



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:35 PM UTC

PDB ID : 1KXT / pdb_00001kxt
Title : Camelid VHH Domains in Complex with Porcine Pancreatic alpha-Amylase
Authors : Desmyter, A.; Spinelli, S.; Payan, F.; Lauwereys, M.; Wyns, L.; Muyldermans, S.; Cambillau, C.
Deposited on : 2002-02-01
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

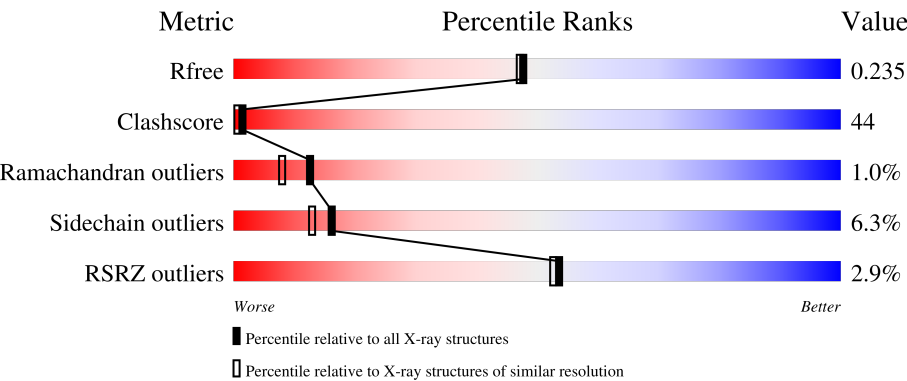
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	496	
1	C	496	
1	E	496	
2	B	127	
2	D	127	

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Mol	Chain	Length	Quality of chain
2	F	127	9% 37% 52% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16172 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 ALPHA-AMYLASE, PANCREATIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3910	2471	688	730	21			
1	C	496	Total	C	N	O	S	0	0	0
			3910	2471	688	730	21			
1	E	496	Total	C	N	O	S	0	0	0
			3910	2471	688	730	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	LYS	GLN	SEE REMARK 999	UNP P00690
A	310	SER	ALA	SEE REMARK 999	UNP P00690
A	323	ILE	VAL	SEE REMARK 999	UNP P00690
A	404	GLN	GLU	SEE REMARK 999	UNP P00690
C	243	LYS	GLN	SEE REMARK 999	UNP P00690
C	310	SER	ALA	SEE REMARK 999	UNP P00690
C	323	ILE	VAL	SEE REMARK 999	UNP P00690
C	404	GLN	GLU	SEE REMARK 999	UNP P00690
E	243	LYS	GLN	SEE REMARK 999	UNP P00690
E	310	SER	ALA	SEE REMARK 999	UNP P00690
E	323	ILE	VAL	SEE REMARK 999	UNP P00690
E	404	GLN	GLU	SEE REMARK 999	UNP P00690

- Molecule 2 is a protein called IMMUNOGLOBULIN VHH FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total	C	N	O	S	0	0	0
			903	560	158	179	6			
2	D	123	Total	C	N	O	S	0	0	0
			903	560	158	179	6			
2	F	123	Total	C	N	O	S	0	0	0
			903	560	158	179	6			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	E	1	Total 1	Ca 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0

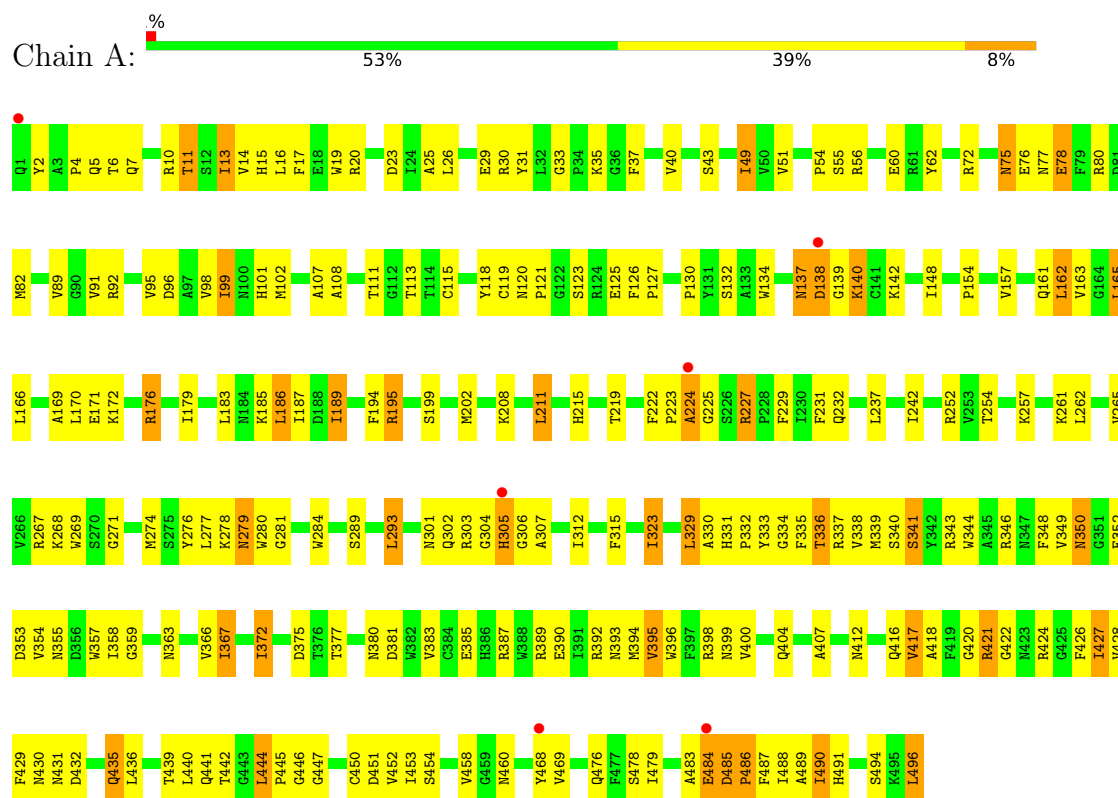
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	479	Total 479	O 479	0	0
5	B	131	Total 131	O 131	0	0
5	C	391	Total 391	O 391	0	0
5	D	120	Total 120	O 120	0	0
5	E	491	Total 491	O 491	0	0
5	F	115	Total 115	O 115	0	0

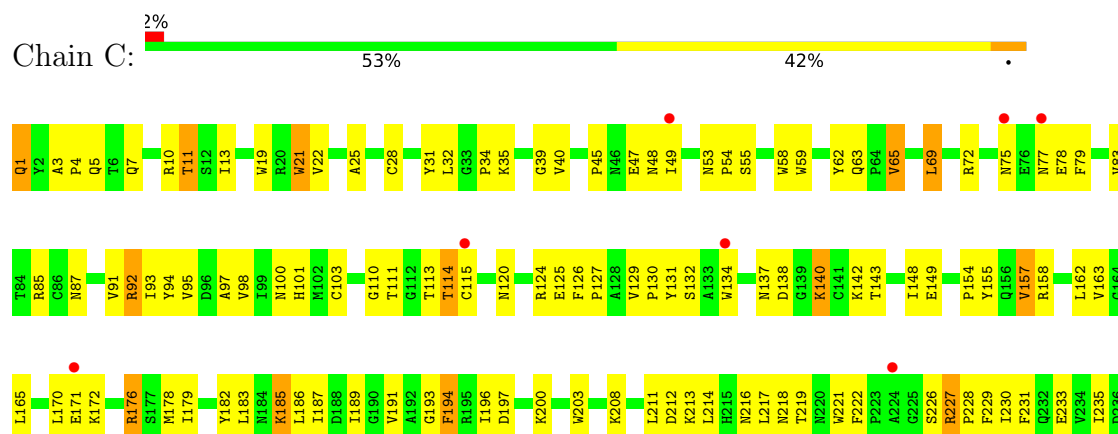
3 Residue-property plots

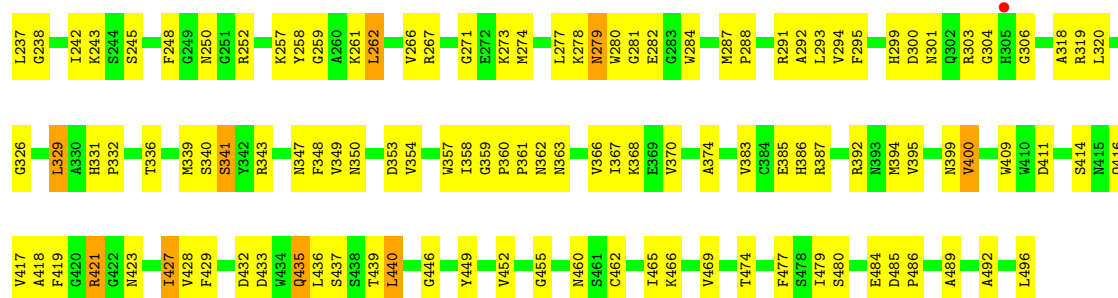
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ALPHA-AMYLASE, PANCREATIC

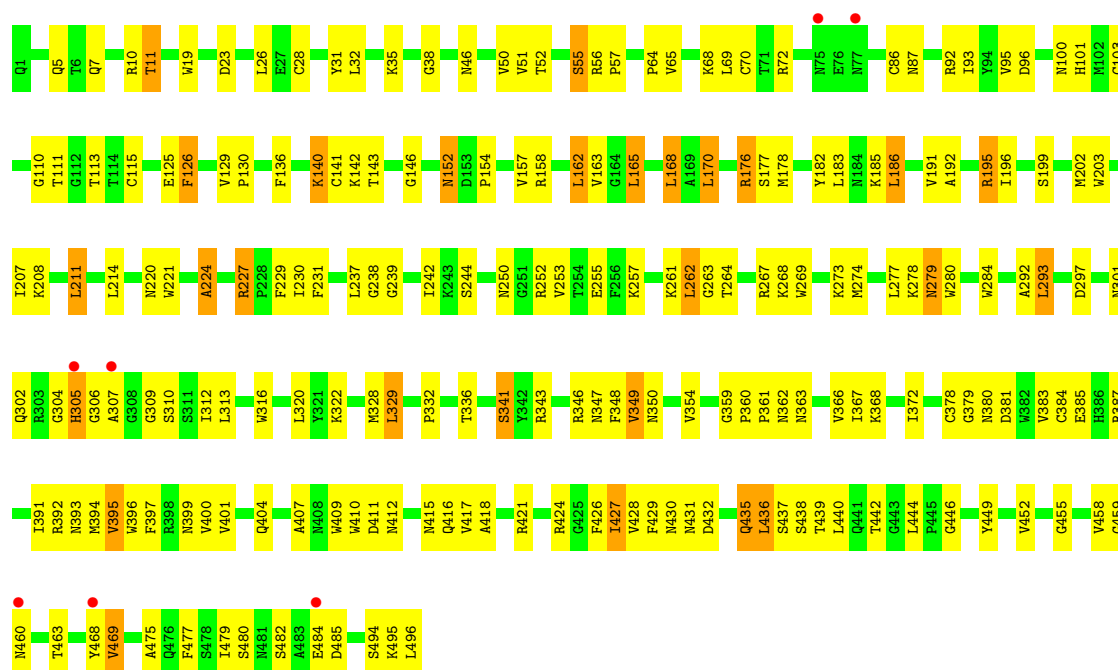


• Molecule 1: ALPHA-AMYLASE, PANCREATIC

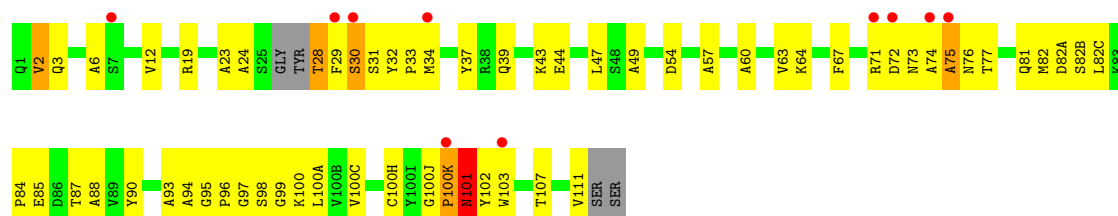




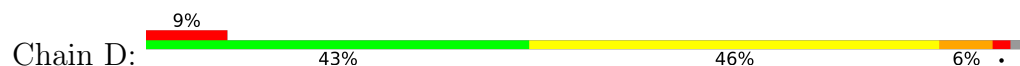
• Molecule 1: ALPHA-AMYLASE, PANCREATIC

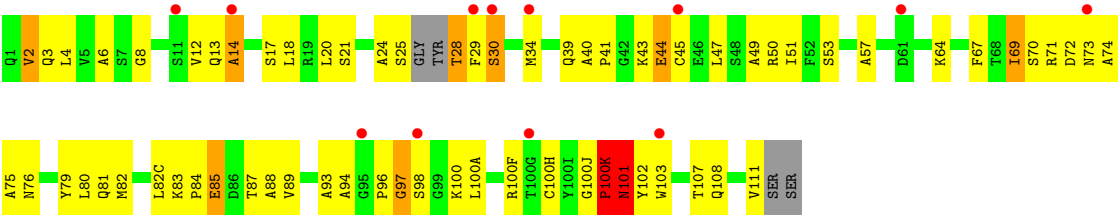


• Molecule 2: IMMUNOGLOBULIN VHH FRAGMENT

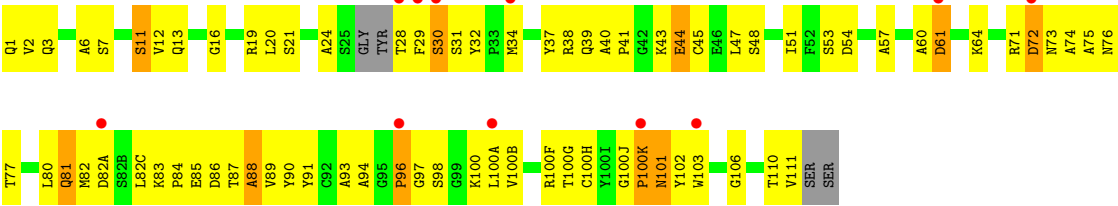


• Molecule 2: IMMUNOGLOBULIN VHH FRAGMENT





• Molecule 2: IMMUNOGLOBULIN VHH FRAGMENT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.78Å 286.85Å 65.98Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	19.95 – 2.00 19.95 – 2.00	Depositor EDS
% Data completeness (in resolution range)	50.1 (19.95-2.00) 50.1 (19.95-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 2.00Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.203 , 0.236 0.203 , 0.235	Depositor DCC
R_{free} test set	1659 reflections (2.52%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.0	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	0.92	EDS
Total number of atoms	16172	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CA

