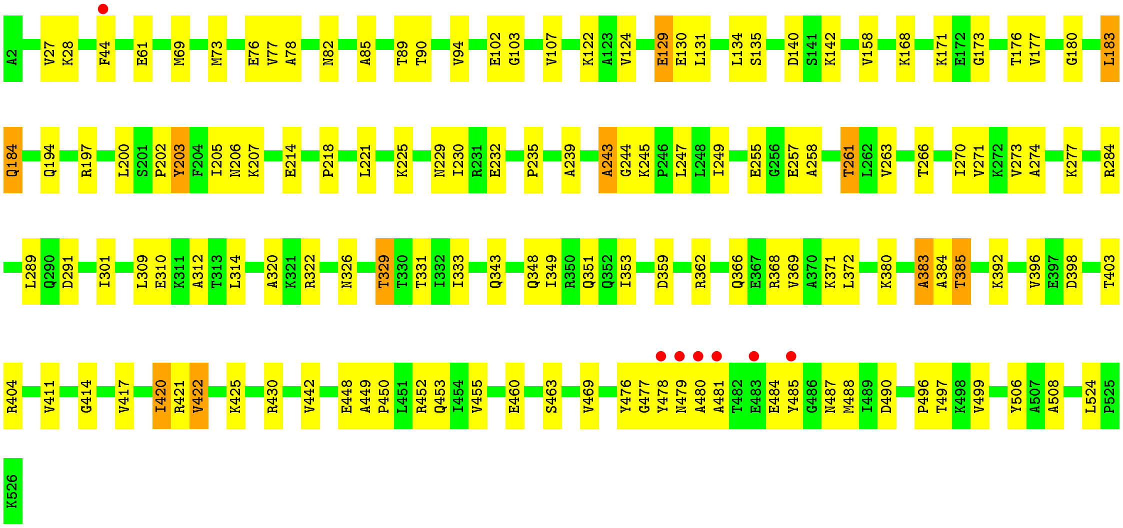
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	60	Total O 60 60	0	0
2	B	83	Total O 83 83	0	0
2	C	65	Total O 65 65	0	0
2	D	62	Total O 62 62	0	0
2	E	79	Total O 79 79	0	0
2	F	53	Total O 53 53	0	0
2	G	74	Total O 74 74	0	0
2	H	52	Total O 52 52	0	0
2	I	64	Total O 64 64	0	0
2	J	75	Total O 75 75	0	0
2	K	55	Total O 55 55	0	0
2	L	64	Total O 64 64	0	0
2	M	57	Total O 57 57	0	0
2	N	58	Total O 58 58	0	0

3 Residue-property plots ⓘ

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

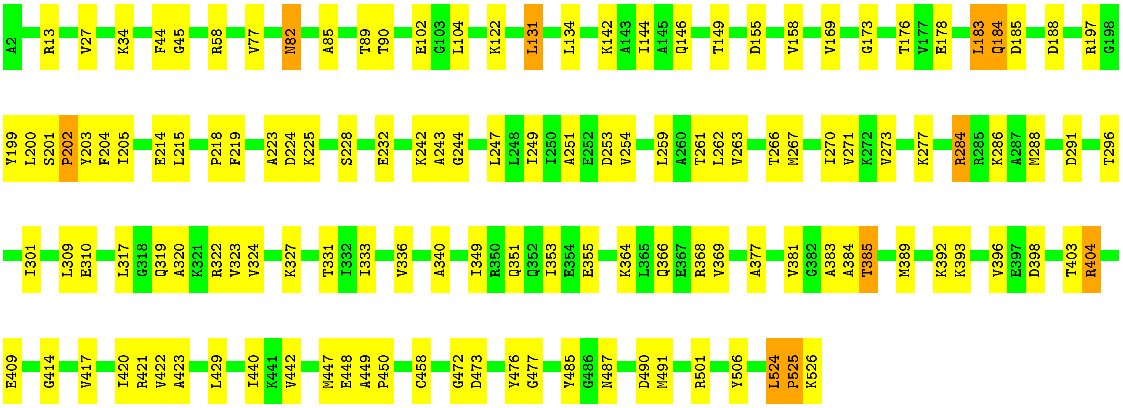
- Molecule 1: 60 kDa chaperonin 4

Chain A:

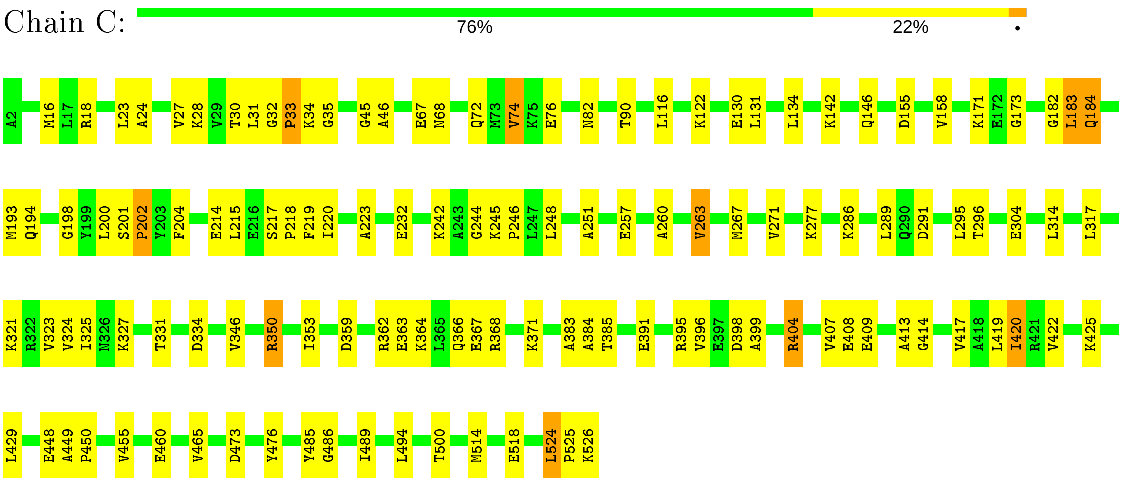


- Molecule 1: 60 kDa chaperonin 4

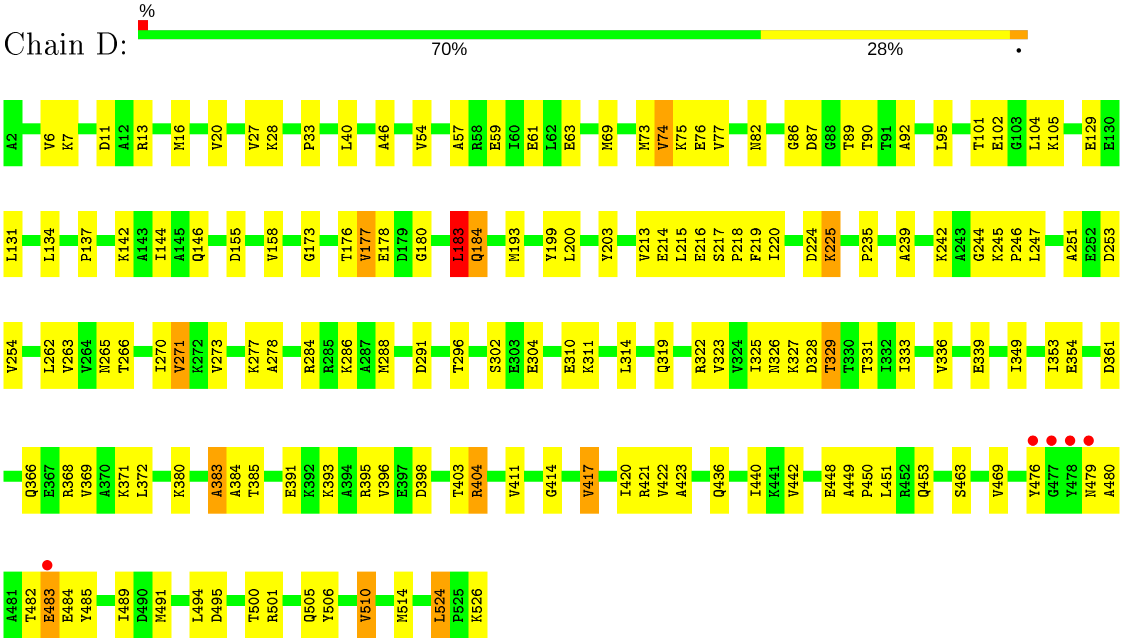
Chain B:



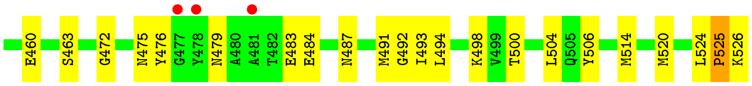
- Molecule 1: 60 kDa chaperonin 4



- Molecule 1: 60 kDa chaperonin 4

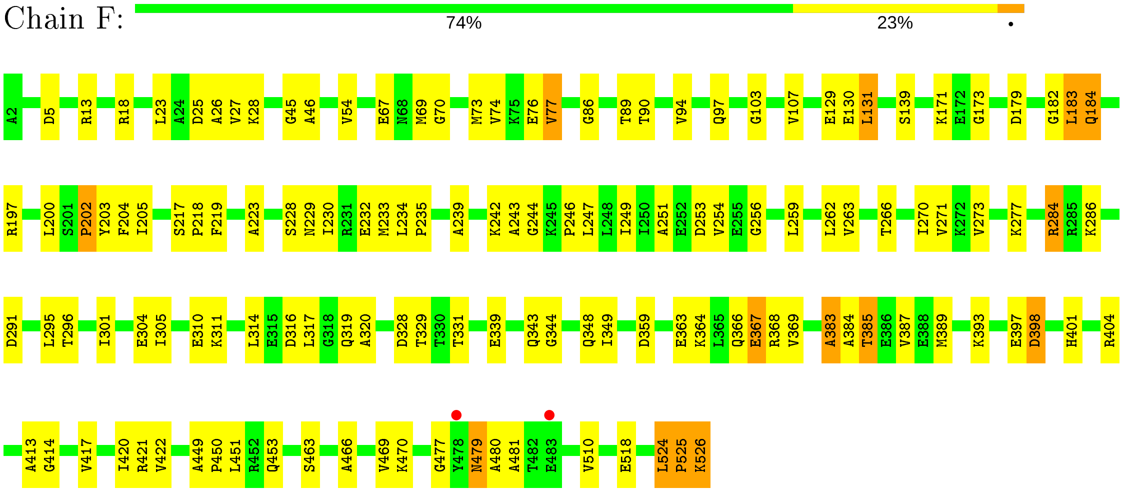


- Molecule 1: 60 kDa chaperonin 4



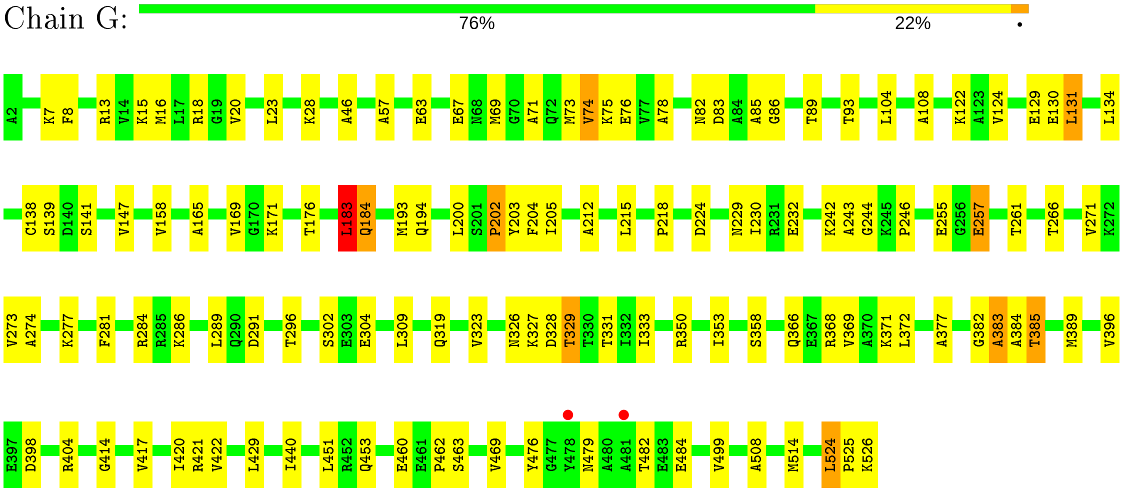
- Molecule 1: 60 kDa chaperonin 4

Chain F:



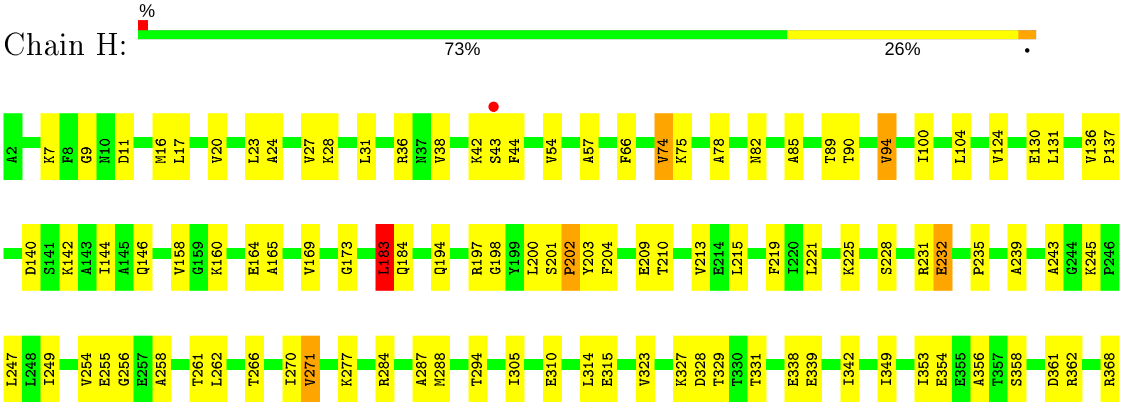
- Molecule 1: 60 kDa chaperonin 4

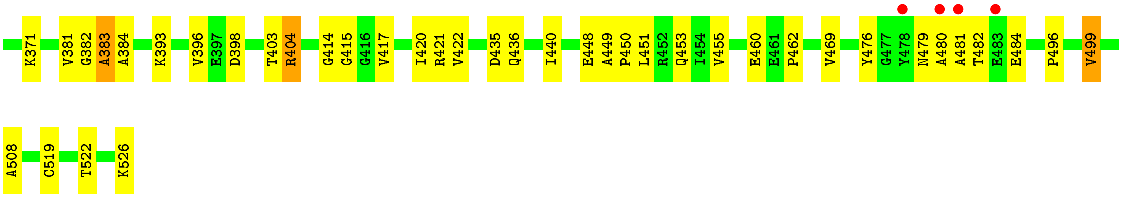
Chain G:



- Molecule 1: 60 kDa chaperonin 4

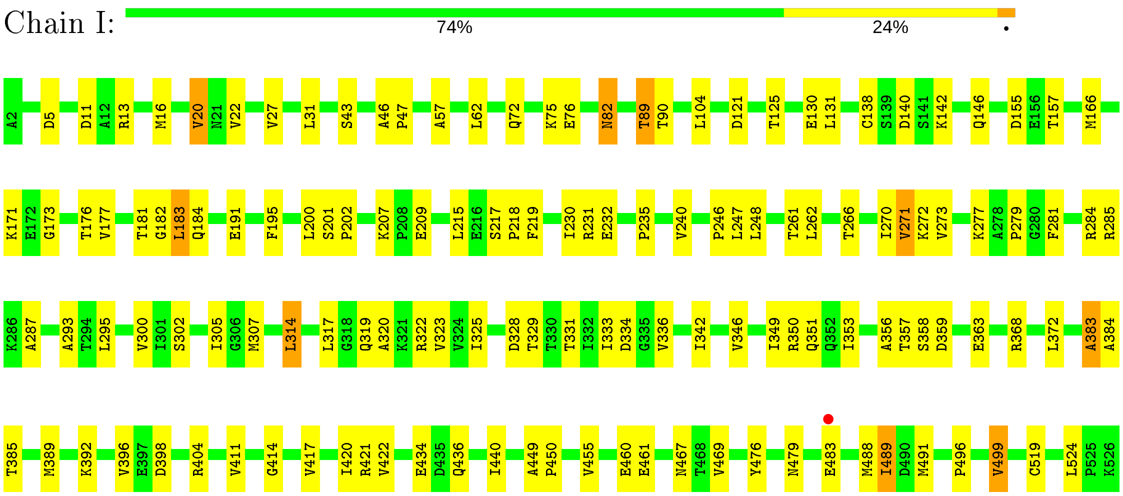
Chain H:





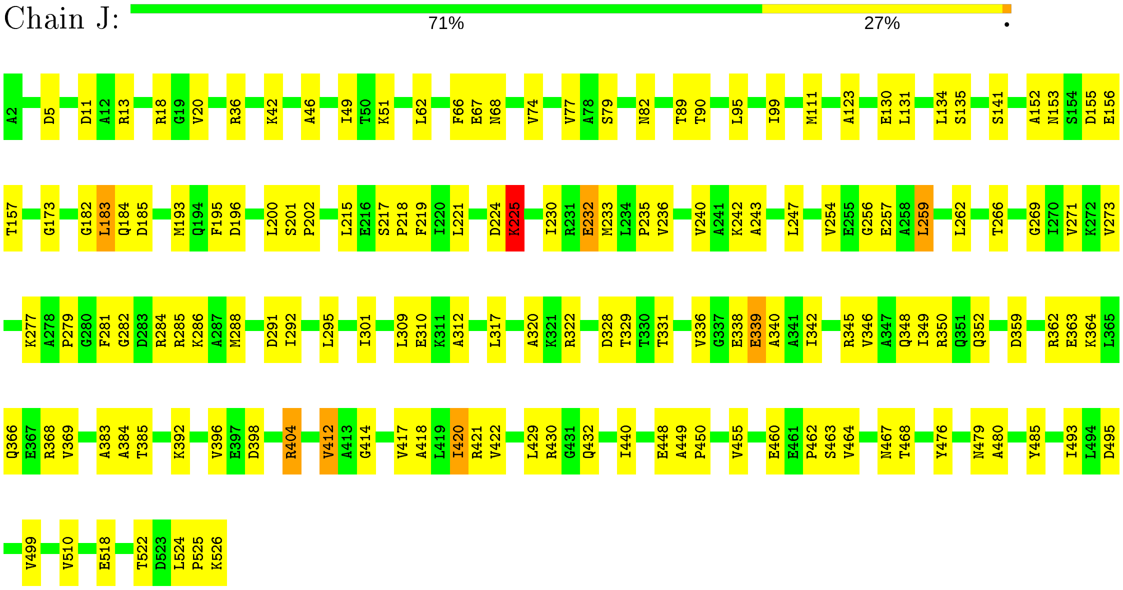
- Molecule 1: 60 kDa chaperonin 4

Chain I:



