



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:30 AM UTC

PDB ID : 1M1G / pdb_00001m1g
Title : Crystal Structure of Aquifex aeolicus N-utilization substance G (NusG), Space Group P2(1)
Authors : Steiner, T.; Kaiser, J.T.; Marinkovic, S.; Huber, R.; Wahl, M.C.
Deposited on : 2002-06-19
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

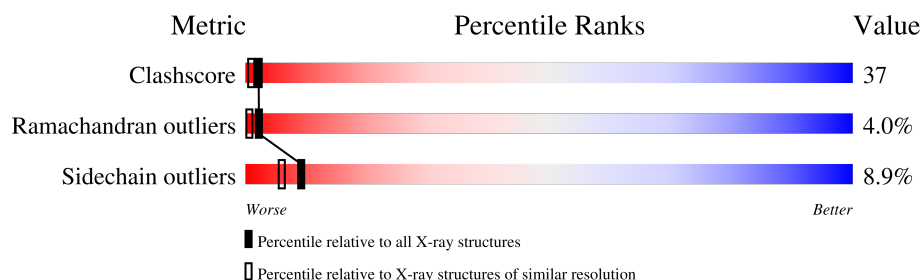
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	248	 38% 50% 8% . .
1	B	248	 34% 54% 8% . .
1	C	248	 35% 51% 11% . .
1	D	248	 40% 45% 11% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8718 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 Transcription antitermination protein nusG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1899	1214	323	354	8			
1	B	242	Total	C	N	O	S	0	0	0
			1917	1224	326	359	8			
1	C	244	Total	C	N	O	S	0	0	0
			1933	1234	329	362	8			
1	D	239	Total	C	N	O	S	0	0	0
			1891	1208	322	353	8			

- Molecule 2 is water.

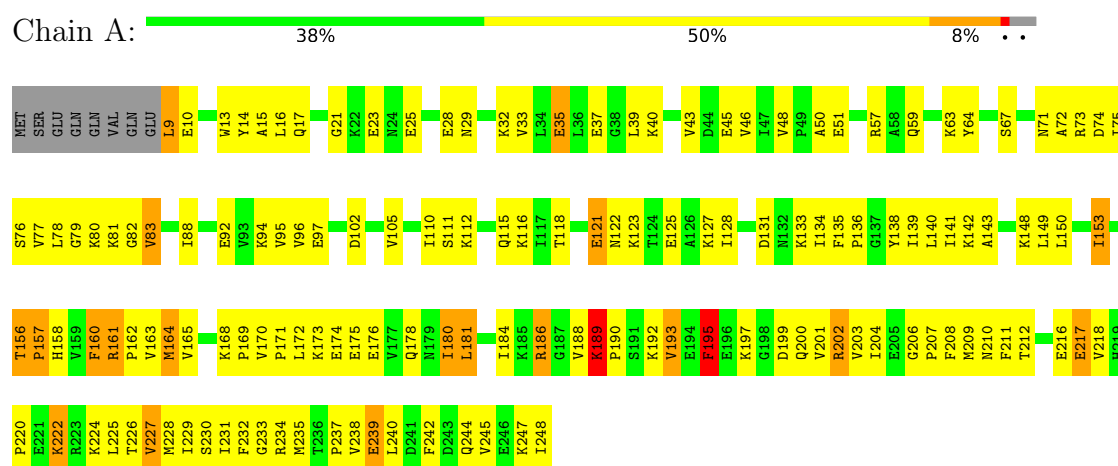
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	220	Total	O	0	0
			220	220		
2	B	338	Total	O	0	0
			338	338		
2	C	300	Total	O	0	0
			300	300		
2	D	220	Total	O	0	0
			220	220		

3 Residue-property plots

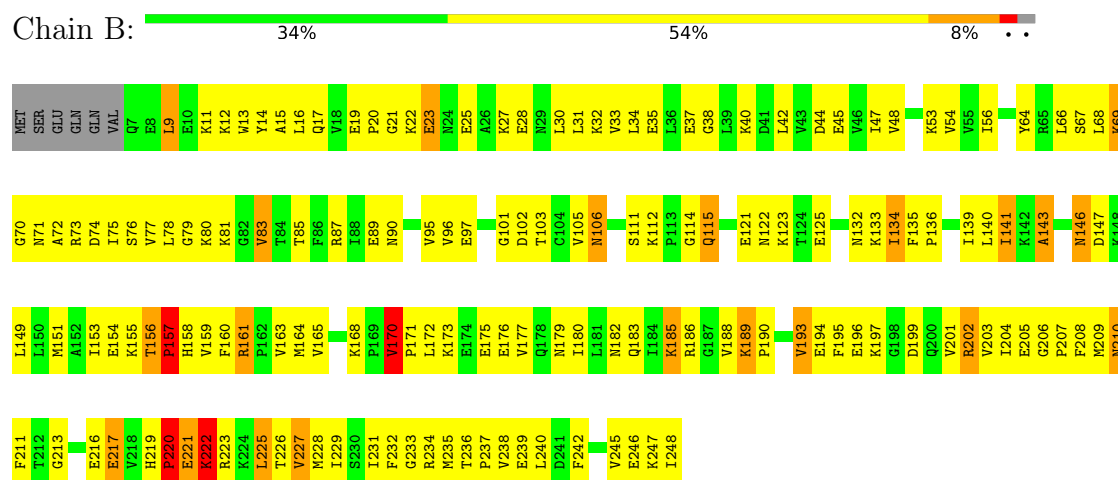
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: Transcription antitermination protein nusG

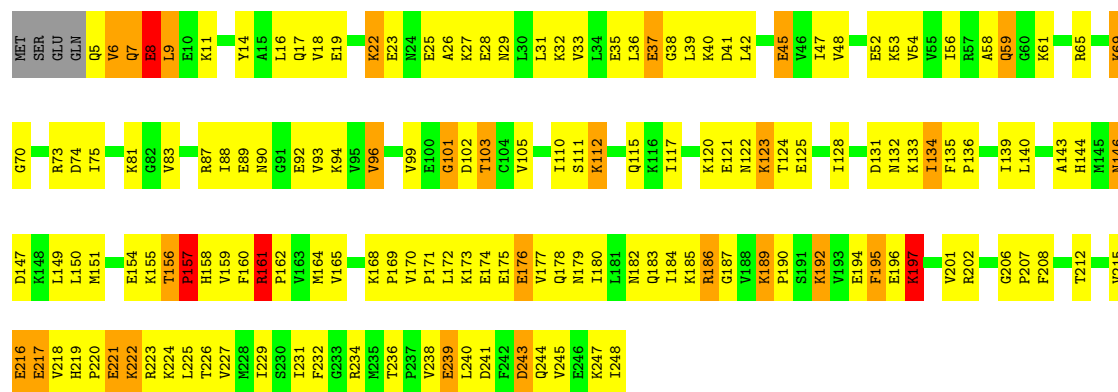


• Molecule 1: Transcription antitermination protein nusG



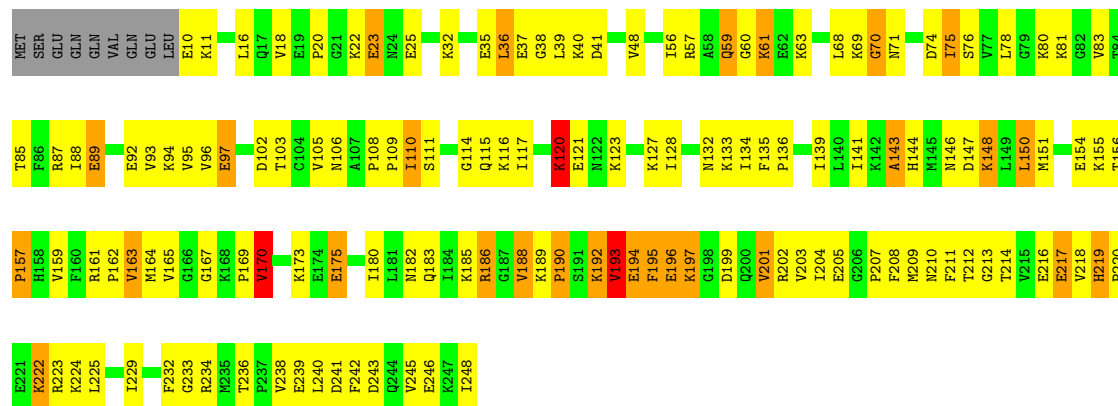
• Molecule 1: Transcription antitermination protein nusG





• Molecule 1: Transcription antitermination protein nusG

Chain D: 40% 45% 11% . .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.50Å 54.40Å 113.20Å 90.00° 89.30° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	94.9 (30.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.251 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8718	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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	0.48	0/1928	0.99	7/2592 (0.3%)
1	B	0.49	0/1946	1.01	12/2616 (0.5%)
1	C	0.47	0/1962	0.98	9/2638 (0.3%)
1	D	0.47	0/1920	1.00	11/2581 (0.4%)
All	All	0.48	0/7756	0.99	39/10427 (0.4%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	LYS	N-CA-C	-10.82	100.11	113.20
1	A	153	ILE	N-CA-C	-6.77	104.17	110.53
1	B	48	VAL	N-CA-C	-6.73	100.89	107.55
1	D	143	ALA	N-CA-C	6.59	117.27	108.38
1	D	163	VAL	N-CA-C	-6.39	100.45	108.89
1	B	222	LYS	N-CA-C	-6.38	104.65	112.88
1	A	156	THR	CA-C-N	6.36	127.79	119.84
1	A	156	THR	C-N-CA	6.36	127.79	119.84
1	D	170	VAL	N-CA-C	6.35	114.18	107.76
1	B	227	VAL	N-CA-C	6.35	117.73	108.58
1	C	83	VAL	N-CA-C	6.13	117.41	108.58
1	D	222	LYS	N-CA-C	-6.11	105.31	112.89
1	C	206	GLY	CA-C-N	6.06	125.95	119.28
1	C	206	GLY	C-N-CA	6.06	125.95	119.28
1	A	21	GLY	N-CA-C	-5.73	108.26	115.08
1	A	143	ALA	N-CA-C	5.63	116.70	108.14
1	B	101	GLY	N-CA-C	-5.62	107.28	114.37
1	D	201	VAL	N-CA-C	5.62	115.38	108.53
1	D	120	LYS	N-CA-C	5.60	119.22	112.38
1	D	156	THR	CA-C-N	5.54	126.77	119.84
1	D	156	THR	C-N-CA	5.54	126.77	119.84
1	B	47	ILE	N-CA-C	5.54	115.86	108.11
1	B	143	ALA	N-CA-C	5.53	116.37	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	HIS	CA-C-N	5.43	125.44	119.90
1	D	219	HIS	C-N-CA	5.43	125.44	119.90
1	B	114	GLY	N-CA-C	-5.39	107.24	114.25
1	A	43	VAL	N-CA-C	5.33	115.25	107.37
1	B	170	VAL	N-CA-C	5.14	112.95	107.76
1	B	156	THR	CA-C-N	5.11	126.22	119.84
1	B	156	THR	C-N-CA	5.11	126.22	119.84
1	C	45	GLU	N-CA-C	5.10	117.88	109.72
1	B	134	ILE	N-CA-C	5.07	115.74	110.82
1	C	156	THR	CA-C-N	5.07	126.18	119.84
1	C	156	THR	C-N-CA	5.07	126.18	119.84
1	C	101	GLY	N-CA-C	-5.07	107.99	114.37
1	B	170	VAL	CB-CA-C	-5.06	105.30	110.71
1	D	114	GLY	N-CA-C	-5.05	108.47	114.48
1	A	164	MET	N-CA-C	5.03	116.70	108.76
1	C	103	THR	N-CA-C	-5.01	107.02	113.23

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	1899	0	1994	112	322
1	B	1917	0	2008	163	388
1	C	1933	0	2025	161	134
1	D	1891	0	1983	144	102
2	A	220	0	0	29	50
2	B	338	0	0	51	69
2	C	300	0	0	48	42
2	D	220	0	0	45	9
All	All	8718	0	8010	580	598

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 37.