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	0.47	0/4020	0.98	17/5461 (0.3%)
1	C	0.41	0/4020	0.96	16/5461 (0.3%)
1	E	0.44	0/4020	0.98	17/5461 (0.3%)
2	B	0.46	0/921	0.88	1/1247 (0.1%)
2	D	0.42	0/921	0.94	1/1247 (0.1%)
2	F	0.45	0/921	0.95	4/1247 (0.3%)
All	All	0.44	0/14823	0.96	56/20124 (0.3%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	GLY	N-CA-C	8.77	125.66	114.25
1	A	336	THR	N-CA-C	7.58	122.70	109.96
2	B	100(K)	PRO	N-CA-C	7.39	127.70	112.47
1	A	395	VAL	N-CA-C	-7.14	103.51	110.72
2	D	100(K)	PRO	N-CA-C	6.79	126.45	112.47
1	C	341	SER	N-CA-C	6.67	117.08	108.34
1	E	146	GLY	N-CA-C	-6.62	106.31	114.92
1	A	400	VAL	N-CA-C	6.54	117.29	110.62
2	F	100(K)	PRO	N-CA-C	6.48	121.60	112.26
1	A	485	ASP	CA-C-N	6.45	127.90	119.84
1	A	485	ASP	C-N-CA	6.45	127.90	119.84
1	E	195	ARG	N-CA-C	-6.27	98.30	108.52
2	F	96	PRO	N-CA-C	-6.21	101.51	111.38
1	E	359	GLY	CA-C-N	6.04	126.61	120.38
1	E	359	GLY	C-N-CA	6.04	126.61	120.38
1	A	161	GLN	N-CA-C	5.90	118.28	109.25
1	E	55	SER	N-CA-C	5.84	117.98	108.63
1	E	395	VAL	N-CA-C	-5.80	104.71	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ARG	N-CA-C	-5.71	99.42	108.73
1	E	126	PHE	CA-C-N	5.66	125.33	119.56
1	E	126	PHE	C-N-CA	5.66	125.33	119.56
1	A	11	THR	N-CA-C	5.66	120.92	112.94
1	C	55	SER	N-CA-C	5.65	117.29	109.15
1	C	194	PHE	N-CA-C	5.61	117.71	109.24
1	E	292	ALA	N-CA-C	5.59	119.36	109.96
1	E	302	GLN	N-CA-C	-5.57	106.56	113.19
1	E	11	THR	N-CA-C	5.53	120.71	113.30
1	E	336	THR	N-CA-C	5.51	118.90	110.20
1	C	11	THR	N-CA-C	5.44	119.90	112.88
1	C	185	LYS	N-CA-C	-5.44	105.35	111.28
1	E	152	ASN	N-CA-C	-5.44	106.64	113.28
1	C	292	ALA	N-CA-C	5.43	118.58	109.95
1	C	301	ASN	N-CA-C	5.42	119.00	112.38
1	C	306	GLY	N-CA-C	-5.42	105.33	112.81
1	A	102	MET	N-CA-C	-5.42	100.59	109.80
1	A	334	GLY	N-CA-C	5.41	122.11	112.22
1	C	359	GLY	CA-C-N	5.40	123.55	119.66
1	C	359	GLY	C-N-CA	5.40	123.55	119.66
1	C	336	THR	N-CA-C	5.39	118.72	110.20
1	C	267	ARG	N-CA-C	-5.38	106.67	113.18
1	A	293	LEU	N-CA-C	-5.30	98.74	108.02
2	F	60	ALA	N-CA-C	-5.30	102.54	110.23
1	C	65	VAL	N-CA-C	-5.28	108.14	113.47
1	A	78	GLU	N-CA-C	-5.25	105.63	111.36
1	E	95	VAL	N-CA-C	5.20	116.77	108.87
1	A	137	ASN	N-CA-C	5.12	118.78	112.54
1	A	55	SER	N-CA-C	5.09	116.77	108.63
1	A	359	GLY	CA-C-N	5.08	125.61	120.38
1	A	359	GLY	C-N-CA	5.08	125.61	120.38
1	E	293	LEU	N-CA-C	-5.08	100.14	108.41
1	C	400	VAL	N-CA-C	5.07	115.79	110.62
1	A	302	GLN	N-CA-C	-5.06	107.06	113.18
1	E	214	LEU	N-CA-C	5.06	117.77	110.28
1	E	494	SER	N-CA-C	-5.05	107.16	113.38
2	F	57	ALA	N-CA-C	5.05	116.74	109.07
1	C	492	ALA	N-CA-C	5.03	118.18	111.75

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	3910	0	3693	329	0
1	C	3910	0	3693	303	0
1	E	3910	0	3693	270	1
2	B	903	0	859	112	0
2	D	903	0	859	122	0
2	F	903	0	859	111	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
4	A	1	0	0	1	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	A	479	0	0	142	1
5	B	131	0	0	60	0
5	C	391	0	0	135	0
5	D	120	0	0	58	0
5	E	491	0	0	128	0
5	F	115	0	0	62	0
All	All	16172	0	13656	1232	1

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 44.