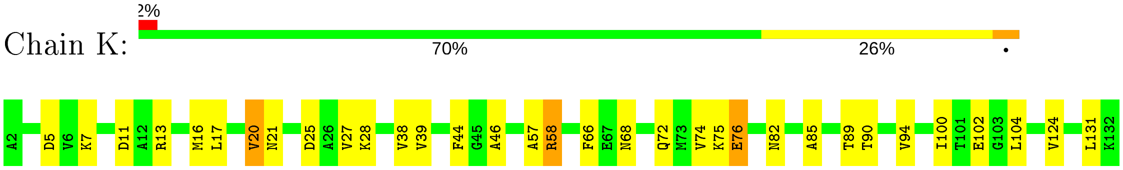
- Molecule 1: 60 kDa chaperonin 4

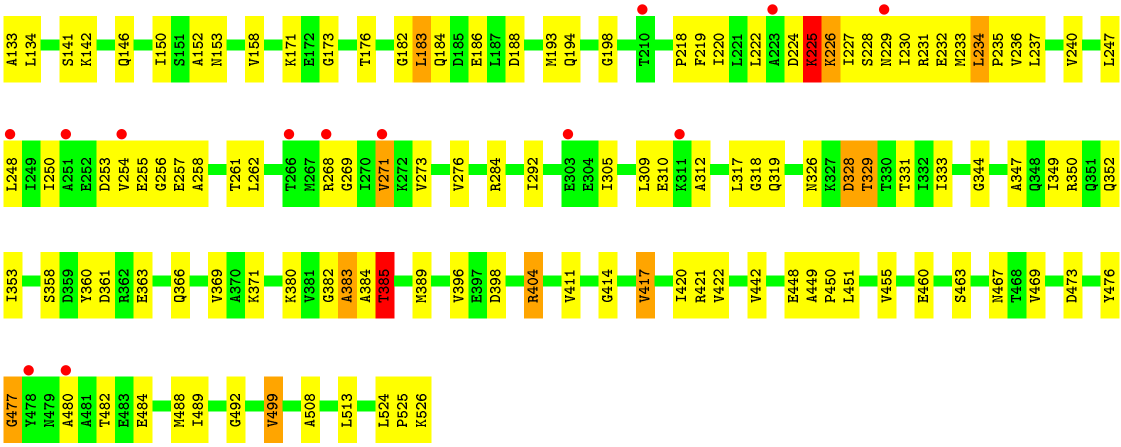
Chain J:



- Molecule 1: 60 kDa chaperonin 4

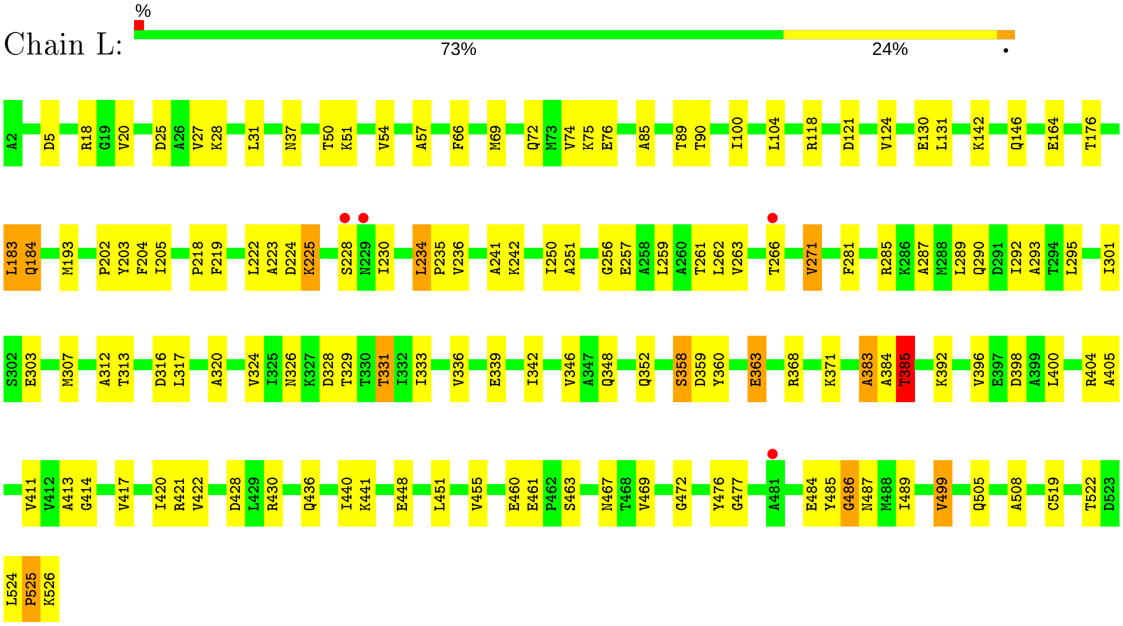
Chain K:





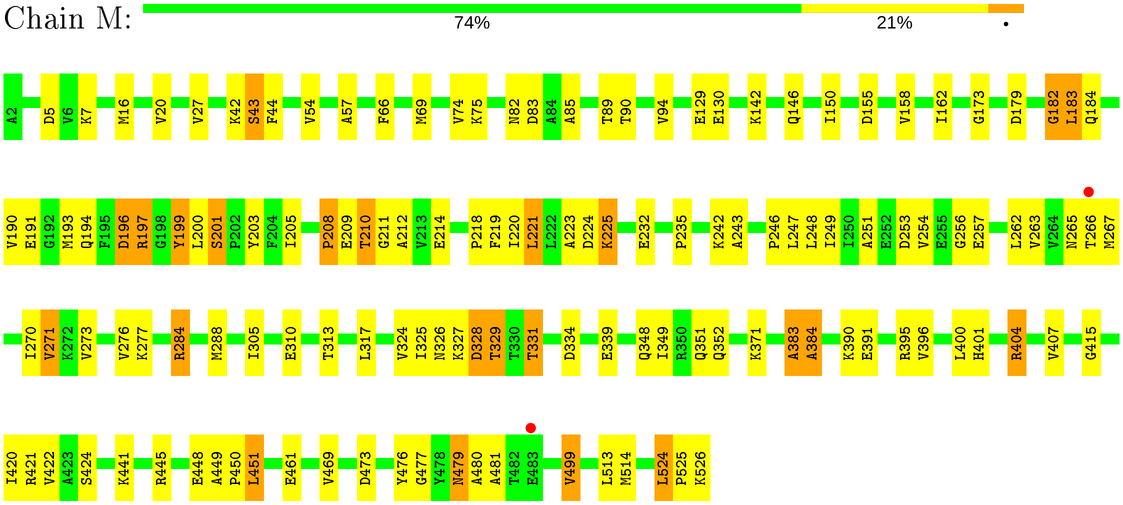
- Molecule 1: 60 kDa chaperonin 4

Chain L:

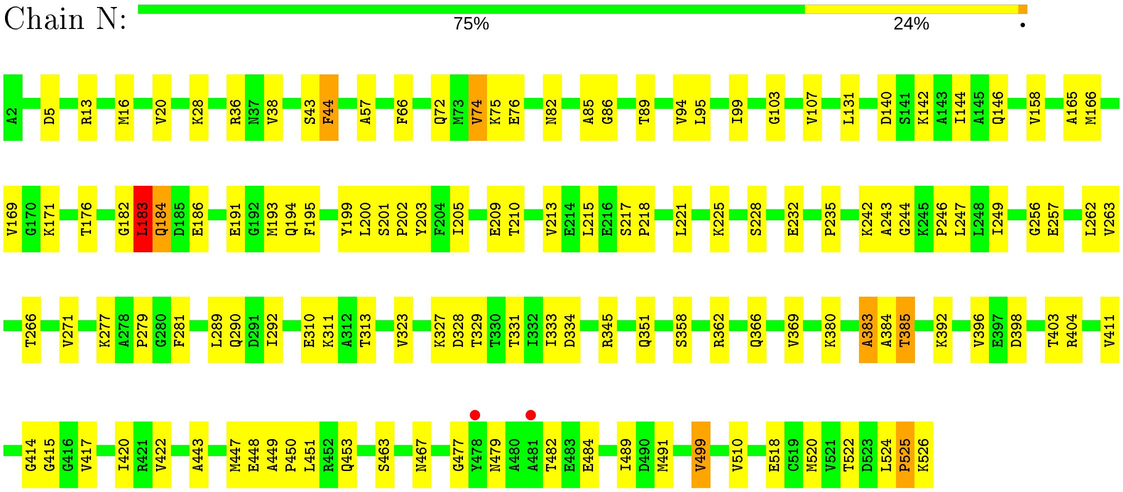


- Molecule 1: 60 kDa chaperonin 4

Chain M:



- Molecule 1: 60 kDa chaperonin 4



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.24Å 261.83Å 282.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.38 – 3.20 59.09 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.38-3.20) 100.0 (59.09-3.20)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.198 , 0.223 0.189 , 0.190	Depositor DCC
R_{free} test set	8373 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	48.3	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 38.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	54997	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0/3892	0.72	1/5254 (0.0%)
1	B	0.59	0/3892	0.69	0/5254
1	C	0.55	0/3892	0.70	2/5254 (0.0%)
1	D	0.56	0/3892	0.70	0/5254
1	E	0.61	0/3892	0.73	0/5254
1	F	0.58	0/3892	0.71	2/5254 (0.0%)
1	G	0.59	0/3892	0.70	1/5254 (0.0%)
1	H	0.58	0/3892	0.71	1/5254 (0.0%)
1	I	0.56	0/3892	0.68	2/5254 (0.0%)
1	J	0.55	0/3892	0.68	1/5254 (0.0%)
1	K	0.52	0/3892	0.67	1/5254 (0.0%)
1	L	0.55	0/3892	0.70	2/5254 (0.0%)
1	M	0.60	0/3892	0.74	1/5254 (0.0%)
1	N	0.58	0/3892	0.70	1/5254 (0.0%)
All	All	0.57	0/54488	0.70	15/73556 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	477	GLY	N-CA-C	6.93	130.42	113.10
1	C	295	LEU	CA-CB-CG	6.61	130.49	115.30
1	N	477	GLY	N-CA-C	6.48	129.29	113.10
1	J	295	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	477	GLY	N-CA-C	6.25	128.73	113.10
1	F	477	GLY	N-CA-C	5.79	127.58	113.10
1	C	134	LEU	CA-CB-CG	5.64	128.27	115.30
1	L	295	LEU	CA-CB-CG	5.43	127.78	115.30
1	F	295	LEU	CA-CB-CG	5.42	127.77	115.30
1	I	314	LEU	CA-CB-CG	5.40	127.72	115.30
1	H	36	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	M	477	GLY	N-CA-C	5.33	126.43	113.10
1	L	131	LEU	CA-CB-CG	5.18	127.21	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	295	LEU	CA-CB-CG	5.13	127.11	115.30
1	G	385	THR	N-CA-CB	5.06	119.92	110.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3864	0	3989	93	0
1	B	3864	0	3989	103	0
1	C	3864	0	3989	92	0
1	D	3864	0	3989	127	0
1	E	3864	0	3989	108	0
1	F	3864	0	3989	97	0
1	G	3864	0	3989	86	0
1	H	3864	0	3989	97	0
1	I	3864	0	3989	100	0
1	J	3864	0	3989	118	0
1	K	3864	0	3989	140	0
1	L	3864	0	3989	105	0
1	M	3864	0	3989	93	0
1	N	3864	0	3989	81	0
2	A	60	0	0	17	0
2	B	83	0	0	32	0
2	C	65	0	0	14	0
2	D	62	0	0	32	0
2	E	79	0	0	32	0
2	F	53	0	0	5	0
2	G	74	0	0	10	0
2	H	52	0	0	20	0
2	I	64	0	0	24	0
2	J	75	0	0	43	0
2	K	55	0	0	33	0
2	L	64	0	0	28	0
2	M	57	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	58	0	0	13	0
All	All	54997	0	55846	1407	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 13.