All (580) 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:D:212:THR:C	2:D:320:HOH:O	1.75	1.26
1:D:207:PRO:CG	2:D:365:HOH:O	1.84	1.24
1:B:235:MET:HB3	2:B:267:HOH:O	1.09	1.23
1:B:228:MET:HE2	2:B:267:HOH:O	1.40	1.18
1:D:213:GLY:N	2:D:320:HOH:O	1.74	1.18
1:D:217:GLU:HB2	2:D:423:HOH:O	1.44	1.15
1:B:168:LYS:O	2:B:362:HOH:O	1.68	1.10
1:C:103:THR:HG23	2:C:445:HOH:O	1.53	1.07
1:D:207:PRO:HG2	2:D:365:HOH:O	1.44	1.06
1:B:201:VAL:HG13	2:B:260:HOH:O	1.53	1.05
1:D:190:PRO:HA	2:D:395:HOH:O	1.57	1.04
1:D:151:MET:O	1:D:155:LYS:HD3	1.62	1.00
1:D:243:ASP:OD2	2:D:373:HOH:O	1.84	0.94
1:C:215:VAL:HB	2:C:522:HOH:O	1.67	0.93
1:C:247:LYS:O	1:C:248:ILE:HG12	1.68	0.93
1:C:112:LYS:H	1:C:112:LYS:HD2	1.32	0.93
1:B:67:SER:OG	2:B:395:HOH:O	1.87	0.92
1:B:140:LEU:HD11	1:B:180:ILE:HD11	1.51	0.92
1:D:213:GLY:CA	2:D:320:HOH:O	2.09	0.92
1:A:195:PHE:O	1:A:218:VAL:HG21	1.70	0.92
1:D:189:LYS:HB3	2:D:395:HOH:O	1.69	0.91
1:B:205:GLU:OE1	2:B:297:HOH:O	1.87	0.91
1:A:206:GLY:C	2:A:267:HOH:O	2.15	0.90
1:C:111:SER:H	1:C:115:GLN:HE22	1.12	0.89
1:B:219:HIS:O	2:B:426:HOH:O	1.90	0.89
1:D:214:THR:HG21	2:D:277:HOH:O	1.74	0.87
1:B:42:LEU:HB2	2:B:295:HOH:O	1.74	0.86
1:A:204:ILE:HG12	2:A:439:HOH:O	1.76	0.85
1:B:197:LYS:CE	2:B:330:HOH:O	2.24	0.84
1:B:67:SER:CB	2:B:395:HOH:O	2.25	0.84
1:B:69:LYS:HD3	1:B:70:GLY:N	1.92	0.84
1:C:111:SER:H	1:C:115:GLN:NE2	1.74	0.84
1:C:202:ARG:HG3	2:C:314:HOH:O	1.77	0.83
1:B:197:LYS:HE3	2:B:330:HOH:O	1.78	0.82
1:D:189:LYS:HB3	1:D:190:PRO:HA	1.61	0.82
1:D:92:GLU:HG2	2:D:448:HOH:O	1.79	0.81
1:A:201:VAL:HG12	1:A:247:LYS:HA	1.61	0.81
1:C:212:THR:HG23	2:C:314:HOH:O	1.80	0.80
1:B:197:LYS:NZ	1:B:216:GLU:HG3	1.97	0.80
1:D:213:GLY:HA2	2:D:320:HOH:O	1.75	0.80
1:B:202:ARG:HH22	1:B:204:ILE:HG22	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ILE:HG12	2:C:381:HOH:O	1.82	0.79
1:D:11:LYS:HD3	1:D:143:ALA:HA	1.63	0.79
1:C:239:GLU:HG3	2:C:299:HOH:O	1.82	0.79
1:A:186:ARG:HD3	1:A:186:ARG:N	1.97	0.78
1:B:16:LEU:HB2	1:B:139:ILE:CG2	2.14	0.78
1:A:228:MET:HE1	1:A:237:PRO:HB3	1.63	0.78
1:C:105:VAL:HB	2:C:265:HOH:O	1.84	0.78
1:C:146:ASN:ND2	1:C:149:LEU:H	1.80	0.77
1:C:192:LYS:HD3	1:C:192:LYS:H	1.49	0.77
1:B:112:LYS:O	1:B:115:GLN:HB2	1.85	0.76
1:D:163:VAL:O	1:D:170:VAL:HG23	1.86	0.76
1:D:111:SER:HA	2:D:436:HOH:O	1.86	0.76
1:B:74:ASP:CG	2:B:257:HOH:O	2.28	0.75
1:C:146:ASN:HD21	1:C:149:LEU:H	1.34	0.75
1:C:32:LYS:O	1:C:36:LEU:HD23	1.87	0.75
1:A:186:ARG:HD3	1:A:186:ARG:H	1.51	0.75
1:C:112:LYS:NZ	2:C:451:HOH:O	2.20	0.75
1:D:175:GLU:CD	1:D:175:GLU:H	1.92	0.74
1:A:188:VAL:O	1:A:189:LYS:HB2	1.87	0.74
1:B:32:LYS:HD3	2:B:273:HOH:O	1.87	0.74
1:B:228:MET:SD	2:B:267:HOH:O	2.40	0.74
1:B:199:ASP:O	2:B:260:HOH:O	2.06	0.73
1:D:164:MET:HE1	1:D:169:PRO:HG3	1.70	0.73
1:A:201:VAL:HB	1:A:245:VAL:HG22	1.71	0.73
1:D:207:PRO:CD	2:D:365:HOH:O	2.25	0.73
1:D:147:ASP:O	1:D:151:MET:HG3	1.87	0.73
1:B:11:LYS:HD3	1:B:143:ALA:HA	1.71	0.73
1:B:67:SER:HB2	2:B:395:HOH:O	1.85	0.73
1:B:197:LYS:HZ1	1:B:216:GLU:HG3	1.52	0.73
1:C:48:VAL:HG22	2:C:546:HOH:O	1.89	0.72
1:A:202:ARG:HG3	2:A:445:HOH:O	1.88	0.72
1:D:74:ASP:OD1	1:D:87:ARG:HD3	1.90	0.72
1:C:59:GLN:HG2	1:C:123:LYS:HB3	1.71	0.72
1:A:112:LYS:O	1:A:115:GLN:HG2	1.89	0.72
1:A:71:ASN:HB2	2:A:295:HOH:O	1.90	0.71
1:B:78:LEU:HD23	1:B:83:VAL:HG12	1.71	0.71
1:B:111:SER:H	1:B:115:GLN:HE22	1.38	0.71
1:B:227:VAL:HG21	1:B:240:LEU:HD12	1.72	0.71
1:A:227:VAL:HG13	1:A:238:VAL:HG13	1.72	0.71
1:B:165:VAL:HB	2:B:406:HOH:O	1.89	0.71
1:C:19:GLU:HG2	1:C:22:LYS:HD2	1.69	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LYS:HB2	2:A:296:HOH:O	1.90	0.71
1:B:205:GLU:HA	1:B:209:MET:HE2	1.71	0.71
1:D:190:PRO:CA	2:D:395:HOH:O	2.27	0.71
1:D:141:ILE:HB	2:D:450:HOH:O	1.91	0.70
1:B:163:VAL:O	1:B:170:VAL:HG23	1.90	0.70
1:B:196:GLU:HG2	1:B:199:ASP:OD2	1.91	0.70
1:A:16:LEU:HD11	1:A:141:ILE:HD13	1.73	0.70
1:D:195:PHE:O	1:D:218:VAL:HG21	1.92	0.70
1:C:172:LEU:HG	2:C:509:HOH:O	1.90	0.69
1:B:228:MET:CE	2:B:267:HOH:O	2.09	0.69
1:D:68:LEU:HD11	2:D:436:HOH:O	1.92	0.69
1:B:35:GLU:N	1:B:40:LYS:HE2	2.07	0.69
1:B:69:LYS:HD3	1:B:70:GLY:H	1.57	0.69
1:C:161:ARG:HD2	1:C:164:MET:HE3	1.74	0.69
1:B:31:LEU:C	2:B:477:HOH:O	2.37	0.68
1:D:134:ILE:HG12	2:D:301:HOH:O	1.93	0.68
1:A:222:LYS:O	1:A:224:LYS:HG2	1.94	0.68
1:A:127:LYS:HB2	2:A:265:HOH:O	1.93	0.68
1:C:222:LYS:O	1:C:224:LYS:HG2	1.95	0.67
1:A:180:ILE:O	1:A:184:ILE:HG12	1.94	0.67
1:B:170:VAL:HG13	2:B:406:HOH:O	1.94	0.67
1:C:173:LYS:HB3	2:C:489:HOH:O	1.94	0.67
1:D:162:PRO:HD2	1:D:164:MET:CE	2.25	0.67
1:B:197:LYS:HE2	2:B:330:HOH:O	1.93	0.67
1:D:208:PHE:CE1	1:D:238:VAL:HG21	2.30	0.66
1:C:201:VAL:HB	1:C:245:VAL:HG22	1.77	0.66
1:B:149:LEU:HD22	2:B:295:HOH:O	1.95	0.66
1:D:56:ILE:HD13	1:D:75:ILE:HD12	1.78	0.66
1:C:112:LYS:H	1:C:112:LYS:CD	2.05	0.66
1:D:207:PRO:HD2	2:D:365:HOH:O	1.91	0.66
1:D:241:ASP:O	1:D:245:VAL:HG12	1.96	0.66
1:D:194:GLU:CD	2:D:364:HOH:O	2.40	0.66
1:B:23:GLU:HG3	1:B:132:ASN:OD1	1.96	0.65
1:D:148:LYS:HE3	1:D:148:LYS:O	1.96	0.65
1:B:74:ASP:OD2	2:B:257:HOH:O	2.13	0.65
1:C:244:GLN:HG3	2:C:530:HOH:O	1.95	0.65
1:D:205:GLU:HA	1:D:209:MET:HE2	1.78	0.65
1:C:146:ASN:C	1:C:146:ASN:HD22	2.03	0.65
1:B:27:LYS:HE2	1:B:31:LEU:HD11	1.78	0.65
1:B:186:ARG:NH1	2:B:338:HOH:O	2.29	0.65
1:B:34:LEU:N	2:B:477:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:VAL:HG23	2:B:547:HOH:O	1.97	0.64
1:C:134:ILE:O	1:C:136:PRO:HD3	1.97	0.64
1:A:227:VAL:HB	2:A:451:HOH:O	1.97	0.64
1:B:223:ARG:HG3	2:B:523:HOH:O	1.97	0.64
1:D:59:GLN:NE2	1:D:80:LYS:HB2	2.12	0.64
1:B:199:ASP:C	2:B:260:HOH:O	2.41	0.64
1:B:80:LYS:HE3	1:B:123:LYS:HG3	1.79	0.63
1:B:235:MET:CB	2:B:267:HOH:O	1.89	0.63
1:C:5:GLN:HG2	1:C:6:VAL:HG23	1.80	0.63
1:D:154:GLU:HB2	2:D:355:HOH:O	1.98	0.63
1:B:53:LYS:HE2	2:B:325:HOH:O	1.99	0.63
1:D:132:ASN:O	1:D:136:PRO:HG3	1.99	0.63
1:C:248:ILE:HG13	1:C:248:ILE:O	1.96	0.63
1:C:194:GLU:O	1:C:195:PHE:HB2	1.98	0.62
1:B:111:SER:H	1:B:115:GLN:NE2	1.96	0.62
1:B:16:LEU:HB2	1:B:139:ILE:HG22	1.82	0.62
1:D:61:LYS:HD3	1:D:63:LYS:HE3	1.81	0.62
1:B:201:VAL:HB	1:B:245:VAL:HG13	1.81	0.62
1:C:218:VAL:O	1:C:220:PRO:HD3	1.99	0.62
1:D:204:ILE:HG12	2:D:432:HOH:O	1.99	0.62
1:B:133:LYS:NZ	1:B:189:LYS:HZ1	1.97	0.62
1:A:9:LEU:N	1:A:9:LEU:HD23	2.15	0.62
1:A:164:MET:HB2	1:A:168:LYS:O	2.00	0.62
1:A:48:VAL:HG13	2:A:446:HOH:O	2.00	0.61
1:D:59:GLN:HE21	1:D:80:LYS:HB2	1.64	0.61
1:B:68:LEU:N	2:B:547:HOH:O	2.33	0.61
1:D:182:ASN:O	1:D:186:ARG:HB2	2.00	0.61
1:B:64:TYR:CE1	1:B:75:ILE:HD11	2.35	0.61
1:B:201:VAL:HB	1:B:245:VAL:CG1	2.30	0.61
1:B:219:HIS:O	1:B:221:GLU:N	2.34	0.61
1:C:6:VAL:O	1:C:8:GLU:N	2.34	0.61
1:C:151:MET:O	1:C:155:LYS:HG2	2.00	0.61
1:D:141:ILE:O	1:D:141:ILE:HG13	2.00	0.61
1:D:167:GLY:HA2	2:D:273:HOH:O	2.00	0.61
1:C:150:LEU:O	1:C:154:GLU:HG3	2.01	0.60
1:D:162:PRO:HD2	1:D:164:MET:HE3	1.82	0.60
1:A:164:MET:HG2	2:A:258:HOH:O	2.01	0.60
1:C:182:ASN:ND2	1:C:186:ARG:HB2	2.17	0.60
1:D:203:VAL:HB	1:D:208:PHE:O	2.00	0.60
1:D:110:ILE:HG12	1:D:128:ILE:HD11	1.82	0.60
1:D:194:GLU:O	1:D:195:PHE:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ILE:HG13	1:A:204:ILE:O	2.00	0.60
1:A:228:MET:HE1	1:A:237:PRO:CB	2.31	0.60
1:D:57:ARG:HB3	1:D:57:ARG:NH2	2.17	0.59
1:A:142:LYS:NZ	2:A:306:HOH:O	2.33	0.59
1:C:158:HIS:HB2	2:C:352:HOH:O	2.03	0.59
1:C:74:ASP:C	1:C:75:ILE:HD12	2.26	0.59
1:D:69:LYS:HD3	1:D:69:LYS:C	2.27	0.59
1:B:183:GLN:O	1:B:189:LYS:HD3	2.03	0.59
1:C:234:ARG:HH21	1:C:234:ARG:HG3	1.67	0.59
1:C:160:PHE:C	1:C:161:ARG:HG3	2.27	0.59
1:B:134:ILE:C	1:B:136:PRO:HD3	2.28	0.59
1:B:196:GLU:HG2	1:B:199:ASP:CG	2.27	0.59
1:D:120:LYS:NZ	1:D:120:LYS:HB3	2.18	0.59
1:D:165:VAL:HG23	1:D:170:VAL:HG21	1.84	0.59
1:A:164:MET:HB3	1:A:169:PRO:HA	1.84	0.59
1:A:206:GLY:O	2:A:267:HOH:O	2.16	0.59
1:D:190:PRO:CB	2:D:395:HOH:O	2.48	0.59
1:D:216:GLU:O	1:D:217:GLU:HB3	2.03	0.59
1:A:174:GLU:O	1:A:178:GLN:HG3	2.03	0.58
1:B:68:LEU:HB2	2:B:547:HOH:O	2.03	0.58
1:C:69:LYS:HE2	1:C:70:GLY:H	1.67	0.58
1:A:161:ARG:HG3	1:A:162:PRO:O	2.02	0.58
1:B:146:ASN:ND2	1:B:149:LEU:H	2.01	0.58
1:D:196:GLU:HG2	2:D:462:HOH:O	2.01	0.58
1:A:48:VAL:HG22	2:A:446:HOH:O	2.02	0.58
1:A:245:VAL:HG13	1:A:245:VAL:O	2.03	0.58
1:B:165:VAL:HG23	1:B:170:VAL:CG2	2.33	0.58
1:C:222:LYS:HA	2:C:541:HOH:O	2.03	0.58
1:D:18:VAL:HG12	1:D:159:VAL:HG22	1.84	0.58
1:A:207:PRO:N	2:A:267:HOH:O	2.34	0.58
1:A:218:VAL:HG13	1:A:225:LEU:CD1	2.34	0.58
1:D:209:MET:HG2	1:D:210:ASN:OD1	2.04	0.58
1:B:112:LYS:H	1:B:115:GLN:NE2	2.02	0.58
1:B:112:LYS:H	1:B:115:GLN:HE21	1.52	0.57
1:D:22:LYS:HB3	1:D:25:GLU:HB2	1.86	0.57
1:D:196:GLU:HB2	2:D:439:HOH:O	2.04	0.57
1:C:184:ILE:HG21	2:C:504:HOH:O	2.04	0.57
1:C:131:ASP:OD1	1:C:133:LYS:HE2	2.05	0.57
1:C:161:ARG:HD2	1:C:164:MET:CE	2.34	0.57
1:D:185:LYS:HG2	2:D:255:HOH:O	2.05	0.57
1:B:16:LEU:HB2	1:B:139:ILE:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:NZ	1:A:222:LYS:HB3	2.20	0.57
1:D:69:LYS:HD3	1:D:70:GLY:N	2.20	0.57
1:C:221:GLU:OE1	1:C:221:GLU:HA	2.04	0.57
1:D:10:GLU:HA	2:D:409:HOH:O	2.04	0.57
1:A:203:VAL:HB	1:A:208:PHE:O	2.05	0.56
1:A:216:GLU:O	1:A:217:GLU:HB3	2.05	0.56
1:A:110:ILE:CD1	1:A:116:LYS:HA	2.35	0.56
1:D:85:THR:HB	1:D:97:GLU:HG3	1.86	0.56
1:D:201:VAL:HB	1:D:245:VAL:HG23	1.87	0.56
1:C:160:PHE:HB2	2:C:310:HOH:O	2.03	0.56
1:C:185:LYS:HZ2	1:C:186:ARG:NE	2.03	0.56
1:C:144:HIS:HD2	2:C:520:HOH:O	1.87	0.56
1:A:95:VAL:HG12	1:A:105:VAL:HG12	1.86	0.56
1:B:182:ASN:O	1:B:186:ARG:HD3	2.06	0.56
1:C:88:ILE:HA	1:C:92:GLU:O	2.06	0.56
1:D:204:ILE:HG23	2:D:432:HOH:O	2.05	0.56
1:A:180:ILE:HG13	1:A:181:LEU:N	2.19	0.56
1:C:16:LEU:HD23	1:C:162:PRO:HB3	1.88	0.56
1:C:216:GLU:O	1:C:226:THR:HB	2.05	0.56
1:D:110:ILE:HB	1:D:115:GLN:HB3	1.86	0.56
1:D:197:LYS:HD2	1:D:216:GLU:HA	1.88	0.56
1:B:219:HIS:NE2	1:B:226:THR:OG1	2.39	0.55
1:A:231:ILE:O	1:A:232:PHE:HB2	2.06	0.55
1:B:228:MET:HE3	1:B:228:MET:HA	1.89	0.55
1:C:69:LYS:HE2	1:C:69:LYS:HA	1.88	0.55
1:C:101:GLY:C	1:C:121:GLU:HG3	2.31	0.55
1:D:80:LYS:NZ	1:D:81:LYS:HE3	2.22	0.55
1:A:188:VAL:O	1:A:190:PRO:HA	2.05	0.55
1:B:23:GLU:H	1:B:23:GLU:CD	2.13	0.55
1:B:53:LYS:HA	2:B:547:HOH:O	2.06	0.55
1:D:193:VAL:HB	1:D:196:GLU:HB3	1.89	0.55
1:B:165:VAL:HG23	1:B:170:VAL:HG22	1.88	0.55
1:C:23:GLU:HB3	2:C:546:HOH:O	2.05	0.55
1:A:110:ILE:HD13	1:A:116:LYS:HA	1.89	0.55
1:C:19:GLU:HB3	1:C:22:LYS:HG3	1.88	0.55
1:B:235:MET:CA	2:B:267:HOH:O	2.37	0.55
1:B:163:VAL:HG12	1:B:170:VAL:CG2	2.36	0.55
1:C:17:GLN:HB2	1:C:161:ARG:HH11	1.72	0.55
1:C:22:LYS:HE2	2:C:345:HOH:O	2.06	0.55
1:C:26:ALA:N	2:C:352:HOH:O	2.39	0.55
1:B:44:ASP:C	1:B:45:GLU:HG2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:VAL:HB	1:C:245:VAL:CG2	2.36	0.54
1:B:239:GLU:HG2	2:B:580:HOH:O	2.08	0.54
1:D:87:ARG:HG2	1:D:89:GLU:HG3	1.88	0.54
1:D:120:LYS:H	1:D:120:LYS:HD2	1.73	0.54
1:C:194:GLU:O	1:C:195:PHE:CB	2.54	0.54
1:C:220:PRO:HG3	2:C:374:HOH:O	2.06	0.54
1:D:224:LYS:HD2	1:D:241:ASP:OD2	2.07	0.54
1:C:112:LYS:HD2	1:C:112:LYS:N	2.12	0.54
1:C:185:LYS:O	1:C:186:ARG:HB2	2.07	0.54
1:D:110:ILE:HG12	1:D:128:ILE:CD1	2.37	0.54
1:C:229:ILE:HD12	1:C:238:VAL:HG11	1.89	0.54
1:D:183:GLN:HB2	2:D:256:HOH:O	2.08	0.53
1:C:160:PHE:O	1:C:161:ARG:HG3	2.08	0.53
1:D:80:LYS:HZ2	1:D:81:LYS:HE3	1.73	0.53
1:A:202:ARG:CG	2:A:445:HOH:O	2.49	0.53
1:C:182:ASN:ND2	1:C:186:ARG:CB	2.72	0.53
1:B:15:ALA:HB2	1:B:172:LEU:HD11	1.90	0.53
1:C:6:VAL:O	1:C:8:GLU:HG2	2.09	0.53
1:C:11:LYS:HD3	1:C:143:ALA:HA	1.89	0.53
1:D:193:VAL:HG11	2:D:439:HOH:O	2.08	0.53
1:D:75:ILE:C	1:D:75:ILE:HD13	2.34	0.53
1:C:161:ARG:HG2	2:C:447:HOH:O	2.09	0.52
1:B:9:LEU:HA	2:B:363:HOH:O	2.10	0.52
1:B:216:GLU:O	1:B:217:GLU:HB3	2.08	0.52
1:C:81:LYS:HD2	2:C:484:HOH:O	2.09	0.52
1:C:182:ASN:HD22	1:C:186:ARG:HB2	1.74	0.52
1:D:151:MET:HE2	2:D:253:HOH:O	2.09	0.52
1:A:71:ASN:O	1:A:73:ARG:HG2	2.09	0.52
1:A:110:ILE:HD12	1:A:128:ILE:HG12	1.91	0.52
1:C:73:ARG:HD3	2:C:482:HOH:O	2.09	0.52
1:A:23:GLU:HB3	2:A:446:HOH:O	2.09	0.52
1:B:30:LEU:O	1:B:33:VAL:HG12	2.10	0.52
1:C:176:GLU:HA	1:C:176:GLU:OE1	2.08	0.52
1:A:75:ILE:HG23	1:A:75:ILE:O	2.10	0.52
1:B:54:VAL:HG12	1:B:56:ILE:CD1	2.39	0.52
1:B:78:LEU:CD2	1:B:83:VAL:HG12	2.37	0.52
1:B:102:ASP:CG	1:B:121:GLU:HB3	2.35	0.52
1:B:195:PHE:O	1:B:196:GLU:HB3	2.10	0.51
1:B:235:MET:HE3	2:B:267:HOH:O	2.09	0.51
1:C:185:LYS:NZ	1:C:186:ARG:NE	2.58	0.51
1:D:248:ILE:HG22	1:D:248:ILE:OXT	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLU:HG2	1:A:111:SER:HB3	1.91	0.51
1:A:139:ILE:HG22	2:A:446:HOH:O	2.09	0.51
1:B:189:LYS:HB2	1:B:189:LYS:HZ2	1.75	0.51