All (1232) 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)
2:B:77:THR:HG22	5:B:205:HOH:O	1.37	1.24
1:E:185:LYS:HD2	5:E:4460:HOH:O	1.38	1.23
1:A:29:GLU:HG2	5:A:4430:HOH:O	1.34	1.22
1:C:278:LYS:HE2	5:C:4326:HOH:O	1.40	1.22
1:C:294:VAL:HB	5:C:4294:HOH:O	1.42	1.19
2:D:43:LYS:HE2	5:D:199:HOH:O	1.36	1.18
1:C:98:VAL:HG22	5:C:4324:HOH:O	1.44	1.18
1:C:367:ILE:HG13	5:C:4323:HOH:O	1.42	1.18
1:A:121:PRO:HA	5:A:4385:HOH:O	1.42	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:LEU:HA	5:E:4456:HOH:O	1.44	1.17
1:C:58:TRP:HA	5:C:4273:HOH:O	1.41	1.16
1:C:91:VAL:HG13	5:C:4371:HOH:O	1.46	1.16
1:E:111:THR:HG21	5:E:4421:HOH:O	1.41	1.16
1:E:278:LYS:HG2	5:E:4382:HOH:O	1.46	1.15
1:C:383:VAL:HB	5:C:4316:HOH:O	1.44	1.15
2:B:32:TYR:HA	5:B:231:HOH:O	1.45	1.13
1:A:148:ILE:HG12	5:A:4406:HOH:O	1.48	1.13
2:F:31:SER:HA	5:F:215:HOH:O	1.46	1.12
2:F:53:SER:HB2	5:F:180:HOH:O	1.46	1.12
1:E:383:VAL:HB	5:E:4418:HOH:O	1.51	1.11
1:E:407:ALA:HB3	5:E:4416:HOH:O	1.47	1.11
1:C:421:ARG:HG2	5:C:4320:HOH:O	1.51	1.09
1:A:82:MET:HA	5:A:4468:HOH:O	1.49	1.08
1:E:186:LEU:HD23	5:E:4456:HOH:O	1.53	1.07
5:C:4287:HOH:O	2:D:45:CYS:HB3	1.52	1.06
1:E:391:ILE:HG12	5:E:4385:HOH:O	1.55	1.06
1:E:177:SER:HB2	5:E:4491:HOH:O	1.56	1.06
1:C:400:VAL:HA	5:C:4279:HOH:O	1.55	1.05
2:D:53:SER:HB2	5:D:196:HOH:O	1.55	1.04
1:A:323:ILE:HA	5:A:4338:HOH:O	1.58	1.04
2:F:84:PRO:HD2	5:F:205:HOH:O	1.57	1.04
2:F:100(G):THR:HB	5:F:221:HOH:O	1.56	1.03
1:C:49:ILE:HG21	5:C:4391:HOH:O	1.58	1.03
1:A:25:ALA:HB2	5:A:4468:HOH:O	1.58	1.03
1:C:349:VAL:HG23	5:C:4345:HOH:O	1.57	1.01
2:D:96:PRO:HB2	5:D:152:HOH:O	1.59	1.01
1:C:179:ILE:HA	5:C:4252:HOH:O	1.59	1.01
1:E:239:GLY:HA2	5:F:192:HOH:O	1.60	1.01
1:E:428:VAL:HB	5:E:4244:HOH:O	1.58	1.01
1:E:458:VAL:HB	5:E:4399:HOH:O	1.58	1.00
1:E:52:THR:HG23	5:E:4293:HOH:O	1.60	1.00
1:C:22:VAL:HG11	5:C:4310:HOH:O	1.61	1.00
1:C:252:ARG:HA	5:C:4205:HOH:O	1.61	1.00
1:C:49:ILE:HG22	1:C:65:VAL:CG1	1.92	0.99
1:C:110:GLY:HA2	5:C:4230:HOH:O	1.62	0.99
1:E:7:GLN:HB3	1:E:10:ARG:HD2	1.44	0.99
1:E:309:GLY:HA3	5:E:4447:HOH:O	1.62	0.98
1:A:490:ILE:HG13	5:A:4416:HOH:O	1.62	0.98
1:A:7:GLN:HG2	5:A:4420:HOH:O	1.63	0.97
1:C:423:ASN:HB3	5:C:4288:HOH:O	1.63	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ILE:HG13	5:A:4230:HOH:O	1.62	0.97
1:E:343:ARG:HB3	5:E:4343:HOH:O	1.65	0.97
1:A:162:LEU:O	1:A:165:LEU:HD22	1.64	0.96
1:E:110:GLY:HA3	5:E:4481:HOH:O	1.62	0.96
1:E:368:LYS:HD3	5:E:4396:HOH:O	1.63	0.96
2:B:100:LYS:HD3	5:B:220:HOH:O	1.65	0.96
2:F:45:CYS:HB2	5:F:206:HOH:O	1.63	0.96
2:F:71:ARG:HB3	5:F:193:HOH:O	1.64	0.96
2:F:89:VAL:HG12	5:F:220:HOH:O	1.63	0.96
1:C:196:ILE:HG12	5:C:4083:HOH:O	1.63	0.96
2:D:69:ILE:HG21	5:D:179:HOH:O	1.66	0.95
1:A:108:ALA:HB2	5:A:4418:HOH:O	1.65	0.95
1:A:363:ASN:O	1:A:366:VAL:HG22	1.67	0.95
2:D:75:ALA:HB1	5:D:197:HOH:O	1.65	0.95
1:A:421:ARG:HH21	1:A:421:ARG:HB3	1.29	0.95
1:E:50:VAL:HG12	5:E:4293:HOH:O	1.65	0.94
2:D:69:ILE:HG13	5:D:219:HOH:O	1.67	0.94
1:A:428:VAL:HB	5:A:4250:HOH:O	1.68	0.94
1:A:163:VAL:HG23	1:A:165:LEU:CD2	1.97	0.94
1:A:257:LYS:HE2	5:A:4344:HOH:O	1.66	0.93
1:A:185:LYS:O	1:A:189:ILE:HD13	1.69	0.93
1:E:293:LEU:HD11	5:E:4321:HOH:O	1.67	0.93
1:C:350:ASN:HA	5:C:4355:HOH:O	1.68	0.92
1:E:440:LEU:HG	5:E:4434:HOH:O	1.67	0.92
1:A:14:VAL:HB	5:A:4233:HOH:O	1.67	0.92
1:E:255:GLU:HG2	5:E:4202:HOH:O	1.69	0.92
1:E:378:CYS:HB2	5:E:4359:HOH:O	1.69	0.92
1:E:366:VAL:HG21	5:E:4486:HOH:O	1.69	0.91
1:A:211:LEU:HB3	5:A:4297:HOH:O	1.71	0.91
1:C:257:LYS:HE2	5:D:152:HOH:O	1.70	0.91
1:E:142:LYS:HG2	5:E:4243:HOH:O	1.69	0.91
1:E:23:ASP:HB3	5:E:4325:HOH:O	1.71	0.91
1:E:346:ARG:HD2	5:E:4496:HOH:O	1.71	0.91
1:C:49:ILE:CG2	1:C:65:VAL:CG1	2.47	0.90
1:C:79:PHE:HA	5:C:4239:HOH:O	1.70	0.90
2:D:64:LYS:HE2	5:D:218:HOH:O	1.69	0.90
1:A:343:ARG:HD3	5:A:4223:HOH:O	1.70	0.90
1:A:383:VAL:HB	5:A:4238:HOH:O	1.71	0.90
1:A:486:PRO:HA	5:A:4261:HOH:O	1.71	0.89
1:A:307:ALA:O	1:A:312:ILE:HD11	1.72	0.89
1:E:100:ASN:HD22	1:E:101:HIS:HD2	1.18	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:O	1:A:165:LEU:CD2	2.21	0.89
1:E:293:LEU:CD1	5:E:4321:HOH:O	2.19	0.89
1:C:49:ILE:HD13	1:C:103:CYS:HB2	1.53	0.89
2:F:34:MET:HE1	5:F:200:HOH:O	1.73	0.88
1:C:21:TRP:HB2	5:C:4172:HOH:O	1.73	0.88
1:A:341:SER:O	1:A:383:VAL:HG12	1.73	0.88
2:B:19:ARG:HD3	5:B:183:HOH:O	1.71	0.88
2:D:28:THR:HG22	5:D:147:HOH:O	1.74	0.88
1:A:60:GLU:HB2	5:A:4317:HOH:O	1.74	0.88
1:A:340:SER:HB2	5:A:4233:HOH:O	1.74	0.87
2:B:100(K):PRO:O	2:B:101:ASN:HB2	1.72	0.87
1:C:185:LYS:O	1:C:189:ILE:HG12	1.75	0.87
2:D:108:GLN:HG2	5:D:232:HOH:O	1.74	0.87
1:C:363:ASN:O	1:C:366:VAL:HG22	1.74	0.87
2:D:51:ILE:HB	2:D:69:ILE:HD12	1.56	0.87
1:C:363:ASN:HB2	5:C:4366:HOH:O	1.75	0.86
1:A:392:ARG:O	1:A:395:VAL:HG22	1.75	0.86
1:E:31:TYR:OH	1:E:392:ARG:HG3	1.75	0.86
1:C:274:MET:HE1	1:C:429:PHE:HB2	1.58	0.86
2:F:82(C):LEU:HG	5:F:164:HOH:O	1.76	0.86
1:E:261:LYS:HE3	2:F:98:SER:HB3	1.57	0.85
1:E:320:LEU:HG	5:E:4275:HOH:O	1.74	0.85
1:A:429:PHE:HE2	5:A:4338:HOH:O	1.57	0.85
2:F:83:LYS:HA	5:F:205:HOH:O	1.76	0.85
1:A:460:ASN:HB3	5:A:4422:HOH:O	1.75	0.85
1:C:341:SER:O	1:C:383:VAL:HG12	1.77	0.85
1:A:130:PRO:HD2	5:A:4471:HOH:O	1.76	0.85
1:A:323:ILE:HD11	1:A:486:PRO:HG2	1.56	0.85
2:D:96:PRO:HG2	5:D:220:HOH:O	1.75	0.85
2:F:75:ALA:HB2	5:F:158:HOH:O	1.75	0.85
1:A:268:LYS:HB2	5:A:4407:HOH:O	1.75	0.85
2:D:49:ALA:HB1	5:D:179:HOH:O	1.76	0.85
1:E:387:ARG:HB3	5:E:4352:HOH:O	1.74	0.85
1:A:29:GLU:HB2	5:A:4253:HOH:O	1.78	0.84
2:B:100:LYS:HD2	5:B:225:HOH:O	1.75	0.84
1:A:170:LEU:O	1:A:176:ARG:HD2	1.78	0.84
2:B:93:ALA:HB1	2:B:103:TRP:CZ3	2.12	0.84
1:A:26:LEU:HA	5:A:4253:HOH:O	1.77	0.83
1:A:427:ILE:HG13	5:A:4480:HOH:O	1.77	0.83
1:A:31:TYR:OH	1:A:392:ARG:HG3	1.79	0.83
1:C:374:ALA:CB	5:C:4313:HOH:O	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:GLU:HB2	5:C:4162:HOH:O	1.79	0.82
2:D:64:LYS:CE	5:D:218:HOH:O	2.26	0.82
1:A:427:ILE:CD1	5:A:4480:HOH:O	2.26	0.82
2:F:20:LEU:HG	5:F:228:HOH:O	1.78	0.82
2:B:82:MET:C	5:B:215:HOH:O	2.23	0.82
1:E:343:ARG:CD	5:E:4380:HOH:O	2.28	0.82
1:E:267:ARG:HD2	5:E:4432:HOH:O	1.78	0.82
1:A:427:ILE:HD11	5:A:4480:HOH:O	1.78	0.81
2:B:93:ALA:HB1	2:B:103:TRP:HZ3	1.44	0.81
2:B:98:SER:HB3	5:B:200:HOH:O	1.80	0.81
1:C:394:MET:SD	5:C:4284:HOH:O	2.38	0.81
2:D:100(K):PRO:O	2:D:101:ASN:HB2	1.78	0.81
2:F:30:SER:HB2	2:F:71:ARG:HH21	1.44	0.81
1:E:343:ARG:HD3	5:E:4380:HOH:O	1.80	0.81
2:F:1:GLN:HB3	5:F:186:HOH:O	1.80	0.81
1:E:220:ASN:HB3	5:E:4353:HOH:O	1.80	0.81
1:E:427:ILE:HD13	1:E:428:VAL:N	1.96	0.81
2:D:69:ILE:CD1	5:D:219:HOH:O	2.27	0.81
1:A:77:ASN:HB3	5:A:4216:HOH:O	1.80	0.80
1:C:287:MET:HB2	5:C:4344:HOH:O	1.81	0.80
1:A:162:LEU:HD22	1:A:163:VAL:HG22	1.62	0.80
1:C:49:ILE:HD11	1:C:63:GLN:OE1	1.81	0.80
1:E:307:ALA:O	1:E:312:ILE:HD11	1.81	0.80
1:A:163:VAL:HG23	1:A:165:LEU:HD21	1.64	0.80
1:C:273:LYS:HE3	5:C:4195:HOH:O	1.81	0.80
1:A:43:SER:CB	5:A:4460:HOH:O	2.28	0.80
1:A:427:ILE:HD13	1:A:428:VAL:N	1.97	0.79
2:B:107:THR:CG2	5:B:224:HOH:O	2.29	0.79
1:E:69:LEU:HD11	1:E:185:LYS:HE3	1.62	0.79
2:F:34:MET:HG2	2:F:94:ALA:HB2	1.64	0.79
2:B:64:LYS:HG3	5:B:154:HOH:O	1.81	0.79
2:D:84:PRO:HG2	2:D:85:GLU:OE1	1.82	0.79
2:F:34:MET:HG2	2:F:94:ALA:CB	2.12	0.79
1:C:111:THR:HG23	5:C:4338:HOH:O	1.83	0.79
1:C:179:ILE:CA	5:C:4252:HOH:O	2.23	0.79
1:C:155:TYR:HB3	5:C:4152:HOH:O	1.82	0.79
2:D:34:MET:HG2	2:D:94:ALA:HB1	1.65	0.79
1:E:427:ILE:HD12	1:E:429:PHE:CE1	2.17	0.79
1:A:390:GLU:HG3	5:A:4392:HOH:O	1.81	0.78
1:A:118:TYR:CD2	5:A:4402:HOH:O	2.36	0.78
1:C:49:ILE:HG23	1:C:65:VAL:HG13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:SER:CB	5:B:200:HOH:O	2.32	0.78
2:D:100(A):LEU:HB2	2:D:103:TRP:NE1	1.97	0.78
2:B:72:ASP:HB3	5:B:158:HOH:O	1.82	0.78
2:D:12:VAL:HG22	2:D:13:GLN:H	1.48	0.78
2:B:82(B):SER:HB2	5:B:236:HOH:O	1.83	0.78
1:E:273:LYS:HE3	5:E:4398:HOH:O	1.82	0.78
2:F:51:ILE:HG21	5:F:193:HOH:O	1.83	0.78
1:A:107:ALA:HB3	1:A:121:PRO:HG2	1.65	0.78
2:F:100(K):PRO:HD2	2:F:103:TRP:HZ3	1.49	0.78
1:C:460:ASN:HA	5:C:4184:HOH:O	1.83	0.78
1:A:483:ALA:HB3	5:A:4261:HOH:O	1.84	0.77
1:E:224:ALA:HB3	5:E:4349:HOH:O	1.84	0.77
1:A:140:LYS:HD3	5:A:4302:HOH:O	1.82	0.77
2:D:100:LYS:HD2	5:D:182:HOH:O	1.84	0.77
1:E:100:ASN:HD22	1:E:101:HIS:CD2	2.03	0.77
2:B:100(A):LEU:HB2	2:B:103:TRP:NE1	1.99	0.77
1:A:460:ASN:CB	5:A:4422:HOH:O	2.28	0.77
2:B:96:PRO:CA	5:B:210:HOH:O	2.33	0.77
1:E:70:CYS:HB3	5:E:4409:HOH:O	1.83	0.77
1:A:427:ILE:CG1	5:A:4480:HOH:O	2.30	0.77
2:B:100:LYS:CD	5:B:220:HOH:O	2.25	0.77
1:C:392:ARG:O	1:C:395:VAL:HG22	1.85	0.77
1:E:227:ARG:HH21	1:E:227:ARG:HG3	1.49	0.77
1:E:208:LYS:HD3	1:E:250:ASN:OD1	1.86	0.76
1:A:163:VAL:CG2	1:A:165:LEU:CD2	2.62	0.76
1:C:409:TRP:CH2	1:C:417:VAL:HG11	2.20	0.76
1:E:479:ILE:HD12	5:E:4208:HOH:O	1.84	0.76
1:A:89:VAL:HG11	5:A:4430:HOH:O	1.85	0.76
1:E:428:VAL:HG22	5:E:4208:HOH:O	1.85	0.76
1:C:49:ILE:HG22	1:C:65:VAL:HG11	1.68	0.76
1:C:211:LEU:HD23	5:C:4272:HOH:O	1.85	0.76
1:E:426:PHE:HE2	5:E:4244:HOH:O	1.68	0.76
1:A:99:ILE:HB	1:A:179:ILE:HD13	1.68	0.76
1:A:490:ILE:CG1	5:A:4416:HOH:O	2.27	0.76
1:C:433:ASP:HA	5:C:4278:HOH:O	1.84	0.76
2:F:40:ALA:HB1	5:F:176:HOH:O	1.86	0.76
1:A:163:VAL:HG23	1:A:165:LEU:HD22	1.68	0.75
1:A:17:PHE:HA	5:A:4149:HOH:O	1.86	0.75
1:A:279:ASN:HD22	1:A:279:ASN:H	1.32	0.75
1:C:49:ILE:CG2	5:C:4391:HOH:O	2.26	0.75
1:C:486:PRO:HB3	5:C:4128:HOH:O	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:GLN:CD	5:C:4272:HOH:O	2.28	0.74
1:E:348:PHE:CZ	5:E:4496:HOH:O	2.39	0.74
1:C:427:ILE:HG13	5:C:4284:HOH:O	1.88	0.74
2:B:32:TYR:CD2	5:B:231:HOH:O	2.41	0.74
1:E:392:ARG:O	1:E:395:VAL:HG22	1.88	0.73
1:A:108:ALA:CB	5:A:4418:HOH:O	2.28	0.73
2:F:7:SER:HB2	2:F:21:SER:HB2	1.68	0.73
1:A:254:THR:HG22	1:A:293:LEU:HD23	1.69	0.73
1:A:421:ARG:HB3	1:A:421:ARG:NH2	2.03	0.73
2:B:71:ARG:NH2	5:B:159:HOH:O	2.20	0.73
1:A:7:GLN:CG	5:A:4420:HOH:O	2.28	0.73
1:A:17:PHE:HD2	5:A:4149:HOH:O	1.72	0.73
2:B:32:TYR:HB3	2:B:33:PRO:HD2	1.70	0.73
2:F:100(B):VAL:HG22	2:F:100(G):THR:HG22	1.69	0.73
1:E:70:CYS:CB	5:E:4409:HOH:O	2.35	0.73
1:E:86:CYS:HB2	1:E:93:ILE:HD11	1.70	0.73
1:E:230:ILE:HG23	5:E:4278:HOH:O	1.89	0.73
2:B:6:ALA:HB1	5:B:224:HOH:O	1.89	0.72
2:B:82(B):SER:CB	5:B:236:HOH:O	2.37	0.72
2:B:107:THR:HB	5:B:224:HOH:O	1.89	0.72
2:D:29:PHE:CZ	5:D:229:HOH:O	2.41	0.72
1:A:78:GLU:HG3	5:A:4218:HOH:O	1.87	0.72
2:D:75:ALA:CB	5:D:197:HOH:O	2.29	0.72
5:A:4270:HOH:O	2:B:47:LEU:HB3	1.88	0.72
1:C:5:GLN:HE21	1:C:5:GLN:HA	1.55	0.72
1:C:349:VAL:CG2	5:C:4345:HOH:O	2.26	0.72
1:C:178:MET:HE1	5:C:4219:HOH:O	1.89	0.72
1:C:197:ASP:CG	5:C:4324:HOH:O	2.33	0.72
2:D:108:GLN:HG3	5:D:175:HOH:O	1.87	0.72
1:E:143:THR:N	5:E:4426:HOH:O	2.23	0.72
1:A:25:ALA:CB	5:A:4468:HOH:O	2.24	0.72
1:A:7:GLN:CD	5:A:4420:HOH:O	2.32	0.72
1:E:341:SER:O	1:E:383:VAL:HG12	1.90	0.72
1:C:162:LEU:CD2	1:C:163:VAL:HG22	2.19	0.71
2:D:30:SER:HB3	5:D:150:HOH:O	1.90	0.71
1:E:152:ASN:HB3	5:E:4391:HOH:O	1.89	0.71
1:E:391:ILE:CG1	5:E:4385:HOH:O	2.25	0.71
1:A:33:GLY:HA2	5:A:4316:HOH:O	1.89	0.71
2:F:100(H):CYS:HB2	5:F:206:HOH:O	1.90	0.71
1:C:287:MET:CG	5:C:4344:HOH:O	2.38	0.71
1:E:446:GLY:HA2	1:E:469:VAL:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASP:HB3	5:C:4234:HOH:O	1.88	0.71
1:C:299:HIS:HD2	5:C:4293:HOH:O	1.74	0.71
1:A:289:SER:HB3	5:A:4325:HOH:O	1.89	0.71
1:A:75:ASN:HB2	5:A:4218:HOH:O	1.90	0.71
1:E:442:THR:HG21	5:E:4310:HOH:O	1.88	0.71
1:C:39:GLY:N	5:C:4371:HOH:O	2.23	0.71
1:A:231:PHE:CD1	1:A:293:LEU:HD22	2.26	0.71
2:D:69:ILE:CG1	5:D:219:HOH:O	2.29	0.71
1:A:99:ILE:HD11	1:A:202:MET:HE1	1.73	0.70
1:C:243:LYS:HG2	5:C:4220:HOH:O	1.90	0.70
1:C:300:ASP:CB	5:C:4311:HOH:O	2.38	0.70
1:E:183:LEU:HD23	5:E:4456:HOH:O	1.90	0.70
1:A:372:ILE:HD12	1:A:372:ILE:N	2.05	0.70
2:B:34:MET:SD	5:B:156:HOH:O	2.47	0.70
1:E:409:TRP:CH2	1:E:417:VAL:HG11	2.26	0.70
1:A:91:VAL:HG23	5:A:4316:HOH:O	1.90	0.70
1:A:301:ASN:HB2	1:A:312:ILE:HD13	1.73	0.70
2:D:69:ILE:HD13	2:D:70:SER:N	2.07	0.70
1:A:432:ASP:N	5:A:4300:HOH:O	2.23	0.70
2:D:100(A):LEU:CA	2:D:103:TRP:HE1	2.04	0.70
1:C:303:ARG:CB	5:C:4327:HOH:O	2.39	0.70
1:C:437:SER:N	5:C:4336:HOH:O	2.25	0.70
2:D:20:LEU:HD22	2:D:107:THR:HG21	1.74	0.69
1:A:490:ILE:CD1	5:A:4416:HOH:O	2.39	0.69
2:B:76:ASN:HB2	5:B:212:HOH:O	1.93	0.69
1:A:281:GLY:N	5:A:4376:HOH:O	2.25	0.69
2:B:74:ALA:HB3	5:B:158:HOH:O	1.92	0.69
1:C:366:VAL:HG23	5:C:4366:HOH:O	1.92	0.69
2:F:100(G):THR:CB	5:F:221:HOH:O	2.25	0.69
1:C:162:LEU:HD22	1:C:163:VAL:HG22	1.75	0.69
1:C:300:ASP:HB2	5:C:4311:HOH:O	1.91	0.69
1:C:436:LEU:HD23	1:C:436:LEU:C	2.17	0.69
1:A:261:LYS:HE3	2:B:98:SER:HB3	1.73	0.69
1:C:303:ARG:HB2	5:C:4327:HOH:O	1.92	0.69
1:A:123:SER:HB3	5:A:4222:HOH:O	1.93	0.69
1:C:400:VAL:CA	5:C:4279:HOH:O	2.26	0.69
1:A:279:ASN:ND2	1:A:284:TRP:HE1	1.91	0.69
1:A:427:ILE:HD12	1:A:429:PHE:CE1	2.27	0.69
1:C:217:LEU:HB2	1:C:226:SER:HB2	1.75	0.69
2:B:29:PHE:HD2	2:B:30:SER:H	1.40	0.68
1:E:305:HIS:HB2	5:E:4332:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LYS:C	2:B:103:TRP:HE1	2.02	0.68
2:D:12:VAL:HG22	2:D:13:GLN:N	2.06	0.68
1:C:230:ILE:HG22	5:C:4083:HOH:O	1.94	0.68
1:A:78:GLU:CB	5:A:4218:HOH:O	2.41	0.68
1:E:343:ARG:NH1	5:E:4411:HOH:O	2.27	0.68
1:C:437:SER:HB3	5:C:4336:HOH:O	1.94	0.68
2:B:100(K):PRO:HD2	2:B:103:TRP:CZ3	2.29	0.68
1:E:264:THR:CG2	5:E:4451:HOH:O	2.42	0.68
1:A:11:THR:H	1:A:399:ASN:HD21	1.39	0.68
2:F:100(K):PRO:HD2	2:F:103:TRP:CZ3	2.28	0.68