All (1407) 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:234:LEU:HA	2:K:630:HOH:O	1.37	1.24
1:K:234:LEU:HD23	2:K:630:HOH:O	1.35	1.24
1:K:384:ALA:HA	2:L:635:HOH:O	1.36	1.22
1:K:219:PHE:HA	2:K:636:HOH:O	1.39	1.18
1:H:261:THR:HB	2:H:647:HOH:O	1.47	1.12
1:M:421:ARG:HD3	2:M:656:HOH:O	1.52	1.10
1:D:95:LEU:HB2	2:D:661:HOH:O	1.50	1.09
1:B:491:MET:SD	2:B:680:HOH:O	2.10	1.08
1:J:18:ARG:HB2	2:J:650:HOH:O	1.53	1.06
1:E:526:LYS:HG3	2:E:649:HOH:O	1.53	1.06
1:L:486:GLY:CA	2:L:660:HOH:O	2.04	1.05
1:D:95:LEU:N	2:D:661:HOH:O	1.87	1.04
1:D:173:GLY:O	1:D:404:ARG:NH2	1.90	1.04
1:B:203:TYR:N	2:B:661:HOH:O	1.91	1.03
1:J:82:ASN:HB2	2:J:628:HOH:O	1.57	1.02
1:A:417:VAL:HG11	1:A:488:MET:HE1	1.40	1.02
1:H:261:THR:CA	2:H:647:HOH:O	2.08	1.00
1:G:514:MET:SD	2:G:666:HOH:O	2.21	0.98
1:M:265:ASN:HB3	1:M:271:VAL:HG21	1.46	0.98
1:B:45:GLY:N	2:B:667:HOH:O	1.96	0.97
1:D:11:ASP:HB3	2:D:637:HOH:O	1.63	0.97
1:F:46:ALA:HB2	1:G:76:GLU:HG3	1.45	0.96
1:B:223:ALA:HA	2:B:658:HOH:O	1.67	0.95
1:K:477:GLY:HA3	1:K:488:MET:HE2	1.49	0.94
1:A:385:THR:N	2:A:632:HOH:O	1.98	0.94
1:J:184:GLN:HB2	2:J:645:HOH:O	1.67	0.94
1:D:137:PRO:HD2	2:D:644:HOH:O	1.67	0.93
1:L:487:ASN:N	2:L:660:HOH:O	2.01	0.93
1:J:385:THR:N	2:J:644:HOH:O	2.00	0.93
1:K:254:VAL:HB	2:K:629:HOH:O	1.69	0.93
1:L:313:THR:N	2:L:643:HOH:O	1.98	0.93
1:L:234:LEU:H	1:L:235:PRO:HD2	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:271:VAL:N	2:I:645:HOH:O	2.02	0.92
1:D:484:GLU:HG2	2:D:656:HOH:O	1.69	0.91
1:B:224:ASP:N	2:B:658:HOH:O	2.04	0.90
1:B:366:GLN:NE2	2:B:651:HOH:O	2.03	0.90
1:B:301:ILE:O	2:B:658:HOH:O	1.89	0.90
1:H:258:ALA:O	2:H:647:HOH:O	1.89	0.89
1:D:137:PRO:CD	2:D:644:HOH:O	2.20	0.89
1:F:54:VAL:HG22	1:F:89:THR:HG21	1.53	0.89
1:D:489:ILE:HG23	1:D:494:LEU:HD21	1.54	0.89
1:H:173:GLY:O	1:H:404:ARG:NH2	2.06	0.89
1:I:285:ARG:NE	2:I:643:HOH:O	2.06	0.88
1:H:200:LEU:HD21	1:H:277:LYS:HG3	1.56	0.88
1:B:173:GLY:O	1:B:404:ARG:NH2	2.06	0.87
1:H:262:LEU:N	2:H:647:HOH:O	2.07	0.87
1:E:420:ILE:HD12	1:E:451:LEU:HD13	1.55	0.87
1:G:78:ALA:O	1:G:89:THR:HG22	1.75	0.87
1:H:261:THR:CB	2:H:647:HOH:O	2.08	0.87
1:N:247:LEU:HD21	1:N:249:ILE:HD11	1.57	0.87
1:K:233:MET:O	2:K:630:HOH:O	1.93	0.86
1:G:421:ARG:NH1	1:G:469:VAL:O	2.08	0.86
1:J:235:PRO:HG3	1:J:310:GLU:HA	1.55	0.86
1:J:67:GLU:OE1	2:J:657:HOH:O	1.93	0.86
1:J:173:GLY:O	1:J:404:ARG:NH2	2.08	0.86
1:C:32:GLY:N	2:C:643:HOH:O	2.06	0.86
1:D:92:ALA:O	2:D:661:HOH:O	1.92	0.86
1:E:76:GLU:CG	2:E:657:HOH:O	2.23	0.86
1:K:230:ILE:HG21	2:K:644:HOH:O	1.77	0.85
1:K:421:ARG:NH1	1:K:469:VAL:O	2.09	0.85
1:A:235:PRO:HG3	1:A:310:GLU:HA	1.58	0.85
1:L:54:VAL:HG22	1:L:89:THR:HG21	1.55	0.85
1:J:269:GLY:HA3	1:K:257:GLU:HG3	1.59	0.85
1:C:30:THR:C	2:C:651:HOH:O	2.14	0.85
1:H:142:LYS:O	2:H:633:HOH:O	1.95	0.84
1:I:350:ARG:O	2:I:637:HOH:O	1.93	0.84
1:L:348:GLN:HB3	2:L:647:HOH:O	1.75	0.84
1:N:327:LYS:NZ	2:N:640:HOH:O	2.08	0.83
1:C:31:LEU:N	2:C:651:HOH:O	2.11	0.83
1:H:421:ARG:NH1	1:H:469:VAL:O	2.12	0.83
1:K:218:PRO:O	2:K:649:HOH:O	1.95	0.83
1:M:401:HIS:HB3	2:M:647:HOH:O	1.77	0.83
1:A:82:ASN:HB2	1:A:89:THR:HG23	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:SER:HB3	2:N:650:HOH:O	1.78	0.83
1:K:58:ARG:HH11	1:K:58:ARG:HB3	1.43	0.82
1:H:339:GLU:N	2:H:637:HOH:O	2.11	0.82
1:I:353:ILE:O	2:I:653:HOH:O	1.97	0.82
1:K:236:VAL:HG23	2:K:638:HOH:O	1.78	0.82
1:M:324:VAL:HG23	1:M:331:THR:HG23	1.62	0.82
1:A:168:LYS:C	2:A:640:HOH:O	2.19	0.81
1:F:45:GLY:O	2:F:644:HOH:O	1.99	0.81
1:J:232:GLU:OE1	2:J:629:HOH:O	1.97	0.81
1:C:31:LEU:C	2:C:651:HOH:O	2.18	0.81
1:D:421:ARG:NH1	1:D:469:VAL:O	2.14	0.81
1:A:421:ARG:NH1	1:A:469:VAL:O	2.13	0.81
1:K:420:ILE:HD12	1:K:451:LEU:HD13	1.64	0.80
1:F:398:ASP:OD1	2:F:635:HOH:O	2.00	0.80
1:I:421:ARG:NH2	1:I:476:TYR:O	2.14	0.80
1:E:76:GLU:HB3	2:E:657:HOH:O	1.81	0.80
1:N:76:GLU:OE1	2:N:633:HOH:O	2.00	0.80
1:C:131:LEU:HD13	1:C:422:VAL:HG21	1.63	0.80
1:D:421:ARG:NH2	1:D:476:TYR:O	2.13	0.80
1:H:42:LYS:O	1:H:44:PHE:N	2.14	0.80
1:J:18:ARG:CB	2:J:650:HOH:O	2.18	0.80
1:A:384:ALA:C	2:A:632:HOH:O	2.19	0.79
1:L:202:PRO:O	1:L:205:ILE:HG13	1.83	0.79
1:C:404:ARG:HH11	1:C:404:ARG:HG2	1.46	0.79
1:J:156:GLU:OE2	2:J:667:HOH:O	2.00	0.79
1:C:518:GLU:OE2	2:C:653:HOH:O	1.99	0.79
1:F:131:LEU:HD13	1:F:422:VAL:HG21	1.65	0.79
1:C:31:LEU:CA	2:C:651:HOH:O	2.29	0.79
1:G:158:VAL:HG13	1:G:396:VAL:HG22	1.65	0.78
1:L:316:ASP:OD2	2:L:643:HOH:O	2.01	0.78
1:B:85:ALA:O	2:B:673:HOH:O	2.01	0.78
1:L:485:TYR:CD1	2:L:646:HOH:O	2.36	0.78
1:M:421:ARG:NH2	1:M:476:TYR:O	2.15	0.78
1:J:350:ARG:NE	2:J:643:HOH:O	2.13	0.78
1:A:359:ASP:N	2:A:620:HOH:O	2.16	0.78
1:D:420:ILE:HD12	1:D:451:LEU:HD13	1.66	0.78
1:E:362:ARG:HD2	2:E:674:HOH:O	1.82	0.78
1:C:350:ARG:HH11	1:C:350:ARG:CG	1.98	0.77
1:E:272:LYS:NZ	2:E:665:HOH:O	2.10	0.77
1:D:101:THR:O	2:D:640:HOH:O	2.01	0.77
1:E:209:GLU:O	2:E:679:HOH:O	2.02	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ASP:HB2	1:F:524:LEU:HD23	1.67	0.77
1:K:227:ILE:O	1:K:254:VAL:HA	1.83	0.77
1:D:183:LEU:O	1:D:184:GLN:HB2	1.81	0.77
1:E:130:GLU:HB3	1:E:422:VAL:HG22	1.65	0.77
2:E:665:HOH:O	1:F:256:GLY:HA3	1.82	0.77
1:I:284:ARG:NH2	2:I:601:HOH:O	2.17	0.77
1:A:44:PHE:HB2	2:A:660:HOH:O	1.85	0.76
1:F:130:GLU:HB3	1:F:422:VAL:HG22	1.67	0.76
1:I:353:ILE:N	2:I:637:HOH:O	2.17	0.76
1:K:58:ARG:HH11	1:K:58:ARG:CB	1.97	0.76
1:F:420:ILE:HD12	1:F:451:LEU:HD13	1.66	0.76
1:M:288:MET:HE3	2:M:653:HOH:O	1.85	0.76
1:B:183:LEU:O	1:B:184:GLN:HB2	1.84	0.76
1:G:484:GLU:O	2:G:653:HOH:O	2.02	0.76
1:D:61:GLU:OE1	2:D:652:HOH:O	2.04	0.76
1:F:262:LEU:HD22	1:F:273:VAL:HG21	1.66	0.76
1:K:318:GLY:O	2:K:636:HOH:O	2.04	0.76
1:F:173:GLY:O	1:F:404:ARG:NH2	2.19	0.76
1:G:169:VAL:HG11	1:G:377:ALA:HB2	1.68	0.76
1:M:54:VAL:HG22	1:M:89:THR:HG21	1.68	0.76
1:G:171:LYS:O	1:G:404:ARG:NH2	2.19	0.75
1:E:183:LEU:HD22	2:E:670:HOH:O	1.87	0.74
1:F:286:LYS:NZ	1:F:304:GLU:OE1	2.19	0.74
1:M:44:PHE:CD2	2:M:651:HOH:O	2.39	0.74
1:K:232:GLU:HB3	1:K:309:LEU:HB2	1.69	0.74
1:K:254:VAL:N	2:K:629:HOH:O	2.20	0.74
1:M:208:PRO:O	1:M:210:THR:N	2.20	0.74
1:B:185:ASP:O	2:B:665:HOH:O	2.06	0.74
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.70	0.74
1:K:44:PHE:O	2:K:632:HOH:O	2.06	0.74
1:D:7:LYS:NZ	2:D:637:HOH:O	2.19	0.74
1:I:270:ILE:HA	2:I:645:HOH:O	1.86	0.74
1:B:44:PHE:CA	2:B:667:HOH:O	2.35	0.74
1:E:3:ALA:O	2:E:677:HOH:O	2.04	0.74
1:A:44:PHE:O	2:A:660:HOH:O	2.05	0.74
1:D:271:VAL:HB	2:D:651:HOH:O	1.86	0.74
1:D:95:LEU:CA	2:D:661:HOH:O	2.26	0.74
1:K:232:GLU:HA	1:K:310:GLU:CD	2.08	0.74
1:E:235:PRO:HG3	1:E:310:GLU:HA	1.69	0.74
1:C:173:GLY:O	1:C:404:ARG:NH2	2.20	0.73
1:C:46:ALA:N	2:C:658:HOH:O	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:428:ASP:OD2	2:L:663:HOH:O	2.04	0.73
1:D:54:VAL:HG22	1:D:89:THR:HG21	1.68	0.73
1:G:18:ARG:NH2	2:G:654:HOH:O	2.19	0.73
1:G:326:ASN:ND2	1:G:329:THR:OG1	2.21	0.73
1:E:463:SER:OG	2:E:643:HOH:O	2.06	0.73
1:M:421:ARG:NH1	1:M:469:VAL:O	2.22	0.73
1:G:398:ASP:OD2	2:G:648:HOH:O	2.05	0.73
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.70	0.73
1:I:207:LYS:NZ	2:I:646:HOH:O	2.22	0.73
1:H:78:ALA:O	1:H:89:THR:HG22	1.89	0.73
1:N:327:LYS:O	2:N:648:HOH:O	2.06	0.73
1:M:158:VAL:HG13	1:M:396:VAL:HG22	1.70	0.73
1:H:261:THR:C	2:H:647:HOH:O	2.25	0.72
1:L:505:GLN:O	2:L:662:HOH:O	2.07	0.72
1:B:205:ILE:HG13	2:B:661:HOH:O	1.89	0.72
1:K:414:GLY:O	1:K:417:VAL:HG13	1.90	0.72
1:A:168:LYS:O	2:A:640:HOH:O	2.07	0.72
1:K:360:TYR:HB3	2:K:633:HOH:O	1.89	0.72
1:K:131:LEU:HD13	1:K:422:VAL:HG21	1.70	0.72
1:K:228:SER:O	1:K:257:GLU:HB3	1.90	0.72
1:F:171:LYS:O	1:F:404:ARG:NH1	2.22	0.72
1:K:228:SER:N	2:K:631:HOH:O	2.09	0.72
1:K:319:GLN:HG3	2:K:649:HOH:O	1.90	0.72
1:M:66:PHE:HA	1:M:69:MET:HE3	1.72	0.72
1:C:257:GLU:OE1	2:C:656:HOH:O	2.07	0.71
1:E:78:ALA:O	1:E:89:THR:HG22	1.89	0.71
1:H:339:GLU:HG2	2:H:634:HOH:O	1.89	0.71
1:K:358:SER:OG	2:K:633:HOH:O	2.07	0.71
1:L:485:TYR:OH	2:L:652:HOH:O	2.06	0.71
1:B:223:ALA:CA	2:B:658:HOH:O	2.30	0.71
1:M:235:PRO:HG3	1:M:310:GLU:HA	1.72	0.71
1:K:236:VAL:N	2:K:638:HOH:O	2.23	0.71
1:D:354:GLU:OE2	2:D:654:HOH:O	2.08	0.71
1:N:327:LYS:HD3	2:N:640:HOH:O	1.91	0.71
1:D:46:ALA:HB2	1:E:76:GLU:HG3	1.73	0.71
1:J:185:ASP:OD2	2:J:646:HOH:O	2.07	0.71
1:B:259:LEU:O	1:B:263:VAL:HG23	1.91	0.71
1:E:525:PRO:O	2:E:649:HOH:O	2.08	0.70
1:H:371:LYS:O	2:H:643:HOH:O	2.09	0.70
1:A:129:GLU:OE1	2:A:658:HOH:O	2.08	0.70
1:C:413:ALA:O	2:C:605:HOH:O	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:GLN:HG3	2:H:633:HOH:O	1.90	0.70
1:J:266:THR:O	2:J:647:HOH:O	2.08	0.70
1:L:285:ARG:HD2	2:L:651:HOH:O	1.92	0.70
1:K:229:ASN:O	2:K:640:HOH:O	2.10	0.70
1:I:479:ASN:O	1:I:483:GLU:N	2.24	0.70
1:B:423:ALA:O	2:B:664:HOH:O	2.10	0.69
1:K:235:PRO:C	2:K:638:HOH:O	2.30	0.69
1:K:44:PHE:HB3	2:K:632:HOH:O	1.90	0.69
1:K:482:THR:OG1	1:K:484:GLU:HG2	1.92	0.69
1:M:328:ASP:OD2	1:M:328:ASP:N	2.21	0.69
1:E:76:GLU:OE1	2:E:657:HOH:O	2.10	0.69
1:K:420:ILE:HG12	1:K:448:GLU:HG2	1.74	0.69
1:M:247:LEU:HB3	1:M:273:VAL:HG22	1.73	0.69
1:L:485:TYR:HD1	2:L:646:HOH:O	1.70	0.69
1:A:173:GLY:O	1:A:404:ARG:NH2	2.26	0.69
1:I:173:GLY:O	1:I:404:ARG:NH2	2.25	0.69
1:E:359:ASP:O	1:E:363:GLU:HG3	1.93	0.69
1:I:421:ARG:NH1	1:I:469:VAL:O	2.26	0.69
1:M:288:MET:CE	2:M:649:HOH:O	2.41	0.69
1:B:487:ASN:CB	2:B:652:HOH:O	2.41	0.68
1:G:514:MET:CG	2:G:666:HOH:O	2.40	0.68
1:B:490:ASP:OD1	2:B:679:HOH:O	2.11	0.68
1:N:194:GLN:NE2	2:N:643:HOH:O	2.25	0.68
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.74	0.68
1:E:239:ALA:HB1	1:E:314:LEU:HG	1.75	0.68
1:E:348:GLN:OE1	2:E:663:HOH:O	2.10	0.68
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.74	0.68
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.76	0.68
1:K:173:GLY:O	1:K:404:ARG:NH2	2.27	0.68
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.75	0.68
1:B:44:PHE:HA	2:B:667:HOH:O	1.92	0.68
1:C:183:LEU:O	1:C:184:GLN:HB2	1.92	0.68
1:C:408:GLU:OE1	2:C:642:HOH:O	2.10	0.68
1:J:288:MET:HE1	2:J:639:HOH:O	1.94	0.68
1:L:228:SER:O	1:L:257:GLU:HB3	1.94	0.68
1:H:219:PHE:CE2	1:H:245:LYS:HD2	2.29	0.68
1:I:270:ILE:C	2:I:645:HOH:O	2.31	0.68
1:N:411:VAL:HG23	1:N:489:ILE:HD13	1.76	0.68
1:A:183:LEU:O	1:A:184:GLN:HB2	1.94	0.68
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.24	0.68
1:M:173:GLY:O	1:M:404:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:327:LYS:NZ	2:N:633:HOH:O	2.18	0.68
1:H:254:VAL:O	2:H:632:HOH:O	2.10	0.67
1:D:28:LYS:HD2	1:D:453:GLN:OE1	1.94	0.67
1:D:420:ILE:HG12	1:D:448:GLU:HG2	1.77	0.67
1:E:420:ILE:HG12	1:E:448:GLU:HG2	1.74	0.67
1:B:340:ALA:N	2:B:655:HOH:O	2.09	0.67
1:L:411:VAL:HG23	1:L:489:ILE:HD13	1.77	0.67
1:M:43:SER:OG	2:M:651:HOH:O	2.13	0.67
1:N:13:ARG:NH2	1:N:518:GLU:OE2	2.25	0.67
1:C:346:VAL:HG12	1:C:350:ARG:HD2	1.76	0.67
1:D:6:VAL:O	2:D:660:HOH:O	2.13	0.67
1:K:254:VAL:CA	2:K:629:HOH:O	2.43	0.67
1:D:391:GLU:OE1	1:D:395:ARG:NH1	2.28	0.67
1:C:419:LEU:HD11	1:C:500:THR:HG23	1.77	0.66
1:K:46:ALA:HB2	1:L:76:GLU:HG3	1.76	0.66
1:L:384:ALA:O	1:L:385:THR:HG23	1.93	0.66
1:E:284:ARG:NH2	2:E:602:HOH:O	2.18	0.66
1:G:414:GLY:O	1:G:417:VAL:HG13	1.95	0.66
1:A:421:ARG:NH2	1:A:476:TYR:O	2.28	0.66
1:N:86:GLY:O	2:N:630:HOH:O	2.12	0.66
1:A:78:ALA:O	1:A:89:THR:HG22	1.95	0.66
1:H:42:LYS:C	1:H:44:PHE:H	1.99	0.66
1:K:358:SER:HB3	2:K:645:HOH:O	1.95	0.66
1:A:359:ASP:HA	1:A:362:ARG:NH1	2.11	0.66
1:I:460:GLU:OE2	2:I:659:HOH:O	2.13	0.66
1:N:94:VAL:O	2:N:632:HOH:O	2.14	0.66
1:J:193:MET:CE	1:J:292:ILE:HG12	2.26	0.66
1:C:30:THR:O	2:C:651:HOH:O	2.13	0.65
1:D:354:GLU:O	2:D:650:HOH:O	2.14	0.65
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.79	0.65
1:B:286:LYS:NZ	2:B:683:HOH:O	2.29	0.65
1:K:247:LEU:HB3	1:K:273:VAL:HG22	1.77	0.65
1:D:95:LEU:CB	2:D:661:HOH:O	2.16	0.65
1:G:319:GLN:OE1	2:G:670:HOH:O	2.15	0.65
1:K:227:ILE:HB	1:K:254:VAL:HG22	1.77	0.65
1:C:404:ARG:NH1	1:C:404:ARG:HG2	2.07	0.65
1:I:270:ILE:CA	2:I:645:HOH:O	2.43	0.65
1:K:232:GLU:HG3	2:K:640:HOH:O	1.97	0.65
1:G:82:ASN:H	1:G:89:THR:HG23	1.61	0.65
1:B:200:LEU:HD21	1:B:277:LYS:HG3	1.79	0.65
1:M:158:VAL:O	1:M:162:ILE:HG12	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:82:ASN:HB2	1:G:89:THR:CG2	2.27	0.64
1:H:338:GLU:OE1	2:H:634:HOH:O	2.15	0.64
1:J:183:LEU:O	2:J:645:HOH:O	2.15	0.64
1:L:312:ALA:HA	2:L:643:HOH:O	1.96	0.64
1:B:262:LEU:O	1:B:266:THR:HG23	1.98	0.64
1:B:447:MET:O	2:B:649:HOH:O	2.14	0.64
1:G:224:ASP:HB3	1:G:302:SER:HA	1.79	0.64
1:F:13:ARG:NH2	1:F:518:GLU:OE2	2.30	0.64
1:H:261:THR:N	2:H:647:HOH:O	2.26	0.64
1:J:262:LEU:O	1:J:266:THR:HG23	1.98	0.64
1:J:480:ALA:CB	2:J:661:HOH:O	2.45	0.64
1:J:479:ASN:HD22	1:J:493:ILE:HG13	1.63	0.64
1:I:302:SER:H	1:I:307:MET:HE3	1.63	0.64
1:J:18:ARG:CG	2:J:650:HOH:O	2.40	0.64
1:D:137:PRO:O	2:D:644:HOH:O	2.15	0.64
1:H:239:ALA:HB1	1:H:314:LEU:HD11	1.78	0.64
1:I:231:ARG:NE	2:I:639:HOH:O	2.29	0.64
1:J:183:LEU:HD22	1:J:184:GLN:H	1.63	0.64
1:G:122:LYS:HE2	1:G:429:LEU:HD11	1.79	0.63
1:I:414:GLY:O	1:I:417:VAL:HG13	1.98	0.63
1:M:208:PRO:O	1:M:211:GLY:N	2.24	0.63
1:L:54:VAL:HG22	1:L:89:THR:CG2	2.28	0.63
1:B:253:ASP:OD2	1:B:254:VAL:N	2.29	0.63
1:K:319:GLN:OE1	2:K:652:HOH:O	2.15	0.63
1:B:202:PRO:C	2:B:661:HOH:O	2.31	0.63
1:G:86:GLY:O	2:G:648:HOH:O	2.16	0.63
1:M:129:GLU:OE2	2:M:648:HOH:O	2.15	0.63
1:M:42:LYS:O	1:M:44:PHE:N	2.24	0.63
1:C:130:GLU:HB3	1:C:422:VAL:HG22	1.80	0.63
1:D:224:ASP:HB3	1:D:302:SER:HA	1.80	0.63
1:F:202:PRO:O	1:F:205:ILE:HG13	1.99	0.63
1:H:11:ASP:OD2	2:H:645:HOH:O	2.16	0.63
1:K:349:ILE:O	1:K:353:ILE:HG13	1.98	0.63
1:L:219:PHE:HB3	1:L:317:LEU:HD23	1.80	0.63
1:E:231:ARG:NH1	2:E:671:HOH:O	2.23	0.63
1:M:404:ARG:HG2	1:M:404:ARG:HH11	1.64	0.63
1:A:171:LYS:O	1:A:404:ARG:NH1	2.32	0.63
1:B:176:THR:HG21	1:B:333:ILE:HD11	1.80	0.63
1:I:166:MET:CE	1:I:171:LYS:HA	2.27	0.63
1:L:358:SER:OG	1:L:359:ASP:N	2.30	0.63
1:D:137:PRO:CB	2:D:644:HOH:O	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:ILE:HA	2:E:644:HOH:O	1.99	0.63
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.29	0.63
1:K:236:VAL:HG12	1:K:236:VAL:O	1.98	0.63
1:L:360:TYR:OH	2:L:635:HOH:O	2.15	0.63
1:E:433:ASN:HD21	1:E:435:ASP:HB2	1.64	0.62
1:F:183:LEU:O	1:F:184:GLN:HB2	1.97	0.62
1:K:236:VAL:CG2	2:K:638:HOH:O	2.39	0.62
1:G:420:ILE:HD12	1:G:451:LEU:HD13	1.81	0.62
1:J:339:GLU:C	2:J:656:HOH:O	2.38	0.62
1:K:194:GLN:O	1:K:371:LYS:HE3	1.99	0.62
1:J:384:ALA:C	2:J:644:HOH:O	2.32	0.62
1:B:404:ARG:HH11	1:B:404:ARG:HG2	1.63	0.62
1:J:184:GLN:OE1	2:J:645:HOH:O	2.16	0.62
1:M:199:TYR:HB3	1:M:201:SER:H	1.65	0.62
1:B:218:PRO:HD2	1:B:320:ALA:O	2.00	0.62
1:E:76:GLU:CB	2:E:657:HOH:O	2.38	0.62
1:L:234:LEU:H	1:L:235:PRO:CD	2.11	0.62
1:I:207:LYS:CE	2:I:646:HOH:O	2.48	0.62
1:L:486:GLY:C	2:L:660:HOH:O	2.23	0.62
1:M:415:GLY:O	1:M:451:LEU:HD12	2.00	0.62
1:K:310:GLU:OE1	1:K:310:GLU:N	2.32	0.62
1:L:463:SER:O	1:L:467:ASN:HB2	1.99	0.62
1:J:342:ILE:O	1:J:346:VAL:HG23	2.00	0.61
1:M:288:MET:CE	2:M:653:HOH:O	2.47	0.61
1:D:155:ASP:OD2	1:D:395:ARG:NH2	2.32	0.61
1:E:433:ASN:ND2	1:E:435:ASP:HB2	2.15	0.61
1:E:494:LEU:N	2:E:644:HOH:O	2.09	0.61
1:A:243:ALA:O	1:A:245:LYS:N	2.33	0.61
1:J:349:ILE:HA	1:J:352:GLN:HG3	1.83	0.61
1:J:266:THR:HA	2:J:647:HOH:O	2.01	0.61
1:J:285:ARG:NH1	2:J:649:HOH:O	2.05	0.61
1:D:137:PRO:CA	2:D:644:HOH:O	2.49	0.61
1:E:414:GLY:O	1:E:417:VAL:HG13	2.01	0.61
1:B:404:ARG:HG2	1:B:404:ARG:NH1	2.14	0.61
1:I:131:LEU:HD13	1:I:422:VAL:HG21	1.81	0.61
1:G:183:LEU:O	1:G:382:GLY:HA3	2.00	0.61
1:H:197:ARG:NH1	2:H:607:HOH:O	2.29	0.61
1:N:158:VAL:HG13	1:N:396:VAL:HG22	1.81	0.61
1:I:183:LEU:HD22	1:I:184:GLN:H	1.65	0.61
1:J:340:ALA:N	2:J:656:HOH:O	2.33	0.61
1:N:131:LEU:HD13	1:N:422:VAL:HG21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ALA:O	1:D:384:ALA:HB3	2.01	0.61
1:F:54:VAL:CG2	1:F:89:THR:HG21	2.30	0.61
1:H:130:GLU:HB3	1:H:422:VAL:HG22	1.82	0.61
1:J:414:GLY:O	1:J:417:VAL:HG13	2.00	0.61
1:A:131:LEU:HD13	1:A:422:VAL:HG21	1.82	0.60
1:D:366:GLN:HA	1:D:369:VAL:HG22	1.82	0.60
1:E:349:ILE:O	1:E:353:ILE:HG13	2.00	0.60
1:H:247:LEU:HD21	1:H:249:ILE:HD11	1.83	0.60
1:B:102:GLU:HB2	1:B:442:VAL:HG13	1.83	0.60
1:K:58:ARG:HB3	1:K:58:ARG:NH1	2.15	0.60
1:L:421:ARG:NH2	1:L:476:TYR:O	2.23	0.60
1:B:420:ILE:HG13	1:B:448:GLU:HG2	1.82	0.60
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.83	0.60
1:K:417:VAL:HG21	1:K:488:MET:HE3	1.83	0.60
1:N:235:PRO:HG3	1:N:310:GLU:HA	1.83	0.60
1:B:524:LEU:O	1:B:526:LYS:N	2.34	0.60
1:K:328:ASP:OD1	1:K:328:ASP:N	2.34	0.60
1:N:200:LEU:HD21	1:N:277:LYS:HG3	1.81	0.60
1:L:525:PRO:HD3	2:L:632:HOH:O	2.01	0.60
1:B:228:SER:N	2:B:672:HOH:O	2.07	0.60
1:G:169:VAL:CG1	1:G:377:ALA:HB2	2.32	0.60
1:A:82:ASN:HB2	1:A:89:THR:CG2	2.30	0.60
1:C:350:ARG:HH11	1:C:350:ARG:HG2	1.66	0.60
1:F:202:PRO:O	1:F:204:PHE:N	2.34	0.60
1:M:262:LEU:O	1:M:266:THR:HG23	2.01	0.60
1:M:404:ARG:HG2	1:M:404:ARG:NH1	2.17	0.60
1:C:45:GLY:HA3	2:C:658:HOH:O	2.00	0.59
1:B:131:LEU:HD13	1:B:422:VAL:HG21	1.83	0.59
1:H:314:LEU:H	1:H:314:LEU:HD12	1.67	0.59
1:I:353:ILE:HB	2:I:637:HOH:O	2.00	0.59
1:J:224:ASP:O	1:J:225:LYS:HB3	2.01	0.59
1:C:200:LEU:HD21	1:C:277:LYS:HG3	1.83	0.59
1:D:495:ASP:OD2	2:D:636:HOH:O	2.16	0.59
1:G:286:LYS:NZ	1:G:304:GLU:OE2	2.32	0.59
1:K:384:ALA:O	1:K:385:THR:HG23	2.02	0.59
1:L:121:ASP:OD1	2:L:630:HOH:O	2.16	0.59
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.84	0.59
1:E:158:VAL:HG13	1:E:396:VAL:HG22	1.83	0.59
1:H:479:ASN:HB2	1:H:484:GLU:O	2.02	0.59
1:H:420:ILE:HG12	1:H:448:GLU:HG2	1.85	0.59
1:I:322:ARG:HD2	2:I:658:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:LEU:O	1:C:526:LYS:N	2.36	0.59
1:H:287:ALA:HB1	1:H:368:ARG:NH1	2.18	0.59
1:M:218:PRO:HB3	1:M:246:PRO:HG2	1.85	0.59
1:D:291:ASP:OD2	1:D:368:ARG:HD2	2.03	0.59
1:B:44:PHE:C	2:B:667:HOH:O	2.33	0.59
1:E:183:LEU:HD13	1:E:184:GLN:HG3	1.83	0.59
1:E:524:LEU:O	1:E:526:LYS:N	2.36	0.59
1:H:448:GLU:OE2	2:H:625:HOH:O	2.17	0.59
1:G:429:LEU:HG	1:G:440:ILE:HD13	1.83	0.58
1:K:225:LYS:HD3	1:K:226:LYS:O	2.03	0.58
1:B:202:PRO:O	1:B:204:PHE:N	2.33	0.58
1:B:215:LEU:HB2	1:B:323:VAL:HG22	1.85	0.58
1:B:82:ASN:HB2	1:B:89:THR:OG1	2.03	0.58
1:G:131:LEU:HD13	1:G:422:VAL:HG21	1.85	0.58
1:K:182:GLY:HA2	1:L:281:PHE:CZ	2.38	0.58
1:G:200:LEU:HD21	1:G:277:LYS:HG3	1.86	0.58
1:H:414:GLY:O	1:H:417:VAL:HG13	2.03	0.58
1:J:155:ASP:OD1	1:J:157:THR:OG1	2.15	0.58
1:D:213:VAL:HB	1:D:325:ILE:HB	1.84	0.58
1:F:291:ASP:OD2	1:F:368:ARG:HD2	2.04	0.58
1:I:130:GLU:HB3	1:I:422:VAL:HG22	1.85	0.58
1:J:134:LEU:HD12	1:J:412:VAL:HG22	1.85	0.58
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.84	0.58