1:A:25:GLU:HB2	2:A:253:HOH:O	2.10	0.51
1:A:64:TYR:CZ	1:A:75:ILE:HD11	2.45	0.51
1:A:199:ASP:CG	1:A:247:LYS:NZ	2.68	0.51
1:B:16:LEU:HD21	1:B:153:ILE:HD13	1.92	0.51
1:B:245:VAL:HG12	1:B:246:GLU:N	2.25	0.51
1:A:29:ASN:HB3	1:A:156:THR:HG23	1.93	0.51
1:D:57:ARG:NH2	1:D:60:GLY:O	2.43	0.51
1:A:164:MET:HA	1:A:170:VAL:HG23	1.91	0.51
1:A:201:VAL:HB	1:A:245:VAL:CG2	2.40	0.51
1:C:146:ASN:ND2	1:C:146:ASN:C	2.69	0.51
1:C:182:ASN:HD21	1:C:186:ARG:HG2	1.76	0.51
1:C:207:PRO:HG2	1:C:208:PHE:CD1	2.46	0.51
1:C:224:LYS:HD2	1:C:241:ASP:OD2	2.11	0.51
1:C:241:ASP:HB2	2:C:530:HOH:O	2.11	0.50
1:A:37:GLU:HB3	1:A:39:LEU:HG	1.94	0.50
1:C:53:LYS:HG3	1:C:131:ASP:OD1	2.11	0.50
1:A:29:ASN:O	1:A:33:VAL:HG23	2.10	0.50
1:B:28:GLU:OE1	1:B:28:GLU:HA	2.12	0.50
1:B:175:GLU:CD	1:B:175:GLU:H	2.20	0.50
1:D:87:ARG:HB2	1:D:96:VAL:CG2	2.41	0.50
1:A:45:GLU:HB2	2:A:307:HOH:O	2.10	0.50
1:A:176:GLU:O	1:A:180:ILE:HG23	2.11	0.50
1:B:147:ASP:O	1:B:151:MET:HG3	2.12	0.50
1:B:228:MET:HG3	1:B:235:MET:HE3	1.94	0.50
1:A:9:LEU:O	1:A:10:GLU:HB3	2.11	0.50
1:A:164:MET:HB2	1:A:168:LYS:C	2.37	0.50
1:D:48:VAL:HG22	1:D:139:ILE:HG22	1.92	0.50
1:D:238:VAL:HG22	1:D:239:GLU:N	2.26	0.50
1:B:220:PRO:O	1:B:221:GLU:C	2.53	0.50
1:C:172:LEU:N	1:C:172:LEU:HD22	2.26	0.50
1:D:110:ILE:O	1:D:128:ILE:HD11	2.11	0.50
1:B:245:VAL:CG1	1:B:246:GLU:N	2.74	0.50
1:C:61:LYS:HB2	2:C:413:HOH:O	2.12	0.50
1:C:140:LEU:HD13	1:C:177:VAL:HG13	1.94	0.50
1:D:155:LYS:HE2	2:D:253:HOH:O	2.12	0.50
1:A:64:TYR:CE1	1:A:75:ILE:HD11	2.46	0.49
1:D:165:VAL:HG23	1:D:170:VAL:CG2	2.41	0.49
1:A:239:GLU:O	1:A:240:LEU:HD23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:LYS:C	1:D:225:LEU:HD22	2.36	0.49
1:D:245:VAL:HA	2:D:432:HOH:O	2.12	0.49
1:C:190:PRO:HD2	2:C:544:HOH:O	2.12	0.49
1:D:57:ARG:HB3	1:D:57:ARG:HH21	1.77	0.49
1:D:88:ILE:HA	1:D:92:GLU:O	2.12	0.49
1:B:85:THR:O	1:B:96:VAL:HG22	2.12	0.49
1:B:219:HIS:O	1:B:220:PRO:C	2.55	0.49
1:B:95:VAL:HG12	1:B:105:VAL:HG12	1.93	0.49
1:B:135:PHE:N	1:B:136:PRO:HD3	2.27	0.49
1:B:228:MET:HE1	1:B:237:PRO:HD3	1.95	0.49
1:D:225:LEU:O	1:D:239:GLU:HA	2.12	0.49
1:A:244:GLN:C	2:A:439:HOH:O	2.55	0.49
1:B:97:GLU:HG3	2:B:291:HOH:O	2.13	0.49
1:C:189:LYS:HB2	1:C:189:LYS:NZ	2.28	0.49
1:D:218:VAL:HG12	1:D:219:HIS:N	2.28	0.49
1:B:34:LEU:HB3	1:B:40:LYS:HD3	1.95	0.48
1:C:208:PHE:HD2	2:C:502:HOH:O	1.97	0.48
1:D:57:ARG:HH21	1:D:57:ARG:CB	2.26	0.48
1:D:150:LEU:O	1:D:154:GLU:HG2	2.12	0.48
1:B:25:GLU:OE2	1:B:25:GLU:N	2.43	0.48
1:B:201:VAL:CG1	2:B:260:HOH:O	2.32	0.48
1:C:164:MET:HA	1:C:170:VAL:HG23	1.95	0.48
1:A:50:ALA:HB1	1:A:131:ASP:C	2.38	0.48
1:A:186:ARG:NH2	2:A:257:HOH:O	2.45	0.48
1:C:215:VAL:HG13	1:C:225:LEU:HD22	1.95	0.48
1:D:25:GLU:HG2	2:D:257:HOH:O	2.13	0.48
1:D:173:LYS:HG2	2:D:431:HOH:O	2.13	0.48
1:B:103:THR:O	1:B:106:ASN:HB2	2.14	0.48
1:B:160:PHE:HA	2:B:251:HOH:O	2.13	0.48
1:C:135:PHE:HD2	2:C:450:HOH:O	1.96	0.48
1:D:94:LYS:HB3	1:D:109:PRO:HB3	1.95	0.48
1:A:225:LEU:O	1:A:239:GLU:HA	2.14	0.48
1:D:135:PHE:CZ	1:D:183:GLN:HG2	2.49	0.48
1:A:45:GLU:CB	2:A:307:HOH:O	2.61	0.48
1:A:248:ILE:OXT	1:A:248:ILE:HG22	2.14	0.48
1:D:116:LYS:HE2	1:D:127:LYS:HD2	1.95	0.48
1:B:222:LYS:NZ	1:B:222:LYS:CB	2.76	0.48
1:D:110:ILE:HD12	1:D:117:ILE:HG13	1.96	0.48
1:C:28:GLU:HG3	2:C:263:HOH:O	2.13	0.48
1:A:218:VAL:O	1:A:220:PRO:HD3	2.14	0.48
1:B:163:VAL:HG12	1:B:170:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LYS:CE	1:C:70:GLY:H	2.25	0.48
1:C:69:LYS:HG3	2:C:397:HOH:O	2.13	0.48
1:D:192:LYS:O	1:D:193:VAL:C	2.56	0.48
1:B:164:MET:CB	2:B:362:HOH:O	2.45	0.47
1:B:103:THR:HA	2:C:506:HOH:O	2.14	0.47
1:C:111:SER:HB2	1:C:112:LYS:HD2	1.97	0.47
1:C:156:THR:HG23	1:C:157:PRO:HD2	1.96	0.47
1:A:94:LYS:HG2	2:A:443:HOH:O	2.13	0.47
1:A:186:ARG:O	1:A:186:ARG:HG2	2.14	0.47
1:B:146:ASN:HD22	1:B:146:ASN:H	1.60	0.47
1:C:171:PRO:HB2	2:C:513:HOH:O	2.13	0.47
1:B:164:MET:HB3	2:B:362:HOH:O	2.13	0.47
1:B:202:ARG:NH2	1:B:204:ILE:HG22	2.23	0.47
1:B:225:LEU:HD22	1:B:242:PHE:HD1	1.80	0.47
1:D:16:LEU:CD2	1:D:162:PRO:HG3	2.44	0.47
1:D:110:ILE:HD13	1:D:110:ILE:H	1.79	0.47
1:D:173:LYS:HD2	1:D:175:GLU:HG2	1.97	0.47
1:D:212:THR:O	2:D:320:HOH:O	2.01	0.47
1:C:134:ILE:C	1:C:136:PRO:HD3	2.39	0.47
1:A:202:ARG:CD	2:A:445:HOH:O	2.48	0.47
1:B:28:GLU:O	1:B:32:LYS:HG2	2.14	0.47
1:B:79:GLY:HA3	1:B:122:ASN:ND2	2.30	0.47
1:B:175:GLU:O	1:B:179:ASN:ND2	2.48	0.47
1:B:197:LYS:HZ3	1:B:216:GLU:HG3	1.74	0.47
1:B:222:LYS:NZ	1:B:222:LYS:HB3	2.28	0.47
1:C:131:ASP:HB3	1:C:133:LYS:HG3	1.97	0.47
1:D:234:ARG:HG2	1:D:236:THR:OG1	2.15	0.47
1:C:140:LEU:HD22	2:C:509:HOH:O	2.13	0.47
1:D:192:LYS:NZ	1:D:192:LYS:HB3	2.30	0.47
1:B:189:LYS:HB2	1:B:189:LYS:NZ	2.29	0.47
1:C:52:GLU:OE2	1:C:185:LYS:HG3	2.15	0.47
1:C:165:VAL:HG23	1:C:170:VAL:HG21	1.96	0.47
1:D:105:VAL:HG21	2:D:269:HOH:O	2.15	0.46
1:B:193:VAL:HG13	1:B:193:VAL:O	2.15	0.46
1:C:196:GLU:O	1:C:197:LYS:C	2.58	0.46
1:A:149:LEU:O	1:A:153:ILE:HG12	2.15	0.46
1:B:156:THR:HG23	1:B:157:PRO:HD2	1.98	0.46
1:A:46:VAL:HG22	1:A:141:ILE:HG22	1.98	0.46
1:A:160:PHE:HB3	2:A:356:HOH:O	2.16	0.46
1:A:180:ILE:CG1	1:A:181:LEU:N	2.78	0.46
1:B:80:LYS:CE	1:B:123:LYS:HG3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:THR:HG23	2:C:351:HOH:O	2.15	0.46
1:B:202:ARG:HH22	1:B:204:ILE:CG2	2.24	0.46
1:C:17:GLN:HG2	2:C:272:HOH:O	2.14	0.46
1:C:140:LEU:HD13	1:C:177:VAL:CG1	2.46	0.46
1:C:221:GLU:C	1:C:223:ARG:H	2.19	0.46
1:C:234:ARG:HG3	1:C:234:ARG:NH2	2.31	0.46
1:B:80:LYS:HD2	2:B:382:HOH:O	2.16	0.46
1:B:176:GLU:O	1:B:180:ILE:HG23	2.14	0.46
1:C:33:VAL:O	1:C:37:GLU:HB2	2.15	0.46
1:C:192:LYS:HD3	1:C:192:LYS:N	2.25	0.46
1:D:188:VAL:HG21	2:D:338:HOH:O	2.15	0.46
1:D:223:ARG:HA	1:D:242:PHE:CE1	2.51	0.46
1:A:127:LYS:HB3	2:A:405:HOH:O	2.16	0.46
1:B:54:VAL:N	2:B:547:HOH:O	2.49	0.46
1:A:39:LEU:HD21	1:A:148:LYS:CD	2.46	0.46
1:C:158:HIS:CD2	2:C:352:HOH:O	2.69	0.46
1:C:75:ILE:HD12	1:C:75:ILE:N	2.32	0.45
1:D:163:VAL:HG21	2:D:430:HOH:O	2.16	0.45
1:A:57:ARG:HG3	1:A:125:GLU:HG2	1.97	0.45
1:A:116:LYS:HB2	2:A:405:HOH:O	2.17	0.45
1:A:192:LYS:O	1:A:192:LYS:HG3	2.16	0.45
1:C:47:ILE:HG13	2:C:308:HOH:O	2.17	0.45
1:D:56:ILE:CD1	1:D:75:ILE:HD12	2.46	0.45
1:D:189:LYS:CB	1:D:190:PRO:HA	2.41	0.45
1:C:164:MET:HB2	1:C:168:LYS:C	2.41	0.45
1:C:216:GLU:O	1:C:226:THR:O	2.34	0.45
1:D:173:LYS:CD	1:D:175:GLU:HG2	2.46	0.45
1:A:78:LEU:HD23	1:A:83:VAL:HG12	1.98	0.45
1:A:197:LYS:HG3	1:A:217:GLU:H	1.81	0.45
1:B:141:ILE:HG13	1:B:141:ILE:O	2.16	0.45
1:C:247:LYS:O	1:C:248:ILE:CG1	2.52	0.45
1:A:51:GLU:OE1	1:A:67:SER:HB2	2.16	0.45
1:B:163:VAL:HG12	1:B:170:VAL:HG21	1.99	0.45
1:D:127:LYS:HE3	2:D:291:HOH:O	2.17	0.45
1:D:246:GLU:O	1:D:246:GLU:HG3	2.17	0.45
1:A:160:PHE:O	1:A:161:ARG:HG2	2.17	0.45
1:D:20:PRO:HB3	2:D:416:HOH:O	2.17	0.45
1:A:17:GLN:NE2	1:A:161:ARG:NH2	2.65	0.45
1:A:102:ASP:OD2	1:A:121:GLU:HB2	2.16	0.45
1:C:215:VAL:CG1	1:C:225:LEU:HD22	2.47	0.45
1:C:221:GLU:C	1:C:223:ARG:N	2.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LYS:O	1:A:193:VAL:C	2.60	0.45
1:B:247:LYS:O	1:B:248:ILE:O	2.35	0.45
1:C:217:GLU:CD	1:C:219:HIS:HE1	2.24	0.45
1:A:13:TRP:HE1	1:A:174:GLU:HG3	1.81	0.44
1:B:204:ILE:CG2	1:B:246:GLU:HB2	2.47	0.44
1:D:102:ASP:OD2	1:D:121:GLU:HB3	2.17	0.44
1:B:64:TYR:CZ	1:B:75:ILE:HD11	2.52	0.44
1:B:133:LYS:HZ1	1:B:189:LYS:HZ1	1.63	0.44
1:B:213:GLY:HA3	1:B:229:ILE:HA	1.98	0.44
1:C:14:TYR:HA	1:C:172:LEU:CD2	2.46	0.44
1:C:184:ILE:HD13	2:C:504:HOH:O	2.16	0.44
1:B:87:ARG:HG2	1:B:89:GLU:HG3	1.99	0.44
1:B:189:LYS:NZ	1:B:189:LYS:CB	2.80	0.44
1:B:185:LYS:HG2	2:B:552:HOH:O	2.18	0.44
1:C:16:LEU:HA	1:C:162:PRO:HA	2.00	0.44
1:C:27:LYS:O	1:C:31:LEU:HG	2.18	0.44
1:B:209:MET:O	1:B:210:ASN:HB2	2.17	0.44
1:C:215:VAL:HG22	1:C:227:VAL:HG12	2.00	0.44
1:D:133:LYS:HG3	1:D:190:PRO:HD2	1.99	0.44
1:D:135:PHE:CE1	1:D:180:ILE:HG23	2.52	0.44
1:D:241:ASP:C	1:D:243:ASP:N	2.72	0.44
1:A:133:LYS:HD2	2:A:268:HOH:O	2.16	0.44
1:B:64:TYR:HB3	1:B:66:LEU:CD1	2.47	0.44
1:B:203:VAL:HA	2:B:385:HOH:O	2.17	0.44
1:C:25:GLU:HG3	2:C:524:HOH:O	2.17	0.44
1:C:196:GLU:HA	1:C:218:VAL:HG21	1.98	0.44
2:C:276:HOH:O	1:D:155:LYS:HE3	2.17	0.44
1:B:16:LEU:HD22	1:B:153:ILE:HG21	1.99	0.44
1:B:219:HIS:NE2	1:B:239:GLU:OE1	2.51	0.44
1:B:219:HIS:CD2	1:B:239:GLU:OE1	2.71	0.44
1:D:192:LYS:O	1:D:192:LYS:HG3	2.18	0.44
1:A:16:LEU:HD21	1:A:141:ILE:HD11	2.00	0.43
1:D:59:GLN:NE2	1:D:123:LYS:HG3	2.33	0.43
1:C:54:VAL:CG1	1:C:93:VAL:HG21	2.48	0.43
1:A:242:PHE:N	1:A:242:PHE:CD1	2.87	0.43
1:A:195:PHE:HD2	1:A:195:PHE:HA	1.70	0.43
1:B:216:GLU:O	1:B:217:GLU:CB	2.66	0.43
1:C:87:ARG:HB2	1:C:96:VAL:CG2	2.49	0.43
1:D:162:PRO:HB2	1:D:164:MET:HE2	2.00	0.43
1:D:196:GLU:N	1:D:199:ASP:OD2	2.51	0.43
1:D:218:VAL:HG13	1:D:225:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLU:O	1:A:32:LYS:HG3	2.18	0.43
1:B:204:ILE:HG12	2:B:385:HOH:O	2.17	0.43
1:C:182:ASN:HD21	1:C:186:ARG:CB	2.30	0.43
1:B:13:TRP:CG	1:B:177:VAL:HG21	2.53	0.43
1:B:54:VAL:HG22	1:B:68:LEU:HD13	2.00	0.43
1:B:69:LYS:HD3	1:B:69:LYS:C	2.42	0.43
1:C:19:GLU:HB3	1:C:158:HIS:HB3	2.01	0.43
1:A:226:THR:OG1	1:A:239:GLU:OE2	2.29	0.43
1:C:37:GLU:HB3	1:C:39:LEU:HG	2.01	0.43
1:A:135:PHE:N	1:A:136:PRO:HD3	2.34	0.42
1:A:216:GLU:O	1:A:217:GLU:CB	2.67	0.42
1:A:220:PRO:C	1:A:222:LYS:H	2.27	0.42
1:A:227:VAL:HG22	1:A:229:ILE:HG13	2.01	0.42
1:B:160:PHE:O	1:B:160:PHE:CG	2.72	0.42
1:A:13:TRP:HD1	2:A:280:HOH:O	2.02	0.42
1:C:58:ALA:O	1:C:59:GLN:HB2	2.20	0.42
1:D:211:PHE:HB3	1:D:229:ILE:HG23	2.01	0.42
1:B:194:GLU:HB3	1:B:242:PHE:CE2	2.54	0.42
1:A:199:ASP:CG	1:A:247:LYS:HZ1	2.27	0.42
1:C:56:ILE:HD12	1:C:56:ILE:N	2.34	0.42
1:C:185:LYS:C	1:C:187:GLY:H	2.28	0.42
1:B:74:ASP:OD1	1:B:87:ARG:HB2	2.18	0.42
1:C:29:ASN:HB3	1:C:157:PRO:HG2	2.01	0.42
1:B:38:GLY:HA2	2:B:256:HOH:O	2.19	0.42
1:C:164:MET:HB3	1:C:169:PRO:HA	2.02	0.42
1:B:12:LYS:HB2	1:B:14:TYR:CE1	2.55	0.42
1:C:164:MET:HB2	1:C:168:LYS:O	2.20	0.42
1:C:243:ASP:OD2	1:C:243:ASP:N	2.33	0.42
1:D:120:LYS:HB3	1:D:120:LYS:HZ3	1.85	0.42
1:B:160:PHE:O	1:B:161:ARG:HG3	2.20	0.42
1:C:54:VAL:O	1:C:65:ARG:HA	2.19	0.42
1:C:175:GLU:HA	1:C:178:GLN:HG2	2.01	0.42
1:C:179:ASN:HB3	2:C:371:HOH:O	2.18	0.42
1:C:231:ILE:O	1:C:232:PHE:HB2	2.20	0.42
1:D:141:ILE:HD12	2:D:450:HOH:O	2.20	0.42
1:B:175:GLU:HG3	2:B:421:HOH:O	2.20	0.42
1:C:40:LYS:HG2	2:C:278:HOH:O	2.19	0.42
1:C:99:VAL:O	1:C:102:ASP:HB2	2.20	0.42
1:C:195:PHE:O	1:C:218:VAL:HG11	2.20	0.42
1:D:87:ARG:CG	1:D:89:GLU:HG3	2.49	0.42
1:D:162:PRO:HD2	1:D:164:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LYS:HB3	1:C:22:LYS:NZ	2.35	0.42
1:D:165:VAL:HB	1:D:170:VAL:HG22	2.01	0.42
1:A:35:GLU:HG2	1:A:40:LYS:HE3	2.02	0.41
1:B:32:LYS:C	2:B:477:HOH:O	2.63	0.41
1:C:173:LYS:HE2	1:C:174:GLU:HB3	2.01	0.41
1:C:192:LYS:HD3	2:C:457:HOH:O	2.19	0.41
1:C:18:VAL:HG12	1:C:159:VAL:HG22	2.02	0.41
1:C:202:ARG:NH2	2:C:314:HOH:O	2.53	0.41
1:B:225:LEU:HD22	1:B:242:PHE:CD1	2.55	0.41
1:B:228:MET:HE2	1:B:235:MET:C	2.45	0.41
1:C:139:ILE:HG22	2:C:546:HOH:O	2.19	0.41
1:D:23:GLU:HG2	2:D:286:HOH:O	2.20	0.41
1:D:76:SER:HB3	1:D:83:VAL:CG1	2.50	0.41
1:D:95:VAL:HG23	1:D:117:ILE:HG21	2.03	0.41
1:B:34:LEU:CB	1:B:40:LYS:HD3	2.49	0.41
1:D:87:ARG:HD2	2:D:466:HOH:O	2.20	0.41
1:A:25:GLU:HB3	1:A:158:HIS:CD2	2.56	0.41
1:A:122:ASN:O	1:A:123:LYS:HB2	2.20	0.41
1:B:193:VAL:O	1:B:194:GLU:HB2	2.21	0.41
1:C:124:THR:O	1:C:125:GLU:HB3	2.20	0.41
1:D:220:PRO:C	1:D:222:LYS:H	2.29	0.41
1:B:31:LEU:O	1:B:40:LYS:NZ	2.40	0.41
1:D:59:GLN:HE22	1:D:123:LYS:HG3	1.85	0.41
1:A:230:SER:O	1:A:231:ILE:HD13	2.21	0.41
1:B:53:LYS:CA	2:B:547:HOH:O	2.68	0.41
1:C:28:GLU:O	1:C:32:LYS:HD3	2.20	0.41
1:C:103:THR:C	1:C:105:VAL:N	2.78	0.41
1:C:122:ASN:O	1:C:123:LYS:HB2	2.20	0.41
1:C:156:THR:HG22	2:C:293:HOH:O	2.21	0.41
1:A:207:PRO:CA	2:A:267:HOH:O	2.67	0.41
1:A:242:PHE:N	1:A:242:PHE:HD1	2.18	0.41
1:C:94:LYS:HA	1:C:117:ILE:CD1	2.51	0.41
1:C:239:GLU:O	1:C:240:LEU:HD23	2.21	0.41
1:A:72:ALA:HA	1:A:88:ILE:O	2.21	0.41
1:D:61:LYS:CD	1:D:63:LYS:HE3	2.49	0.41
1:D:196:GLU:HA	1:D:218:VAL:HG23	2.03	0.41
1:C:16:LEU:CD2	1:C:162:PRO:HB3	2.51	0.40
1:C:110:ILE:HG13	1:C:128:ILE:HD11	2.02	0.40
1:D:87:ARG:O	1:D:93:VAL:HA	2.22	0.40
1:D:241:ASP:C	1:D:243:ASP:H	2.28	0.40
1:C:222:LYS:HG3	2:C:286:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:VAL:HG22	1:D:240:LEU:HD11	2.03	0.40
1:A:134:ILE:C	1:A:136:PRO:HD3	2.46	0.40
1:A:222:LYS:HB3	1:A:222:LYS:HZ3	1.85	0.40
1:B:133:LYS:HE2	1:B:134:ILE:HD11	2.03	0.40
1:B:146:ASN:HD22	1:B:146:ASN:C	2.29	0.40
1:C:160:PHE:O	1:C:161:ARG:O	2.40	0.40