1:E:384:CYS:HB2	5:E:4359:HOH:O	1.94	0.68
2:F:64:LYS:HE3	5:F:169:HOH:O	1.93	0.68
1:A:5:GLN:HA	1:A:5:GLN:HE21	1.58	0.68
1:C:287:MET:CB	5:C:4344:HOH:O	2.40	0.68
1:C:303:ARG:C	5:C:4327:HOH:O	2.37	0.67
1:E:279:ASN:H	1:E:279:ASN:HD22	1.42	0.67
1:E:417:VAL:HG12	1:E:418:ALA:N	2.09	0.67
1:A:13:ILE:HD11	1:A:337:ARG:HB2	1.76	0.67
1:C:49:ILE:HG21	1:C:103:CYS:CB	2.24	0.67
1:C:347:ASN:HD22	1:C:354:VAL:CG2	2.06	0.67
1:E:391:ILE:CD1	5:E:4385:HOH:O	2.43	0.67
2:B:3:GLN:HB2	5:B:216:HOH:O	1.93	0.67
1:A:56:ARG:NH1	1:A:72:ARG:HD2	2.09	0.67
1:C:360:PRO:HG2	1:C:367:ILE:HD12	1.77	0.67
1:C:417:VAL:HB	5:C:4145:HOH:O	1.94	0.67
1:E:261:LYS:HE3	2:F:98:SER:CB	2.25	0.67
2:B:30:SER:HA	5:B:156:HOH:O	1.95	0.67
1:E:263:GLY:C	5:E:4432:HOH:O	2.37	0.67
5:A:4270:HOH:O	2:B:47:LEU:HD23	1.94	0.66
1:E:185:LYS:HD3	5:E:4344:HOH:O	1.95	0.66
1:A:315:PHE:CE2	5:A:4238:HOH:O	2.47	0.66
2:B:28:THR:HB	5:B:162:HOH:O	1.93	0.66
1:A:157:VAL:HG11	1:A:242:ILE:CD1	2.24	0.66
1:A:453:ILE:HG22	5:A:4392:HOH:O	1.95	0.66
2:B:74:ALA:HB2	5:B:180:HOH:O	1.93	0.66
1:E:19:TRP:CZ3	5:E:4325:HOH:O	2.47	0.66
1:E:68:LYS:HB3	5:E:4409:HOH:O	1.94	0.66
2:B:100:LYS:CD	5:B:225:HOH:O	2.35	0.66
2:B:96:PRO:HA	5:B:210:HOH:O	1.92	0.66
1:C:299:HIS:CD2	5:C:4293:HOH:O	2.48	0.66
1:E:460:ASN:HB3	5:E:4247:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:LYS:CB	5:B:220:HOH:O	2.44	0.66
2:D:41:PRO:HD3	5:D:164:HOH:O	1.95	0.66
2:B:6:ALA:HB2	5:B:151:HOH:O	1.96	0.66
1:C:259:GLY:HA3	5:C:4308:HOH:O	1.95	0.66
1:A:453:ILE:CG2	5:A:4392:HOH:O	2.45	0.65
1:E:231:PHE:CD1	1:E:293:LEU:HD22	2.32	0.65
1:A:127:PRO:CD	5:A:4402:HOH:O	2.45	0.65
1:C:78:GLU:HB3	5:C:4172:HOH:O	1.95	0.65
2:D:82:MET:HB3	2:D:82(C):LEU:HD21	1.78	0.65
1:E:11:THR:H	1:E:399:ASN:HD21	1.43	0.65
2:B:95:GLY:HA2	5:B:167:HOH:O	1.96	0.65
1:E:410:TRP:CE2	5:E:4274:HOH:O	2.49	0.65
1:C:134:TRP:HB3	5:C:4151:HOH:O	1.96	0.65
1:E:140:LYS:NZ	1:E:140:LYS:HB2	2.11	0.65
1:A:281:GLY:CA	5:A:4376:HOH:O	2.45	0.65
1:A:279:ASN:HD21	1:A:284:TRP:HE1	1.44	0.65
1:E:458:VAL:C	5:E:4399:HOH:O	2.39	0.65
1:E:163:VAL:CG2	1:E:165:LEU:HD22	2.27	0.64
1:A:89:VAL:CG1	5:A:4430:HOH:O	2.42	0.64
1:C:427:ILE:HD13	1:C:428:VAL:N	2.12	0.64
1:A:227:ARG:HH21	1:A:227:ARG:HG3	1.61	0.64
1:A:421:ARG:HH21	1:A:421:ARG:CB	2.08	0.64
1:C:417:VAL:HG12	1:C:418:ALA:N	2.12	0.64
1:A:271:GLY:O	5:A:4270:HOH:O	2.15	0.64
1:C:212:ASP:HB2	5:C:4353:HOH:O	1.96	0.64
1:E:110:GLY:CA	5:E:4481:HOH:O	2.34	0.64
2:F:82(A):ASP:C	5:F:164:HOH:O	2.40	0.64
1:A:166:LEU:HD11	5:A:4385:HOH:O	1.96	0.64
2:B:24:ALA:O	5:B:157:HOH:O	2.15	0.64
2:B:84:PRO:HG2	2:B:85:GLU:OE1	1.97	0.64
1:A:30:ARG:CZ	1:A:372:ILE:HD11	2.27	0.64
1:A:166:LEU:CD1	5:A:4385:HOH:O	2.46	0.64
2:B:84:PRO:HA	2:B:111:VAL:HB	1.80	0.64
1:C:329:LEU:HD23	5:C:4084:HOH:O	1.97	0.64
1:E:341:SER:HA	5:E:4256:HOH:O	1.97	0.64
1:A:43:SER:HB3	5:A:4460:HOH:O	1.93	0.64
1:C:140:LYS:HB2	1:C:140:LYS:NZ	2.12	0.64
2:B:96:PRO:CB	5:B:210:HOH:O	2.46	0.64
1:C:49:ILE:CG2	1:C:65:VAL:HG13	2.21	0.64
1:C:279:ASN:H	1:C:279:ASN:HD22	1.45	0.64
1:C:427:ILE:HD12	1:C:429:PHE:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:HD3	5:A:4328:HOH:O	1.97	0.64
1:C:148:ILE:HG12	1:C:157:VAL:HA	1.80	0.64
1:C:235:ILE:HG13	5:C:4169:HOH:O	1.97	0.64
1:A:163:VAL:CG2	1:A:165:LEU:HD21	2.27	0.63
2:B:76:ASN:HB3	5:B:157:HOH:O	1.97	0.63
2:F:31:SER:C	5:F:180:HOH:O	2.40	0.63
2:F:94:ALA:O	2:F:100(K):PRO:O	2.17	0.63
2:F:100(A):LEU:HG	2:F:103:TRP:CD1	2.33	0.63
1:C:419:PHE:CE1	5:C:4320:HOH:O	2.51	0.63
1:A:478:SER:O	1:A:479:ILE:HD13	1.98	0.63
2:D:44:GLU:HG2	5:D:206:HOH:O	1.97	0.63
2:F:110:THR:HG23	5:F:191:HOH:O	1.97	0.63
1:A:14:VAL:HG12	1:A:338:VAL:HB	1.81	0.63
2:D:34:MET:SD	5:D:150:HOH:O	2.56	0.63
1:A:51:VAL:HG23	5:A:4317:HOH:O	1.99	0.63
1:A:424:ARG:NH1	5:A:4466:HOH:O	2.32	0.63
1:E:427:ILE:HD13	1:E:428:VAL:H	1.63	0.63
1:E:274:MET:HG3	1:E:277:LEU:HD12	1.81	0.63
1:A:132:SER:HB2	1:A:134:TRP:CD1	2.34	0.62
1:C:49:ILE:HG22	1:C:65:VAL:HG12	1.81	0.62
1:A:268:LYS:C	5:A:4441:HOH:O	2.42	0.62
1:A:453:ILE:HD13	1:A:487:PHE:CD1	2.34	0.62
1:A:468:TYR:HB2	5:A:4217:HOH:O	1.97	0.62
2:B:97:GLY:N	5:B:210:HOH:O	2.28	0.62
1:C:28:CYS:HA	1:C:32:LEU:HB2	1.80	0.62
1:E:363:ASN:O	1:E:366:VAL:HG22	1.99	0.62
1:C:219:THR:HA	1:C:222:PHE:O	1.99	0.62
2:D:34:MET:HG2	2:D:94:ALA:CB	2.29	0.62
2:D:50:ARG:CB	5:D:167:HOH:O	2.47	0.62
2:B:100(K):PRO:O	2:B:101:ASN:CB	2.45	0.62
1:C:4:PRO:HA	1:C:229:PHE:CG	2.34	0.62
1:E:125:GLU:HB3	5:E:4288:HOH:O	1.99	0.62
1:E:162:LEU:O	1:E:165:LEU:HD22	1.99	0.62
1:E:381:ASP:HB3	5:E:4343:HOH:O	1.98	0.62
1:E:426:PHE:CE2	5:E:4244:HOH:O	2.47	0.62
1:C:120:ASN:HB3	1:C:125:GLU:HB2	1.80	0.62
1:C:134:TRP:HE3	5:C:4151:HOH:O	1.83	0.62
1:C:374:ALA:HB3	5:C:4313:HOH:O	1.93	0.62
1:E:5:GLN:HE21	1:E:5:GLN:HA	1.65	0.62
2:D:80:LEU:HD21	5:D:192:HOH:O	2.00	0.62
1:E:329:LEU:HD23	1:E:394:MET:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ARG:HG3	1:E:227:ARG:NH2	2.14	0.61
1:A:227:ARG:HG3	1:A:227:ARG:NH2	2.14	0.61
1:A:404:GLN:OE1	1:A:422:GLY:HA3	2.00	0.61
2:F:32:TYR:N	5:F:180:HOH:O	2.31	0.61
1:A:76:GLU:HB3	5:A:4306:HOH:O	1.99	0.61
1:A:278:LYS:HD2	5:A:4236:HOH:O	2.00	0.61
1:E:343:ARG:HG2	1:E:343:ARG:HH21	1.66	0.61
2:F:31:SER:HB3	5:F:127:HOH:O	1.99	0.61
1:A:134:TRP:HB2	5:A:4343:HOH:O	2.01	0.61
1:A:394:MET:HE2	5:A:4230:HOH:O	1.99	0.61
1:A:483:ALA:CB	5:A:4261:HOH:O	2.44	0.61
2:B:34:MET:HG2	2:B:94:ALA:CB	2.30	0.61
1:A:7:GLN:HB3	1:A:10:ARG:HD2	1.81	0.61
1:A:407:ALA:HB2	5:A:4415:HOH:O	2.01	0.61
2:D:71:ARG:HB2	5:D:128:HOH:O	1.99	0.61
1:A:242:ILE:HD12	5:A:4248:HOH:O	2.01	0.61
1:E:273:LYS:HZ1	2:F:61:ASP:H	1.48	0.61
1:C:208:LYS:HD3	1:C:250:ASN:OD1	2.01	0.60
1:C:49:ILE:HD11	1:C:63:GLN:CD	2.26	0.60
2:F:32:TYR:CE2	2:F:96:PRO:HB3	2.36	0.60
1:C:349:VAL:HG23	1:C:349:VAL:O	2.00	0.60
1:C:484:GLU:OE2	1:C:484:GLU:N	2.34	0.60
2:D:82:MET:HE2	2:D:82(C):LEU:HD21	1.82	0.60
1:E:463:THR:C	5:E:4488:HOH:O	2.45	0.60
1:A:435:GLN:HE21	1:A:436:LEU:N	2.00	0.60
2:B:6:ALA:CB	5:B:224:HOH:O	2.47	0.60
1:C:295:PHE:N	5:C:4294:HOH:O	2.34	0.60
2:D:100(A):LEU:CB	2:D:103:TRP:NE1	2.65	0.60
2:B:23:ALA:HA	5:B:205:HOH:O	2.00	0.60
1:C:348:PHE:CE1	1:C:353:ASP:HB2	2.36	0.60
2:D:100(K):PRO:O	2:D:101:ASN:CB	2.50	0.60
1:E:69:LEU:N	1:E:69:LEU:HD12	2.16	0.60
1:C:7:GLN:HB2	5:C:4147:HOH:O	2.02	0.60
2:D:82:MET:HG2	5:D:192:HOH:O	2.01	0.60
1:E:154:PRO:O	1:E:157:VAL:HG12	2.01	0.60
1:C:465:ILE:HD13	5:C:4191:HOH:O	2.01	0.60
1:A:72:ARG:HD3	5:A:4219:HOH:O	2.02	0.60
1:C:158:ARG:NH1	1:C:242:ILE:HD12	2.17	0.60
1:A:13:ILE:HD12	1:A:335:PHE:HE2	1.67	0.59
2:F:37:TYR:CZ	2:F:47:LEU:HD13	2.37	0.59
2:F:100:LYS:CE	5:F:204:HOH:O	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:THR:H	1:A:399:ASN:ND2	2.00	0.59
2:B:37:TYR:CZ	2:B:47:LEU:HD13	2.37	0.59
2:F:12:VAL:HG22	2:F:13:GLN:N	2.18	0.59
1:C:11:THR:H	1:C:399:ASN:HD21	1.50	0.59
1:E:328:MET:HE1	5:E:4257:HOH:O	2.02	0.59
1:A:393:ASN:HB3	1:A:452:VAL:HB	1.84	0.59
1:C:111:THR:CG2	5:C:4338:HOH:O	2.45	0.59
1:A:2:TYR:O	1:A:252:ARG:HD2	2.01	0.59
1:A:276:TYR:HE1	5:A:4270:HOH:O	1.86	0.59
1:A:490:ILE:HD13	1:A:490:ILE:N	2.17	0.59
1:C:126:PHE:O	1:C:130:PRO:HA	2.02	0.59
1:C:427:ILE:CG1	5:C:4284:HOH:O	2.45	0.59
2:D:40:ALA:HB3	2:D:43:LYS:HB2	1.85	0.59
2:F:11:SER:HB3	2:F:110:THR:HB	1.83	0.59
2:B:57:ALA:HB1	5:B:149:HOH:O	2.03	0.59
1:C:100:ASN:HD22	1:C:101:HIS:HD2	1.50	0.59
1:C:170:LEU:O	1:C:176:ARG:HD2	2.03	0.59
1:A:435:GLN:NE2	1:A:436:LEU:N	2.50	0.58
1:A:367:ILE:N	1:A:367:ILE:HD12	2.18	0.58
1:A:394:MET:CE	5:A:4230:HOH:O	2.51	0.58
1:C:179:ILE:N	5:C:4252:HOH:O	2.33	0.58
2:D:44:GLU:CG	5:D:206:HOH:O	2.49	0.58
1:E:92:ARG:HD3	1:E:192:ALA:HB2	1.84	0.58
1:E:349:VAL:HG12	5:E:4338:HOH:O	2.03	0.58
2:F:30:SER:CB	2:F:71:ARG:HH21	2.13	0.58
2:B:32:TYR:CG	5:B:231:HOH:O	2.55	0.58
2:B:29:PHE:CD2	2:B:30:SER:N	2.68	0.58
1:E:341:SER:C	1:E:383:VAL:HG12	2.29	0.58
1:A:157:VAL:HG11	1:A:242:ILE:HD11	1.85	0.58
1:C:127:PRO:O	1:C:130:PRO:HB3	2.03	0.58
1:E:417:VAL:CG1	1:E:418:ALA:N	2.67	0.58
1:E:163:VAL:HG22	1:E:165:LEU:HD22	1.85	0.58
2:F:100:LYS:HE3	5:F:204:HOH:O	2.04	0.58
1:C:62:TYR:HD2	5:C:4324:HOH:O	1.87	0.58
1:C:436:LEU:CD2	5:C:4250:HOH:O	2.52	0.58
1:A:132:SER:HB2	1:A:134:TRP:NE1	2.18	0.58
1:A:165:LEU:HD13	5:A:4314:HOH:O	2.03	0.58
1:A:257:LYS:HE3	2:B:97:GLY:N	2.17	0.58
2:D:72:ASP:HB2	5:D:153:HOH:O	2.03	0.58
1:A:281:GLY:HA2	5:A:4376:HOH:O	2.04	0.58
2:D:100(J):GLY:C	2:D:103:TRP:HH2	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ALA:HB1	1:A:171:GLU:OE1	2.03	0.58
1:A:279:ASN:HD22	1:A:279:ASN:N	2.01	0.58
2:B:29:PHE:HD2	2:B:30:SER:N	2.00	0.58
1:C:462:CYS:SG	1:C:466:LYS:HG2	2.44	0.58
1:E:178:MET:SD	5:E:4268:HOH:O	2.57	0.58
1:A:140:LYS:HB2	1:A:140:LYS:NZ	2.18	0.57
1:A:195:ARG:NH2	4:A:4002:CL:CL	2.74	0.57
1:E:93:ILE:CD1	5:E:4350:HOH:O	2.52	0.57
1:A:78:GLU:N	5:A:4218:HOH:O	2.07	0.57
1:C:303:ARG:HH21	1:C:303:ARG:HG3	1.69	0.57
2:D:93:ALA:HB1	2:D:103:TRP:CZ3	2.39	0.57
1:E:430:ASN:HB2	1:E:436:LEU:HD13	1.84	0.57
1:E:329:LEU:HD23	1:E:394:MET:CB	2.34	0.57
1:A:10:ARG:NH1	5:A:4316:HOH:O	2.37	0.57
2:B:100(A):LEU:HG	2:B:103:TRP:CD1	2.39	0.57
1:E:10:ARG:HB3	1:E:38:GLY:HA2	1.86	0.57
1:E:177:SER:CB	5:E:4491:HOH:O	2.32	0.57
1:E:436:LEU:C	1:E:436:LEU:HD23	2.30	0.57
1:C:231:PHE:C	5:C:4083:HOH:O	2.48	0.57
2:D:69:ILE:HD11	5:D:219:HOH:O	1.97	0.57
1:A:137:ASN:O	1:A:139:GLY:N	2.38	0.57
2:F:45:CYS:CB	5:F:206:HOH:O	2.32	0.57
1:A:119:CYS:HA	5:A:4402:HOH:O	2.05	0.57
1:A:429:PHE:CE2	5:A:4338:HOH:O	2.43	0.57
1:E:11:THR:H	1:E:399:ASN:ND2	2.02	0.57
1:E:383:VAL:C	5:E:4359:HOH:O	2.48	0.57
1:E:435:GLN:HE22	1:E:436:LEU:C	2.12	0.57
1:C:303:ARG:CA	5:C:4327:HOH:O	2.52	0.57
1:C:427:ILE:HD13	1:C:428:VAL:H	1.70	0.57
1:C:436:LEU:HD22	5:C:4250:HOH:O	2.03	0.57
1:E:458:VAL:CA	5:E:4399:HOH:O	2.52	0.57
1:A:490:ILE:HD13	1:A:490:ILE:H	1.68	0.56
1:C:341:SER:C	1:C:383:VAL:HG12	2.29	0.56
1:E:264:THR:HG23	5:E:4451:HOH:O	2.03	0.56
2:F:87:THR:O	2:F:88:ALA:HB2	2.05	0.56
1:A:15:HIS:CE1	5:A:4149:HOH:O	2.58	0.56
1:C:258:TYR:HE1	1:C:262:LEU:HD12	1.69	0.56
2:D:83:LYS:NZ	5:D:173:HOH:O	2.34	0.56
1:E:310:SER:N	5:E:4447:HOH:O	2.37	0.56
2:F:82:MET:SD	5:F:228:HOH:O	2.58	0.56
1:A:49:ILE:HG23	5:A:4317:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:29:PHE:HZ	5:D:229:HOH:O	1.83	0.56
2:F:83:LYS:C	2:F:111:VAL:HG11	2.31	0.56
1:A:78:GLU:CG	5:A:4218:HOH:O	2.47	0.56
1:A:349:VAL:HG22	1:A:354:VAL:HG13	1.88	0.56
1:E:301:ASN:CG	1:E:312:ILE:HD13	2.31	0.56
2:D:100(A):LEU:HD23	2:D:103:TRP:HD1	1.70	0.56
2:D:100(F):ARG:HD3	5:D:206:HOH:O	2.05	0.56
1:E:362:ASN:ND2	5:E:4239:HOH:O	2.35	0.56
2:F:54:ASP:HB3	5:F:171:HOH:O	2.06	0.56
2:F:34:MET:HG2	2:F:94:ALA:HB1	1.87	0.56
2:F:84:PRO:HG2	2:F:85:GLU:OE1	2.06	0.56
1:A:72:ARG:NH2	5:A:4381:HOH:O	2.38	0.56
1:A:162:LEU:O	1:A:165:LEU:HD23	2.04	0.56
2:B:100(A):LEU:CB	2:B:103:TRP:NE1	2.69	0.56
1:C:400:VAL:HG13	5:C:4279:HOH:O	2.06	0.56
1:E:475:ALA:CB	5:E:4310:HOH:O	2.54	0.56
1:A:13:ILE:HD13	1:A:336:THR:O	2.06	0.56
1:A:140:LYS:HB2	1:A:140:LYS:HZ2	1.70	0.56
2:D:40:ALA:HB1	2:D:41:PRO:HD2	1.88	0.56
1:A:72:ARG:HB3	1:A:367:ILE:HD13	1.87	0.56
1:A:366:VAL:HG23	1:A:366:VAL:O	2.04	0.56
2:B:75:ALA:O	2:B:77:THR:HG23	2.06	0.56
2:D:47:LEU:HD21	5:D:167:HOH:O	2.06	0.56
1:E:142:LYS:HD3	5:E:4497:HOH:O	2.06	0.56
1:E:468:TYR:HB2	5:E:4035:HOH:O	2.04	0.56
2:B:3:GLN:CB	5:B:216:HOH:O	2.52	0.55
2:B:34:MET:HG2	2:B:94:ALA:HB2	1.87	0.55
1:A:30:ARG:NH1	1:A:372:ILE:HD11	2.21	0.55
1:C:469:VAL:O	1:C:469:VAL:HG13	2.06	0.55
2:F:19:ARG:CZ	5:F:184:HOH:O	2.54	0.55
2:F:84:PRO:HA	2:F:111:VAL:HB	1.88	0.55
2:F:100(K):PRO:O	2:F:102:TYR:N	2.38	0.55
1:A:426:PHE:CE2	5:A:4250:HOH:O	2.53	0.55
2:D:100:LYS:HA	2:D:100(H):CYS:O	2.07	0.55
2:B:100(A):LEU:HD22	2:B:100(C):VAL:HG23	1.87	0.55
1:C:49:ILE:CG2	1:C:103:CYS:HB3	2.37	0.55
1:C:343:ARG:HG2	1:C:343:ARG:HH21	1.71	0.55
2:D:89:VAL:HG13	2:D:107:THR:O	2.06	0.55
1:E:7:GLN:OE1	1:E:10:ARG:NH2	2.39	0.55
2:B:29:PHE:O	5:B:156:HOH:O	2.18	0.55
1:C:25:ALA:HB1	1:C:85:ARG:CZ	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:GLN:NE2	5:D:178:HOH:O	2.38	0.55
1:E:412:ASN:ND2	1:E:416:GLN:HG3	2.22	0.55
2:F:32:TYR:CZ	2:F:96:PRO:HB3	2.42	0.55
1:A:315:PHE:CZ	5:A:4238:HOH:O	2.60	0.55
1:A:416:GLN:CG	5:A:4300:HOH:O	2.55	0.55
2:D:70:SER:HB3	5:D:181:HOH:O	2.07	0.55
1:A:412:ASN:CG	1:A:416:GLN:HB2	2.32	0.55
2:F:93:ALA:HB1	2:F:103:TRP:CZ3	2.42	0.55
1:A:187:ILE:HD11	1:A:194:PHE:HE1	1.70	0.54
1:C:48:ASN:OD1	1:C:114:THR:HG21	2.07	0.54
1:C:214:LEU:O	1:C:227:ARG:NH1	2.40	0.54
1:C:279:ASN:HD22	1:C:279:ASN:N	2.03	0.54
1:C:291:ARG:HB2	5:C:4344:HOH:O	2.07	0.54
2:F:20:LEU:CD2	5:F:228:HOH:O	2.54	0.54
1:A:183:LEU:O	1:A:187:ILE:HG12	2.07	0.54
2:D:72:ASP:OD1	2:D:79:TYR:HE2	1.91	0.54
1:A:82:MET:CA	5:A:4468:HOH:O	2.27	0.54
2:F:43:LYS:HE2	5:F:174:HOH:O	2.06	0.54
1:C:271:GLY:N	5:C:4378:HOH:O	2.40	0.54
1:C:288:PRO:HD2	5:C:4344:HOH:O	2.08	0.54
1:E:367:ILE:HG12	5:E:4022:HOH:O	2.07	0.54
1:E:469:VAL:HG12	5:E:4310:HOH:O	2.08	0.54
1:E:484:GLU:HG2	1:E:485:ASP:N	2.23	0.54
2:B:72:ASP:C	2:B:74:ALA:H	2.16	0.54
2:B:100(K):PRO:HD2	2:B:103:TRP:HZ3	1.71	0.54
1:C:245:SER:HA	1:C:248:PHE:CE2	2.43	0.54
1:E:142:LYS:C	5:E:4426:HOH:O	2.49	0.54
1:E:257:LYS:HE2	2:F:97:GLY:HA2	1.90	0.54
1:A:416:GLN:HG2	5:A:4300:HOH:O	2.07	0.54
1:C:5:GLN:HA	1:C:5:GLN:NE2	2.21	0.54
1:E:446:GLY:HA2	1:E:469:VAL:CG2	2.38	0.54
1:A:4:PRO:HB2	1:A:6:THR:HG23	1.90	0.54