1:E:76:GLU:HG3	2:E:657:HOH:O	1.97	0.58
1:H:202:PRO:O	1:H:203:TYR:HB2	2.04	0.58
1:H:421:ARG:NH2	1:H:476:TYR:O	2.35	0.58
1:J:285:ARG:HD2	2:J:649:HOH:O	2.03	0.58
1:K:326:ASN:OD1	1:K:329:THR:N	2.36	0.58
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.86	0.58
1:E:525:PRO:C	2:E:649:HOH:O	2.40	0.58
1:D:411:VAL:HB	1:D:494:LEU:HD22	1.85	0.58
1:H:131:LEU:HD13	1:H:422:VAL:HG21	1.86	0.58
1:J:11:ASP:OD2	2:J:633:HOH:O	2.17	0.58
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.58
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.86	0.58
1:N:215:LEU:HB2	1:N:323:VAL:HG22	1.86	0.58
1:K:133:ALA:O	2:K:625:HOH:O	2.17	0.57
1:D:46:ALA:CB	1:E:76:GLU:HG3	2.33	0.57
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.86	0.57
1:K:13:ARG:HD2	1:K:104:LEU:HD22	1.85	0.57
1:M:248:LEU:HD13	1:M:325:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:MET:CE	2:B:680:HOH:O	2.47	0.57
1:C:142:LYS:O	1:C:146:GLN:HG3	2.05	0.57
1:E:13:ARG:HD2	1:E:104:LEU:HD22	1.86	0.57
1:K:361:ASP:OD2	2:K:645:HOH:O	2.17	0.57
1:D:92:ALA:C	2:D:661:HOH:O	2.38	0.57
1:H:194:GLN:O	1:H:371:LYS:HE3	2.04	0.57
1:L:486:GLY:HA2	2:L:660:HOH:O	1.83	0.57
1:N:247:LEU:CD2	1:N:249:ILE:HD11	2.33	0.57
1:D:414:GLY:O	1:D:417:VAL:HG13	2.04	0.57
1:H:435:ASP:OD2	2:H:624:HOH:O	2.18	0.57
1:J:131:LEU:HD13	1:J:422:VAL:HG21	1.86	0.57
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.85	0.57
1:B:242:LYS:C	1:B:244:GLY:H	2.08	0.57
1:I:262:LEU:O	1:I:266:THR:HG23	2.05	0.57
1:L:25:ASP:HA	1:L:28:LYS:HE2	1.85	0.57
1:N:414:GLY:O	1:N:417:VAL:HG13	2.04	0.57
1:D:239:ALA:HB1	1:D:314:LEU:HG	1.87	0.57
1:E:479:ASN:HB2	1:E:491:MET:HE1	1.86	0.57
1:L:225:LYS:HE3	1:L:303:GLU:HB2	1.85	0.57
1:M:193:MET:HE1	2:M:646:HOH:O	2.05	0.57
1:M:421:ARG:CD	2:M:656:HOH:O	2.25	0.57
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.85	0.56
1:D:203:TYR:HB2	1:D:263:VAL:HG13	1.87	0.56
1:N:262:LEU:O	1:N:266:THR:HG23	2.05	0.56
1:C:194:GLN:O	1:C:371:LYS:HE3	2.05	0.56
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.35	0.56
1:J:141:SER:CB	2:J:635:HOH:O	2.53	0.56
1:K:268:ARG:NH2	2:K:637:HOH:O	2.37	0.56
1:K:358:SER:CB	2:K:645:HOH:O	2.51	0.56
1:K:46:ALA:CB	1:L:76:GLU:HG3	2.34	0.56
1:M:421:ARG:NH1	2:M:656:HOH:O	2.11	0.56
1:D:57:ALA:O	1:D:75:LYS:HE3	2.05	0.56
1:G:291:ASP:OD2	1:G:368:ARG:HD2	2.05	0.56
1:L:312:ALA:CA	2:L:643:HOH:O	2.52	0.56
1:A:257:GLU:O	1:A:261:THR:OG1	2.23	0.56
1:B:472:GLY:HA3	1:B:476:TYR:CD2	2.40	0.56
1:D:423:ALA:O	2:D:657:HOH:O	2.17	0.56
1:F:200:LEU:HD21	1:F:277:LYS:HG3	1.86	0.56
1:I:411:VAL:HG23	1:I:489:ILE:HD13	1.86	0.56
1:A:420:ILE:CG1	1:A:448:GLU:HG2	2.35	0.56
1:D:82:ASN:HB2	1:D:89:THR:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:185:ASP:CG	2:J:646:HOH:O	2.43	0.56
1:D:214:GLU:OE2	1:D:322:ARG:NH2	2.39	0.56
1:F:94:VAL:O	2:F:645:HOH:O	2.18	0.56
1:J:62:LEU:HD13	1:J:68:ASN:HA	1.87	0.56
1:D:235:PRO:HG3	1:D:310:GLU:HA	1.88	0.56
1:E:231:ARG:HD2	2:E:671:HOH:O	2.06	0.56
1:N:327:LYS:CD	2:N:640:HOH:O	2.51	0.56
1:G:57:ALA:O	1:G:75:LYS:HE3	2.06	0.56
1:H:381:VAL:HG21	1:H:393:LYS:HB2	1.88	0.56
1:J:18:ARG:HG2	2:J:650:HOH:O	2.05	0.56
1:K:7:LYS:HG3	1:K:66:PHE:CZ	2.40	0.56
1:L:100:ILE:O	1:L:104:LEU:HG	2.06	0.56
1:M:179:ASP:OD1	1:M:390:LYS:NZ	2.39	0.56
1:J:82:ASN:CB	2:J:628:HOH:O	2.31	0.55
1:D:326:ASN:HD22	1:D:329:THR:HB	1.72	0.55
1:G:383:ALA:HB3	1:G:389:MET:HB2	1.88	0.55
1:K:421:ARG:NH2	1:K:476:TYR:O	2.39	0.55
1:B:491:MET:HE1	2:B:680:HOH:O	2.06	0.55
1:C:155:ASP:OD2	1:C:395:ARG:NH2	2.40	0.55
1:D:451:LEU:HD11	1:D:469:VAL:HG21	1.89	0.55
1:I:479:ASN:HB2	1:I:491:MET:SD	2.46	0.55
1:K:235:PRO:CG	1:K:310:GLU:HA	2.36	0.55
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.89	0.55
1:A:452:ARG:NH1	2:A:604:HOH:O	2.36	0.55
1:D:266:THR:HG22	1:D:273:VAL:H	1.71	0.55
1:N:95:LEU:O	1:N:99:ILE:HG13	2.06	0.55
1:B:34:LYS:HD2	1:B:458:CYS:HA	1.89	0.55
1:E:200:LEU:HD21	1:E:277:LYS:HG3	1.87	0.55
1:F:366:GLN:HA	1:F:369:VAL:HG22	1.89	0.55
1:H:358:SER:HB3	1:H:361:ASP:OD2	2.05	0.55
1:L:5:ASP:OD2	2:L:632:HOH:O	2.18	0.55
1:M:253:ASP:OD2	1:M:254:VAL:N	2.39	0.55
1:N:221:LEU:HD23	1:N:249:ILE:HD12	1.87	0.55
1:D:158:VAL:HG13	1:D:396:VAL:HG22	1.89	0.55
1:H:144:ILE:HG23	1:H:403:THR:HG21	1.87	0.55
1:C:214:GLU:HG3	1:C:324:VAL:HG22	1.88	0.55
1:A:353:ILE:HG23	1:A:362:ARG:HG3	1.88	0.55
1:D:54:VAL:CG2	1:D:89:THR:HG21	2.36	0.55
1:I:183:LEU:O	1:I:184:GLN:HB2	2.06	0.55
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.37	0.55
1:A:239:ALA:HB1	1:A:314:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASN:C	1:A:481:ALA:H	2.11	0.55
1:G:366:GLN:HA	1:G:369:VAL:HG22	1.88	0.55
1:N:415:GLY:O	1:N:451:LEU:HD12	2.06	0.55
1:B:487:ASN:N	2:B:652:HOH:O	1.99	0.54
1:F:259:LEU:O	1:F:263:VAL:HG23	2.07	0.54
1:I:287:ALA:HB1	1:I:368:ARG:NH1	2.22	0.54
1:J:359:ASP:OD1	1:J:362:ARG:NH1	2.39	0.54
1:K:44:PHE:CB	2:K:632:HOH:O	2.52	0.54
1:A:69:MET:O	1:A:73:MET:HG3	2.07	0.54
1:L:352:GLN:HA	2:L:638:HOH:O	2.07	0.54
1:L:421:ARG:NH1	1:L:469:VAL:O	2.40	0.54
1:M:473:ASP:O	1:M:476:TYR:HB3	2.07	0.54
1:G:524:LEU:O	1:G:526:LYS:N	2.37	0.54
1:I:166:MET:HE2	1:I:171:LYS:HA	1.88	0.54
1:A:202:PRO:O	1:A:205:ILE:HG13	2.07	0.54
1:B:225:LYS:NZ	1:B:232:GLU:OE2	2.32	0.54
1:C:33:PRO:O	1:C:35:GLY:N	2.40	0.54
1:C:353:ILE:HD13	1:C:366:GLN:HG3	1.89	0.54
1:D:105:LYS:HG3	2:D:640:HOH:O	2.07	0.54
1:E:142:LYS:O	1:E:146:GLN:HG3	2.07	0.54
1:J:5:ASP:OD1	2:J:671:HOH:O	2.18	0.54
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.90	0.54
1:N:186:GLU:HB2	1:N:380:LYS:HB2	1.90	0.54
1:F:69:MET:O	1:F:73:MET:HG3	2.06	0.54
1:A:479:ASN:O	1:A:481:ALA:N	2.41	0.54
1:B:349:ILE:O	1:B:353:ILE:HG13	2.08	0.54
1:G:23:LEU:HD23	1:G:74:VAL:HG22	1.88	0.54
1:G:479:ASN:ND2	1:G:482:THR:OG1	2.41	0.54
1:J:364:LYS:NZ	2:J:639:HOH:O	2.39	0.54
1:D:218:PRO:HB3	1:D:246:PRO:HG2	1.89	0.54
1:E:76:GLU:OE2	2:E:668:HOH:O	2.18	0.54
1:C:414:GLY:O	1:C:417:VAL:HG13	2.08	0.54
1:F:524:LEU:O	1:F:526:LYS:N	2.40	0.54
1:G:82:ASN:HB2	1:G:89:THR:HG23	1.88	0.54
1:K:102:GLU:HB2	1:K:442:VAL:HG13	1.90	0.54
1:K:411:VAL:HG23	1:K:489:ILE:HD13	1.89	0.54
1:C:23:LEU:HD23	1:C:74:VAL:HG22	1.90	0.54
1:I:181:THR:O	1:J:282:GLY:HA3	2.08	0.54
1:K:142:LYS:HE3	1:K:146:GLN:NE2	2.23	0.54
1:K:44:PHE:C	2:K:632:HOH:O	2.45	0.54
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HD13	1:A:366:GLN:HG3	1.89	0.53
1:G:82:ASN:HB2	1:G:89:THR:HG21	1.89	0.53
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.90	0.53
1:K:349:ILE:HA	1:K:352:GLN:HG3	1.89	0.53
1:K:350:ARG:HG3	1:K:353:ILE:HD12	1.89	0.53
1:K:183:LEU:O	1:K:382:GLY:HA3	2.08	0.53
1:N:28:LYS:HD2	1:N:453:GLN:OE1	2.08	0.53
1:C:202:PRO:O	1:C:204:PHE:N	2.39	0.53
1:I:215:LEU:HB2	1:I:323:VAL:HG22	1.91	0.53
1:K:38:VAL:HG13	1:L:519:CYS:HB3	1.88	0.53
1:A:366:GLN:HA	1:A:369:VAL:HG22	1.90	0.53
1:H:258:ALA:O	1:H:262:LEU:HG	2.08	0.53
1:I:27:VAL:CG1	1:I:90:THR:HG23	2.38	0.53
1:L:420:ILE:HG12	1:L:448:GLU:HG2	1.90	0.53
1:L:5:ASP:HB2	1:L:524:LEU:HD12	1.90	0.53
1:M:199:TYR:CZ	1:M:205:ILE:HD11	2.44	0.53
1:A:168:LYS:HB3	2:A:640:HOH:O	2.09	0.53
1:A:257:GLU:OE1	2:A:652:HOH:O	2.19	0.53
1:E:455:VAL:HG13	1:E:460:GLU:HB2	1.89	0.53
1:I:207:LYS:HE3	2:I:646:HOH:O	2.08	0.53
1:A:194:GLN:O	1:A:371:LYS:HE3	2.09	0.53
1:E:492:GLY:O	2:E:644:HOH:O	2.19	0.53
1:I:496:PRO:HB2	1:I:499:VAL:HG13	1.91	0.53
1:A:206:ASN:O	1:A:207:LYS:HD2	2.09	0.53
1:B:414:GLY:O	1:B:417:VAL:HG13	2.09	0.53
1:F:314:LEU:HD23	1:F:317:LEU:HD12	1.91	0.53
1:K:344:GLY:O	1:K:347:ALA:HB3	2.09	0.53
1:F:86:GLY:O	2:F:635:HOH:O	2.19	0.53
1:H:183:LEU:O	1:H:382:GLY:HA3	2.08	0.53
1:J:480:ALA:HB2	2:J:661:HOH:O	2.06	0.53
1:B:487:ASN:HB3	2:B:652:HOH:O	2.07	0.53
1:I:140:ASP:OD2	1:I:142:LYS:HB3	2.09	0.53
1:K:420:ILE:HD12	1:K:451:LEU:CD1	2.38	0.53
1:K:82:ASN:HB2	1:K:89:THR:OG1	2.08	0.53
1:J:464:VAL:O	1:J:468:THR:HG23	2.09	0.52
1:M:420:ILE:HG12	1:M:448:GLU:HG2	1.92	0.52
1:F:247:LEU:HD21	1:F:249:ILE:HD11	1.90	0.52
1:E:493:ILE:CA	2:E:644:HOH:O	2.57	0.52
1:M:5:ASP:HB2	1:M:524:LEU:HD12	1.92	0.52
1:N:383:ALA:O	1:N:384:ALA:HB3	2.09	0.52
1:J:82:ASN:ND2	2:J:628:HOH:O	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:236:VAL:HG22	1:L:312:ALA:O	2.10	0.52
1:N:82:ASN:HB2	1:N:89:THR:HB	1.90	0.52
1:M:220:ILE:O	1:M:220:ILE:HG22	2.09	0.52
1:D:219:PHE:CE2	1:D:245:LYS:HD2	2.45	0.52
1:D:131:LEU:HD13	1:D:422:VAL:HG21	1.91	0.52
1:E:76:GLU:CD	2:E:657:HOH:O	2.40	0.52
1:I:176:THR:HG21	1:I:333:ILE:HD13	1.92	0.52
1:N:176:THR:HG21	1:N:333:ILE:HD13	1.91	0.52
1:C:409:GLU:OE1	2:C:649:HOH:O	2.19	0.52
1:D:137:PRO:N	2:D:644:HOH:O	2.36	0.52
1:I:72:GLN:HE22	1:I:75:LYS:HE3	1.74	0.52
1:B:266:THR:HG21	1:B:273:VAL:HB	1.91	0.52
1:C:248:LEU:HD13	1:C:325:ILE:HD11	1.91	0.52
1:E:262:LEU:O	1:E:266:THR:HG23	2.10	0.52
1:H:140:ASP:OD2	1:H:142:LYS:HB3	2.09	0.52
1:I:218:PRO:HB3	1:I:246:PRO:HG2	1.91	0.52
1:I:350:ARG:HA	1:I:353:ILE:HD12	1.91	0.52
1:J:193:MET:HE3	1:J:292:ILE:HG12	1.91	0.52
1:H:225:LYS:NZ	1:H:232:GLU:OE1	2.35	0.52
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.92	0.52
1:K:158:VAL:HG13	1:K:396:VAL:HG22	1.92	0.52
1:K:420:ILE:CD1	1:K:451:LEU:HD13	2.38	0.52
1:F:219:PHE:HB3	1:F:317:LEU:HD13	1.92	0.52
1:I:200:LEU:HD21	1:I:277:LYS:HG3	1.91	0.52
1:N:479:ASN:HB3	1:N:484:GLU:H	1.75	0.52
1:B:142:LYS:O	1:B:146:GLN:HG3	2.10	0.51
1:C:217:SER:O	1:C:245:LYS:HD3	2.10	0.51
1:C:383:ALA:O	1:C:384:ALA:HB3	2.09	0.51
1:G:296:THR:HB	1:G:319:GLN:H	1.75	0.51
1:M:476:TYR:HB2	2:M:632:HOH:O	2.09	0.51
1:D:200:LEU:HD21	1:D:277:LYS:HG3	1.91	0.51
1:F:301:ILE:HD11	1:F:316:ASP:HB3	1.91	0.51
1:H:23:LEU:CD2	1:H:74:VAL:HG22	2.41	0.51
1:I:11:ASP:OD2	2:I:640:HOH:O	2.18	0.51
1:C:291:ASP:OD2	1:C:368:ARG:HD2	2.10	0.51
1:D:178:GLU:HA	1:D:393:LYS:HE3	1.92	0.51
1:D:411:VAL:HG23	1:D:489:ILE:HD13	1.90	0.51
1:D:69:MET:O	1:D:73:MET:HG3	2.09	0.51
1:I:488:MET:HA	1:I:491:MET:HE2	1.92	0.51
1:K:176:THR:HG21	1:K:333:ILE:HD13	1.92	0.51
1:L:72:GLN:OE1	1:L:75:LYS:HE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ASN:HB3	2:A:652:HOH:O	2.11	0.51
1:A:76:GLU:HG3	1:G:46:ALA:HB2	1.93	0.51
1:G:202:PRO:O	1:G:204:PHE:N	2.41	0.51
1:M:184:GLN:OE1	1:M:184:GLN:HA	2.09	0.51
1:A:28:LYS:HD2	1:A:453:GLN:OE1	2.10	0.51
1:A:348:GLN:NE2	2:A:606:HOH:O	2.37	0.51
1:E:288:MET:HG2	1:E:368:ARG:HD3	1.93	0.51
1:E:291:ASP:OD2	1:E:368:ARG:HD2	2.11	0.51
1:I:314:LEU:HA	1:I:317:LEU:HD22	1.93	0.51
1:J:141:SER:HB3	2:J:635:HOH:O	2.10	0.51
1:B:291:ASP:OD2	1:B:368:ARG:HD2	2.11	0.51
1:B:421:ARG:NH2	1:B:476:TYR:O	2.43	0.51
1:I:217:SER:HA	1:I:320:ALA:O	2.11	0.51
1:K:27:VAL:CG1	1:K:90:THR:HG23	2.40	0.51
1:K:417:VAL:HG11	1:K:488:MET:CE	2.41	0.51
1:L:486:GLY:HA3	2:L:660:HOH:O	1.85	0.51
1:K:193:MET:HG3	1:K:371:LYS:HB3	1.92	0.51
1:A:247:LEU:HD21	1:A:249:ILE:HD11	1.91	0.51
1:B:247:LEU:HD21	1:B:249:ILE:HD11	1.92	0.51
1:C:215:LEU:HB2	1:C:323:VAL:HG22	1.92	0.51
1:C:33:PRO:C	1:C:35:GLY:H	2.14	0.51
1:C:420:ILE:HG13	1:C:448:GLU:HG2	1.93	0.51
1:E:355:GLU:HB3	2:E:648:HOH:O	2.10	0.51
1:M:57:ALA:O	1:M:75:LYS:HD2	2.11	0.51
1:E:215:LEU:HB2	1:E:323:VAL:HG22	1.91	0.51
1:E:455:VAL:CG1	1:E:460:GLU:HB2	2.41	0.51
1:G:353:ILE:HD13	1:G:366:GLN:HG3	1.92	0.51
1:G:383:ALA:O	1:G:384:ALA:HB3	2.10	0.51
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.93	0.51
1:C:31:LEU:HD13	1:C:90:THR:HG21	1.92	0.51
1:E:28:LYS:HD2	1:E:453:GLN:OE1	2.11	0.51
1:F:284:ARG:NH1	1:F:367:GLU:OE1	2.40	0.51
1:M:221:LEU:HD23	1:M:249:ILE:HG12	1.92	0.51
1:N:165:ALA:O	1:N:169:VAL:HG22	2.12	0.50
1:N:183:LEU:O	1:N:184:GLN:HB2	2.10	0.50
1:C:350:ARG:HH11	1:C:350:ARG:HG3	1.76	0.50
1:E:176:THR:HG21	1:E:333:ILE:HD13	1.92	0.50
1:E:383:ALA:O	1:E:384:ALA:HB3	2.11	0.50
1:E:82:ASN:HB2	1:E:89:THR:HG23	1.93	0.50
1:L:202:PRO:O	1:L:204:PHE:N	2.44	0.50
1:B:266:THR:CG2	1:B:273:VAL:HB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:ALA:O	1:B:385:THR:HG23	2.11	0.50
1:D:500:THR:HG22	2:D:638:HOH:O	2.10	0.50
1:F:23:LEU:HD23	1:F:74:VAL:HG22	1.93	0.50
1:G:130:GLU:HB3	1:G:422:VAL:HG22	1.92	0.50
1:H:496:PRO:HB2	1:H:499:VAL:HG13	1.94	0.50
1:L:218:PRO:HD2	1:L:320:ALA:O	2.12	0.50
1:A:372:LEU:O	2:A:633:HOH:O	2.20	0.50
1:F:479:ASN:O	1:F:481:ALA:N	2.43	0.50
1:I:342:ILE:O	1:I:346:VAL:HG23	2.11	0.50
1:J:111:MET:O	2:J:651:HOH:O	2.19	0.50
1:K:240:VAL:HG21	1:K:247:LEU:HB2	1.93	0.50
1:L:336:VAL:HG12	1:L:336:VAL:O	2.11	0.50
1:M:7:LYS:HG3	1:M:66:PHE:CZ	2.47	0.50
1:D:137:PRO:HB2	2:D:644:HOH:O	2.10	0.50
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.92	0.50
1:D:63:GLU:HB2	1:E:524:LEU:HD11	1.94	0.50
1:G:242:LYS:C	1:G:244:GLY:H	2.15	0.50
1:J:359:ASP:O	1:J:363:GLU:HG3	2.12	0.50
1:L:414:GLY:O	1:L:417:VAL:HG13	2.11	0.50
1:N:242:LYS:C	1:N:244:GLY:H	2.15	0.50
1:N:193:MET:CE	1:N:292:ILE:HG12	2.42	0.50
1:N:310:GLU:OE1	1:N:310:GLU:N	2.43	0.50
1:A:383:ALA:O	1:A:384:ALA:HB3	2.11	0.50
1:G:202:PRO:O	1:G:203:TYR:HB2	2.12	0.50
1:H:160:LYS:O	1:H:164:GLU:HG3	2.11	0.50
1:H:383:ALA:O	1:H:384:ALA:HB3	2.12	0.50
1:M:326:ASN:OD1	1:M:329:THR:N	2.45	0.50
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.94	0.50
1:J:141:SER:HB2	2:J:635:HOH:O	2.11	0.50
1:J:42:LYS:NZ	1:J:46:ALA:O	2.45	0.50
1:C:314:LEU:HD23	1:C:317:LEU:HD22	1.93	0.49
1:D:16:MET:HB3	1:D:514:MET:CE	2.41	0.49
1:F:383:ALA:O	1:F:384:ALA:HB3	2.12	0.49
1:A:524:LEU:HD11	1:G:63:GLU:HB2	1.93	0.49
1:J:200:LEU:HD21	1:J:277:LYS:HG3	1.94	0.49
1:J:479:ASN:ND2	1:J:493:ILE:HG13	2.26	0.49
1:K:236:VAL:HG21	1:K:312:ALA:HB3	1.94	0.49
1:H:90:THR:O	1:H:94:VAL:HG13	2.11	0.49
1:K:198:GLY:O	1:K:276:VAL:HG12	2.12	0.49
1:K:68:ASN:O	1:K:72:GLN:HG2	2.12	0.49
1:M:348:GLN:O	1:M:351:GLN:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:ILE:CG1	1:C:448:GLU:HG2	2.43	0.49
1:C:476:TYR:HA	1:C:486:GLY:O	2.11	0.49
1:G:93:THR:OG1	2:G:669:HOH:O	2.20	0.49
1:J:495:ASP:OD1	2:J:660:HOH:O	2.20	0.49
1:L:383:ALA:O	1:L:384:ALA:HB3	2.11	0.49
1:M:220:ILE:O	1:M:220:ILE:CG2	2.60	0.49
1:A:359:ASP:HA	1:A:362:ARG:HH12	1.76	0.49
1:B:351:GLN:NE2	1:B:355:GLU:OE1	2.45	0.49
1:C:158:VAL:HG13	1:C:396:VAL:HG22	1.94	0.49
1:E:266:THR:HG21	1:E:273:VAL:O	2.12	0.49
1:E:498:LYS:NZ	2:E:661:HOH:O	2.44	0.49
1:F:70:GLY:HA2	1:F:73:MET:HE2	1.94	0.49
1:H:82:ASN:HB3	1:H:89:THR:HG23	1.95	0.49
1:A:76:GLU:HG3	1:G:46:ALA:CB	2.41	0.49
1:C:242:LYS:C	1:C:244:GLY:H	2.15	0.49
1:C:321:LYS:HB2	1:C:334:ASP:HB3	1.93	0.49
1:M:219:PHE:HB3	1:M:317:LEU:HD23	1.95	0.49
1:D:242:LYS:C	1:D:244:GLY:H	2.15	0.49
1:E:362:ARG:HG2	1:E:366:GLN:NE2	2.27	0.49
1:J:266:THR:CA	2:J:647:HOH:O	2.60	0.49
1:M:183:LEU:O	1:M:184:GLN:HB2	2.12	0.49
1:N:525:PRO:HD3	2:N:645:HOH:O	2.11	0.49
1:B:409:GLU:OE2	1:B:501:ARG:NH2	2.33	0.49
1:E:242:LYS:C	1:E:244:GLY:H	2.15	0.49
1:F:421:ARG:NH1	1:F:469:VAL:O	2.46	0.49
1:A:455:VAL:HG13	1:A:460:GLU:HB2	1.93	0.49
1:B:383:ALA:HB3	1:B:389:MET:HB2	1.94	0.49
1:C:260:ALA:O	1:C:263:VAL:HG12	2.12	0.49
1:F:242:LYS:C	1:F:244:GLY:H	2.16	0.49
1:G:82:ASN:N	1:G:89:THR:HG23	2.28	0.49
1:J:366:GLN:HA	1:J:369:VAL:HG22	1.95	0.49
1:K:524:LEU:O	1:K:526:LYS:N	2.45	0.49
1:F:25:ASP:OD1	1:F:28:LYS:HE2	2.12	0.49
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.95	0.49
1:I:436:GLN:O	1:I:440:ILE:HG13	2.13	0.49
1:J:134:LEU:CD1	1:J:412:VAL:HG22	2.42	0.49
1:E:78:ALA:O	1:E:89:THR:CG2	2.60	0.49
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.94	0.49
1:K:57:ALA:O	1:K:75:LYS:HD2	2.13	0.49
1:M:130:GLU:HB3	1:M:422:VAL:HG22	1.95	0.49
1:H:262:LEU:O	1:H:266:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:226:LYS:HG3	1:K:253:ASP:HB3	1.95	0.48
1:L:485:TYR:O	1:L:486:GLY:O	2.31	0.48
1:N:203:TYR:HB2	1:N:263:VAL:HG13	1.95	0.48
1:B:242:LYS:O	1:B:243:ALA:HB3	2.12	0.48
1:J:193:MET:HE1	1:J:292:ILE:HG12	1.93	0.48
1:J:254:VAL:HG12	1:J:259:LEU:HB2	1.95	0.48
1:J:281:PHE:HD1	1:J:284:ARG:HH21	1.60	0.48
1:M:479:ASN:C	1:M:481:ALA:H	2.15	0.48
1:A:200:LEU:HD21	1:A:277:LYS:HG3	1.93	0.48
1:F:466:ALA:O	1:F:470:LYS:HG3	2.13	0.48
1:H:455:VAL:HG13	1:H:460:GLU:HB2	1.95	0.48
1:I:176:THR:HG22	1:I:177:VAL:N	2.27	0.48
1:J:288:MET:O	1:J:292:ILE:HG13	2.14	0.48
1:B:383:ALA:O	1:B:384:ALA:HB3	2.13	0.48
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.43	0.48
1:F:524:LEU:HD22	1:F:525:PRO:HD2	1.96	0.48
1:H:353:ILE:HG23	1:H:362:ARG:HG3	1.94	0.48
1:I:353:ILE:CA	2:I:637:HOH:O	2.57	0.48
1:K:230:ILE:N	1:K:257:GLU:OE1	2.42	0.48
1:L:25:ASP:OD1	1:L:28:LYS:HE2	2.14	0.48
1:A:221:LEU:HD23	1:A:249:ILE:HD12	1.96	0.48
1:G:83:ASP:OD2	1:G:327:LYS:HD3	2.14	0.48
1:J:219:PHE:HB3	1:J:317:LEU:HD23	1.96	0.48
1:D:265:ASN:ND2	2:D:612:HOH:O	2.46	0.48
1:G:242:LYS:O	1:G:243:ALA:HB3	2.14	0.48
1:A:102:GLU:HB2	1:A:442:VAL:HG13	1.96	0.48
1:H:354:GLU:C	1:H:356:ALA:H	2.17	0.48
1:J:240:VAL:HG11	1:J:247:LEU:HB2	1.95	0.48
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.44	0.48
1:N:66:PHE:CZ	1:N:522:THR:HG22	2.49	0.48
1:C:183:LEU:HA	1:C:383:ALA:N	2.29	0.48
1:D:217:SER:N	1:D:218:PRO:CD	2.76	0.48
1:D:349:ILE:O	1:D:353:ILE:HG13	2.13	0.48
1:D:46:ALA:HB2	1:E:76:GLU:CG	2.43	0.48
1:K:224:ASP:O	1:K:225:LYS:HB3	2.13	0.48
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.44	0.48
1:C:476:TYR:HB3	1:C:485:TYR:OH	2.14	0.48
1:F:179:ASP:OD2	1:F:393:LYS:HE3	2.14	0.48
1:F:28:LYS:HD2	1:F:453:GLN:OE1	2.14	0.48
1:J:46:ALA:HB2	1:K:76:GLU:HG3	1.96	0.48
1:K:366:GLN:HA	1:K:369:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:PRO:HB3	1:C:246:PRO:HG2	1.94	0.48
1:I:142:LYS:O	1:I:146:GLN:HG3	2.14	0.48
1:I:392:LYS:O	1:I:396:VAL:HG23	2.14	0.48
1:K:326:ASN:HD21	1:K:329:THR:HB	1.79	0.48
1:K:358:SER:N	2:K:645:HOH:O	2.47	0.48
1:N:218:PRO:HB3	1:N:246:PRO:HG2	1.94	0.48
1:A:124:VAL:HG21	1:A:508:ALA:HB2	1.96	0.47
1:F:349:ILE:CG2	1:F:369:VAL:HG13	2.44	0.47
1:F:451:LEU:HD11	1:F:469:VAL:HG21	1.95	0.47
1:I:359:ASP:O	1:I:363:GLU:HG2	2.14	0.47
1:I:383:ALA:HB3	1:I:389:MET:HA	1.96	0.47
1:J:412:VAL:HG13	1:J:418:ALA:HB2	1.96	0.47
1:K:219:PHE:O	1:K:247:LEU:HD12	2.15	0.47
1:L:118:ARG:HD2	1:L:436:GLN:HE22	1.78	0.47
1:L:477:GLY:O	1:L:485:TYR:HA	2.14	0.47
1:C:18:ARG:HG2	1:C:67:GLU:CD	2.35	0.47
1:F:420:ILE:CD1	1:F:451:LEU:HD13	2.42	0.47
1:G:232:GLU:HB3	1:G:309:LEU:HB3	1.95	0.47
1:G:460:GLU:O	1:G:462:PRO:HD3	2.14	0.47
1:I:16:MET:O	1:I:20:VAL:HG13	2.14	0.47
1:I:235:PRO:HG2	2:I:634:HOH:O	2.12	0.47
1:J:524:LEU:O	1:J:526:LYS:N	2.47	0.47
1:K:183:LEU:HG	1:K:384:ALA:HB2	1.96	0.47
1:C:24:ALA:HA	1:C:27:VAL:HG12	1.97	0.47
1:D:33:PRO:HG3	1:D:480:ALA:HB1	1.96	0.47
1:F:139:SER:O	1:F:171:LYS:NZ	2.29	0.47
1:E:484:GLU:HG3	2:E:645:HOH:O	2.15	0.47
1:M:349:ILE:HA	1:M:352:GLN:HG3	1.96	0.47
1:M:155:ASP:OD2	1:M:395:ARG:NH2	2.48	0.47
1:D:319:GLN:O	1:D:336:VAL:HG23	2.14	0.47