All (598) 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:A:165:VAL:CB	1:B:238:VAL:CG1[2_757]	0.11	2.09
1:D:195:PHE:CD2	2:A:260:HOH:O[2_646]	0.20	2.00
1:B:207:PRO:C	2:A:258:HOH:O[2_747]	0.44	1.76
1:C:29:ASN:OD1	1:C:178:GLN:OE1[2_756]	0.45	1.75
1:B:71:ASN:CG	1:B:160:PHE:CA[2_757]	0.47	1.73
1:B:161:ARG:NH1	2:B:293:HOH:O[2_747]	0.47	1.73
1:A:232:PHE:O	2:B:255:HOH:O[2_757]	0.50	1.70
1:B:71:ASN:CA	1:B:160:PHE:CG[2_757]	0.50	1.70
1:A:170:VAL:CB	1:B:231:ILE:CG1[2_757]	0.52	1.68
1:A:172:LEU:CB	1:B:232:PHE:C[2_757]	0.53	1.67
1:B:234:ARG:CZ	2:A:300:HOH:O[2_747]	0.55	1.65
1:D:146:ASN:CB	2:B:434:HOH:O[2_746]	0.58	1.62
1:A:138:TYR:CZ	1:B:210:ASN:CB[2_757]	0.59	1.61
1:A:164:MET:O	1:B:208:PHE:CD1[2_757]	0.59	1.61
1:A:211:PHE:CD2	1:B:176:GLU:CB[2_757]	0.62	1.58
1:A:232:PHE:CG	1:B:15:ALA:CA[2_757]	0.62	1.58
1:A:170:VAL:O	1:B:231:ILE:CG2[2_757]	0.63	1.57
1:A:231:ILE:CD1	1:B:176:GLU:OE2[2_757]	0.64	1.56
1:A:232:PHE:CD2	1:B:15:ALA:CB[2_757]	0.64	1.56
1:A:234:ARG:CB	1:B:163:VAL:CG1[2_757]	0.66	1.54
1:C:90:ASN:O	1:C:151:MET:CE[2_746]	0.66	1.54
1:A:172:LEU:CG	1:B:232:PHE:N[2_757]	0.70	1.50
1:D:242:PHE:O	2:A:364:HOH:O[2_646]	0.70	1.50
1:A:17:GLN:OE1	1:B:209:MET:CG[2_757]	0.76	1.44
1:A:233:GLY:N	1:B:170:VAL:O[2_757]	0.77	1.43
1:A:138:TYR:OH	1:B:210:ASN:CA[2_757]	0.79	1.41
1:A:211:PHE:CE2	1:B:176:GLU:CB[2_757]	0.79	1.41
1:A:212:THR:N	2:B:413:HOH:O[2_757]	0.79	1.41
1:C:232:PHE:CE2	1:D:135:PHE:CD2[2_656]	0.79	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:O	1:B:208:PHE:CG[2_757]	0.80	1.40
1:A:164:MET:CA	1:B:208:PHE:CD2[2_757]	0.80	1.40
1:A:172:LEU:CG	1:B:232:PHE:CA[2_757]	0.81	1.39
1:B:22:LYS:CD	1:B:186:ARG:CD[2_747]	0.82	1.38
2:B:296:HOH:O	2:B:299:HOH:O[2_747]	0.82	1.38
1:B:234:ARG:NE	2:A:300:HOH:O[2_747]	0.83	1.37
1:B:240:LEU:N	2:B:264:HOH:O[2_757]	0.86	1.34
1:A:233:GLY:C	1:B:170:VAL:CB[2_757]	0.87	1.33
1:A:73:ARG:NH1	1:C:36:LEU:CD1[2_756]	0.88	1.32
1:A:232:PHE:C	2:B:255:HOH:O[2_757]	0.88	1.32
2:A:381:HOH:O	2:C:334:HOH:O[2_756]	0.88	1.32
1:A:138:TYR:CE1	1:B:210:ASN:ND2[2_757]	0.89	1.31
1:A:172:LEU:CD2	1:B:232:PHE:N[2_757]	0.89	1.31
1:C:185:LYS:CE	2:C:307:HOH:O[2_746]	0.89	1.31
1:B:72:ALA:CA	1:B:160:PHE:CZ[2_757]	0.90	1.30
1:B:217:GLU:OE1	2:D:310:HOH:O[2_756]	0.92	1.28
1:B:237:PRO:CD	1:D:103:THR:CB[2_756]	0.92	1.28
1:A:211:PHE:CE1	1:B:176:GLU:C[2_757]	0.93	1.27
1:A:14:TYR:C	1:B:232:PHE:CE2[2_757]	0.94	1.26
1:A:211:PHE:CE1	1:B:176:GLU:O[2_757]	0.95	1.25
1:A:163:VAL:CG1	1:B:211:PHE:CD1[2_757]	0.96	1.24
1:A:233:GLY:CA	1:B:170:VAL:CA[2_757]	0.97	1.23
1:D:233:GLY:CA	2:C:395:HOH:O[2_646]	0.97	1.23
1:A:163:VAL:CB	1:B:211:PHE:CD1[2_757]	0.98	1.22
1:B:74:ASP:O	1:D:38:GLY:N[2_756]	0.98	1.22
1:A:164:MET:C	1:B:208:PHE:CD2[2_757]	0.99	1.21
1:A:138:TYR:CE2	1:B:210:ASN:CB[2_757]	1.00	1.20
1:A:172:LEU:CB	1:B:232:PHE:CA[2_757]	1.00	1.20
1:B:208:PHE:N	2:A:258:HOH:O[2_747]	1.00	1.20
1:A:232:PHE:CG	1:B:15:ALA:N[2_757]	1.01	1.19
1:B:238:VAL:CA	1:D:106:ASN:OD1[2_756]	1.01	1.19
1:B:71:ASN:CA	1:B:160:PHE:CB[2_757]	1.03	1.17
1:B:71:ASN:C	1:B:160:PHE:CG[2_757]	1.04	1.16
2:B:369:HOH:O	2:C:315:HOH:O[1_556]	1.06	1.14
1:C:186:ARG:CG	2:C:474:HOH:O[2_746]	1.06	1.14
1:A:138:TYR:CD1	1:B:210:ASN:ND2[2_757]	1.07	1.13
1:B:22:LYS:CE	1:B:186:ARG:CZ[2_747]	1.07	1.13
1:B:75:ILE:C	1:D:38:GLY:O[2_756]	1.07	1.13
1:A:170:VAL:C	1:B:231:ILE:CB[2_757]	1.08	1.12
1:C:40:LYS:CA	2:A:251:HOH:O[2_746]	1.08	1.12
1:C:155:LYS:CB	1:C:186:ARG:CZ[2_756]	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:LYS:CG	1:C:186:ARG:NH1[2_756]	1.08	1.12
1:A:210:ASN:CA	2:B:253:HOH:O[2_757]	1.09	1.11
1:A:231:ILE:CD1	1:B:176:GLU:CD[2_757]	1.09	1.11
1:B:72:ALA:N	1:B:160:PHE:CE2[2_757]	1.09	1.11
1:D:148:LYS:NZ	2:B:340:HOH:O[2_746]	1.09	1.11
1:D:40:LYS:CG	2:B:271:HOH:O[2_746]	1.10	1.10
1:B:75:ILE:CA	1:D:38:GLY:O[2_756]	1.11	1.09
1:A:170:VAL:CB	1:B:231:ILE:CD1[2_757]	1.12	1.08
1:A:163:VAL:CB	1:B:211:PHE:CE1[2_757]	1.13	1.07
1:C:232:PHE:CZ	1:D:135:PHE:CG[2_656]	1.13	1.07
1:A:75:ILE:CA	1:C:38:GLY:O[2_756]	1.14	1.06
1:A:75:ILE:C	1:C:38:GLY:O[2_756]	1.14	1.06
1:A:232:PHE:CD1	1:B:15:ALA:N[2_757]	1.15	1.05
1:B:73:ARG:NH2	1:D:35:GLU:O[2_756]	1.15	1.05
1:A:233:GLY:CA	1:B:170:VAL:C[2_757]	1.16	1.04
1:B:22:LYS:CE	1:B:186:ARG:NH2[2_747]	1.16	1.04
1:A:74:ASP:CG	2:C:292:HOH:O[2_756]	1.17	1.03
1:A:165:VAL:CG1	1:B:238:VAL:CA[2_757]	1.17	1.03
1:A:17:GLN:CD	1:B:209:MET:SD[2_757]	1.18	1.02
1:A:138:TYR:CE1	1:B:210:ASN:CG[2_757]	1.19	1.01
1:A:164:MET:C	1:B:208:PHE:CG[2_757]	1.19	1.01
1:A:211:PHE:CZ	1:B:176:GLU:C[2_757]	1.19	1.01
1:A:17:GLN:CD	1:B:209:MET:CG[2_757]	1.20	1.00
1:A:234:ARG:N	1:B:170:VAL:CG2[2_757]	1.20	1.00
1:A:15:ALA:N	1:B:232:PHE:CE2[2_757]	1.21	0.99
1:A:170:VAL:CA	1:B:231:ILE:CG1[2_757]	1.21	0.99
1:B:71:ASN:C	1:B:160:PHE:CD1[2_757]	1.21	0.99
1:A:138:TYR:CZ	1:B:210:ASN:CG[2_757]	1.22	0.98
1:A:165:VAL:CG1	1:D:106:ASN:OD1[1_566]	1.22	0.98
1:A:172:LEU:CA	1:B:232:PHE:C[2_757]	1.22	0.98
1:B:161:ARG:CZ	2:B:293:HOH:O[2_747]	1.22	0.98
1:A:80:LYS:CG	1:C:8:GLU:OE1[2_756]	1.24	0.96
1:A:171:PRO:C	1:B:231:ILE:O[2_757]	1.24	0.96
1:A:231:ILE:CA	1:B:172:LEU:CD2[2_757]	1.24	0.96
1:B:74:ASP:O	1:D:37:GLU:C[2_756]	1.24	0.96
1:A:74:ASP:O	1:C:38:GLY:N[2_756]	1.25	0.95
1:A:170:VAL:O	1:B:231:ILE:CB[2_757]	1.25	0.95
1:A:209:MET:O	1:B:179:ASN:ND2[2_757]	1.25	0.95
1:A:211:PHE:CD1	1:B:176:GLU:CA[2_757]	1.25	0.95
1:A:232:PHE:CD2	1:B:15:ALA:CA[2_757]	1.26	0.94
1:C:40:LYS:N	2:A:251:HOH:O[2_746]	1.26	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:C	1:B:231:ILE:CG2[2_757]	1.27	0.93
1:A:233:GLY:C	1:B:170:VAL:CG2[2_757]	1.27	0.93
1:B:71:ASN:ND2	1:B:160:PHE:C[2_757]	1.27	0.93
1:A:165:VAL:CG1	1:B:238:VAL:CB[2_757]	1.28	0.92
1:A:232:PHE:CD1	1:B:14:TYR:C[2_757]	1.28	0.92
1:C:40:LYS:CG	2:A:255:HOH:O[2_746]	1.28	0.92
2:A:302:HOH:O	2:C:291:HOH:O[2_756]	1.28	0.92
1:B:22:LYS:CE	1:B:186:ARG:NE[2_747]	1.29	0.91
1:A:74:ASP:CB	2:C:292:HOH:O[2_756]	1.30	0.90
1:A:74:ASP:O	1:C:38:GLY:CA[2_756]	1.30	0.90
1:C:40:LYS:C	2:A:251:HOH:O[2_746]	1.30	0.90
1:B:22:LYS:NZ	1:B:186:ARG:NH2[2_747]	1.30	0.90
1:B:71:ASN:C	1:B:160:PHE:CD2[2_757]	1.30	0.90
1:A:211:PHE:N	2:B:546:HOH:O[2_757]	1.31	0.89
1:A:233:GLY:C	1:B:170:VAL:CA[2_757]	1.31	0.89
1:D:242:PHE:C	2:A:364:HOH:O[2_646]	1.31	0.89
1:B:219:HIS:CE1	1:D:108:PRO:CB[2_756]	1.31	0.89
1:D:233:GLY:C	2:C:395:HOH:O[2_646]	1.31	0.89
1:A:164:MET:C	1:B:208:PHE:CE2[2_757]	1.32	0.88
1:A:165:VAL:N	1:B:208:PHE:CZ[2_757]	1.32	0.88
1:A:172:LEU:CD2	1:B:231:ILE:C[2_757]	1.32	0.88
1:B:71:ASN:N	1:B:160:PHE:CB[2_757]	1.32	0.88
1:B:71:ASN:CB	1:B:160:PHE:CA[2_757]	1.32	0.88
1:A:64:TYR:OH	1:C:40:LYS:CB[2_756]	1.33	0.87
1:A:232:PHE:CD1	1:B:15:ALA:CA[2_757]	1.33	0.87
1:B:19:GLU:OE1	2:B:466:HOH:O[2_747]	1.33	0.87
1:B:237:PRO:CD	1:D:103:THR:CG2[2_756]	1.33	0.87
1:A:172:LEU:N	1:B:231:ILE:O[2_757]	1.34	0.86
1:A:211:PHE:C	2:B:413:HOH:O[2_757]	1.34	0.86
1:B:71:ASN:OD1	1:B:159:VAL:O[2_757]	1.34	0.86
1:B:76:SER:OG	1:D:39:LEU:CD2[2_756]	1.34	0.86
1:D:41:ASP:N	2:B:254:HOH:O[2_746]	1.34	0.86
2:B:268:HOH:O	2:B:359:HOH:O[2_747]	1.34	0.86
1:C:36:LEU:O	2:C:262:HOH:O[2_756]	1.34	0.86
1:A:165:VAL:CG2	1:B:238:VAL:CG2[2_757]	1.35	0.85
1:B:72:ALA:N	1:B:160:PHE:CZ[2_757]	1.35	0.85
1:A:76:SER:OG	1:C:39:LEU:CD2[2_756]	1.36	0.84
1:A:80:LYS:O	1:C:9:LEU:CD2[2_756]	1.36	0.84
1:A:211:PHE:CG	1:B:176:GLU:CA[2_757]	1.36	0.84
1:B:71:ASN:CG	1:B:160:PHE:N[2_757]	1.36	0.84
1:B:73:ARG:CZ	1:D:35:GLU:O[2_756]	1.36	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASP:O	1:D:38:GLY:CA[2_756]	1.36	0.84
1:A:164:MET:CA	1:B:208:PHE:CE2[2_757]	1.37	0.83
1:A:165:VAL:N	1:B:208:PHE:CE2[2_757]	1.37	0.83
1:B:71:ASN:ND2	1:B:160:PHE:CA[2_757]	1.37	0.83
1:B:207:PRO:O	2:A:258:HOH:O[2_747]	1.38	0.82
1:D:195:PHE:CE2	2:A:260:HOH:O[2_646]	1.38	0.82
1:B:71:ASN:ND2	1:B:160:PHE:N[2_757]	1.38	0.82
1:B:165:VAL:CG1	2:C:545:HOH:O[1_556]	1.38	0.82
1:D:40:LYS:C	2:B:254:HOH:O[2_746]	1.38	0.82
1:A:76:SER:N	1:C:38:GLY:O[2_756]	1.39	0.81
1:A:233:GLY:O	1:B:170:VAL:CG2[2_757]	1.39	0.81
1:B:20:PRO:CG	2:B:535:HOH:O[2_747]	1.39	0.81
1:B:22:LYS:CD	1:B:186:ARG:NE[2_747]	1.39	0.81
1:A:14:TYR:O	1:B:232:PHE:CE2[2_757]	1.40	0.80
1:A:74:ASP:OD2	2:C:292:HOH:O[2_756]	1.40	0.80
2:A:254:HOH:O	2:C:516:HOH:O[2_756]	1.40	0.80
1:C:232:PHE:CZ	1:D:135:PHE:CD2[2_656]	1.40	0.80
1:A:162:PRO:O	1:B:207:PRO:O[2_757]	1.41	0.79
1:A:210:ASN:CG	1:B:175:GLU:CG[2_757]	1.41	0.79
1:C:9:LEU:O	2:A:254:HOH:O[2_746]	1.41	0.79
1:D:195:PHE:CG	2:A:260:HOH:O[2_646]	1.41	0.79
1:B:71:ASN:OD1	1:B:159:VAL:C[2_757]	1.41	0.79
1:B:76:SER:N	1:D:38:GLY:O[2_756]	1.41	0.79
1:A:77:VAL:CB	1:C:41:ASP:OD2[2_756]	1.42	0.78
1:A:172:LEU:C	1:B:232:PHE:O[2_757]	1.42	0.78
1:A:234:ARG:CA	1:B:170:VAL:CG2[2_757]	1.42	0.78
1:B:72:ALA:C	1:B:160:PHE:CZ[2_757]	1.42	0.78
1:C:90:ASN:C	1:C:151:MET:CE[2_746]	1.42	0.78
1:A:17:GLN:OE1	1:B:209:MET:SD[2_757]	1.43	0.77
1:A:173:LYS:N	1:B:233:GLY:CA[2_757]	1.43	0.77
1:A:233:GLY:O	1:B:170:VAL:CB[2_757]	1.43	0.77
1:B:72:ALA:CA	1:B:160:PHE:CE2[2_757]	1.43	0.77
1:A:165:VAL:CB	1:B:238:VAL:CB[2_757]	1.44	0.76
2:A:303:HOH:O	2:C:306:HOH:O[2_756]	1.44	0.76
1:C:90:ASN:O	1:C:151:MET:SD[2_746]	1.44	0.76
1:C:135:PHE:CD2	1:D:232:PHE:CZ[2_656]	1.44	0.76
1:A:170:VAL:CG1	1:B:231:ILE:CG1[2_757]	1.45	0.75
1:B:21:GLY:O	2:B:348:HOH:O[2_747]	1.45	0.75
1:B:240:LEU:CG	2:B:551:HOH:O[2_757]	1.45	0.75
1:A:232:PHE:CD1	1:B:14:TYR:O[2_757]	1.46	0.74
1:D:40:LYS:CB	2:B:271:HOH:O[2_746]	1.46	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TYR:C	1:B:232:PHE:CD2[2_757]	1.47	0.73
1:A:209:MET:CB	1:B:179:ASN:OD1[2_757]	1.48	0.72
1:B:71:ASN:OD1	1:B:160:PHE:N[2_757]	1.48	0.72
1:B:72:ALA:N	1:B:160:PHE:CD2[2_757]	1.48	0.72
1:D:202:ARG:CD	2:C:503:HOH:O[2_646]	1.48	0.72