1:A:390:GLU:CG	5:A:4392:HOH:O	2.47	0.54
1:C:132:SER:HB2	1:C:134:TRP:NE1	2.22	0.54
2:D:4:LEU:N	5:D:189:HOH:O	2.41	0.54
1:E:86:CYS:CB	1:E:93:ILE:HD11	2.38	0.54
1:A:77:ASN:ND2	5:A:4234:HOH:O	2.40	0.53
1:E:186:LEU:HB3	1:E:191:VAL:HG21	1.90	0.53
1:A:78:GLU:HB2	5:A:4218:HOH:O	2.06	0.53
1:A:118:TYR:HD2	5:A:4402:HOH:O	1.79	0.53
2:B:82(A):ASP:CG	5:B:211:HOH:O	2.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:VAL:HB	1:C:93:ILE:HD13	1.90	0.53
1:C:229:PHE:HE2	1:C:252:ARG:HD3	1.73	0.53
1:E:332:PRO:HA	1:E:421:ARG:NH1	2.23	0.53
1:A:349:VAL:HG23	1:A:349:VAL:O	2.07	0.53
1:E:393:ASN:HB3	1:E:452:VAL:HB	1.90	0.53
2:F:91:TYR:CD2	5:F:220:HOH:O	2.54	0.53
1:A:340:SER:HA	1:A:385:GLU:OE2	2.07	0.53
1:C:11:THR:H	1:C:399:ASN:ND2	2.06	0.53
1:A:484:GLU:HG2	1:A:485:ASP:N	2.24	0.53
1:E:304:GLY:O	1:E:306:GLY:N	2.37	0.53
2:F:100:LYS:NZ	5:F:204:HOH:O	2.34	0.53
1:A:5:GLN:HA	1:A:5:GLN:NE2	2.22	0.53
1:E:343:ARG:HD2	5:E:4380:HOH:O	2.00	0.53
1:A:341:SER:C	1:A:383:VAL:HG12	2.32	0.53
2:D:73:ASN:N	5:D:153:HOH:O	2.41	0.53
1:E:157:VAL:HG13	1:E:158:ARG:HG3	1.89	0.53
2:F:34:MET:HE1	5:F:157:HOH:O	2.08	0.53
1:A:303:ARG:HH21	1:A:303:ARG:HG3	1.73	0.53
1:C:233:GLU:HG2	5:C:4169:HOH:O	2.09	0.53
2:D:50:ARG:O	2:D:57:ALA:HA	2.08	0.53
2:D:100(K):PRO:N	2:D:103:TRP:HH2	2.05	0.53
1:A:447:GLY:N	1:A:469:VAL:HG13	2.23	0.53
2:D:50:ARG:N	5:D:179:HOH:O	2.42	0.53
2:D:84:PRO:HA	2:D:111:VAL:HB	1.91	0.53
1:A:340:SER:CB	5:A:4233:HOH:O	2.46	0.53
1:C:49:ILE:CG2	1:C:65:VAL:HG12	2.36	0.53
1:C:203:TRP:HZ3	5:C:4314:HOH:O	1.92	0.53
1:E:268:LYS:HE2	5:E:4390:HOH:O	2.08	0.53
1:E:380:ASN:ND2	5:E:4396:HOH:O	2.42	0.53
2:F:20:LEU:CG	5:F:228:HOH:O	2.49	0.53
1:A:4:PRO:O	1:A:5:GLN:HB2	2.08	0.52
1:C:242:ILE:HG12	5:C:4381:HOH:O	2.09	0.52
2:D:80:LEU:CD2	5:D:192:HOH:O	2.56	0.52
1:A:215:HIS:O	5:A:4341:HOH:O	2.19	0.52
2:D:102:TYR:O	2:D:103:TRP:HE3	1.93	0.52
1:C:39:GLY:CA	5:C:4371:HOH:O	2.56	0.52
2:D:94:ALA:O	2:D:100(K):PRO:O	2.27	0.52
1:E:273:LYS:NZ	2:F:61:ASP:H	2.07	0.52
1:C:75:ASN:HB2	1:C:77:ASN:OD1	2.10	0.52
1:A:404:GLN:O	1:A:421:ARG:NH2	2.42	0.52
1:C:274:MET:HE1	1:C:429:PHE:CB	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:SER:HB2	5:E:4328:HOH:O	2.09	0.52
1:E:126:PHE:O	1:E:130:PRO:HA	2.10	0.52
1:A:13:ILE:HD13	1:A:13:ILE:H	1.74	0.52
1:A:301:ASN:HB2	1:A:312:ILE:CD1	2.39	0.52
2:B:100:LYS:HB3	5:B:220:HOH:O	2.08	0.52
2:B:100(K):PRO:HD2	2:B:103:TRP:CH2	2.44	0.52
1:C:92:ARG:HB2	1:C:94:TYR:CE1	2.45	0.52
2:D:12:VAL:CG2	2:D:13:GLN:H	2.20	0.52
1:E:401:VAL:HB	1:E:421:ARG:HB3	1.92	0.52
1:E:410:TRP:NE1	5:E:4274:HOH:O	2.43	0.52
1:C:350:ASN:CA	5:C:4355:HOH:O	2.43	0.52
2:D:17:SER:HA	2:D:82:MET:O	2.10	0.52
1:E:301:ASN:ND2	1:E:312:ILE:HD13	2.24	0.52
1:A:355:ASN:O	1:A:358:ILE:HG13	2.09	0.52
1:C:440:LEU:O	1:C:474:THR:HA	2.10	0.52
1:E:349:VAL:HB	5:E:4372:HOH:O	2.09	0.52
2:F:32:TYR:CA	5:F:180:HOH:O	2.58	0.52
1:A:487:PHE:CE1	5:A:4338:HOH:O	2.63	0.52
2:B:98:SER:HB2	5:B:200:HOH:O	2.02	0.52
1:C:124:ARG:NH1	1:C:138:ASP:OD2	2.43	0.52
1:E:231:PHE:N	5:E:4278:HOH:O	2.43	0.52
1:E:396:TRP:O	1:E:400:VAL:HG23	2.09	0.52
2:F:3:GLN:HB2	5:F:188:HOH:O	2.10	0.52
1:A:280:TRP:CD1	5:A:4376:HOH:O	2.63	0.51
2:B:96:PRO:HB2	5:B:210:HOH:O	2.08	0.51
2:F:100(J):GLY:C	2:F:103:TRP:HH2	2.17	0.51
1:A:269:TRP:C	5:A:4441:HOH:O	2.53	0.51
1:C:237:LEU:N	1:C:237:LEU:HD22	2.26	0.51
1:E:196:ILE:HG12	5:E:4278:HOH:O	2.11	0.51
1:E:435:GLN:NE2	1:E:436:LEU:O	2.43	0.51
1:A:13:ILE:HD12	1:A:335:PHE:CE2	2.45	0.51
1:A:72:ARG:NE	1:A:367:ILE:HD11	2.26	0.51
1:A:348:PHE:CE1	1:A:353:ASP:HB2	2.44	0.51
2:B:71:ARG:NH1	5:B:201:HOH:O	2.32	0.51
2:B:93:ALA:CB	2:B:103:TRP:CZ3	2.90	0.51
2:D:53:SER:HA	2:D:71:ARG:HH12	1.75	0.51
1:E:381:ASP:CB	5:E:4343:HOH:O	2.56	0.51
1:E:458:VAL:CB	5:E:4399:HOH:O	2.34	0.51
2:F:19:ARG:HG3	2:F:81:GLN:HG2	1.92	0.51
1:E:435:GLN:NE2	1:E:436:LEU:N	2.58	0.51
1:E:439:THR:C	1:E:440:LEU:HD12	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:VAL:HG11	1:C:113:THR:HG22	1.93	0.51
1:C:409:TRP:CH2	1:C:417:VAL:CG1	2.93	0.51
1:E:140:LYS:HB2	1:E:140:LYS:HZ3	1.73	0.51
1:E:409:TRP:CH2	1:E:417:VAL:CG1	2.93	0.51
2:F:12:VAL:HG22	2:F:13:GLN:H	1.75	0.51
1:A:16:LEU:HD12	1:A:40:VAL:HG11	1.92	0.51
1:C:217:LEU:HB2	1:C:226:SER:CB	2.41	0.51
1:C:428:VAL:CG2	5:C:4250:HOH:O	2.58	0.51
1:A:195:ARG:HG3	1:A:231:PHE:CE1	2.45	0.51
1:A:330:ALA:HB2	5:A:4230:HOH:O	2.10	0.51
1:C:162:LEU:HD23	1:C:163:VAL:HG22	1.91	0.51
2:D:18:LEU:HD12	2:D:82(C):LEU:CD1	2.40	0.51
1:C:216:ASN:C	5:C:4218:HOH:O	2.54	0.51
1:C:360:PRO:HG2	1:C:367:ILE:CD1	2.39	0.51
2:F:86:ASP:C	5:F:209:HOH:O	2.53	0.51
1:A:98:VAL:HG13	5:A:4139:HOH:O	2.09	0.51
1:C:1:GLN:NE2	5:C:4272:HOH:O	2.42	0.51
1:E:142:LYS:HE2	5:E:4200:HOH:O	2.11	0.51
2:B:32:TYR:CB	5:B:231:HOH:O	2.58	0.50
1:C:257:LYS:HE3	2:D:97:GLY:CA	2.41	0.50
1:E:332:PRO:HA	1:E:421:ARG:HH11	1.76	0.50
1:C:231:PHE:CG	1:C:293:LEU:HD13	2.45	0.50
1:E:56:ARG:NH1	1:E:72:ARG:HD2	2.26	0.50
2:D:76:ASN:N	5:D:153:HOH:O	2.45	0.50
2:D:96:PRO:CG	5:D:220:HOH:O	2.44	0.50
1:E:459:GLY:N	5:E:4399:HOH:O	2.44	0.50
1:A:148:ILE:HD12	1:A:148:ILE:N	2.26	0.50
1:C:132:SER:HB2	1:C:134:TRP:CD1	2.47	0.50
2:D:50:ARG:HB3	5:D:167:HOH:O	2.09	0.50
1:E:381:ASP:CA	5:E:4343:HOH:O	2.59	0.50
1:A:301:ASN:CB	1:A:312:ILE:HD13	2.41	0.50
2:B:100(A):LEU:CA	2:B:103:TRP:HE1	2.25	0.50
1:C:49:ILE:CD1	1:C:63:GLN:OE1	2.57	0.50
1:C:427:ILE:HD12	1:C:429:PHE:CZ	2.46	0.50
1:C:417:VAL:CG1	1:C:418:ALA:N	2.75	0.50
2:D:50:ARG:HB2	5:D:167:HOH:O	2.12	0.50
1:E:322:LYS:HG2	1:E:391:ILE:HD11	1.92	0.50
1:C:446:GLY:HA2	1:C:469:VAL:HG13	1.93	0.50
1:E:35:LYS:HE3	5:E:4394:HOH:O	2.12	0.50
1:C:437:SER:HA	1:C:477:PHE:O	2.12	0.50
2:D:101:ASN:ND2	5:D:214:HOH:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:TRP:HB2	5:A:4178:HOH:O	2.12	0.50
1:A:447:GLY:H	1:A:469:VAL:HG13	1.77	0.50
1:C:21:TRP:CG	5:C:4239:HOH:O	2.64	0.49
1:C:340:SER:HA	1:C:385:GLU:OE2	2.12	0.49
1:C:419:PHE:CD1	5:C:4320:HOH:O	2.64	0.49
2:D:100(A):LEU:N	2:D:103:TRP:HE1	2.10	0.49
1:E:31:TYR:OH	1:E:387:ARG:HA	2.11	0.49
2:F:100:LYS:HA	2:F:100(H):CYS:O	2.12	0.49
1:E:401:VAL:HG21	1:E:421:ARG:HG3	1.94	0.49
1:A:383:VAL:HG13	1:A:385:GLU:OE2	2.13	0.49
1:C:435:GLN:HG2	1:C:480:SER:HA	1.94	0.49
1:A:367:ILE:CD1	1:A:367:ILE:H	2.26	0.49
1:C:366:VAL:HG23	1:C:366:VAL:O	2.12	0.49
1:C:392:ARG:HD2	5:C:4236:HOH:O	2.11	0.49
1:E:278:LYS:CG	5:E:4382:HOH:O	2.28	0.49
1:A:127:PRO:HD3	5:A:4402:HOH:O	2.11	0.49
1:A:417:VAL:CG1	1:A:418:ALA:N	2.75	0.49
1:C:279:ASN:ND2	1:C:284:TRP:HE1	2.10	0.49
1:C:394:MET:CE	5:C:4284:HOH:O	2.60	0.49
2:D:100(A):LEU:HD23	2:D:103:TRP:CD1	2.48	0.49
1:C:245:SER:N	5:C:4254:HOH:O	2.39	0.49
1:C:320:LEU:HD11	5:C:4021:HOH:O	2.12	0.49
1:C:427:ILE:HG12	1:C:489:ALA:HB2	1.93	0.49
1:E:244:SER:HB2	1:E:253:VAL:HG11	1.95	0.49
2:F:84:PRO:CD	5:F:205:HOH:O	2.35	0.49
2:B:100(J):GLY:HA3	2:B:103:TRP:HH2	1.76	0.49
1:E:437:SER:HA	1:E:477:PHE:O	2.13	0.49
1:A:375:ASP:OD2	1:A:377:THR:HG23	2.13	0.49
1:A:439:THR:OG1	1:A:476:GLN:NE2	2.46	0.49
1:C:49:ILE:HG12	1:C:63:GLN:HB2	1.95	0.49
2:D:12:VAL:CG2	2:D:13:GLN:N	2.75	0.49
2:D:51:ILE:HD11	5:D:168:HOH:O	2.12	0.49
1:E:87:ASN:CG	5:E:4350:HOH:O	2.55	0.49
1:E:238:GLY:HA3	2:F:101:ASN:HD21	1.78	0.49
2:F:91:TYR:CE2	5:F:220:HOH:O	2.66	0.49
1:A:268:LYS:HE3	5:A:4407:HOH:O	2.12	0.49
1:A:431:ASN:N	5:A:4300:HOH:O	2.45	0.49
1:C:392:ARG:O	1:C:395:VAL:CG2	2.59	0.49
1:E:349:VAL:HG22	1:E:354:VAL:HG13	1.94	0.49
1:A:274:MET:HG3	1:A:277:LEU:HD12	1.94	0.49
1:A:331:HIS:CG	1:A:332:PRO:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:MET:HG3	5:C:4344:HOH:O	2.09	0.49
1:C:300:ASP:CA	5:C:4311:HOH:O	2.61	0.48
2:F:31:SER:CA	5:F:215:HOH:O	2.27	0.48
2:B:32:TYR:HB3	2:B:33:PRO:CD	2.42	0.48
1:C:87:ASN:HB3	1:C:221:TRP:CD1	2.48	0.48
1:C:183:LEU:O	1:C:187:ILE:HG12	2.13	0.48
1:E:279:ASN:ND2	1:E:284:TRP:HE1	2.11	0.48
1:E:347:ASN:O	1:E:354:VAL:HG22	2.13	0.48
1:A:137:ASN:O	1:A:138:ASP:C	2.57	0.48
1:A:357:TRP:HA	5:A:4355:HOH:O	2.13	0.48
2:B:100(K):PRO:HB3	5:B:165:HOH:O	2.13	0.48
1:A:127:PRO:HD2	5:A:4402:HOH:O	2.11	0.48
1:A:451:ASP:OD1	1:A:488:ILE:HD12	2.13	0.48
1:C:170:LEU:HD12	5:C:4275:HOH:O	2.14	0.48
1:C:279:ASN:H	1:C:279:ASN:ND2	2.12	0.48
1:E:203:TRP:O	1:E:207:ILE:HG12	2.13	0.48
1:C:484:GLU:HG2	1:C:485:ASP:OD2	2.13	0.48
1:A:488:ILE:HG22	1:A:489:ALA:N	2.28	0.48
2:B:100(A):LEU:N	2:B:103:TRP:HE1	2.12	0.48
1:E:484:GLU:CB	5:E:4437:HOH:O	2.61	0.48
2:F:100:LYS:C	2:F:103:TRP:HE1	2.21	0.48
1:C:229:PHE:O	1:C:230:ILE:HD13	2.14	0.48
1:C:331:HIS:CG	1:C:332:PRO:HD2	2.49	0.48
1:A:257:LYS:HE3	2:B:97:GLY:CA	2.44	0.48
1:C:435:GLN:NE2	1:C:435:GLN:C	2.72	0.48
2:D:100(K):PRO:N	2:D:103:TRP:CH2	2.81	0.48
1:E:28:CYS:HA	1:E:32:LEU:HB2	1.96	0.48
1:E:368:LYS:CD	5:E:4396:HOH:O	2.37	0.48
1:A:187:ILE:HG13	5:A:4341:HOH:O	2.13	0.48
1:C:191:VAL:HG12	1:C:193:GLY:H	1.79	0.48
2:D:2:VAL:HG11	2:D:102:TYR:CZ	2.49	0.48
1:E:262:LEU:HG	1:E:280:TRP:CZ2	2.49	0.48
2:F:82(C):LEU:N	5:F:164:HOH:O	2.46	0.48
1:C:200:LYS:HE3	5:C:4130:HOH:O	2.14	0.48
1:C:435:GLN:HE22	1:C:437:SER:HB2	1.78	0.48
2:D:29:PHE:HE2	5:D:138:HOH:O	1.97	0.48
1:E:229:PHE:CE2	1:E:252:ARG:HD3	2.49	0.48
1:A:490:ILE:HD12	5:A:4416:HOH:O	2.09	0.47
1:C:271:GLY:HA3	2:D:47:LEU:H	1.78	0.47
2:D:100:LYS:C	2:D:103:TRP:HE1	2.22	0.47
2:D:100(A):LEU:CB	2:D:103:TRP:HE1	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:CYS:C	5:E:4426:HOH:O	2.57	0.47
1:E:442:THR:O	1:E:444:LEU:HD12	2.14	0.47
1:A:62:TYR:HD2	5:A:4139:HOH:O	1.96	0.47
1:A:267:ARG:HD3	1:A:269:TRP:CZ2	2.49	0.47
1:A:280:TRP:C	5:A:4376:HOH:O	2.57	0.47
1:A:366:VAL:HG21	5:A:4128:HOH:O	2.13	0.47
2:B:34:MET:HG2	2:B:94:ALA:HB1	1.95	0.47
1:C:257:LYS:CE	5:D:152:HOH:O	2.46	0.47
1:E:163:VAL:HG23	1:E:165:LEU:HD22	1.95	0.47
1:E:429:PHE:C	5:E:4208:HOH:O	2.57	0.47
1:A:137:ASN:O	1:A:140:LYS:N	2.47	0.47
1:A:154:PRO:O	1:A:157:VAL:HG12	2.15	0.47
1:A:427:ILE:HD13	1:A:428:VAL:H	1.78	0.47
1:C:300:ASP:HA	5:C:4311:HOH:O	2.13	0.47
1:E:379:GLY:HA3	5:E:4478:HOH:O	2.14	0.47
2:F:12:VAL:HG21	2:F:16:GLY:HA3	1.96	0.47
1:E:475:ALA:HB2	5:E:4310:HOH:O	2.15	0.47
2:F:53:SER:HA	2:F:71:ARG:HH12	1.79	0.47
2:F:81:GLN:NE2	5:F:201:HOH:O	2.47	0.47
1:C:49:ILE:HG12	1:C:63:GLN:CB	2.44	0.47
1:C:326:GLY:HA2	5:C:4084:HOH:O	2.14	0.47
1:E:5:GLN:HA	1:E:5:GLN:NE2	2.29	0.47
1:E:182:TYR:CE2	1:E:186:LEU:HD21	2.49	0.47
2:F:64:LYS:HG2	5:F:131:HOH:O	2.14	0.47
1:A:274:MET:HE1	1:A:429:PHE:HB3	1.96	0.47
1:A:420:GLY:HA3	5:A:4015:HOH:O	2.14	0.47
1:A:460:ASN:CG	1:A:460:ASN:O	2.56	0.47
1:A:257:LYS:HG2	2:B:97:GLY:HA2	1.97	0.47
1:A:485:ASP:C	5:A:4261:HOH:O	2.57	0.47
1:C:294:VAL:CB	5:C:4294:HOH:O	2.24	0.47
1:C:339:MET:HE3	1:C:341:SER:HB3	1.97	0.47
1:C:386:HIS:N	5:C:4162:HOH:O	2.47	0.47
2:D:102:TYR:C	2:D:103:TRP:CE3	2.93	0.47
1:E:415:ASN:HB2	1:E:432:ASP:CG	2.40	0.47
2:F:30:SER:HA	5:F:116:HOH:O	2.14	0.47
1:A:75:ASN:N	1:A:75:ASN:ND2	2.63	0.47
1:A:111:THR:O	1:A:113:THR:N	2.47	0.47
1:A:171:GLU:HG3	5:A:4154:HOH:O	2.14	0.47
1:A:427:ILE:HG12	1:A:489:ALA:HB2	1.96	0.47
1:C:360:PRO:CG	1:C:367:ILE:HD12	2.44	0.47
1:C:423:ASN:CB	5:C:4288:HOH:O	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:GLN:NE2	1:E:436:LEU:HB2	2.30	0.47
1:A:331:HIS:HE1	5:A:4348:HOH:O	1.98	0.47
1:A:187:ILE:HD11	1:A:194:PHE:CE1	2.48	0.47
1:A:426:PHE:HB3	1:A:490:ILE:HD11	1.96	0.47
1:E:415:ASN:HB2	1:E:432:ASP:OD2	2.15	0.47
1:A:223:PRO:O	1:A:224:ALA:C	2.57	0.46
1:E:238:GLY:HA3	2:F:101:ASN:ND2	2.30	0.46
1:A:237:LEU:N	1:A:237:LEU:HD22	2.29	0.46
1:A:430:ASN:HB2	1:A:436:LEU:HD13	1.98	0.46
1:C:19:TRP:CH2	1:C:370:VAL:HG11	2.50	0.46
2:D:49:ALA:C	5:D:167:HOH:O	2.58	0.46
1:E:229:PHE:HE2	1:E:252:ARG:CD	2.28	0.46
1:A:95:VAL:HG21	1:A:186:LEU:HG	1.98	0.46
1:C:13:ILE:HG22	1:C:39:GLY:CA	2.45	0.46
2:D:30:SER:HA	5:D:114:HOH:O	2.14	0.46
2:D:67:PHE:CE2	5:D:192:HOH:O	2.67	0.46
1:A:479:ILE:HD11	1:A:488:ILE:CG1	2.46	0.46
1:C:140:LYS:HB2	1:C:140:LYS:HZ2	1.77	0.46
1:C:362:ASN:HA	1:C:368:LYS:HG3	1.97	0.46
1:E:293:LEU:HD13	5:E:4321:HOH:O	1.98	0.46
1:E:349:VAL:CG1	5:E:4338:HOH:O	2.62	0.46
1:E:411:ASP:HA	1:E:416:GLN:O	2.16	0.46
1:A:7:GLN:HB3	1:A:10:ARG:CD	2.46	0.46
1:A:20:ARG:HD3	1:A:23:ASP:OD1	2.16	0.46
2:F:72:ASP:O	2:F:73:ASN:HB2	2.15	0.46
1:A:372:ILE:N	1:A:372:ILE:CD1	2.76	0.46
1:A:389:ARG:NH2	1:A:453:ILE:O	2.47	0.46
1:C:279:ASN:HD21	1:C:284:TRP:HE1	1.64	0.46
1:C:320:LEU:CD1	5:C:4175:HOH:O	2.63	0.46
2:F:6:ALA:HA	2:F:21:SER:O	2.15	0.46
1:A:185:LYS:HB3	1:A:185:LYS:HE2	1.73	0.46
2:D:34:MET:CG	5:D:146:HOH:O	2.63	0.46
1:E:199:SER:HB3	5:E:4295:HOH:O	2.15	0.46
1:E:211:LEU:CD2	1:E:250:ASN:HB3	2.46	0.46
2:F:100(B):VAL:HA	2:F:100(F):ARG:O	2.16	0.46
1:A:208:LYS:CE	5:A:4350:HOH:O	2.64	0.46
2:B:87:THR:O	2:B:88:ALA:HB2	2.16	0.46
1:C:258:TYR:CE1	1:C:262:LEU:HD12	2.51	0.46
1:E:442:THR:O	1:E:444:LEU:CD1	2.64	0.46
1:A:120:ASN:HB3	1:A:125:GLU:HB2	1.97	0.46
1:A:229:PHE:CE2	1:A:252:ARG:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:TYR:C	1:C:34:PRO:HD2	2.41	0.46
2:D:4:LEU:HD23	2:D:24:ALA:HB2	1.98	0.46
2:F:3:GLN:CB	5:F:188:HOH:O	2.63	0.46
1:A:333:TYR:HB2	5:A:4348:HOH:O	2.16	0.46
1:A:352:GLU:HG2	5:A:4285:HOH:O	2.16	0.46
1:A:436:LEU:O	1:A:478:SER:HA	2.16	0.46
1:A:460:ASN:HB2	5:A:4422:HOH:O	2.00	0.46
2:B:100:LYS:HA	2:B:100(H):CYS:O	2.16	0.46
2:D:29:PHE:HB2	5:D:151:HOH:O	2.15	0.46
2:D:85:GLU:CD	2:D:85:GLU:H	2.23	0.46
1:E:383:VAL:HG13	1:E:385:GLU:OE2	2.15	0.46
1:E:401:VAL:HB	1:E:421:ARG:CB	2.45	0.46
1:C:281:GLY:O	1:C:282:GLU:C	2.59	0.45