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.95	0.47
1:M:205:ILE:HG23	1:M:212:ALA:O	2.14	0.47
1:M:271:VAL:HG12	1:M:273:VAL:HG23	1.97	0.47
1:F:413:ALA:HB3	1:F:417:VAL:HG22	1.95	0.47
1:I:319:GLN:HB3	1:I:336:VAL:HG21	1.96	0.47
1:I:5:ASP:HB2	1:I:524:LEU:HD12	1.96	0.47
1:K:186:GLU:HB2	1:K:380:LYS:HB2	1.97	0.47
1:L:230:ILE:HG21	1:L:261:THR:HG21	1.96	0.47
1:L:118:ARG:HD2	1:L:436:GLN:NE2	2.29	0.47
1:B:263:VAL:O	1:B:267:MET:HB2	2.15	0.47
1:B:270:ILE:H	1:B:270:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:ILE:HG23	1:C:494:LEU:HD23	1.95	0.47
1:D:484:GLU:CG	2:D:656:HOH:O	2.44	0.47
1:E:25:ASP:HA	1:E:28:LYS:HE2	1.95	0.47
1:K:473:ASP:OD2	1:K:473:ASP:N	2.47	0.47
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.97	0.47
1:K:360:TYR:CB	2:K:633:HOH:O	2.55	0.47
1:N:205:ILE:HA	1:N:213:VAL:HG22	1.97	0.47
1:B:197:ARG:HD2	1:B:277:LYS:HB2	1.96	0.47
1:B:219:PHE:HB3	1:B:317:LEU:HD23	1.96	0.47
1:C:122:LYS:HE2	1:C:429:LEU:HD11	1.96	0.47
1:D:451:LEU:HD23	1:D:451:LEU:C	2.35	0.47
1:H:526:LYS:HD3	1:H:526:LYS:HA	1.69	0.47
1:J:135:SER:HA	1:J:412:VAL:HG23	1.97	0.47
1:C:413:ALA:CB	1:C:417:VAL:HG22	2.43	0.47
1:C:473:ASP:O	1:C:476:TYR:HB2	2.15	0.47
1:E:421:ARG:NH2	1:E:476:TYR:O	2.48	0.47
1:L:392:LYS:O	1:L:396:VAL:HG23	2.15	0.47
1:M:441:LYS:O	1:M:445:ARG:HB2	2.15	0.47
1:B:524:LEU:HD12	1:B:525:PRO:HD2	1.97	0.47
1:D:20:VAL:HB	1:D:74:VAL:HG11	1.97	0.47
1:G:273:VAL:HG12	1:G:274:ALA:N	2.30	0.47
1:K:7:LYS:HD3	1:K:11:ASP:OD1	2.15	0.47
1:N:142:LYS:O	1:N:146:GLN:HG3	2.15	0.47
1:N:290:GLN:HB3	1:N:345:ARG:NH2	2.30	0.47
2:H:652:HOH:O	1:N:36:ARG:NH2	2.48	0.47
1:A:301:ILE:HD12	1:A:312:ALA:HB2	1.98	0.46
1:D:176:THR:HG21	1:D:333:ILE:HD13	1.97	0.46
1:D:339:GLU:CD	1:D:339:GLU:H	2.18	0.46
1:G:229:ASN:HA	2:G:616:HOH:O	2.15	0.46
1:N:366:GLN:HA	1:N:369:VAL:HG22	1.97	0.46
1:B:178:GLU:HA	1:B:393:LYS:HE3	1.97	0.46
1:B:349:ILE:CG2	1:B:369:VAL:HG13	2.45	0.46
1:C:31:LEU:HD13	1:C:90:THR:CG2	2.45	0.46
1:G:16:MET:O	1:G:20:VAL:HG13	2.15	0.46
1:K:193:MET:CE	1:K:292:ILE:HG12	2.45	0.46
1:A:301:ILE:HG21	1:A:309:LEU:HD23	1.97	0.46
1:D:262:LEU:O	1:D:266:THR:HG23	2.14	0.46
1:E:149:THR:HG23	1:E:155:ASP:C	2.36	0.46
1:E:526:LYS:HE2	2:E:649:HOH:O	2.16	0.46
1:H:202:PRO:C	1:H:204:PHE:H	2.19	0.46
1:N:463:SER:O	1:N:467:ASN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASN:HB2	1:A:484:GLU:H	1.80	0.46
1:F:397:GLU:O	1:F:401:HIS:ND1	2.47	0.46
1:F:97:GLN:HB3	2:F:645:HOH:O	2.15	0.46
1:K:319:GLN:HA	2:K:636:HOH:O	2.14	0.46
1:K:463:SER:O	1:K:467:ASN:HB2	2.15	0.46
1:F:359:ASP:O	1:F:363:GLU:HG3	2.16	0.46
1:K:258:ALA:O	1:K:262:LEU:HG	2.16	0.46
1:L:430:ARG:HD2	2:L:633:HOH:O	2.16	0.46
1:D:501:ARG:NH1	1:D:505:GLN:OE1	2.46	0.46
1:F:223:ALA:O	1:F:251:ALA:HA	2.15	0.46
1:G:28:LYS:HD2	1:G:453:GLN:OE1	2.16	0.46
1:H:31:LEU:HD13	1:H:90:THR:CG2	2.45	0.46
1:L:222:LEU:HD23	1:L:250:ILE:HB	1.96	0.46
1:L:400:LEU:O	1:L:404:ARG:HG2	2.16	0.46
1:A:203:TYR:HB2	1:A:263:VAL:HG13	1.97	0.46
1:H:198:GLY:HA3	1:H:327:LYS:O	2.16	0.46
1:K:222:LEU:HD23	1:K:250:ILE:HB	1.97	0.46
1:L:472:GLY:HA3	1:L:476:TYR:CD2	2.51	0.46
1:L:484:GLU:HA	2:L:646:HOH:O	2.14	0.46
1:M:54:VAL:HG22	1:M:89:THR:CG2	2.44	0.46
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.97	0.46
1:E:131:LEU:HD13	1:E:422:VAL:HG21	1.97	0.46
1:E:472:GLY:HA3	1:E:476:TYR:CD2	2.51	0.46
1:E:40:LEU:HD13	1:E:59:GLU:HG3	1.98	0.46
1:G:202:PRO:C	1:G:204:PHE:H	2.18	0.46
1:I:183:LEU:HD23	1:I:383:ALA:HA	1.98	0.46
1:M:27:VAL:CG1	1:M:90:THR:HG23	2.46	0.46
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.70	0.46
1:C:398:ASP:OD2	1:C:399:ALA:N	2.49	0.46
1:L:193:MET:CE	1:L:292:ILE:HG12	2.45	0.46
1:N:225:LYS:NZ	1:N:232:GLU:OE2	2.48	0.46
1:N:358:SER:O	1:N:362:ARG:HB2	2.16	0.46
1:B:77:VAL:HG12	1:B:506:TYR:HB3	1.97	0.46
1:C:359:ASP:HA	1:C:362:ARG:HH11	1.81	0.46
1:E:372:LEU:HA	1:E:372:LEU:HD12	1.75	0.46
1:F:131:LEU:HA	1:F:131:LEU:HD12	1.77	0.46
1:I:121:ASP:O	1:I:125:THR:HG23	2.16	0.46
1:J:201:SER:HA	1:J:202:PRO:HD3	1.81	0.46
1:K:235:PRO:HG2	1:K:310:GLU:HA	1.98	0.46
1:L:57:ALA:O	1:L:75:LYS:HD2	2.16	0.46
1:A:85:ALA:HB1	1:A:499:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:SER:O	1:C:202:PRO:O	2.34	0.45
1:C:220:ILE:HD12	1:C:296:THR:HG21	1.97	0.45
1:D:253:ASP:OD1	1:D:254:VAL:N	2.50	0.45
1:E:350:ARG:O	1:E:353:ILE:HB	2.16	0.45
1:F:266:THR:CG2	1:F:273:VAL:H	2.28	0.45
1:H:315:GLU:O	1:H:315:GLU:HG2	2.16	0.45
1:M:479:ASN:O	1:M:481:ALA:N	2.46	0.45
1:C:409:GLU:HB2	2:C:601:HOH:O	2.15	0.45
1:F:218:PRO:CB	1:F:246:PRO:HG2	2.44	0.45
1:J:257:GLU:C	2:J:670:HOH:O	2.54	0.45
1:J:350:ARG:CD	2:J:643:HOH:O	2.61	0.45
1:K:240:VAL:HG13	1:K:271:VAL:HG11	1.97	0.45
1:B:324:VAL:HB	1:B:331:THR:HG23	1.98	0.45
1:D:216:GLU:C	1:D:218:PRO:HD3	2.37	0.45
1:E:82:ASN:OD1	1:E:89:THR:OG1	2.31	0.45
1:G:524:LEU:HA	1:G:524:LEU:HD12	1.75	0.45
1:I:319:GLN:HB3	1:I:336:VAL:CG2	2.47	0.45
1:J:432:GLN:NE2	2:J:672:HOH:O	2.49	0.45
1:L:339:GLU:OE2	2:L:659:HOH:O	2.20	0.45
1:M:305:ILE:O	1:M:305:ILE:HG22	2.17	0.45
1:N:144:ILE:HG23	1:N:403:THR:HG21	1.97	0.45
1:E:118:ARG:HD2	1:E:436:GLN:HE22	1.81	0.45
1:F:266:THR:CG2	1:F:273:VAL:HG22	2.46	0.45
1:F:218:PRO:HD2	1:F:320:ALA:O	2.17	0.45
1:G:69:MET:O	1:G:73:MET:HG3	2.16	0.45
1:I:82:ASN:HB2	1:I:89:THR:OG1	2.16	0.45
1:J:421:ARG:NH2	1:J:476:TYR:O	2.49	0.45
1:K:219:PHE:HB3	1:K:317:LEU:HD23	1.97	0.45
1:L:183:LEU:HD13	1:L:184:GLN:N	2.31	0.45
1:N:183:LEU:HD22	1:N:184:GLN:H	1.82	0.45
1:N:5:ASP:HB2	1:N:524:LEU:HD12	1.99	0.45
1:A:372:LEU:HD12	1:A:372:LEU:HA	1.83	0.45
1:B:284:ARG:O	1:B:288:MET:HG3	2.16	0.45
1:D:193:MET:HG3	1:D:371:LYS:HB3	1.98	0.45
1:E:349:ILE:CG2	1:E:369:VAL:HG13	2.47	0.45
1:F:234:LEU:HB2	1:F:235:PRO:HD3	1.97	0.45
1:H:24:ALA:O	1:H:28:LYS:HG2	2.16	0.45
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.98	0.45
1:J:463:SER:O	1:J:467:ASN:HB2	2.17	0.45
1:K:124:VAL:HG21	1:K:508:ALA:HB2	1.98	0.45
1:L:352:GLN:CA	2:L:638:HOH:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:142:LYS:O	1:M:146:GLN:HG3	2.16	0.45
1:C:359:ASP:O	1:C:363:GLU:HG3	2.17	0.45
1:E:169:VAL:CG1	1:E:377:ALA:HB2	2.46	0.45
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.99	0.45
1:G:266:THR:HB	2:G:640:HOH:O	2.16	0.45
1:H:144:ILE:HG23	1:H:403:THR:CG2	2.46	0.45
1:H:519:CYS:HB3	1:N:38:VAL:HB	1.98	0.45
1:K:16:MET:O	1:K:20:VAL:HG13	2.17	0.45
1:L:524:LEU:O	1:L:526:LYS:N	2.46	0.45
1:A:61:GLU:HG2	2:A:638:HOH:O	2.17	0.45
1:B:310:GLU:OE1	1:B:310:GLU:N	2.50	0.45
1:D:16:MET:O	1:D:20:VAL:HG13	2.17	0.45
1:F:463:SER:CB	2:N:650:HOH:O	2.48	0.45
1:G:193:MET:HG3	1:G:371:LYS:HB3	1.98	0.45
1:I:13:ARG:HD2	1:I:104:LEU:HD22	1.98	0.45
1:I:314:LEU:O	1:I:317:LEU:HB2	2.16	0.45
1:I:353:ILE:CB	2:I:637:HOH:O	2.60	0.45
1:I:349:ILE:O	1:I:353:ILE:HG13	2.17	0.45
1:I:157:THR:HG21	1:I:392:LYS:NZ	2.31	0.45
1:J:90:THR:OG1	2:J:640:HOH:O	2.20	0.45
1:N:217:SER:N	1:N:218:PRO:CD	2.80	0.45
1:D:137:PRO:C	2:D:644:HOH:O	2.52	0.45
1:F:247:LEU:HB3	1:F:273:VAL:HG12	1.98	0.45
1:H:270:ILE:O	1:H:271:VAL:HB	2.17	0.45
1:M:391:GLU:OE1	1:M:395:ARG:NH1	2.50	0.45
1:M:54:VAL:CG2	1:M:89:THR:HG21	2.42	0.45
1:B:301:ILE:HG21	1:B:309:LEU:HD23	1.97	0.45
1:B:296:THR:HB	1:B:319:GLN:H	1.82	0.45
1:B:364:LYS:HD3	1:B:364:LYS:HA	1.68	0.45
1:B:473:ASP:OD2	2:B:678:HOH:O	2.21	0.45
1:C:131:LEU:HD21	1:C:500:THR:HG22	1.99	0.45
1:D:271:VAL:O	2:D:651:HOH:O	2.21	0.45
1:F:524:LEU:HD23	1:F:524:LEU:HA	1.83	0.45
1:L:37:ASN:OD1	1:L:51:LYS:HE3	2.16	0.45
1:M:224:ASP:O	1:M:225:LYS:HB3	2.17	0.45
1:N:16:MET:HG3	1:N:520:MET:SD	2.56	0.45
1:F:247:LEU:CD2	1:F:249:ILE:HD11	2.47	0.45
1:G:138:CYS:SG	1:G:147:VAL:HG21	2.57	0.45
1:G:183:LEU:O	1:G:184:GLN:O	2.35	0.45
1:H:284:ARG:O	1:H:288:MET:HG3	2.16	0.45
1:J:5:ASP:HB2	1:J:524:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:229:ASN:C	1:K:231:ARG:H	2.21	0.45
1:K:404:ARG:HH11	1:K:404:ARG:CG	2.30	0.45
1:L:176:THR:HG21	1:L:333:ILE:HD11	1.99	0.45
1:L:455:VAL:HG13	1:L:460:GLU:HB2	2.00	0.45
1:A:266:THR:CG2	1:A:273:VAL:H	2.31	0.44
1:A:392:LYS:O	1:A:396:VAL:HG23	2.17	0.44
1:A:77:VAL:HG12	1:A:506:TYR:HB3	1.99	0.44
1:C:219:PHE:CE2	1:C:245:LYS:HD2	2.52	0.44
1:D:479:ASN:OD1	1:D:483:GLU:HA	2.16	0.44
1:E:475:ASN:ND2	2:E:608:HOH:O	2.30	0.44
1:F:183:LEU:O	1:F:184:GLN:CB	2.65	0.44
1:F:364:LYS:O	1:F:367:GLU:HG3	2.17	0.44
1:F:26:ALA:HA	1:G:8:PHE:HE1	1.82	0.44
1:I:336:VAL:O	1:I:336:VAL:HG12	2.16	0.44
1:J:235:PRO:CG	1:J:310:GLU:HA	2.38	0.44
1:L:50:THR:OG1	1:L:51:LYS:N	2.49	0.44
1:N:201:SER:HA	1:N:202:PRO:HD3	1.85	0.44
1:N:420:ILE:HG12	1:N:448:GLU:HG2	2.00	0.44
1:A:130:GLU:HG3	1:A:425:LYS:NZ	2.33	0.44
1:A:214:GLU:OE2	1:A:322:ARG:NH2	2.40	0.44
1:C:391:GLU:OE1	1:C:395:ARG:NH1	2.50	0.44
1:E:487:ASN:O	1:E:491:MET:HG3	2.17	0.44
1:F:239:ALA:HB1	1:F:314:LEU:HG	1.99	0.44
1:J:338:GLU:C	1:J:340:ALA:H	2.20	0.44
1:J:384:ALA:CA	2:J:644:HOH:O	2.65	0.44
1:K:100:ILE:O	1:K:104:LEU:HG	2.18	0.44
1:B:204:PHE:CD1	1:B:273:VAL:O	2.70	0.44
1:E:169:VAL:HG11	1:E:377:ALA:HB2	1.99	0.44
1:H:165:ALA:O	1:H:169:VAL:HG22	2.18	0.44
1:I:356:ALA:HB3	2:I:653:HOH:O	2.16	0.44
1:J:196:ASP:OD2	2:J:641:HOH:O	2.21	0.44
1:A:158:VAL:HG13	1:A:396:VAL:HG22	2.00	0.44
1:D:219:PHE:O	1:D:247:LEU:HD12	2.16	0.44
1:D:220:ILE:HD12	1:D:296:THR:HG21	1.98	0.44
1:I:72:GLN:NE2	1:I:75:LYS:HE3	2.32	0.44
1:K:305:ILE:O	1:K:305:ILE:HG22	2.17	0.44
1:L:142:LYS:O	1:L:146:GLN:HG3	2.17	0.44
1:L:524:LEU:HD12	1:L:524:LEU:HA	1.82	0.44
1:M:183:LEU:HD22	1:M:184:GLN:H	1.82	0.44
1:M:83:ASP:OD2	1:M:327:LYS:HD3	2.17	0.44
1:N:44:PHE:HD1	1:N:44:PHE:H	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG13	1:B:396:VAL:HG22	1.99	0.44
1:C:223:ALA:O	1:C:251:ALA:HA	2.18	0.44
1:F:414:GLY:O	1:F:417:VAL:HG13	2.16	0.44
1:I:350:ARG:C	2:I:637:HOH:O	2.45	0.44
1:D:463:SER:HB3	1:I:461:GLU:OE2	2.17	0.44
1:J:291:ASP:OD1	1:J:368:ARG:NH1	2.51	0.44
1:L:223:ALA:O	1:L:251:ALA:HA	2.17	0.44
1:E:29:VAL:HG11	1:F:518:GLU:HB3	1.99	0.44
1:I:272:LYS:N	1:I:272:LYS:HD2	2.33	0.44
1:I:57:ALA:O	1:I:75:LYS:HD2	2.18	0.44
1:J:13:ARG:NH2	1:J:518:GLU:OE2	2.48	0.44
1:N:482:THR:OG1	1:N:484:GLU:HG2	2.18	0.44
1:D:77:VAL:HG12	1:D:506:TYR:HB3	1.99	0.44
1:H:221:LEU:HD23	1:H:249:ILE:HD12	1.99	0.44
1:J:218:PRO:HD2	1:J:320:ALA:O	2.18	0.44
1:J:242:LYS:O	1:J:243:ALA:HB3	2.18	0.44
1:J:291:ASP:OD2	1:J:368:ARG:HD2	2.18	0.44
1:D:383:ALA:O	1:D:384:ALA:CB	2.65	0.44
1:E:131:LEU:HD21	1:E:500:THR:HG22	1.98	0.44
1:F:103:GLY:O	1:F:107:VAL:HG23	2.18	0.44
1:I:183:LEU:HB2	1:I:384:ALA:H	1.82	0.44
1:I:195:PHE:HB2	1:I:279:PRO:HB3	2.00	0.44
1:K:247:LEU:O	1:K:273:VAL:HG13	2.17	0.44
1:K:417:VAL:HG11	1:K:488:MET:HE3	1.99	0.44
1:L:324:VAL:HB	1:L:331:THR:HG23	1.99	0.44
1:L:27:VAL:HG12	1:L:90:THR:HG23	2.00	0.44
1:A:218:PRO:HD2	1:A:320:ALA:O	2.18	0.44
1:D:77:VAL:HG21	1:D:510:VAL:HG13	1.99	0.44
1:F:197:ARG:HD2	1:F:277:LYS:HB2	2.00	0.44
1:G:165:ALA:O	1:G:169:VAL:HG22	2.18	0.44
1:K:142:LYS:HE3	1:K:146:GLN:HE21	1.82	0.44
1:A:230:ILE:HG12	1:A:258:ALA:HA	1.99	0.43
1:A:124:VAL:HG21	1:A:508:ALA:CB	2.48	0.43
1:B:144:ILE:HG23	1:B:403:THR:HG21	1.99	0.43
1:C:286:LYS:NZ	1:C:304:GLU:OE1	2.51	0.43
1:K:227:ILE:CD1	1:K:309:LEU:HD11	2.48	0.43
1:L:290:GLN:HA	1:L:290:GLN:OE1	2.18	0.43
1:G:463:SER:HB3	1:M:461:GLU:OE2	2.17	0.43
1:N:311:LYS:HE2	1:N:311:LYS:HB3	1.82	0.43
1:A:225:LYS:HB2	1:A:225:LYS:HE3	1.89	0.43
1:A:420:ILE:HG12	1:A:448:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:ILE:HG22	1:F:305:ILE:O	2.18	0.43
1:G:176:THR:HG21	1:G:333:ILE:HD13	2.00	0.43
1:H:404:ARG:HG2	1:H:404:ARG:HH11	1.83	0.43
1:N:191:GLU:O	1:N:334:ASP:HA	2.18	0.43
1:D:311:LYS:HB3	1:D:311:LYS:HE2	1.85	0.43
1:D:74:VAL:HA	1:D:510:VAL:HG11	2.00	0.43
1:E:383:ALA:HB3	1:E:389:MET:HB2	2.00	0.43
1:F:77:VAL:HG11	1:F:510:VAL:HB	2.00	0.43
1:G:215:LEU:HB2	1:G:323:VAL:HG22	2.00	0.43
1:H:100:ILE:O	1:H:104:LEU:HG	2.18	0.43
1:H:158:VAL:HG13	1:H:396:VAL:HG22	2.00	0.43
1:H:202:PRO:O	1:H:203:TYR:CB	2.67	0.43
1:H:204:PHE:O	1:H:213:VAL:HG22	2.18	0.43
1:K:171:LYS:HB2	1:K:171:LYS:HE3	1.84	0.43
1:N:103:GLY:O	1:N:107:VAL:HG23	2.17	0.43
1:N:72:GLN:OE1	1:N:75:LYS:HE2	2.19	0.43
1:A:326:ASN:HD22	1:A:329:THR:HB	1.83	0.43
1:E:314:LEU:HD23	1:E:317:LEU:HD22	2.00	0.43
1:E:219:PHE:HB3	1:E:317:LEU:HD23	2.01	0.43
1:F:18:ARG:HG2	1:F:67:GLU:CD	2.38	0.43
1:H:404:ARG:HG2	1:H:404:ARG:NH1	2.33	0.43
1:I:31:LEU:HA	1:I:31:LEU:HD12	1.85	0.43
1:C:350:ARG:CG	1:C:350:ARG:NH1	2.68	0.43
1:D:286:LYS:HE2	1:D:286:LYS:HB3	1.66	0.43
1:D:215:LEU:HB2	1:D:323:VAL:HG22	2.00	0.43
1:E:180:GLY:HA2	1:E:380:LYS:HB3	2.01	0.43
1:I:176:THR:CG2	1:I:177:VAL:N	2.81	0.43
1:K:284:ARG:CZ	1:K:284:ARG:HB2	2.48	0.43
1:L:262:LEU:O	1:L:266:THR:HG23	2.17	0.43
1:M:16:MET:HB3	1:M:514:MET:CE	2.48	0.43
1:M:200:LEU:HD21	1:M:277:LYS:HG3	2.00	0.43
1:M:194:GLN:O	1:M:371:LYS:HE2	2.17	0.43
1:N:166:MET:CE	1:N:171:LYS:HA	2.48	0.43
1:N:57:ALA:O	1:N:75:LYS:HD2	2.17	0.43
1:H:66:PHE:CZ	1:H:522:THR:HG22	2.54	0.43
1:J:152:ALA:O	1:J:153:ASN:HB2	2.19	0.43
1:K:230:ILE:HG13	1:K:233:MET:HB3	2.00	0.43
1:K:150:ILE:HD13	1:K:492:GLY:HA2	2.00	0.43
1:M:200:LEU:HG	1:M:276:VAL:HA	2.00	0.43
1:C:16:MET:HB3	1:C:514:MET:HE1	2.00	0.43
1:E:42:LYS:HB3	1:E:42:LYS:HE2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:ILE:HD12	1:F:233:MET:HG3	2.00	0.43
1:G:16:MET:HB3	1:G:514:MET:CE	2.49	0.43
1:G:230:ILE:HD12	1:G:261:THR:HB	1.99	0.43
1:G:194:GLN:O	1:G:371:LYS:HE3	2.19	0.43
1:K:383:ALA:HB3	1:K:389:MET:CA	2.49	0.43
1:N:74:VAL:HA	1:N:510:VAL:HG21	1.99	0.43
1:B:205:ILE:CB	2:B:661:HOH:O	2.66	0.43
1:D:224:ASP:O	1:D:225:LYS:HB3	2.19	0.43
1:I:230:ILE:HD13	1:I:261:THR:CG2	2.49	0.43
1:J:49:ILE:HD12	1:K:513:LEU:HD13	1.99	0.43
1:L:301:ILE:HA	1:L:307:MET:SD	2.59	0.43
1:B:288:MET:HG2	1:B:368:ARG:HD3	2.01	0.43
1:C:286:LYS:HB3	1:C:286:LYS:HE2	1.75	0.43
1:C:413:ALA:HB3	1:C:417:VAL:HG22	2.01	0.43
1:C:455:VAL:HG21	1:C:465:VAL:HG11	2.00	0.43
1:E:284:ARG:O	1:E:288:MET:HG3	2.18	0.43
1:G:124:VAL:HG21	1:G:508:ALA:HB2	2.01	0.43
1:H:201:SER:C	1:H:202:PRO:O	2.56	0.43
1:H:27:VAL:CG1	1:H:90:THR:HG23	2.48	0.43
1:M:162:ILE:HD12	1:M:400:LEU:HD13	2.00	0.43
1:D:449:ALA:HB3	1:D:450:PRO:HD3	2.01	0.43
1:E:82:ASN:HB2	1:E:89:THR:CG2	2.49	0.43
1:G:18:ARG:HG2	1:G:67:GLU:CD	2.39	0.43
1:H:57:ALA:O	1:H:75:LYS:HD2	2.19	0.43
1:I:22:VAL:HG11	1:I:62:LEU:HD21	2.01	0.43
1:I:46:ALA:HA	1:I:47:PRO:HD3	1.90	0.43
1:L:130:GLU:HB3	1:L:422:VAL:HG22	2.00	0.43
1:L:66:PHE:CZ	1:L:522:THR:HG22	2.54	0.43
1:M:203:TYR:HB2	1:M:263:VAL:HG13	2.00	0.43
1:A:273:VAL:HG12	1:A:274:ALA:N	2.33	0.42
1:B:205:ILE:CG1	2:B:661:HOH:O	2.57	0.42
1:D:524:LEU:O	1:D:526:LYS:N	2.41	0.42
1:F:311:LYS:HD3	1:F:311:LYS:HA	1.82	0.42
1:F:339:GLU:O	1:F:343:GLN:HG2	2.19	0.42
1:J:36:ARG:O	1:J:51:LYS:HG2	2.19	0.42
1:L:31:LEU:HD13	1:L:90:THR:CG2	2.49	0.42
1:B:34:LYS:HB2	1:B:458:CYS:SG	2.59	0.42
1:E:359:ASP:N	2:E:659:HOH:O	1.98	0.42
1:F:235:PRO:HG2	1:F:310:GLU:HA	2.01	0.42
1:G:372:LEU:HD12	1:G:372:LEU:HA	1.77	0.42
1:I:247:LEU:HB3	1:I:273:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:215:LEU:O	1:J:322:ARG:HA	2.19	0.42
1:J:338:GLU:O	1:J:340:ALA:N	2.52	0.42
1:J:392:LYS:O	1:J:396:VAL:HG23	2.19	0.42
1:L:420:ILE:HD12	1:L:451:LEU:HD13	2.01	0.42
1:N:140:ASP:OD2	1:N:142:LYS:HB3	2.18	0.42
1:A:291:ASP:OD2	1:A:368:ARG:HD2	2.20	0.42
1:B:201:SER:C	1:B:202:PRO:O	2.57	0.42
1:F:463:SER:HA	2:N:650:HOH:O	2.17	0.42
1:J:130:GLU:HB3	1:J:422:VAL:HG22	2.01	0.42
1:J:66:PHE:CZ	1:J:522:THR:HG22	2.54	0.42
1:K:269:GLY:HA3	1:L:257:GLU:HB2	2.02	0.42
1:L:193:MET:HG3	1:L:371:LYS:HB3	2.00	0.42
1:B:429:LEU:HG	1:B:440:ILE:HD13	2.00	0.42
1:D:16:MET:HB3	1:D:514:MET:HE3	2.00	0.42
1:D:270:ILE:O	2:D:651:HOH:O	2.21	0.42
1:E:203:TYR:HB2	1:E:263:VAL:HG13	2.01	0.42
1:F:242:LYS:N	1:F:242:LYS:HD3	2.34	0.42
1:G:421:ARG:NH2	1:G:476:TYR:O	2.46	0.42
1:H:235:PRO:HG3	1:H:310:GLU:HA	2.01	0.42
1:J:221:LEU:HD11	1:J:301:ILE:HD12	2.01	0.42
1:J:232:GLU:OE2	1:J:309:LEU:HD12	2.19	0.42
1:J:262:LEU:HD22	1:J:273:VAL:HG11	2.01	0.42
1:L:241:ALA:HB2	1:L:271:VAL:HG21	2.00	0.42
1:B:223:ALA:O	1:B:251:ALA:HA	2.19	0.42
1:B:247:LEU:CD2	1:B:249:ILE:HD11	2.48	0.42
1:D:13:ARG:HD2	1:D:104:LEU:HD22	2.00	0.42
1:C:46:ALA:HB2	1:D:76:GLU:HG3	2.01	0.42
1:H:136:VAL:HA	1:H:137:PRO:HD3	1.78	0.42
1:H:460:GLU:O	1:H:462:PRO:HD3	2.19	0.42
1:H:124:VAL:HG21	1:H:508:ALA:CB	2.50	0.42
1:K:420:ILE:CG1	1:K:448:GLU:HG2	2.48	0.42
1:M:404:ARG:O	1:M:407:VAL:HG12	2.20	0.42
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.57	0.42
1:C:24:ALA:O	1:C:28:LYS:HG2	2.19	0.42
1:D:251:ALA:O	1:D:278:ALA:N	2.49	0.42
1:D:484:GLU:HG2	2:D:643:HOH:O	2.19	0.42
1:H:28:LYS:HD2	1:H:453:GLN:OE1	2.19	0.42
1:J:286:LYS:HE3	1:J:286:LYS:HB2	1.87	0.42
1:J:462:PRO:HD2	2:J:606:HOH:O	2.20	0.42
1:A:349:ILE:O	1:A:353:ILE:HG13	2.19	0.42
1:C:116:LEU:HA	1:C:116:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:THR:HB	1:D:319:GLN:H	1.84	0.42
1:D:199:TYR:CZ	1:D:327:LYS:HA	2.54	0.42
1:G:326:ASN:HD22	1:G:329:THR:HG1	1.68	0.42
1:H:16:MET:O	1:H:20:VAL:HG12	2.19	0.42
1:I:155:ASP:OD1	1:I:157:THR:HB	2.20	0.42
1:N:228:SER:O	1:N:257:GLU:HB3	2.19	0.42
1:A:135:SER:HB2	1:A:497:THR:OG1	2.19	0.42
1:A:176:THR:HG21	1:A:333:ILE:HD13	2.02	0.42
1:D:142:LYS:O	1:D:146:GLN:HG3	2.20	0.42
1:D:372:LEU:HA	1:D:372:LEU:HD12	1.83	0.42
1:C:46:ALA:CB	1:D:76:GLU:HG3	2.49	0.42
1:E:266:THR:HG22	1:E:273:VAL:H	1.84	0.42
1:E:420:ILE:CD1	1:E:451:LEU:HD13	2.39	0.42
1:F:383:ALA:HB3	1:F:389:MET:HB2	2.01	0.42
1:H:54:VAL:HG21	1:H:82:ASN:HD22	1.83	0.42
1:J:336:VAL:HG12	1:J:336:VAL:O	2.19	0.42
1:L:289:LEU:HA	1:L:289:LEU:HD23	1.86	0.42
1:L:342:ILE:O	1:L:346:VAL:HG23	2.20	0.42
1:A:463:SER:HB3	1:L:461:GLU:OE2	2.20	0.42
1:M:196:ASP:O	1:M:197:ARG:O	2.38	0.42
1:N:289:LEU:HA	1:N:289:LEU:HD23	1.79	0.42
1:A:140:ASP:OD2	1:A:142:LYS:HB3	2.20	0.42
1:B:58:ARG:NH1	2:B:660:HOH:O	2.53	0.42
1:B:82:ASN:HD22	1:B:89:THR:HB	1.85	0.42
1:D:286:LYS:NZ	1:D:304:GLU:OE1	2.46	0.42
1:G:205:ILE:HG23	1:G:212:ALA:O	2.20	0.42
1:F:182:GLY:HA2	1:G:281:PHE:CE2	2.55	0.42
1:G:7:LYS:HE3	1:G:15:LYS:HE3	2.02	0.42
1:I:248:LEU:HD13	1:I:325:ILE:HD11	2.01	0.42
1:K:25:ASP:OD1	1:K:28:LYS:HE2	2.19	0.42
1:L:164:GLU:OE1	2:L:655:HOH:O	2.21	0.42
1:K:39:VAL:HG12	1:L:69:MET:CE	2.50	0.42
1:M:146:GLN:O	1:M:150:ILE:HG13	2.20	0.42
1:M:191:GLU:O	1:M:334:ASP:HA	2.19	0.42
1:N:183:LEU:HA	1:N:383:ALA:N	2.35	0.42
1:A:411:VAL:HG12	1:A:496:PRO:HA	2.02	0.42
1:B:149:THR:HG23	1:B:155:ASP:C	2.40	0.42
1:B:203:TYR:C	2:B:661:HOH:O	2.58	0.42
1:B:242:LYS:C	1:B:244:GLY:N	2.73	0.42
1:E:242:LYS:O	1:E:243:ALA:HB3	2.19	0.42
1:E:178:GLU:HA	1:E:393:LYS:HE2	2.02	0.42