1:A:138:TYR:OH	1:B:210:ASN:CB[2_757]	1.49	0.71
1:A:211:PHE:CE1	1:B:176:GLU:CA[2_757]	1.49	0.71
1:A:211:PHE:CE2	1:B:176:GLU:CG[2_757]	1.49	0.71
1:B:78:LEU:CD1	1:D:11:LYS:CE[2_756]	1.49	0.71
1:C:155:LYS:CB	1:C:186:ARG:NH2[2_756]	1.49	0.71
1:A:172:LEU:CA	1:B:233:GLY:N[2_757]	1.50	0.70
1:A:233:GLY:CA	1:B:170:VAL:N[2_757]	1.50	0.70
1:B:19:GLU:CD	2:B:466:HOH:O[2_747]	1.50	0.70
1:A:172:LEU:CD1	1:B:232:PHE:CA[2_757]	1.51	0.69
1:A:232:PHE:CG	1:B:15:ALA:CB[2_757]	1.51	0.69
1:C:40:LYS:CB	2:A:255:HOH:O[2_746]	1.51	0.69
1:D:40:LYS:CA	2:B:254:HOH:O[2_746]	1.51	0.69
1:A:78:LEU:CD2	1:C:144:HIS:CB[2_756]	1.52	0.68
1:A:208:PHE:O	2:B:349:HOH:O[2_757]	1.52	0.68
1:C:147:ASP:OD1	2:A:413:HOH:O[2_746]	1.52	0.68
1:C:224:LYS:NZ	1:D:248:ILE:OXT[2_656]	1.52	0.68
1:A:209:MET:N	1:B:179:ASN:CG[2_757]	1.53	0.67
1:B:237:PRO:CG	1:D:103:THR:CB[2_756]	1.53	0.67
1:A:77:VAL:CG1	1:C:41:ASP:CB[2_756]	1.54	0.66
1:A:165:VAL:CG1	1:B:238:VAL:CG1[2_757]	1.54	0.66
1:A:232:PHE:CB	1:B:15:ALA:N[2_757]	1.54	0.66
1:A:234:ARG:N	1:B:170:VAL:CB[2_757]	1.54	0.66
1:B:234:ARG:NH2	2:A:300:HOH:O[2_747]	1.54	0.66
1:A:209:MET:CA	1:B:179:ASN:OD1[2_757]	1.55	0.65
1:A:210:ASN:C	1:B:175:GLU:CB[2_757]	1.56	0.64
1:B:71:ASN:OD1	1:B:160:PHE:CA[2_757]	1.56	0.64
1:A:138:TYR:CZ	1:B:210:ASN:CA[2_757]	1.57	0.63
1:A:165:VAL:CA	1:B:238:VAL:CG1[2_757]	1.57	0.63
1:A:233:GLY:CA	1:B:170:VAL:O[2_757]	1.57	0.63
1:C:147:ASP:CB	2:A:413:HOH:O[2_746]	1.57	0.63
1:B:71:ASN:O	1:B:160:PHE:CE1[2_757]	1.57	0.63
1:A:74:ASP:C	1:C:37:GLU:O[2_756]	1.58	0.62
1:A:80:LYS:C	1:C:9:LEU:CG[2_756]	1.58	0.62
1:B:71:ASN:C	1:B:160:PHE:CE1[2_757]	1.58	0.62
1:B:75:ILE:CA	1:D:38:GLY:C[2_756]	1.58	0.62
1:B:77:VAL:CB	1:D:41:ASP:OD1[2_756]	1.58	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LYS:N	2:B:254:HOH:O[2_746]	1.58	0.62
1:A:74:ASP:O	1:C:37:GLU:C[2_756]	1.59	0.61
1:A:164:MET:C	1:B:208:PHE:CD1[2_757]	1.59	0.61
1:A:165:VAL:CG2	1:B:238:VAL:CG1[2_757]	1.59	0.61
1:B:64:TYR:OH	1:D:40:LYS:CB[2_756]	1.59	0.61
1:B:73:ARG:NE	1:D:36:LEU:O[2_756]	1.59	0.61
1:C:135:PHE:CD1	1:D:232:PHE:CE1[2_656]	1.59	0.61
1:A:172:LEU:CB	1:B:232:PHE:O[2_757]	1.60	0.60
1:A:209:MET:C	1:B:179:ASN:ND2[2_757]	1.60	0.60
1:D:245:VAL:O	2:A:436:HOH:O[2_646]	1.60	0.60
1:B:71:ASN:CG	1:B:160:PHE:C[2_757]	1.60	0.60
1:B:233:GLY:CA	2:A:344:HOH:O[2_747]	1.61	0.59
1:B:19:GLU:CG	2:B:466:HOH:O[2_747]	1.61	0.59
1:C:29:ASN:OD1	1:C:178:GLN:CD[2_756]	1.61	0.59
1:A:74:ASP:CB	1:C:37:GLU:O[2_756]	1.62	0.58
1:A:83:VAL:CG1	1:C:144:HIS:ND1[2_756]	1.62	0.58
1:A:172:LEU:CB	1:B:233:GLY:N[2_757]	1.62	0.58
1:A:211:PHE:CD2	1:B:176:GLU:CA[2_757]	1.62	0.58
1:C:39:LEU:CD2	2:A:266:HOH:O[2_746]	1.62	0.58
1:C:232:PHE:CE2	1:D:135:PHE:CE2[2_656]	1.62	0.58
1:A:165:VAL:CG2	1:B:238:VAL:CB[2_757]	1.63	0.57
1:A:172:LEU:CA	1:B:232:PHE:O[2_757]	1.63	0.57
1:C:147:ASP:CG	2:A:413:HOH:O[2_746]	1.63	0.57
1:C:29:ASN:CG	1:C:178:GLN:OE1[2_756]	1.63	0.57
1:A:17:GLN:NE2	1:B:209:MET:SD[2_757]	1.64	0.56
1:C:39:LEU:CG	2:A:266:HOH:O[2_746]	1.64	0.56
1:B:71:ASN:O	1:B:160:PHE:CD1[2_757]	1.64	0.56
1:B:71:ASN:CA	1:B:160:PHE:CD1[2_757]	1.64	0.56
1:B:71:ASN:CB	1:B:160:PHE:CB[2_757]	1.65	0.55
1:B:74:ASP:C	1:D:37:GLU:O[2_756]	1.65	0.55
1:A:14:TYR:CA	1:B:232:PHE:CD2[2_757]	1.66	0.54
1:A:80:LYS:CD	1:C:8:GLU:OE1[2_756]	1.66	0.54
1:A:170:VAL:CG2	1:B:231:ILE:CD1[2_757]	1.66	0.54
1:B:74:ASP:O	1:D:37:GLU:O[2_756]	1.66	0.54
1:A:171:PRO:O	1:B:234:ARG:CB[2_757]	1.67	0.53
1:D:233:GLY:O	2:C:395:HOH:O[2_646]	1.67	0.53
1:A:164:MET:C	1:B:208:PHE:CZ[2_757]	1.68	0.52
1:A:231:ILE:CD1	1:B:176:GLU:OE1[2_757]	1.68	0.52
1:A:232:PHE:CE1	1:B:14:TYR:O[2_757]	1.68	0.52
1:A:233:GLY:N	1:B:170:VAL:C[2_757]	1.68	0.52
1:C:41:ASP:N	2:A:251:HOH:O[2_746]	1.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:LEU:C	2:C:262:HOH:O[2_756]	1.68	0.52
1:C:155:LYS:CG	1:C:186:ARG:CZ[2_756]	1.68	0.52
1:A:75:ILE:CA	1:C:38:GLY:C[2_756]	1.69	0.51
1:A:233:GLY:O	1:B:170:VAL:CA[2_757]	1.69	0.51
1:B:71:ASN:C	1:B:160:PHE:CE2[2_757]	1.69	0.51
1:B:71:ASN:N	1:B:160:PHE:CG[2_757]	1.69	0.51
1:D:32:LYS:CD	2:B:317:HOH:O[1_554]	1.69	0.51
1:C:135:PHE:CG	1:D:232:PHE:CE1[2_656]	1.69	0.51
1:C:185:LYS:CD	2:C:307:HOH:O[2_746]	1.69	0.51
1:A:96:VAL:CG1	2:C:505:HOH:O[2_756]	1.70	0.50
1:A:163:VAL:CG1	1:B:211:PHE:CG[2_757]	1.70	0.50
1:A:231:ILE:CG1	1:B:176:GLU:OE2[2_757]	1.70	0.50
2:A:282:HOH:O	2:D:334:HOH:O[2_656]	1.70	0.50
1:B:158:HIS:NE2	1:B:186:ARG:NH1[2_747]	1.70	0.50
1:A:164:MET:N	1:B:208:PHE:CD2[2_757]	1.72	0.48
1:A:209:MET:N	1:B:179:ASN:OD1[2_757]	1.72	0.48
1:A:234:ARG:NH1	1:B:17:GLN:OE1[2_757]	1.72	0.48
1:C:90:ASN:CB	2:C:287:HOH:O[2_746]	1.72	0.48
1:C:135:PHE:CE1	1:D:232:PHE:CE1[2_656]	1.72	0.48
1:A:14:TYR:O	1:B:232:PHE:CZ[2_757]	1.73	0.47
1:A:234:ARG:CG	1:B:163:VAL:CG1[2_757]	1.73	0.47
1:C:35:GLU:OE2	2:A:323:HOH:O[2_746]	1.73	0.47
1:B:72:ALA:C	1:B:160:PHE:CE1[2_757]	1.73	0.47
1:D:146:ASN:CG	2:B:434:HOH:O[2_746]	1.73	0.47
1:C:155:LYS:CB	1:C:186:ARG:NE[2_756]	1.73	0.47
1:A:97:GLU:OE1	2:C:318:HOH:O[2_756]	1.74	0.46
1:A:164:MET:O	1:B:208:PHE:CE1[2_757]	1.74	0.46
1:A:172:LEU:CG	1:B:231:ILE:C[2_757]	1.74	0.46
1:A:209:MET:O	1:B:179:ASN:CG[2_757]	1.74	0.46
1:A:15:ALA:CB	1:B:211:PHE:CE2[2_757]	1.75	0.45
1:A:80:LYS:C	1:C:9:LEU:CD2[2_756]	1.75	0.45
1:A:80:LYS:CE	1:C:8:GLU:OE1[2_756]	1.75	0.45
1:A:210:ASN:C	2:B:253:HOH:O[2_757]	1.75	0.45
1:A:211:PHE:CD2	1:B:176:GLU:CG[2_757]	1.75	0.45
1:B:22:LYS:CE	1:B:186:ARG:CD[2_747]	1.75	0.45
1:B:71:ASN:CA	1:B:160:PHE:CD2[2_757]	1.75	0.45
1:C:186:ARG:CD	2:C:474:HOH:O[2_746]	1.75	0.45
1:C:186:ARG:CB	2:C:474:HOH:O[2_746]	1.75	0.45
1:A:171:PRO:O	1:B:234:ARG:N[2_757]	1.76	0.44
1:A:210:ASN:OD1	1:B:175:GLU:CG[2_757]	1.76	0.44
1:A:233:GLY:C	1:B:170:VAL:N[2_757]	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ARG:NH1	2:A:300:HOH:O[2_747]	1.76	0.44
1:D:39:LEU:CG	2:B:259:HOH:O[2_746]	1.76	0.44
1:A:211:PHE:CG	1:B:176:GLU:CB[2_757]	1.77	0.43
1:B:71:ASN:CB	1:B:160:PHE:C[2_757]	1.77	0.43
1:B:78:LEU:CD2	1:D:144:HIS:CB[2_756]	1.77	0.43
1:B:239:GLU:C	2:B:264:HOH:O[2_757]	1.77	0.43
1:A:74:ASP:CA	1:C:37:GLU:O[2_756]	1.78	0.42
1:A:170:VAL:CA	1:B:231:ILE:CB[2_757]	1.78	0.42
1:A:211:PHE:CZ	1:B:176:GLU:CA[2_757]	1.78	0.42
1:B:209:MET:CE	2:A:447:HOH:O[2_747]	1.78	0.42
1:A:138:TYR:OH	1:B:210:ASN:N[2_757]	1.79	0.41
1:A:172:LEU:O	1:B:232:PHE:O[2_757]	1.79	0.41
1:A:208:PHE:O	1:B:179:ASN:ND2[2_757]	1.79	0.41
1:A:208:PHE:C	1:B:179:ASN:ND2[2_757]	1.79	0.41
1:B:64:TYR:CE2	1:D:40:LYS:CE[2_756]	1.79	0.41
1:B:74:ASP:CB	1:D:37:GLU:O[2_756]	1.79	0.41
1:A:17:GLN:NE2	1:B:209:MET:CB[2_757]	1.80	0.40
1:A:73:ARG:NH1	1:C:36:LEU:CG[2_756]	1.80	0.40
1:A:164:MET:C	1:B:208:PHE:CE1[2_757]	1.80	0.40
1:A:171:PRO:O	1:B:234:ARG:CA[2_757]	1.80	0.40
1:A:172:LEU:CD1	1:B:232:PHE:N[2_757]	1.80	0.40
1:A:211:PHE:CZ	1:B:176:GLU:O[2_757]	1.80	0.40
1:B:71:ASN:CB	1:B:160:PHE:CG[2_757]	1.80	0.40
1:B:71:ASN:C	1:B:160:PHE:CZ[2_757]	1.80	0.40
1:A:80:LYS:O	1:C:9:LEU:CG[2_756]	1.81	0.39
1:C:90:ASN:OD1	2:C:287:HOH:O[2_746]	1.81	0.39
1:C:151:MET:CG	2:C:470:HOH:O[2_756]	1.81	0.39
1:A:77:VAL:CB	1:C:41:ASP:CG[2_756]	1.82	0.38
1:A:211:PHE:CE2	1:B:176:GLU:CA[2_757]	1.83	0.37
1:A:17:GLN:CD	1:B:209:MET:CB[2_757]	1.84	0.36
1:A:231:ILE:C	1:B:172:LEU:CD2[2_757]	1.84	0.36
2:A:302:HOH:O	2:C:306:HOH:O[2_756]	1.84	0.36
1:A:15:ALA:N	1:B:232:PHE:CD2[2_757]	1.85	0.35
1:A:80:LYS:CE	1:C:8:GLU:OE2[2_756]	1.85	0.35
1:A:172:LEU:CG	1:B:232:PHE:CB[2_757]	1.85	0.35
1:A:210:ASN:C	2:B:546:HOH:O[2_757]	1.85	0.35
1:A:211:PHE:CZ	1:B:177:VAL:N[2_757]	1.85	0.35
1:C:135:PHE:CG	1:D:232:PHE:CZ[2_656]	1.85	0.35
1:C:178:GLN:NE2	2:C:547:HOH:O[2_746]	1.85	0.35
1:C:39:LEU:C	2:A:251:HOH:O[2_746]	1.86	0.34
1:B:72:ALA:N	1:B:160:PHE:CE1[2_757]	1.86	0.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LYS:NZ	2:C:249:HOH:O[2_746]	1.86	0.34
1:C:135:PHE:CD2	1:D:232:PHE:CE1[2_656]	1.86	0.34
1:A:80:LYS:CE	1:C:8:GLU:CD[2_756]	1.87	0.33
1:A:164:MET:CB	1:B:208:PHE:CE2[2_757]	1.87	0.33
1:A:210:ASN:ND2	1:B:175:GLU:CG[2_757]	1.87	0.33
1:C:40:LYS:CA	2:A:255:HOH:O[2_746]	1.87	0.33
1:B:207:PRO:CA	2:A:258:HOH:O[2_747]	1.87	0.33
1:A:74:ASP:O	1:C:37:GLU:O[2_756]	1.88	0.32
1:A:171:PRO:O	1:B:231:ILE:O[2_757]	1.88	0.32
1:A:211:PHE:CZ	1:B:176:GLU:CB[2_757]	1.88	0.32
1:A:233:GLY:CA	1:B:170:VAL:CB[2_757]	1.88	0.32
1:B:155:LYS:CE	1:D:32:LYS:NZ[1_556]	1.88	0.32
1:B:217:GLU:OE2	1:D:108:PRO:CG[2_756]	1.88	0.32
1:A:138:TYR:CE1	1:B:210:ASN:CB[2_757]	1.89	0.31
1:A:165:VAL:N	1:B:208:PHE:CE1[2_757]	1.89	0.31
1:B:237:PRO:CD	1:D:103:THR:OG1[2_756]	1.89	0.31
1:C:90:ASN:CG	2:C:287:HOH:O[2_746]	1.89	0.31
1:C:232:PHE:CE2	1:D:135:PHE:CG[2_656]	1.89	0.31
1:A:15:ALA:CA	1:B:232:PHE:CE2[2_757]	1.90	0.30
1:A:164:MET:O	1:B:208:PHE:CD2[2_757]	1.90	0.30
1:A:207:PRO:CB	1:B:183:GLN:CD[2_757]	1.90	0.30
1:A:210:ASN:O	1:B:175:GLU:CB[2_757]	1.90	0.30
1:A:211:PHE:CB	2:B:349:HOH:O[2_757]	1.90	0.30
1:A:232:PHE:CG	1:B:15:ALA:C[2_757]	1.90	0.30
1:A:234:ARG:CZ	2:B:327:HOH:O[2_757]	1.90	0.30
1:B:77:VAL:CG1	1:D:41:ASP:CB[2_756]	1.90	0.30
1:C:135:PHE:CZ	1:D:232:PHE:CE1[2_656]	1.90	0.30
1:A:171:PRO:C	1:B:234:ARG:CB[2_757]	1.91	0.29
1:A:207:PRO:CB	1:B:183:GLN:NE2[2_757]	1.91	0.29
1:A:232:PHE:CA	2:B:255:HOH:O[2_757]	1.91	0.29
1:B:234:ARG:CD	2:A:300:HOH:O[2_747]	1.91	0.29
1:B:71:ASN:O	1:B:160:PHE:CZ[2_757]	1.91	0.29
1:B:173:LYS:N	2:B:268:HOH:O[2_757]	1.91	0.29
1:C:155:LYS:CB	1:C:186:ARG:NH1[2_756]	1.91	0.29
1:A:163:VAL:CA	1:B:211:PHE:CE1[2_757]	1.92	0.28
1:A:170:VAL:CG1	1:B:231:ILE:N[2_757]	1.92	0.28
1:A:231:ILE:N	1:B:172:LEU:CD2[2_757]	1.92	0.28
1:B:75:ILE:CA	1:D:38:GLY:CA[2_756]	1.92	0.28
1:B:90:ASN:ND2	2:B:399:HOH:O[2_757]	1.92	0.28
1:B:188:VAL:CG2	2:B:305:HOH:O[2_757]	1.92	0.28