1:C:319:ARG:NH1	5:C:4128:HOH:O	2.49	0.45
5:C:4287:HOH:O	2:D:100(H):CYS:HA	2.15	0.45
1:E:195:ARG:HA	1:E:231:PHE:O	2.16	0.45
1:A:80:ARG:HD3	5:A:4269:HOH:O	2.16	0.45
1:A:142:LYS:HE2	5:A:4021:HOH:O	2.15	0.45
1:A:435:GLN:HE21	1:A:435:GLN:C	2.23	0.45
1:A:446:GLY:HA2	1:A:469:VAL:HG13	1.98	0.45
1:C:343:ARG:HD2	5:C:4149:HOH:O	2.15	0.45
2:D:93:ALA:HB1	2:D:103:TRP:CE3	2.51	0.45
2:D:100(K):PRO:HD2	2:D:103:TRP:CZ3	2.51	0.45
1:E:301:ASN:HA	1:E:306:GLY:HA3	1.96	0.45
1:E:395:VAL:HG23	1:E:396:TRP:N	2.31	0.45
1:A:442:THR:O	1:A:444:LEU:HD13	2.17	0.45
2:B:99:GLY:HA3	2:B:101:ASN:HA	1.99	0.45
1:C:97:ALA:HA	5:C:4047:HOH:O	2.16	0.45
1:C:178:MET:HB2	5:C:4204:HOH:O	2.16	0.45
1:C:349:VAL:CG2	1:C:349:VAL:O	2.64	0.45
1:C:360:PRO:O	1:C:361:PRO:C	2.59	0.45
1:C:452:VAL:HA	1:C:455:GLY:O	2.16	0.45
1:E:69:LEU:N	1:E:69:LEU:CD1	2.80	0.45
1:E:211:LEU:HD23	5:E:4180:HOH:O	2.15	0.45
1:A:352:GLU:CG	5:A:4285:HOH:O	2.64	0.45
1:C:227:ARG:HG3	1:C:228:PRO:HD2	1.98	0.45
2:D:40:ALA:HB3	2:D:43:LYS:CB	2.47	0.45
1:E:267:ARG:NH1	1:E:313:LEU:HD23	2.32	0.45
1:A:171:GLU:CD	1:A:171:GLU:H	2.24	0.45
1:A:367:ILE:N	1:A:367:ILE:CD1	2.79	0.45
1:A:367:ILE:HD12	1:A:367:ILE:H	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ASN:O	1:A:381:ASP:HB2	2.17	0.45
2:B:71:ARG:NH2	5:B:201:HOH:O	2.42	0.45
1:C:303:ARG:HG3	1:C:303:ARG:NH2	2.31	0.45
1:C:383:VAL:HG13	1:C:385:GLU:OE2	2.16	0.45
1:C:435:GLN:C	1:C:435:GLN:HE21	2.25	0.45
2:D:51:ILE:HG23	2:D:51:ILE:O	2.15	0.45
2:F:34:MET:HB3	5:F:114:HOH:O	2.16	0.45
1:E:96:ASP:HB2	5:E:4117:HOH:O	2.16	0.45
1:E:391:ILE:HD12	1:E:391:ILE:N	2.32	0.45
1:A:101:HIS:HA	5:A:4089:HOH:O	2.16	0.45
2:B:43:LYS:HB3	5:B:203:HOH:O	2.15	0.45
2:B:67:PHE:HA	2:B:81:GLN:O	2.17	0.45
1:C:187:ILE:HD11	1:C:194:PHE:CE1	2.52	0.45
1:E:301:ASN:HB2	1:E:312:ILE:HD12	1.98	0.45
1:E:435:GLN:NE2	1:E:435:GLN:C	2.75	0.45
2:D:70:SER:CB	5:D:181:HOH:O	2.63	0.45
2:D:83:LYS:HB3	2:D:85:GLU:OE2	2.17	0.45
2:F:30:SER:C	2:F:71:ARG:NH2	2.75	0.45
1:A:453:ILE:HD12	1:A:488:ILE:C	2.41	0.45
2:B:107:THR:HG21	5:B:224:HOH:O	2.05	0.45
2:D:72:ASP:C	2:D:74:ALA:H	2.25	0.45
1:E:142:LYS:HB2	1:E:142:LYS:HE3	1.77	0.45
1:E:267:ARG:HD3	1:E:269:TRP:CZ2	2.52	0.45
1:A:304:GLY:O	1:A:306:GLY:N	2.42	0.44
1:A:458:VAL:HG23	1:A:458:VAL:O	2.16	0.44
1:C:229:PHE:CE2	1:C:252:ARG:HD3	2.50	0.44
1:C:465:ILE:CD1	5:C:4191:HOH:O	2.64	0.44
1:E:163:VAL:HG23	1:E:163:VAL:O	2.17	0.44
1:E:435:GLN:NE2	1:E:436:LEU:C	2.74	0.44
2:F:20:LEU:HD12	2:F:80:LEU:HD23	1.98	0.44
1:C:162:LEU:HD23	1:C:163:VAL:HG13	1.98	0.44
1:C:428:VAL:HG22	5:C:4250:HOH:O	2.16	0.44
1:E:440:LEU:HD22	5:E:4244:HOH:O	2.17	0.44
2:F:44:GLU:HG2	5:F:146:HOH:O	2.17	0.44
1:A:99:ILE:HD11	1:A:202:MET:CE	2.45	0.44
1:A:454:SER:HA	5:A:4061:HOH:O	2.17	0.44
1:C:92:ARG:NH2	5:C:4147:HOH:O	2.49	0.44
1:C:238:GLY:HA3	5:D:220:HOH:O	2.17	0.44
1:C:318:ALA:O	1:C:319:ARG:C	2.60	0.44
1:C:435:GLN:HE22	1:C:436:LEU:C	2.25	0.44
1:A:127:PRO:O	1:A:130:PRO:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:HG13	1:A:418:ALA:N	2.33	0.44
1:A:436:LEU:HD23	1:A:436:LEU:C	2.42	0.44
2:B:82(A):ASP:C	5:B:236:HOH:O	2.60	0.44
1:C:47:GLU:HG2	1:C:65:VAL:CG2	2.47	0.44
1:C:143:THR:HB	1:C:149:GLU:OE1	2.18	0.44
1:C:439:THR:O	1:C:440:LEU:HD12	2.18	0.44
1:E:50:VAL:O	5:E:4293:HOH:O	2.21	0.44
1:E:207:ILE:HG13	5:E:4295:HOH:O	2.17	0.44
1:E:372:ILE:HD12	1:E:387:ARG:CZ	2.47	0.44
1:C:437:SER:CB	5:C:4336:HOH:O	2.57	0.44
2:D:34:MET:HG3	5:D:146:HOH:O	2.18	0.44
1:E:412:ASN:HD21	1:E:416:GLN:HG3	1.81	0.44
2:F:102:TYR:HE2	5:F:192:HOH:O	2.01	0.44
1:A:142:LYS:HE2	5:A:4380:HOH:O	2.18	0.44
1:C:3:ALA:O	1:C:5:GLN:HG2	2.17	0.44
1:C:65:VAL:HG11	1:C:113:THR:CG2	2.48	0.44
1:C:428:VAL:HG21	5:C:4250:HOH:O	2.17	0.44
1:C:435:GLN:NE2	1:C:436:LEU:N	2.66	0.44
1:C:479:ILE:HD12	5:C:4250:HOH:O	2.17	0.44
1:C:213:LYS:HD3	5:C:4368:HOH:O	2.18	0.44
1:A:265:VAL:HG11	1:A:277:LEU:HD21	2.00	0.44
2:B:82:MET:N	5:B:215:HOH:O	2.50	0.44
1:E:343:ARG:HB2	5:E:4418:HOH:O	2.18	0.44
1:A:10:ARG:NH1	1:A:33:GLY:O	2.43	0.43
1:A:30:ARG:NH2	1:A:372:ILE:HD11	2.33	0.43
1:A:99:ILE:HD13	1:A:99:ILE:H	1.82	0.43
1:A:274:MET:HE1	1:A:429:PHE:CB	2.47	0.43
1:A:375:ASP:OD2	1:A:375:ASP:C	2.60	0.43
2:B:72:ASP:O	2:B:73:ASN:HB2	2.17	0.43
1:C:221:TRP:HH2	5:C:4197:HOH:O	2.00	0.43
2:D:64:LYS:HE3	5:D:218:HOH:O	2.07	0.43
1:E:227:ARG:NE	1:E:227:ARG:HA	2.33	0.43
1:E:242:ILE:HD13	5:E:4027:HOH:O	2.16	0.43
1:A:427:ILE:HD13	1:A:427:ILE:C	2.43	0.43
1:A:469:VAL:HG13	1:A:469:VAL:O	2.18	0.43
1:C:53:ASN:HA	1:C:54:PRO:C	2.41	0.43
1:C:178:MET:HE2	5:C:4204:HOH:O	2.17	0.43
2:D:100(A):LEU:CA	2:D:103:TRP:NE1	2.78	0.43
1:E:162:LEU:HD22	1:E:163:VAL:HG22	2.00	0.43
1:E:274:MET:HE2	1:E:415:ASN:O	2.18	0.43
2:B:82:MET:HB3	2:B:82(C):LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:ASN:HB2	5:E:4124:HOH:O	2.18	0.43
1:E:455:GLY:HA3	5:E:4488:HOH:O	2.17	0.43
2:F:31:SER:CB	5:F:215:HOH:O	2.64	0.43
1:A:305:HIS:HB3	5:A:4398:HOH:O	2.19	0.43
1:A:450:CYS:SG	1:A:496:LEU:HD13	2.58	0.43
1:C:31:TYR:OH	1:C:387:ARG:HA	2.18	0.43
1:E:87:ASN:HB3	1:E:221:TRP:CD1	2.53	0.43
1:E:93:ILE:HD13	5:E:4350:HOH:O	2.15	0.43
1:A:349:VAL:CG2	1:A:354:VAL:HG13	2.48	0.43
2:D:6:ALA:HA	2:D:21:SER:O	2.19	0.43
2:F:90:TYR:C	5:F:220:HOH:O	2.60	0.43
1:A:5:GLN:HE21	1:A:5:GLN:CA	2.23	0.43
2:B:100(J):GLY:CA	2:B:103:TRP:HH2	2.32	0.43
1:C:45:PRO:HD3	1:C:95:VAL:HG13	1.99	0.43
1:C:187:ILE:HG23	1:C:217:LEU:HD23	2.01	0.43
2:D:12:VAL:HG11	2:D:82(C):LEU:HD12	1.99	0.43
1:E:407:ALA:CB	5:E:4416:HOH:O	2.31	0.43
2:F:51:ILE:HG12	5:F:193:HOH:O	2.17	0.43
1:A:54:PRO:HB2	1:A:357:TRP:CE3	2.54	0.43
1:A:237:LEU:O	2:B:97:GLY:HA3	2.19	0.43
1:E:129:VAL:HB	1:E:130:PRO:CA	2.48	0.43
1:E:343:ARG:HG2	1:E:343:ARG:NH2	2.34	0.43
2:F:72:ASP:O	2:F:74:ALA:N	2.47	0.43
2:F:93:ALA:HB1	2:F:103:TRP:HZ3	1.81	0.43
1:A:385:GLU:C	1:A:387:ARG:H	2.26	0.43
1:A:451:ASP:CG	1:A:488:ILE:HG23	2.43	0.43
1:C:187:ILE:HD11	1:C:194:PHE:HE1	1.83	0.43
1:C:429:PHE:CD1	5:C:4145:HOH:O	2.57	0.43
1:E:162:LEU:CD2	1:E:163:VAL:HG13	2.49	0.43
1:E:436:LEU:HD13	5:E:4208:HOH:O	2.17	0.43
1:E:458:VAL:O	1:E:458:VAL:HG23	2.18	0.43
1:E:469:VAL:HA	1:E:475:ALA:HB2	2.01	0.43
2:F:82(A):ASP:CA	5:F:164:HOH:O	2.66	0.43
2:B:12:VAL:HG11	2:B:82(C):LEU:HD12	2.01	0.43
1:C:49:ILE:HG23	1:C:103:CYS:HB3	2.01	0.43
2:D:13:GLN:O	2:D:14:ALA:C	2.61	0.43
1:A:35:LYS:HB3	1:A:37:PHE:HE1	1.82	0.43
1:C:69:LEU:N	1:C:69:LEU:CD1	2.82	0.43
1:E:93:ILE:HD12	5:E:4350:HOH:O	2.17	0.43
1:E:182:TYR:O	1:E:186:LEU:HD22	2.19	0.43
1:E:417:VAL:CG1	1:E:418:ALA:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:100(K):PRO:N	2:F:103:TRP:CH2	2.87	0.43
1:A:13:ILE:HD13	1:A:13:ILE:N	2.34	0.42
1:C:129:VAL:HG11	1:C:131:TYR:CE2	2.54	0.42
1:A:208:LYS:HE3	5:A:4350:HOH:O	2.19	0.42
1:C:137:ASN:O	1:C:138:ASP:C	2.61	0.42
1:C:261:LYS:HE3	2:D:98:SER:HB3	2.00	0.42
1:E:142:LYS:CE	5:E:4248:HOH:O	2.66	0.42
1:E:316:TRP:CE2	1:E:346:ARG:HD3	2.55	0.42
1:A:16:LEU:HB3	1:A:19:TRP:CG	2.55	0.42
2:B:72:ASP:O	2:B:74:ALA:N	2.46	0.42
1:C:158:ARG:CZ	1:C:242:ILE:HD12	2.48	0.42
1:C:162:LEU:HD23	1:C:162:LEU:C	2.44	0.42
1:C:262:LEU:HD23	1:C:266:VAL:HG23	2.01	0.42
1:C:343:ARG:NE	5:C:4156:HOH:O	2.48	0.42
2:D:20:LEU:CD2	2:D:107:THR:HG21	2.47	0.42
1:E:46:ASN:ND2	1:E:64:PRO:HB3	2.34	0.42
1:E:440:LEU:HG	5:E:4274:HOH:O	2.19	0.42
1:A:441:GLN:HG2	5:A:4474:HOH:O	2.19	0.42
2:B:76:ASN:CB	5:B:212:HOH:O	2.61	0.42
2:B:82:MET:HE1	2:B:90:TYR:CZ	2.54	0.42
1:C:7:GLN:HB3	1:C:10:ARG:HD2	2.02	0.42
1:C:98:VAL:HG13	5:C:4324:HOH:O	2.19	0.42
1:C:343:ARG:HG2	1:C:343:ARG:NH2	2.32	0.42
1:E:202:MET:HB2	1:E:207:ILE:HD11	2.01	0.42
1:E:394:MET:O	1:E:397:PHE:HB3	2.18	0.42
2:F:110:THR:CG2	5:F:191:HOH:O	2.63	0.42
2:B:49:ALA:HB1	5:B:149:HOH:O	2.18	0.42
1:C:349:VAL:HG22	1:C:354:VAL:HG13	2.01	0.42
1:C:411:ASP:HA	1:C:416:GLN:O	2.20	0.42
1:E:469:VAL:CG1	5:E:4310:HOH:O	2.67	0.42
1:E:480:SER:C	1:E:482:SER:N	2.78	0.42
1:A:329:LEU:HD12	1:A:398:ARG:HD2	2.02	0.42
1:A:339:MET:HE3	1:A:341:SER:HB3	2.00	0.42
1:C:274:MET:HG3	5:C:4069:HOH:O	2.18	0.42
1:C:414:SER:HB3	1:C:432:ASP:OD1	2.19	0.42
2:D:2:VAL:HG11	2:D:102:TYR:CE2	2.55	0.42
1:A:301:ASN:CG	1:A:312:ILE:HD13	2.45	0.42
2:B:93:ALA:CB	2:B:103:TRP:CE3	3.03	0.42
1:C:484:GLU:CD	1:C:485:ASP:H	2.28	0.42
1:E:449:TYR:CE1	1:E:495:LYS:HB2	2.55	0.42
1:A:142:LYS:HE3	5:A:4279:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:O	1:A:176:ARG:HD3	2.20	0.42
1:A:278:LYS:CD	5:A:4236:HOH:O	2.63	0.42
1:A:344:TRP:NE1	1:A:346:ARG:HG2	2.34	0.42
1:C:140:LYS:NZ	1:C:140:LYS:CB	2.80	0.42
1:E:142:LYS:CA	5:E:4426:HOH:O	2.68	0.42
1:E:170:LEU:O	1:E:176:ARG:CD	2.68	0.42
1:E:268:LYS:HE2	1:E:431:ASN:HD21	1.84	0.42
2:F:3:GLN:O	2:F:24:ALA:HA	2.19	0.42
1:A:350:ASN:HD22	1:A:350:ASN:HA	1.53	0.42
1:A:453:ILE:HD12	1:A:488:ILE:CA	2.50	0.42
2:B:31:SER:CB	5:B:199:HOH:O	2.67	0.42
1:C:59:TRP:CD1	5:C:4251:HOH:O	2.72	0.42
2:D:82:MET:HE2	2:D:82(C):LEU:CD2	2.50	0.42
1:E:170:LEU:O	1:E:176:ARG:HD3	2.20	0.42
2:F:48:SER:HB2	5:F:179:HOH:O	2.19	0.42
1:C:230:ILE:CG2	5:C:4083:HOH:O	2.60	0.42
1:A:31:TYR:CE2	1:A:35:LYS:HG2	2.54	0.41
2:B:2:VAL:HG11	2:B:102:TYR:CZ	2.55	0.41
1:C:1:GLN:CB	5:C:4256:HOH:O	2.68	0.41
1:C:77:ASN:CG	1:C:78:GLU:N	2.78	0.41
1:C:142:LYS:CE	5:C:4152:HOH:O	2.68	0.41
1:C:357:TRP:O	1:C:358:ILE:C	2.63	0.41
1:E:360:PRO:O	1:E:361:PRO:C	2.63	0.41
2:F:100(K):PRO:CD	2:F:103:TRP:CZ3	3.01	0.41
2:F:106:GLY:CA	5:F:220:HOH:O	2.68	0.41
2:B:67:PHE:CD1	2:B:82:MET:HA	2.55	0.41
1:E:297:ASP:HB3	1:E:313:LEU:O	2.20	0.41
1:A:219:THR:HA	1:A:222:PHE:O	2.20	0.41
1:A:303:ARG:HG3	1:A:303:ARG:NH2	2.33	0.41
2:B:30:SER:CA	5:B:156:HOH:O	2.63	0.41
1:C:49:ILE:HG23	1:C:65:VAL:CG1	2.23	0.41
1:C:79:PHE:O	1:C:83:VAL:HG23	2.20	0.41
1:C:231:PHE:CD1	1:C:293:LEU:HD13	2.56	0.41
2:D:96:PRO:O	2:D:97:GLY:C	2.63	0.41
1:E:237:LEU:N	1:E:237:LEU:HD22	2.35	0.41
1:C:13:ILE:HG22	1:C:39:GLY:HA3	2.02	0.41
1:C:436:LEU:HD23	1:C:437:SER:N	2.35	0.41
1:C:484:GLU:CG	1:C:485:ASP:N	2.83	0.41
1:E:279:ASN:HD22	1:E:279:ASN:N	2.08	0.41
1:E:366:VAL:O	1:E:366:VAL:HG23	2.20	0.41
2:F:41:PRO:HD2	5:F:176:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:ALA:O	2:F:77:THR:HG23	2.20	0.41
1:A:142:LYS:HD3	5:A:4268:HOH:O	2.21	0.41
1:A:305:HIS:HD1	1:A:305:HIS:C	2.28	0.41
1:A:442:THR:HB	1:A:444:LEU:HD22	2.02	0.41
1:C:72:ARG:CZ	1:C:367:ILE:HD11	2.50	0.41
1:E:26:LEU:HD11	5:E:4301:HOH:O	2.20	0.41
1:E:404:GLN:HG3	1:E:424:ARG:HB2	2.03	0.41
2:F:38:ARG:NE	5:F:179:HOH:O	2.53	0.41
2:F:43:LYS:CE	5:F:174:HOH:O	2.65	0.41
1:A:126:PHE:O	1:A:130:PRO:HA	2.21	0.41
1:C:277:LEU:HD22	1:C:280:TRP:CE3	2.56	0.41
1:A:444:LEU:HA	1:A:445:PRO:HD3	1.97	0.41
2:B:107:THR:CB	5:B:224:HOH:O	2.48	0.41
1:C:154:PRO:O	1:C:158:ARG:HD2	2.21	0.41
2:D:72:ASP:C	2:D:74:ALA:N	2.79	0.41
1:E:392:ARG:O	1:E:395:VAL:CG2	2.66	0.41
2:F:100(K):PRO:CD	2:F:103:TRP:HZ3	2.27	0.41
2:B:60:ALA:O	2:B:63:VAL:HG22	2.21	0.41
2:D:3:GLN:HG3	2:D:25:SER:OG	2.20	0.41
1:E:65:VAL:HG11	1:E:113:THR:HG22	2.02	0.41
1:A:142:LYS:HE3	1:A:142:LYS:HB2	1.78	0.41
1:A:416:GLN:HG3	5:A:4300:HOH:O	2.19	0.41
1:C:129:VAL:HB	1:C:130:PRO:CA	2.50	0.41
1:C:179:ILE:O	1:C:182:TYR:HB3	2.21	0.41
1:C:233:GLU:CD	5:C:4169:HOH:O	2.64	0.41
2:D:87:THR:O	2:D:88:ALA:HB2	2.20	0.41
1:E:51:VAL:HB	1:E:57:PRO:HD2	2.03	0.41
1:E:129:VAL:HB	1:E:130:PRO:C	2.46	0.41
1:E:268:LYS:CE	5:E:4390:HOH:O	2.68	0.41
1:E:484:GLU:CG	1:E:485:ASP:N	2.83	0.41
1:A:157:VAL:CG1	1:A:242:ILE:HD11	2.51	0.41
1:A:170:LEU:HD21	1:A:179:ILE:CD1	2.50	0.41
1:A:199:SER:OG	1:A:232:GLN:HB3	2.21	0.41
1:A:208:LYS:HE2	5:A:4305:HOH:O	2.19	0.41
1:A:231:PHE:CD1	1:A:293:LEU:CD2	2.99	0.41
1:A:274:MET:HE3	1:A:417:VAL:HB	2.03	0.41
1:A:304:GLY:C	1:A:306:GLY:H	2.26	0.41
1:A:366:VAL:O	1:A:366:VAL:CG2	2.68	0.41
1:A:491:HIS:CE1	1:A:494:SER:HB3	2.55	0.41
2:D:82:MET:CG	5:D:192:HOH:O	2.63	0.41
1:E:381:ASP:HA	5:E:4343:HOH:O	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:GLU:HB2	5:E:4437:HOH:O	2.19	0.41
2:F:2:VAL:HG21	2:F:102:TYR:CD2	2.56	0.41
2:F:51:ILE:O	2:F:51:ILE:HG23	2.21	0.41
2:F:73:ASN:HA	5:F:162:HOH:O	2.20	0.41
1:A:227:ARG:HH21	1:A:227:ARG:CG	2.26	0.40
2:B:74:ALA:CB	5:B:180:HOH:O	2.63	0.40
1:C:77:ASN:ND2	1:C:78:GLU:HG3	2.36	0.40
1:C:142:LYS:HE3	5:C:4107:HOH:O	2.21	0.40
1:C:171:GLU:HG2	1:C:172:LYS:N	2.35	0.40
2:D:71:ARG:HD3	2:D:73:ASN:HD21	1.86	0.40
2:B:64:LYS:NZ	2:B:64:LYS:HB3	2.36	0.40
1:C:22:VAL:CG1	5:C:4310:HOH:O	2.41	0.40
1:C:484:GLU:OE1	5:C:4274:HOH:O	2.22	0.40
2:D:67:PHE:N	2:D:67:PHE:CD1	2.90	0.40
1:A:54:PRO:HB2	1:A:357:TRP:CZ3	2.56	0.40
1:A:96:ASP:HB2	5:A:4080:HOH:O	2.20	0.40
2:B:30:SER:HB3	5:B:156:HOH:O	2.21	0.40
2:B:32:TYR:CE2	2:B:96:PRO:HB3	2.56	0.40
1:C:217:LEU:HD23	5:C:4218:HOH:O	2.20	0.40
1:C:245:SER:HA	1:C:248:PHE:CZ	2.56	0.40
1:C:437:SER:CA	5:C:4336:HOH:O	2.65	0.40
1:E:136:PHE:CE1	1:E:168:LEU:HD12	2.57	0.40
1:E:142:LYS:HE3	5:E:4248:HOH:O	2.20	0.40
1:A:4:PRO:HA	1:A:229:PHE:CG	2.56	0.40
1:A:430:ASN:HB2	1:A:436:LEU:CD1	2.52	0.40
1:A:468:TYR:CB	5:A:4217:HOH:O	2.64	0.40
1:C:35:LYS:HE2	5:C:4227:HOH:O	2.21	0.40
1:C:129:VAL:HG11	1:C:131:TYR:CZ	2.56	0.40
1:C:349:VAL:CG2	1:C:354:VAL:HG13	2.52	0.40
1:E:70:CYS:HB2	5:E:4409:HOH:O	2.11	0.40
2:F:100(F):ARG:HD3	5:F:146:HOH:O	2.20	0.40
1:C:320:LEU:HD12	1:C:320:LEU:N	2.37	0.40
1:C:449:TYR:HE2	1:C:469:VAL:CG1	2.34	0.40
2:D:102:TYR:O	2:D:103:TRP:CE3	2.73	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:ASN:OD1	5:A:4216:HOH:O[1_655]	2.14	0.06