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
1:H:17:LEU:HD22	1:H:104:LEU:HD12	2.02	0.42
1:H:305:ILE:O	1:H:305:ILE:HG22	2.19	0.42
1:H:436:GLN:O	1:H:440:ILE:HG13	2.20	0.42
1:A:180:GLY:HA2	1:A:380:LYS:HB3	2.01	0.41
1:E:46:ALA:HB2	1:F:76:GLU:HG3	2.01	0.41
1:H:23:LEU:HD23	1:H:74:VAL:HG22	2.01	0.41
1:I:183:LEU:HA	1:I:383:ALA:N	2.35	0.41
1:L:441:LYS:HA	1:L:441:LYS:HD3	1.88	0.41
1:N:392:LYS:O	1:N:396:VAL:HG23	2.19	0.41
1:C:198:GLY:HA3	1:C:327:LYS:O	2.19	0.41
1:D:479:ASN:HD22	1:D:491:MET:CE	2.33	0.41
1:F:449:ALA:HB3	1:F:450:PRO:HD3	2.01	0.41
1:I:434:GLU:HG3	2:I:657:HOH:O	2.20	0.41
1:J:345:ARG:NH1	1:J:348:GLN:OE1	2.53	0.41
1:L:287:ALA:HB1	1:L:368:ARG:NH1	2.34	0.41
1:L:405:ALA:O	2:L:601:HOH:O	2.21	0.41
1:L:413:ALA:HB3	1:L:417:VAL:HG22	2.01	0.41
1:M:242:LYS:O	1:M:243:ALA:HB3	2.20	0.41
1:A:103:GLY:O	1:A:107:VAL:HG23	2.19	0.41
1:B:169:VAL:HG11	1:B:377:ALA:HB2	2.01	0.41
1:B:199:TYR:CZ	1:B:327:LYS:HA	2.55	0.41
1:D:102:GLU:HB2	1:D:442:VAL:HG13	2.01	0.41
1:D:326:ASN:HB2	1:D:329:THR:HB	2.02	0.41
1:E:16:MET:HG3	1:E:520:MET:SD	2.60	0.41
1:F:479:ASN:C	1:F:481:ALA:H	2.23	0.41
1:J:195:PHE:HB2	1:J:279:PRO:HB3	2.02	0.41
1:M:182:GLY:HA2	1:N:281:PHE:CZ	2.55	0.41
1:M:66:PHE:HA	1:M:69:MET:CE	2.47	0.41
1:B:477:GLY:O	1:B:485:TYR:HA	2.20	0.41
1:D:180:GLY:HA2	1:D:380:LYS:HB3	2.01	0.41
1:D:476:TYR:CE1	1:D:485:TYR:HB3	2.55	0.41
1:F:384:ALA:O	1:F:385:THR:HG23	2.20	0.41
1:G:289:LEU:HD23	1:G:289:LEU:HA	1.91	0.41
1:I:281:PHE:HA	1:I:285:ARG:NE	2.35	0.41
1:J:95:LEU:O	1:J:99:ILE:HG13	2.20	0.41
1:L:183:LEU:O	1:L:184:GLN:O	2.38	0.41
1:C:455:VAL:HG13	1:C:460:GLU:HB2	2.02	0.41
1:E:100:ILE:O	1:E:104:LEU:HG	2.21	0.41
1:E:487:ASN:ND2	2:E:673:HOH:O	2.28	0.41
1:L:259:LEU:O	1:L:263:VAL:HG23	2.21	0.41
1:L:326:ASN:HA	1:L:326:ASN:HD22	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:223:ALA:O	1:M:251:ALA:HA	2.21	0.41
1:M:270:ILE:HG13	1:N:257:GLU:HG3	2.02	0.41
1:D:176:THR:HG22	1:D:177:VAL:N	2.35	0.41
1:D:284:ARG:O	1:D:288:MET:HG3	2.21	0.41
1:E:242:LYS:O	1:E:244:GLY:N	2.46	0.41
1:I:293:ALA:HB2	1:I:300:VAL:HG23	2.03	0.41
1:K:220:ILE:HG23	1:K:248:LEU:HD23	2.03	0.41
1:K:230:ILE:HD13	1:K:261:THR:HG21	2.03	0.41
1:L:222:LEU:CD1	1:L:293:ALA:HA	2.51	0.41
1:L:363:GLU:HG2	1:L:363:GLU:H	1.71	0.41
1:L:124:VAL:HG21	1:L:508:ALA:HB2	2.02	0.41
1:M:383:ALA:O	1:M:384:ALA:HB3	2.21	0.41
1:N:384:ALA:O	1:N:385:THR:HG23	2.20	0.41
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.84	0.41
1:C:131:LEU:HD12	1:C:131:LEU:HA	1.76	0.41
1:C:201:SER:C	1:C:202:PRO:O	2.59	0.41
1:D:86:GLY:O	1:D:87:ASP:HB2	2.20	0.41
1:E:183:LEU:O	1:E:184:GLN:HB2	2.20	0.41
1:E:240:VAL:HG11	1:E:247:LEU:HB2	2.03	0.41
1:J:420:ILE:HG12	1:J:448:GLU:HG2	2.02	0.41
1:L:224:ASP:O	1:L:225:LYS:HB3	2.21	0.41
1:N:479:ASN:HB2	1:N:491:MET:SD	2.61	0.41
1:A:122:LYS:NZ	2:A:653:HOH:O	2.40	0.41
1:B:319:GLN:O	1:B:336:VAL:HG23	2.21	0.41
1:C:171:LYS:HB3	1:C:407:VAL:HG11	2.03	0.41
1:F:253:ASP:OD1	1:F:254:VAL:N	2.54	0.41
1:I:240:VAL:HG11	1:I:247:LEU:HB2	2.01	0.41
1:I:404:ARG:NE	2:I:608:HOH:O	2.54	0.41
1:H:38:VAL:HG13	1:I:519:CYS:HB3	2.02	0.41
1:K:152:ALA:O	1:K:153:ASN:HB2	2.21	0.41
1:M:82:ASN:HB2	1:M:89:THR:HB	2.01	0.41
1:D:144:ILE:HG23	1:D:403:THR:HG21	2.03	0.41
1:H:349:ILE:O	1:H:353:ILE:HG13	2.21	0.41
1:I:230:ILE:HG21	1:I:261:THR:HG21	2.03	0.41
1:J:230:ILE:HD12	1:J:233:MET:HG3	2.03	0.41
1:J:236:VAL:HG22	1:J:312:ALA:O	2.21	0.41
1:K:229:ASN:HA	1:K:257:GLU:OE1	2.21	0.41
1:K:237:LEU:O	1:K:240:VAL:HG12	2.21	0.41
1:M:190:VAL:HG21	1:M:334:ASP:HB2	2.02	0.41
1:N:242:LYS:O	1:N:243:ALA:HB3	2.20	0.41
1:A:197:ARG:NH1	2:A:607:HOH:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ARG:NH1	1:C:350:ARG:HG2	2.35	0.41
1:F:242:LYS:O	1:F:243:ALA:HB3	2.21	0.41
1:H:294:THR:HG22	1:H:342:ILE:HD13	2.03	0.41
1:H:415:GLY:O	1:H:451:LEU:HD12	2.20	0.41
1:H:7:LYS:HG3	1:H:66:PHE:CZ	2.55	0.41
1:J:123:ALA:HB2	1:J:440:ILE:HG23	2.02	0.41
1:J:420:ILE:HG13	1:J:448:GLU:HA	2.03	0.41
1:N:443:ALA:O	1:N:447:MET:HG3	2.21	0.41
1:A:478:TYR:HA	1:A:485:TYR:CE2	2.55	0.41
1:C:494:LEU:HD12	1:C:494:LEU:C	2.41	0.41
1:D:16:MET:HB3	1:D:514:MET:HE1	2.02	0.41
1:D:524:LEU:HD12	1:D:524:LEU:HA	1.82	0.41
1:G:230:ILE:HB	1:G:257:GLU:OE2	2.21	0.41
1:G:350:ARG:O	1:G:353:ILE:HB	2.20	0.41
1:I:191:GLU:O	1:I:334:ASP:HA	2.20	0.41
1:J:468:THR:HG1	1:J:485:TYR:HE2	1.59	0.41
1:A:414:GLY:O	1:A:417:VAL:HG13	2.20	0.40
1:B:214:GLU:CD	1:B:322:ARG:HH21	2.25	0.40
1:B:381:VAL:CG1	1:B:392:LYS:HD3	2.51	0.40
1:D:217:SER:N	1:D:218:PRO:HD3	2.35	0.40
1:E:200:LEU:HG	1:E:276:VAL:HA	2.03	0.40
1:E:16:MET:HB3	1:E:514:MET:CE	2.51	0.40
1:E:77:VAL:HG12	1:E:506:TYR:HB3	2.03	0.40
1:F:182:GLY:HA2	1:G:281:PHE:CZ	2.56	0.40
1:F:217:SER:N	1:F:218:PRO:HD3	2.36	0.40
1:M:284:ARG:NE	2:M:653:HOH:O	2.53	0.40
1:M:524:LEU:O	1:M:526:LYS:N	2.50	0.40
1:F:182:GLY:O	1:F:183:LEU:C	2.59	0.40
1:G:218:PRO:HB3	1:G:246:PRO:HG2	2.02	0.40
1:H:231:ARG:HB2	2:H:608:HOH:O	2.22	0.40
1:I:357:THR:OG1	1:I:358:SER:N	2.54	0.40
1:J:200:LEU:HD23	1:J:200:LEU:HA	1.85	0.40
1:N:199:TYR:CE2	1:N:205:ILE:HD11	2.56	0.40
1:C:364:LYS:O	1:C:367:GLU:HB3	2.21	0.40
1:D:436:GLN:O	1:D:440:ILE:HG13	2.21	0.40
1:E:269:GLY:O	1:F:229:ASN:ND2	2.55	0.40
1:F:183:LEU:O	1:F:183:LEU:HD13	2.22	0.40
1:I:201:SER:HA	1:I:202:PRO:HD3	1.89	0.40
1:K:17:LEU:HG	1:K:21:ASN:ND2	2.36	0.40
1:K:5:ASP:HB2	1:K:524:LEU:HD12	2.02	0.40
1:A:203:TYR:CB	1:A:263:VAL:HG13	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:LEU:CD2	1:A:249:ILE:HD11	2.51	0.40
1:B:284:ARG:NH1	2:B:612:HOH:O	2.54	0.40
1:C:263:VAL:O	1:C:267:MET:HB2	2.22	0.40
1:E:95:LEU:HD13	1:E:504:LEU:HA	2.04	0.40
1:F:296:THR:HB	1:F:319:GLN:H	1.86	0.40
1:F:344:GLY:O	1:F:348:GLN:HG3	2.21	0.40
1:J:217:SER:HA	1:J:320:ALA:O	2.22	0.40
1:J:429:LEU:O	1:J:430:ARG:NH1	2.49	0.40
1:J:455:VAL:HG11	1:J:462:PRO:HA	2.01	0.40
1:M:199:TYR:OH	1:M:205:ILE:HD11	2.22	0.40
1:N:195:PHE:HB2	1:N:279:PRO:HB3	2.02	0.40
1:N:404:ARG:HD2	1:N:404:ARG:HA	1.89	0.40
1:N:524:LEU:O	1:N:526:LYS:N	2.55	0.40
1:A:479:ASN:ND2	1:A:484:GLU:O	2.49	0.40
1:A:487:ASN:O	1:A:490:ASP:HB2	2.22	0.40
1:C:68:ASN:O	1:C:72:GLN:HG2	2.21	0.40
1:G:71:ALA:O	1:G:75:LYS:HB2	2.22	0.40
1:I:157:THR:HG21	1:I:392:LYS:HZ1	1.85	0.40
1:I:219:PHE:HB3	1:I:317:LEU:HD23	2.03	0.40
1:K:455:VAL:HG13	1:K:460:GLU:HB2	2.02	0.40
1:M:513:LEU:HD23	1:M:513:LEU:HA	1.79	0.40
1:N:200:LEU:HA	1:N:200:LEU:HD23	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	523/525 (100%)	499 (95%)	15 (3%)	9 (2%)	9	42
1	B	523/525 (100%)	499 (95%)	18 (3%)	6 (1%)	14	51
1	C	523/525 (100%)	496 (95%)	18 (3%)	9 (2%)	9	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	523/525 (100%)	494 (94%)	21 (4%)	8 (2%)	10	44
1	E	523/525 (100%)	493 (94%)	22 (4%)	8 (2%)	10	44
1	F	523/525 (100%)	496 (95%)	17 (3%)	10 (2%)	8	39
1	G	523/525 (100%)	498 (95%)	17 (3%)	8 (2%)	10	44
1	H	523/525 (100%)	488 (93%)	24 (5%)	11 (2%)	7	37
1	I	523/525 (100%)	492 (94%)	26 (5%)	5 (1%)	15	54
1	J	523/525 (100%)	491 (94%)	24 (5%)	8 (2%)	10	44
1	K	523/525 (100%)	486 (93%)	28 (5%)	9 (2%)	9	42
1	L	523/525 (100%)	486 (93%)	25 (5%)	12 (2%)	6	34
1	M	523/525 (100%)	487 (93%)	18 (3%)	18 (3%)	3	24
1	N	523/525 (100%)	492 (94%)	22 (4%)	9 (2%)	9	42
All	All	7322/7350 (100%)	6897 (94%)	295 (4%)	130 (2%)	8	41