1:A:78:LEU:CD1	1:C:11:LYS:CE[2_756]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:MET:N	1:B:179:ASN:ND2[2_757]	1.93	0.27
1:B:71:ASN:CB	1:B:160:PHE:CD1[2_757]	1.93	0.27
1:B:71:ASN:ND2	1:B:161:ARG:N[2_757]	1.93	0.27
1:B:238:VAL:C	1:D:106:ASN:OD1[2_756]	1.93	0.27
1:C:135:PHE:CZ	1:D:232:PHE:CD1[2_656]	1.93	0.27
1:C:147:ASP:OD1	2:C:462:HOH:O[2_756]	1.93	0.27
1:D:202:ARG:NH2	2:C:503:HOH:O[2_646]	1.93	0.27
1:A:78:LEU:CD1	1:C:11:LYS:CG[2_756]	1.94	0.26
1:A:164:MET:CE	1:B:207:PRO:CB[2_757]	1.94	0.26
1:A:165:VAL:N	1:B:208:PHE:CD2[2_757]	1.94	0.26
1:C:37:GLU:OE1	2:C:397:HOH:O[2_756]	1.94	0.26
1:A:138:TYR:OH	1:B:210:ASN:CG[2_757]	1.95	0.25
1:A:210:ASN:N	2:B:253:HOH:O[2_757]	1.95	0.25
1:C:40:LYS:NZ	2:A:323:HOH:O[2_746]	1.95	0.25
1:B:74:ASP:C	1:D:38:GLY:CA[2_756]	1.95	0.25
1:D:40:LYS:CA	2:B:271:HOH:O[2_746]	1.95	0.25
1:C:135:PHE:CE1	1:D:232:PHE:CD1[2_656]	1.95	0.25
1:C:151:MET:SD	2:C:470:HOH:O[2_756]	1.95	0.25
1:A:170:VAL:CG2	1:B:231:ILE:CG1[2_757]	1.96	0.24
1:A:232:PHE:CE2	1:B:15:ALA:CB[2_757]	1.96	0.24
1:A:165:VAL:CA	1:B:208:PHE:CE1[2_757]	1.97	0.23
1:A:170:VAL:CB	1:B:231:ILE:CB[2_757]	1.97	0.23
1:A:209:MET:O	1:B:175:GLU:O[2_757]	1.97	0.23
1:A:210:ASN:ND2	2:B:421:HOH:O[2_757]	1.97	0.23
1:A:230:SER:OG	1:B:171:PRO:O[2_757]	1.97	0.23
1:C:35:GLU:OE1	2:A:323:HOH:O[2_746]	1.97	0.23
1:B:73:ARG:NH1	1:D:35:GLU:O[2_756]	1.97	0.23
1:C:135:PHE:CE2	1:D:232:PHE:CE1[2_656]	1.97	0.23
1:C:185:LYS:NZ	2:C:307:HOH:O[2_746]	1.97	0.23
1:A:77:VAL:CB	1:C:41:ASP:CB[2_756]	1.98	0.22
1:A:210:ASN:O	1:B:175:GLU:CG[2_757]	1.98	0.22
1:C:35:GLU:OE1	2:A:287:HOH:O[2_746]	1.98	0.22
1:B:21:GLY:C	2:B:348:HOH:O[2_747]	1.98	0.22
1:B:81:LYS:C	2:D:271:HOH:O[2_756]	1.98	0.22
1:B:168:LYS:NZ	2:C:317:HOH:O[1_556]	1.98	0.22
1:A:138:TYR:CZ	1:B:210:ASN:ND2[2_757]	1.99	0.21
1:A:164:MET:CA	1:B:208:PHE:CG[2_757]	1.99	0.21
1:A:232:PHE:C	1:B:170:VAL:O[2_757]	1.99	0.21
1:A:232:PHE:CB	1:B:15:ALA:CA[2_757]	1.99	0.21
1:A:234:ARG:NE	2:B:327:HOH:O[2_757]	1.99	0.21
1:C:40:LYS:N	2:A:255:HOH:O[2_746]	1.99	0.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ASN:CG	1:B:160:PHE:CB[2_757]	1.99	0.21
1:B:237:PRO:N	1:D:103:THR:CG2[2_756]	1.99	0.21
1:D:146:ASN:CA	2:B:434:HOH:O[2_746]	1.99	0.21
1:C:232:PHE:CZ	1:D:135:PHE:CD1[2_656]	1.99	0.21
1:C:232:PHE:CZ	1:D:135:PHE:CB[2_656]	1.99	0.21
1:D:233:GLY:O	2:C:473:HOH:O[2_646]	1.99	0.21
1:A:17:GLN:NE2	1:B:209:MET:CG[2_757]	2.00	0.20
1:A:97:GLU:CD	2:C:318:HOH:O[2_756]	2.00	0.20
1:A:140:LEU:CD2	1:B:232:PHE:CE1[2_757]	2.00	0.20
1:A:172:LEU:CD1	1:B:232:PHE:CG[2_757]	2.00	0.20
1:A:172:LEU:C	1:B:232:PHE:C[2_757]	2.00	0.20
1:A:209:MET:CA	1:B:179:ASN:CG[2_757]	2.00	0.20
1:A:232:PHE:N	1:B:172:LEU:CG[2_757]	2.00	0.20
1:C:35:GLU:CD	2:A:323:HOH:O[2_746]	2.00	0.20
1:B:22:LYS:NZ	1:B:182:ASN:O[2_747]	2.00	0.20
1:B:72:ALA:N	1:B:160:PHE:CG[2_757]	2.00	0.20
1:A:77:VAL:N	1:C:42:LEU:CD1[2_756]	2.01	0.19
1:A:81:LYS:N	1:C:9:LEU:CD2[2_756]	2.01	0.19
1:A:161:ARG:NH2	1:B:206:GLY:O[2_757]	2.01	0.19
1:B:71:ASN:O	1:B:160:PHE:CG[2_757]	2.01	0.19
1:B:83:VAL:CG1	1:D:144:HIS:ND1[2_756]	2.01	0.19
1:B:219:HIS:CE1	1:D:108:PRO:CG[2_756]	2.01	0.19
2:B:453:HOH:O	2:D:276:HOH:O[2_756]	2.01	0.19
1:A:17:GLN:NE2	1:B:209:MET:CE[2_757]	2.02	0.18
1:A:165:VAL:CG1	1:B:238:VAL:N[2_757]	2.02	0.18
1:A:172:LEU:CD2	1:B:231:ILE:CA[2_757]	2.02	0.18
1:A:211:PHE:CD1	1:B:176:GLU:C[2_757]	2.02	0.18
1:A:232:PHE:N	1:B:172:LEU:CD2[2_757]	2.02	0.18
1:A:232:PHE:CE2	1:B:15:ALA:CA[2_757]	2.02	0.18
1:B:235:MET:CG	2:B:469:HOH:O[2_757]	2.02	0.18
1:C:25:GLU:OE1	1:C:174:GLU:OE1[2_756]	2.02	0.18
1:A:77:VAL:CG1	1:C:41:ASP:CG[2_756]	2.03	0.17
1:A:81:LYS:CA	1:C:9:LEU:CD2[2_756]	2.03	0.17
1:A:164:MET:O	1:B:208:PHE:CB[2_757]	2.03	0.17
1:A:170:VAL:C	1:B:231:ILE:CG1[2_757]	2.03	0.17
1:B:74:ASP:CA	1:D:37:GLU:O[2_756]	2.03	0.17
1:D:39:LEU:CD2	2:B:259:HOH:O[2_746]	2.03	0.17
1:A:75:ILE:CA	1:C:38:GLY:CA[2_756]	2.04	0.16
1:A:172:LEU:CB	1:B:232:PHE:N[2_757]	2.04	0.16
1:A:172:LEU:CG	1:B:232:PHE:C[2_757]	2.04	0.16
1:A:211:PHE:N	1:B:175:GLU:CB[2_757]	2.04	0.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PHE:CA	1:B:15:ALA:N[2_757]	2.04	0.16
1:B:238:VAL:CB	1:D:106:ASN:OD1[2_756]	2.04	0.16
1:A:81:LYS:N	1:C:9:LEU:CD1[2_756]	2.05	0.15
1:A:161:ARG:CD	1:B:207:PRO:CA[2_757]	2.05	0.15
1:A:170:VAL:O	1:B:231:ILE:CA[2_757]	2.05	0.15
1:A:171:PRO:CB	1:B:234:ARG:CB[2_757]	2.05	0.15
1:A:172:LEU:C	1:B:233:GLY:CA[2_757]	2.05	0.15
1:A:172:LEU:CD1	1:B:232:PHE:CB[2_757]	2.05	0.15
1:A:212:THR:CA	2:B:413:HOH:O[2_757]	2.05	0.15
1:B:208:PHE:CA	2:A:258:HOH:O[2_747]	2.05	0.15
1:B:22:LYS:CD	1:B:186:ARG:CG[2_747]	2.05	0.15
1:C:135:PHE:CE2	1:D:232:PHE:CZ[2_656]	2.05	0.15
1:C:155:LYS:CE	1:C:185:LYS:NZ[2_756]	2.05	0.15
1:D:202:ARG:NE	2:C:503:HOH:O[2_646]	2.05	0.15
1:A:74:ASP:C	1:C:38:GLY:CA[2_756]	2.06	0.14
1:A:211:PHE:CA	2:B:413:HOH:O[2_757]	2.06	0.14
1:D:148:LYS:CD	2:B:336:HOH:O[2_746]	2.06	0.14
1:D:36:LEU:O	2:B:358:HOH:O[2_746]	2.06	0.14
1:A:80:LYS:CG	1:C:8:GLU:CD[2_756]	2.07	0.13
1:A:97:GLU:OE2	2:C:318:HOH:O[2_756]	2.07	0.13
1:A:200:GLN:OE1	1:C:120:LYS:NZ[2_756]	2.07	0.13
1:A:208:PHE:C	1:B:179:ASN:CG[2_757]	2.07	0.13
1:A:211:PHE:O	2:B:546:HOH:O[2_757]	2.07	0.13
1:C:7:GLN:CG	2:A:303:HOH:O[2_746]	2.07	0.13
1:B:73:ARG:N	1:B:160:PHE:CZ[2_757]	2.07	0.13
1:A:211:PHE:CG	1:B:176:GLU:N[2_757]	2.08	0.12
1:C:8:GLU:O	2:A:254:HOH:O[2_746]	2.08	0.12
2:A:384:HOH:O	2:D:328:HOH:O[1_566]	2.08	0.12
1:B:71:ASN:ND2	1:B:160:PHE:O[2_757]	2.08	0.12
1:B:74:ASP:C	1:D:37:GLU:C[2_756]	2.08	0.12
1:B:151:MET:CE	2:D:321:HOH:O[1_556]	2.08	0.12
1:B:161:ARG:NE	2:B:293:HOH:O[2_747]	2.08	0.12
2:B:274:HOH:O	2:B:299:HOH:O[2_747]	2.08	0.12
1:D:148:LYS:CE	2:B:340:HOH:O[2_746]	2.08	0.12
1:A:63:LYS:CG	1:C:41:ASP:OD1[2_756]	2.09	0.11
1:A:78:LEU:CD1	1:C:11:LYS:CD[2_756]	2.09	0.11
1:A:78:LEU:CD2	1:C:144:HIS:CG[2_756]	2.09	0.11
1:A:165:VAL:CA	1:B:208:PHE:CZ[2_757]	2.09	0.11
1:A:209:MET:C	1:B:179:ASN:CG[2_757]	2.09	0.11
1:A:232:PHE:CZ	1:B:140:LEU:CD2[2_757]	2.09	0.11
1:A:233:GLY:N	2:B:255:HOH:O[2_757]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:CB	1:B:163:VAL:CB[2_757]	2.09	0.11
1:B:208:PHE:CE1	2:A:285:HOH:O[2_747]	2.09	0.11
1:A:59:GLN:NE2	1:C:8:GLU:N[2_756]	2.10	0.10
1:A:200:GLN:NE2	2:C:379:HOH:O[2_756]	2.10	0.10
1:A:209:MET:C	1:B:179:ASN:OD1[2_757]	2.10	0.10
1:A:211:PHE:CA	2:B:546:HOH:O[2_757]	2.10	0.10
1:A:232:PHE:CE1	1:B:15:ALA:CA[2_757]	2.10	0.10
1:A:235:MET:N	1:B:165:VAL:CG2[2_757]	2.10	0.10
1:B:154:GLU:OE2	1:D:36:LEU:CD2[1_556]	2.10	0.10
1:B:238:VAL:CA	1:D:106:ASN:CG[2_756]	2.10	0.10
1:C:37:GLU:N	2:C:262:HOH:O[2_756]	2.10	0.10
1:A:163:VAL:CB	1:B:211:PHE:CG[2_757]	2.11	0.09
1:A:170:VAL:CG1	1:B:231:ILE:CB[2_757]	2.11	0.09
1:A:233:GLY:O	1:B:170:VAL:N[2_757]	2.11	0.09
1:C:144:HIS:CE1	2:A:316:HOH:O[2_746]	2.11	0.09
1:B:240:LEU:CB	2:B:551:HOH:O[2_757]	2.11	0.09
1:A:82:GLY:N	1:C:9:LEU:CD1[2_756]	2.12	0.08
1:A:171:PRO:N	1:B:231:ILE:CB[2_757]	2.12	0.08
1:A:211:PHE:CZ	1:B:176:GLU:CG[2_757]	2.12	0.08
1:B:155:LYS:NZ	2:D:363:HOH:O[1_556]	2.12	0.08
1:B:217:GLU:CD	2:D:310:HOH:O[2_756]	2.12	0.08
1:B:240:LEU:CA	2:B:264:HOH:O[2_757]	2.12	0.08
1:D:40:LYS:N	2:B:271:HOH:O[2_746]	2.12	0.08
1:A:81:LYS:N	1:C:9:LEU:CG[2_756]	2.13	0.07
1:A:170:VAL:CA	1:B:231:ILE:CD1[2_757]	2.13	0.07
1:A:209:MET:CA	1:B:179:ASN:ND2[2_757]	2.13	0.07
1:A:234:ARG:CA	1:B:163:VAL:CG1[2_757]	2.13	0.07
1:B:236:THR:CA	1:D:103:THR:CG2[2_756]	2.13	0.07
1:D:39:LEU:C	2:B:254:HOH:O[2_746]	2.13	0.07
1:D:37:GLU:CA	2:B:358:HOH:O[2_746]	2.13	0.07
1:C:90:ASN:CG	1:C:147:ASP:O[2_746]	2.13	0.07
1:A:64:TYR:CE2	1:C:40:LYS:CE[2_756]	2.14	0.06
1:A:74:ASP:C	1:C:37:GLU:C[2_756]	2.14	0.06
1:A:82:GLY:CA	1:C:144:HIS:NE2[2_756]	2.14	0.06
1:A:163:VAL:CG2	1:B:211:PHE:CD1[2_757]	2.14	0.06
1:A:172:LEU:CB	1:B:232:PHE:CB[2_757]	2.14	0.06
1:A:207:PRO:CB	1:B:183:GLN:OE1[2_757]	2.14	0.06
1:A:233:GLY:O	1:B:170:VAL:CG1[2_757]	2.14	0.06
1:B:71:ASN:CA	1:B:160:PHE:CA[2_757]	2.14	0.06
1:B:72:ALA:N	1:B:160:PHE:CD1[2_757]	2.14	0.06
1:B:89:GLU:OE2	2:B:452:HOH:O[2_757]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:LEU:N	2:B:551:HOH:O[2_757]	2.14	0.06
1:A:14:TYR:C	1:B:232:PHE:CZ[2_757]	2.15	0.05
1:A:171:PRO:CB	1:B:234:ARG:CG[2_757]	2.15	0.05
1:C:39:LEU:O	2:A:251:HOH:O[2_746]	2.15	0.05
1:B:72:ALA:CA	1:B:160:PHE:CE1[2_757]	2.15	0.05
1:B:73:ARG:NE	1:D:36:LEU:C[2_756]	2.15	0.05
1:C:182:ASN:ND2	2:C:474:HOH:O[2_746]	2.15	0.05
1:A:59:GLN:NE2	1:C:7:GLN:C[2_756]	2.16	0.04
1:A:77:VAL:CA	1:C:41:ASP:CB[2_756]	2.16	0.04
1:A:79:GLY:O	1:C:9:LEU:CB[2_756]	2.16	0.04
1:A:164:MET:N	1:B:208:PHE:CA[2_757]	2.16	0.04
1:A:172:LEU:CA	1:B:231:ILE:O[2_757]	2.16	0.04
1:B:22:LYS:CD	1:B:186:ARG:CZ[2_747]	2.16	0.04
1:B:235:MET:SD	2:B:469:HOH:O[2_757]	2.16	0.04
1:B:240:LEU:CD2	2:B:551:HOH:O[2_757]	2.16	0.04
1:A:138:TYR:OH	1:B:210:ASN:C[2_757]	2.17	0.03
1:A:170:VAL:CA	1:B:231:ILE:CG2[2_757]	2.17	0.03
1:A:171:PRO:CG	1:B:234:ARG:CG[2_757]	2.17	0.03
1:A:172:LEU:CA	1:B:233:GLY:CA[2_757]	2.17	0.03
1:B:237:PRO:CG	1:D:103:THR:OG1[2_756]	2.17	0.03
1:B:238:VAL:N	1:D:106:ASN:OD1[2_756]	2.17	0.03
1:C:90:ASN:O	1:C:151:MET:CG[2_746]	2.17	0.03
1:A:138:TYR:CD1	1:B:210:ASN:CG[2_757]	2.18	0.02
1:A:172:LEU:CD2	1:B:232:PHE:CA[2_757]	2.18	0.02
1:A:173:LYS:NZ	2:D:387:HOH:O[2_666]	2.18	0.02
1:A:210:ASN:CB	1:B:175:GLU:CB[2_757]	2.18	0.02
1:A:210:ASN:O	2:B:253:HOH:O[2_757]	2.18	0.02
1:B:72:ALA:O	1:B:160:PHE:CE1[2_757]	2.18	0.02
1:B:73:ARG:NH2	1:D:35:GLU:C[2_756]	2.18	0.02
1:B:75:ILE:N	1:D:38:GLY:CA[2_756]	2.18	0.02
1:B:77:VAL:CB	1:D:41:ASP:CG[2_756]	2.18	0.02
1:C:90:ASN:ND2	1:C:147:ASP:O[2_746]	2.18	0.02
1:C:232:PHE:CD2	1:D:135:PHE:CD2[2_656]	2.18	0.02
1:B:21:GLY:CA	2:B:348:HOH:O[2_747]	2.19	0.01
1:B:78:LEU:CD1	1:D:11:LYS:NZ[2_756]	2.19	0.01
1:C:90:ASN:OD1	1:C:147:ASP:CB[2_746]	2.19	0.01