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	494/496 (100%)	458 (93%)	31 (6%)	5 (1%)	12	8
1	C	494/496 (100%)	459 (93%)	33 (7%)	2 (0%)	30	27
1	E	494/496 (100%)	469 (95%)	22 (4%)	3 (1%)	21	17
2	B	119/127 (94%)	110 (92%)	7 (6%)	2 (2%)	7	3
2	D	119/127 (94%)	105 (88%)	9 (8%)	5 (4%)	2	0
2	F	119/127 (94%)	113 (95%)	4 (3%)	2 (2%)	7	3
All	All	1839/1869 (98%)	1714 (93%)	106 (6%)	19 (1%)	12	8

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ASP
1	A	224	ALA
1	E	224	ALA
1	E	305	HIS
2	F	101	ASN
1	A	305	HIS
2	B	101	ASN
1	C	218	ASN
2	D	97	GLY
2	D	8	GLY
2	D	14	ALA
2	D	101	ASN
1	E	103	CYS
2	B	75	ALA
1	C	114	THR
2	F	88	ALA
1	A	225	GLY
1	A	486	PRO
2	D	100(K)	PRO

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	413/413 (100%)	382 (92%)	31 (8%)	12	9
1	C	413/413 (100%)	394 (95%)	19 (5%)	24	22
1	E	413/413 (100%)	392 (95%)	21 (5%)	21	19
2	B	92/95 (97%)	85 (92%)	7 (8%)	12	9
2	D	92/95 (97%)	84 (91%)	8 (9%)	9	6
2	F	92/95 (97%)	82 (89%)	10 (11%)	6	3
All	All	1515/1524 (99%)	1419 (94%)	96 (6%)	16	13