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	ALA
1	B	183	LEU
1	B	184	GLN
1	C	202	PRO
1	E	44	PHE
1	F	184	GLN
1	F	203	TYR
1	G	184	GLN
1	H	43	SER
1	H	184	GLN
1	H	243	ALA
1	I	43	SER
1	K	184	GLN
1	L	184	GLN
1	L	203	TYR
1	L	486	GLY
1	M	43	SER
1	M	199	TYR
1	M	208	PRO
1	M	209	GLU
1	M	221	LEU
1	M	271	VAL

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Mol	Chain	Res	Type
1	A	183	LEU
1	A	244	GLY
1	A	385	THR
1	B	202	PRO
1	B	385	THR
1	C	34	LYS
1	C	385	THR
1	D	385	THR
1	F	183	LEU
1	F	385	THR
1	F	480	ALA
1	G	183	LEU
1	J	183	LEU
1	J	339	GLU
1	K	256	GLY
1	K	480	ALA
1	L	256	GLY
1	M	197	ARG
1	M	256	GLY
1	M	480	ALA
1	A	271	VAL
1	B	271	VAL
1	C	183	LEU
1	C	271	VAL
1	D	183	LEU
1	D	184	GLN
1	D	271	VAL
1	D	482	THR
1	E	183	LEU
1	E	385	THR
1	G	202	PRO
1	G	385	THR
1	H	271	VAL
1	H	481	ALA
1	I	183	LEU
1	I	271	VAL
1	I	383	ALA
1	J	225	LYS
1	J	271	VAL
1	K	271	VAL
1	K	385	THR
1	L	271	VAL