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	238/248 (96%)	214 (90%)	18 (8%)	6 (2%)	4	1
1	B	240/248 (97%)	206 (86%)	27 (11%)	7 (3%)	3	1
1	C	242/248 (98%)	208 (86%)	22 (9%)	12 (5%)	1	0
1	D	237/248 (96%)	205 (86%)	19 (8%)	13 (6%)	1	0
All	All	957/992 (96%)	833 (87%)	86 (9%)	38 (4%)	2	0

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	LYS
1	B	193	VAL
1	B	220	PRO
1	C	8	GLU
1	C	157	PRO
1	C	161	ARG
1	D	186	ARG
1	D	190	PRO
1	D	197	LYS
1	A	193	VAL
1	C	6	VAL
1	C	59	GLN
1	C	195	PHE
1	C	197	LYS
1	D	70	GLY
1	D	71	ASN
1	D	89	GLU
1	A	157	PRO
1	A	195	PHE
1	A	217	GLU
1	B	217	GLU
1	C	7	GLN

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Mol	Chain	Res	Type
1	C	9	LEU
1	D	59	GLN
1	D	161	ARG
1	D	193	VAL
1	B	190	PRO
1	C	217	GLU
1	C	221	GLU
1	D	194	GLU
1	B	161	ARG
1	C	134	ILE
1	D	217	GLU
1	B	221	GLU
1	D	157	PRO
1	D	195	PHE
1	A	161	ARG
1	B	157	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	214/222 (96%)	196 (92%)	18 (8%)	10	7
1	B	216/222 (97%)	197 (91%)	19 (9%)	9	6
1	C	218/222 (98%)	195 (89%)	23 (11%)	6	4
1	D	213/222 (96%)	196 (92%)	17 (8%)	11	8
All	All	861/888 (97%)	784 (91%)	77 (9%)	9	6