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	49	ILE
1	A	75	ASN
1	A	92	ARG
1	A	99	ILE
1	A	115	CYS
1	A	140	LYS
1	A	162	LEU
1	A	165	LEU
1	A	176	ARG
1	A	186	LEU
1	A	189	ILE
1	A	211	LEU
1	A	227	ARG
1	A	262	LEU
1	A	279	ASN
1	A	323	ILE
1	A	329	LEU
1	A	341	SER
1	A	350	ASN
1	A	367	ILE
1	A	372	ILE

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Mol	Chain	Res	Type
1	A	417	VAL
1	A	421	ARG
1	A	427	ILE
1	A	435	GLN
1	A	440	LEU
1	A	444	LEU
1	A	484	GLU
1	A	490	ILE
1	A	496	LEU
2	B	2	VAL
2	B	28	THR
2	B	30	SER
2	B	39	GLN
2	B	44	GLU
2	B	54	ASP
2	B	101	ASN
1	C	1	GLN
1	C	21	TRP
1	C	69	LEU
1	C	92	ARG
1	C	115	CYS
1	C	140	LYS
1	C	157	VAL
1	C	165	LEU
1	C	176	ARG
1	C	186	LEU
1	C	227	ARG
1	C	262	LEU
1	C	279	ASN
1	C	329	LEU
1	C	421	ARG
1	C	427	ILE
1	C	435	GLN
1	C	440	LEU
1	C	496	LEU
2	D	2	VAL
2	D	28	THR
2	D	30	SER
2	D	39	GLN
2	D	44	GLU
2	D	69	ILE
2	D	85	GLU

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Mol	Chain	Res	Type
2	D	101	ASN
1	E	115	CYS
1	E	140	LYS
1	E	162	LEU
1	E	165	LEU
1	E	168	LEU
1	E	170	LEU
1	E	176	ARG
1	E	186	LEU
1	E	211	LEU
1	E	227	ARG
1	E	262	LEU
1	E	279	ASN
1	E	329	LEU
1	E	341	SER
1	E	349	VAL
1	E	427	ILE
1	E	435	GLN
1	E	436	LEU
1	E	438	SER
1	E	469	VAL
1	E	496	LEU
2	F	11	SER
2	F	28	THR
2	F	29	PHE
2	F	30	SER
2	F	39	GLN
2	F	44	GLU
2	F	61	ASP
2	F	72	ASP
2	F	76	ASN
2	F	81	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	15	HIS
1	A	75	ASN
1	A	101	HIS
1	A	161	GLN
1	A	201	HIS

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Mol	Chain	Res	Type
1	A	220	ASN
1	A	279	ASN
1	A	299	HIS
1	A	350	ASN
1	A	363	ASN
1	A	399	ASN
1	A	408	ASN
1	A	435	GLN
1	A	476	GLN
2	B	1	GLN
2	B	81	GLN
2	B	101	ASN
1	C	1	GLN
1	C	5	GLN
1	C	101	HIS
1	C	161	GLN
1	C	279	ASN
1	C	299	HIS
1	C	347	ASN
1	C	350	ASN
1	C	373	ASN
1	C	399	ASN
1	C	416	GLN
1	C	431	ASN
1	C	435	GLN
2	D	1	GLN
2	D	73	ASN
2	D	76	ASN
2	D	81	GLN
2	D	101	ASN
2	D	105	GLN
1	E	5	GLN
1	E	75	ASN
1	E	101	HIS
1	E	161	GLN
1	E	220	ASN
1	E	279	ASN
1	E	299	HIS
1	E	350	ASN
1	E	363	ASN
1	E	364	ASN
1	E	373	ASN

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Mol	Chain	Res	Type
1	E	380	ASN
1	E	399	ASN
1	E	408	ASN
1	E	423	ASN
1	E	435	GLN
1	E	476	GLN
2	F	1	GLN
2	F	3	GLN
2	F	39	GLN
2	F	81	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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, 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	496/496 (100%)	-0.21	6 (1%) 76 76	4, 11, 20, 31	0
1	C	496/496 (100%)	0.09	8 (1%) 70 70	9, 18, 27, 33	0
1	E	496/496 (100%)	-0.14	7 (1%) 73 73	4, 11, 21, 34	0
2	B	123/127 (96%)	0.49	10 (8%) 18 17	9, 22, 31, 36	0
2	D	123/127 (96%)	0.86	12 (9%) 13 12	15, 28, 32, 35	0
2	F	123/127 (96%)	0.75	11 (8%) 15 14	11, 24, 32, 35	0
All	All	1857/1869 (99%)	0.07	54 (2%) 53 52	4, 15, 29, 36	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	34	MET	5.8
2	F	103	TRP	4.9
2	B	29	PHE	4.5
2	D	103	TRP	4.3
2	F	30	SER	4.1
1	A	305	HIS	4.0
2	F	29	PHE	4.0
2	D	34	MET	3.9
1	E	468	TYR	3.8
2	F	72	ASP	3.7
1	A	468	TYR	3.7
2	D	29	PHE	3.3
1	C	134	TRP	3.2
2	F	100(K)	PRO	3.2
1	A	138	ASP	3.0
2	D	73	ASN	3.0
1	C	77	ASN	2.9
1	E	460	ASN	2.9
2	F	61	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	75	ASN	2.8
1	E	484	GLU	2.8
2	F	28	THR	2.8
2	B	74	ALA	2.8
1	E	305	HIS	2.7
2	D	61	ASP	2.7
1	A	224	ALA	2.7
1	E	307	ALA	2.7
2	D	14	ALA	2.7
1	C	49	ILE	2.7
2	D	11	SER	2.7
2	B	100(K)	PRO	2.6
2	B	103	TRP	2.6
1	C	171	GLU	2.5
2	D	30	SER	2.5
2	B	34	MET	2.5
2	D	95	GLY	2.5
1	A	484	GLU	2.4
2	B	72	ASP	2.4
2	B	7	SER	2.4
1	E	77	ASN	2.4
1	C	224	ALA	2.3
2	F	82(A)	ASP	2.3
2	D	100(G)	THR	2.3
1	E	75	ASN	2.3
2	F	96	PRO	2.2
2	B	71	ARG	2.2
2	F	100(A)	LEU	2.2
1	A	1	GLN	2.1
1	C	305	HIS	2.1
2	B	75	ALA	2.1
2	B	30	SER	2.1
2	D	45	CYS	2.1
2	D	98	SER	2.1
1	C	115	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	C	4004	1/1	0.94	0.06	27,27,27,27	0
3	CA	E	4005	1/1	0.95	0.03	17,17,17,17	0
3	CA	A	4001	1/1	0.97	0.03	16,16,16,16	0
3	CA	C	4003	1/1	0.97	0.06	29,29,29,29	0
4	CL	A	4002	1/1	0.98	0.05	22,22,22,22	0
4	CL	E	4006	1/1	0.98	0.04	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.