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Mol	Chain	Res	Type
1	L	385	THR
1	L	525	PRO
1	M	196	ASP
1	M	214	GLU
1	M	525	PRO
1	N	43	SER
1	N	182	GLY
1	N	183	LEU
1	N	256	GLY
1	A	203	TYR
1	A	243	ALA
1	B	525	PRO
1	D	225	LYS
1	E	271	VAL
1	E	483	GLU
1	F	271	VAL
1	F	383	ALA
1	F	479	ASN
1	G	108	ALA
1	G	271	VAL
1	G	383	ALA
1	H	202	PRO
1	H	383	ALA
1	I	182	GLY
1	K	225	LYS
1	K	234	LEU
1	K	525	PRO
1	L	225	LYS
1	L	234	LEU
1	M	183	LEU
1	M	225	LYS
1	N	271	VAL
1	N	383	ALA
1	N	525	PRO
1	A	184	GLN
1	A	383	ALA
1	C	184	GLN
1	C	525	PRO
1	D	383	ALA
1	D	483	GLU
1	E	383	ALA
1	E	525	PRO

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Mol	Chain	Res	Type
1	F	525	PRO
1	G	525	PRO
1	H	9	GLY
1	H	480	ALA
1	J	256	GLY
1	J	383	ALA
1	J	525	PRO
1	K	383	ALA
1	L	183	LEU
1	L	358	SER
1	L	383	ALA
1	M	383	ALA
1	N	385	THR
1	C	182	GLY
1	H	183	LEU
1	H	256	GLY
1	J	182	GLY
1	M	182	GLY
1	M	201	SER
1	M	384	ALA
1	N	184	GLN
1	C	33	PRO
1	F	202	PRO
1	E	182	GLY

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	405/405 (100%)	388 (96%)	17 (4%)	30	65
1	B	405/405 (100%)	395 (98%)	10 (2%)	47	77
1	C	405/405 (100%)	393 (97%)	12 (3%)	41	73
1	D	405/405 (100%)	391 (96%)	14 (4%)	36	69
1	E	405/405 (100%)	393 (97%)	12 (3%)	41	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	405/405 (100%)	390 (96%)	15 (4%)	34	68
1	G	405/405 (100%)	390 (96%)	15 (4%)	34	68
1	H	405/405 (100%)	390 (96%)	15 (4%)	34	68
1	I	405/405 (100%)	386 (95%)	19 (5%)	26	62
1	J	405/405 (100%)	390 (96%)	15 (4%)	34	68
1	K	405/405 (100%)	384 (95%)	21 (5%)	23	59
1	L	405/405 (100%)	393 (97%)	12 (3%)	41	73
1	M	405/405 (100%)	386 (95%)	19 (5%)	26	62
1	N	405/405 (100%)	392 (97%)	13 (3%)	39	71
All	All	5670/5670 (100%)	5461 (96%)	209 (4%)	34	68

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	A	129	GLU
1	A	134	LEU
1	A	177	VAL
1	A	232	GLU
1	A	255	GLU
1	A	261	THR
1	A	270	ILE
1	A	284	ARG
1	A	329	THR
1	A	331	THR
1	A	343	GLN
1	A	351	GLN
1	A	398	ASP
1	A	403	THR
1	A	420	ILE
1	A	422	VAL
1	B	82	ASN
1	B	122	LYS
1	B	131	LEU
1	B	134	LEU
1	B	188	ASP
1	B	261	THR
1	B	284	ARG
1	B	398	ASP

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Mol	Chain	Res	Type
1	B	404	ARG
1	B	524	LEU
1	C	74	VAL
1	C	76	GLU
1	C	82	ASN
1	C	193	MET
1	C	232	GLU
1	C	263	VAL
1	C	331	THR
1	C	350	ARG
1	C	404	ARG
1	C	420	ILE
1	C	425	LYS
1	C	524	LEU
1	D	74	VAL
1	D	129	GLU
1	D	134	LEU
1	D	177	VAL
1	D	183	LEU
1	D	328	ASP
1	D	329	THR
1	D	331	THR
1	D	361	ASP
1	D	398	ASP
1	D	404	ARG
1	D	417	VAL
1	D	510	VAL
1	D	524	LEU
1	E	42	LYS
1	E	82	ASN
1	E	89	THR
1	E	131	LEU
1	E	134	LEU
1	E	177	VAL
1	E	183	LEU
1	E	284	ARG
1	E	319	GLN
1	E	331	THR
1	E	404	ARG
1	E	422	VAL
1	F	77	VAL
1	F	129	GLU

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Mol	Chain	Res	Type
1	F	131	LEU
1	F	228	SER
1	F	232	GLU
1	F	270	ILE
1	F	284	ARG
1	F	328	ASP
1	F	329	THR
1	F	331	THR
1	F	367	GLU
1	F	387	VAL
1	F	398	ASP
1	F	524	LEU
1	F	526	LYS
1	G	74	VAL
1	G	129	GLU
1	G	131	LEU
1	G	134	LEU
1	G	139	SER
1	G	141	SER
1	G	183	LEU
1	G	255	GLU
1	G	257	GLU
1	G	284	ARG
1	G	328	ASP
1	G	329	THR
1	G	331	THR
1	G	358	SER
1	G	524	LEU
1	H	74	VAL
1	H	94	VAL
1	H	183	LEU
1	H	209	GLU
1	H	210	THR
1	H	228	SER
1	H	232	GLU
1	H	255	GLU
1	H	328	ASP
1	H	329	THR
1	H	331	THR
1	H	398	ASP
1	H	404	ARG
1	H	482	THR

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Mol	Chain	Res	Type
1	H	499	VAL
1	I	20	VAL
1	I	76	GLU
1	I	82	ASN
1	I	89	THR
1	I	138	CYS
1	I	209	GLU
1	I	232	GLU
1	I	305	ILE
1	I	328	ASP
1	I	329	THR
1	I	331	THR
1	I	351	GLN
1	I	372	LEU
1	I	385	THR
1	I	398	ASP
1	I	420	ILE
1	I	467	ASN
1	I	489	ILE
1	I	499	VAL
1	J	20	VAL
1	J	74	VAL
1	J	79	SER
1	J	89	THR
1	J	225	LYS
1	J	232	GLU
1	J	259	LEU
1	J	328	ASP
1	J	329	THR
1	J	331	THR
1	J	398	ASP
1	J	404	ARG
1	J	412	VAL
1	J	420	ILE
1	J	499	VAL
1	K	20	VAL
1	K	58	ARG
1	K	74	VAL
1	K	76	GLU
1	K	94	VAL
1	K	134	LEU
1	K	141	SER

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Mol	Chain	Res	Type
1	K	183	LEU
1	K	188	ASP
1	K	225	LYS
1	K	226	LYS
1	K	255	GLU
1	K	328	ASP
1	K	329	THR
1	K	331	THR
1	K	363	GLU
1	K	385	THR
1	K	398	ASP
1	K	404	ARG
1	K	417	VAL
1	K	499	VAL
1	L	18	ARG
1	L	20	VAL
1	L	74	VAL
1	L	242	LYS
1	L	328	ASP
1	L	329	THR
1	L	331	THR
1	L	363	GLU
1	L	385	THR
1	L	398	ASP
1	L	440	ILE
1	L	499	VAL
1	M	20	VAL
1	M	74	VAL
1	M	94	VAL
1	M	210	THR
1	M	232	GLU
1	M	257	GLU
1	M	267	MET
1	M	284	ARG
1	M	313	THR
1	M	328	ASP
1	M	329	THR
1	M	331	THR
1	M	339	GLU
1	M	404	ARG
1	M	424	SER
1	M	451	LEU

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Mol	Chain	Res	Type
1	M	479	ASN
1	M	499	VAL
1	M	524	LEU
1	N	20	VAL
1	N	44	PHE
1	N	74	VAL
1	N	183	LEU
1	N	209	GLU
1	N	210	THR
1	N	313	THR
1	N	328	ASP
1	N	329	THR
1	N	331	THR
1	N	351	GLN
1	N	398	ASP
1	N	499	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	D	326	ASN
1	E	352	GLN
1	E	366	GLN
1	E	433	ASN
1	F	37	ASN
1	G	326	ASN
1	I	72	GLN
1	K	146	GLN
1	L	326	ASN
1	N	326	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95^{th} 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($\AA^2$)	Q<0.9
1	A	525/525 (100%)	-0.47	7 (1%)	77	65	10, 32, 68, 153	0
1	B	525/525 (100%)	-0.41	0	100	100	11, 35, 69, 95	0
1	C	525/525 (100%)	-0.40	0	100	100	13, 40, 77, 102	0
1	D	525/525 (100%)	-0.31	5 (0%)	82	72	13, 39, 88, 153	0
1	E	525/525 (100%)	-0.42	3 (0%)	89	83	11, 30, 63, 180	0
1	F	525/525 (100%)	-0.42	2 (0%)	92	89	9, 38, 73, 163	0
1	G	525/525 (100%)	-0.42	2 (0%)	92	89	10, 34, 74, 122	0
1	H	525/525 (100%)	-0.39	5 (0%)	82	72	11, 38, 74, 140	0
1	I	525/525 (100%)	-0.37	1 (0%)	95	94	12, 41, 79, 170	0
1	J	525/525 (100%)	-0.35	0	100	100	13, 40, 82, 122	0
1	K	525/525 (100%)	-0.10	13 (2%)	57	43	10, 48, 121, 151	0
1	L	525/525 (100%)	-0.25	4 (0%)	86	78	13, 46, 94, 126	0
1	M	525/525 (100%)	-0.35	2 (0%)	92	89	11, 37, 80, 160	0
1	N	525/525 (100%)	-0.35	2 (0%)	92	89	9, 37, 72, 140	0
All	All	7350/7350 (100%)	-0.36	46 (0%)	89	83	9, 38, 85, 180	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	478	TYR	5.1
1	L	481	ALA	4.5
1	K	478	TYR	4.3
1	E	481	ALA	4.2
1	H	43	SER	4.0
1	D	478	TYR	3.9
1	A	481	ALA	3.9
1	I	483	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	483	GLU	3.6
1	D	483	GLU	3.6
1	K	271	VAL	3.6
1	M	483	GLU	3.2
1	H	483	GLU	3.1
1	H	480	ALA	3.0
1	K	480	ALA	2.9
1	A	485	TYR	2.9
1	A	478	TYR	2.8
1	G	481	ALA	2.8
1	K	210	THR	2.8
1	L	228	SER	2.6
1	F	483	GLU	2.6
1	K	229	ASN	2.6
1	N	478	TYR	2.6
1	K	303	GLU	2.5
1	K	268	ARG	2.5
1	H	478	TYR	2.5
1	A	480	ALA	2.4
1	D	477	GLY	2.4
1	A	479	ASN	2.4
1	D	476	TYR	2.4
1	K	311	LYS	2.4
1	K	223	ALA	2.4
1	K	251	ALA	2.4
1	K	266	THR	2.3
1	K	254	VAL	2.3
1	E	478	TYR	2.3
1	H	481	ALA	2.3
1	D	479	ASN	2.2
1	L	266	THR	2.2
1	N	481	ALA	2.2
1	K	248	LEU	2.1
1	A	44	PHE	2.1
1	E	477	GLY	2.1
1	M	266	THR	2.1
1	G	478	TYR	2.1
1	L	229	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.