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	35	GLU
1	A	83	VAL
1	A	118	THR
1	A	121	GLU

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Mol	Chain	Res	Type
1	A	150	LEU
1	A	157	PRO
1	A	160	PHE
1	A	175	GLU
1	A	180	ILE
1	A	181	LEU
1	A	186	ARG
1	A	189	LYS
1	A	195	PHE
1	A	202	ARG
1	A	222	LYS
1	A	227	VAL
1	A	239	GLU
1	B	9	LEU
1	B	23	GLU
1	B	37	GLU
1	B	69	LYS
1	B	83	VAL
1	B	106	ASN
1	B	115	GLN
1	B	125	GLU
1	B	141	ILE
1	B	146	ASN
1	B	157	PRO
1	B	170	VAL
1	B	185	LYS
1	B	189	LYS
1	B	202	ARG
1	B	210	ASN
1	B	220	PRO
1	B	222	LYS
1	B	225	LEU
1	C	8	GLU
1	C	22	LYS
1	C	37	GLU
1	C	45	GLU
1	C	69	LYS
1	C	89	GLU
1	C	96	VAL
1	C	112	LYS
1	C	123	LYS
1	C	132	ASN

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Mol	Chain	Res	Type
1	C	146	ASN
1	C	157	PRO
1	C	161	ARG
1	C	176	GLU
1	C	180	ILE
1	C	183	GLN
1	C	186	ARG
1	C	189	LYS
1	C	192	LYS
1	C	197	LYS
1	C	216	GLU
1	C	239	GLU
1	C	243	ASP
1	D	23	GLU
1	D	36	LEU
1	D	61	LYS
1	D	75	ILE
1	D	78	LEU
1	D	97	GLU
1	D	110	ILE
1	D	120	LYS
1	D	148	LYS
1	D	150	LEU
1	D	157	PRO
1	D	170	VAL
1	D	175	GLU
1	D	188	VAL
1	D	192	LYS
1	D	193	VAL
1	D	196	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	24	ASN
1	A	29	ASN
1	A	90	ASN
1	A	106	ASN
1	A	115	GLN
1	A	158	HIS
1	A	179	ASN

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Mol	Chain	Res	Type
1	A	200	GLN
1	B	17	GLN
1	B	59	GLN
1	B	106	ASN
1	B	115	GLN
1	B	146	ASN
1	B	178	GLN
1	B	182	ASN
1	B	183	GLN
1	C	90	ASN
1	C	106	ASN
1	C	115	GLN
1	C	146	ASN
1	C	178	GLN
1	C	182	ASN
1	C	210	ASN
1	C	219	HIS
1	D	59	GLN
1	D	71	ASN
1	D	106	ASN
1	D	178	GLN
1	D	179	ASN
1	D	183	GLN
1	D	244	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.