Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:34 PM GMT

PDB ID	:	1U76
Title	:	Crystal structure of hPCNA bound to residues 452-466 of the DNA polymerase-delta-p66 subunit
Authors	:	Bruning, J.B.; Shamoo, Y.
Deposited on	:	2004-08-02
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

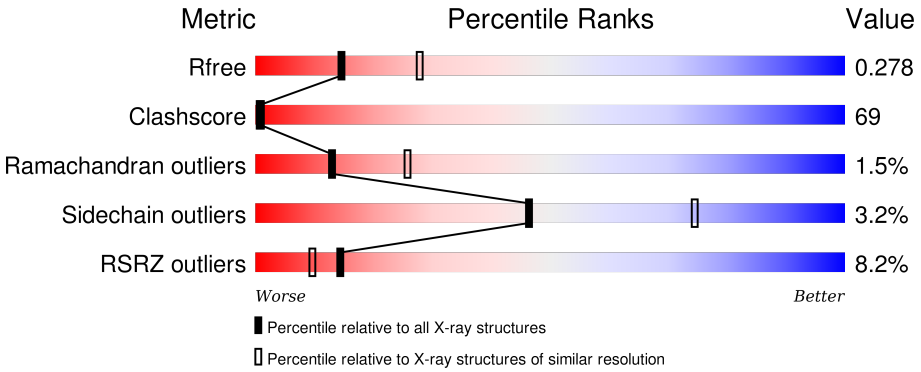
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	261	7% 39% 57%
1	C	261	6% 39% 55%
1	E	261	8% 42% 53%
2	B	15	27% 13% 53% 7% 7% 20%
2	D	15	20% 27% 47% 13% 13%

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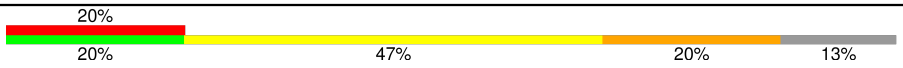
Mol	Chain	Length	Quality of chain
2	F	15	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6701 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	0	0
			1934	1217	316	385	16			
1	C	251	Total	C	N	O	S	0	0	0
			1923	1211	314	382	16			
1	E	253	Total	C	N	O	S	0	0	0
			1933	1216	318	383	16			

- Molecule 2 is a protein called KANRQVSITGFFQRK peptide from DNA polymerase delta subunit 3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	12	Total	C	N	O	0	0	0
			96	61	18	17			
2	D	13	Total	C	N	O	0	0	0
			107	67	22	18			
2	F	13	Total	C	N	O	0	0	0
			107	67	22	18			

- Molecule 3 is water.

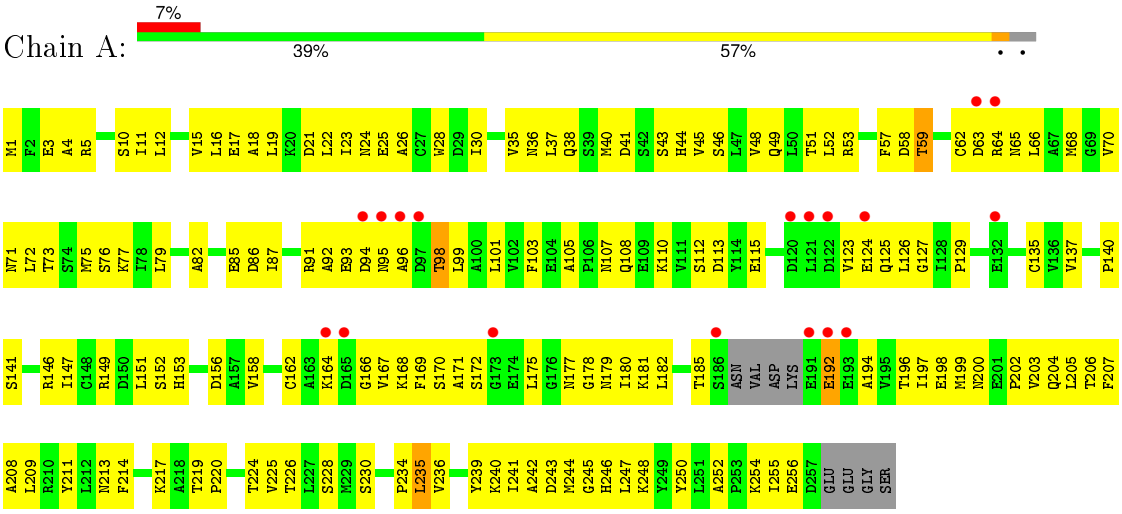
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	181	Total	O	0	0
			181	181		
3	B	10	Total	O	0	0
			10	10		
3	C	197	Total	O	0	0
			197	197		
3	D	11	Total	O	0	0
			11	11		
3	E	187	Total	O	0	0
			187	187		
3	F	15	Total	O	0	0
			15	15		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

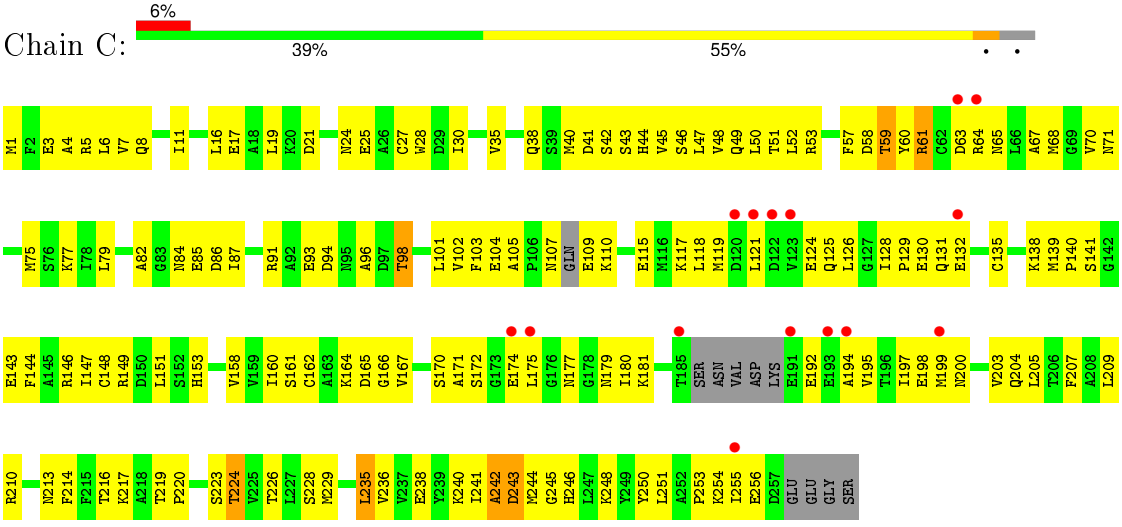
- Molecule 1: Proliferating cell nuclear antigen

Chain A:



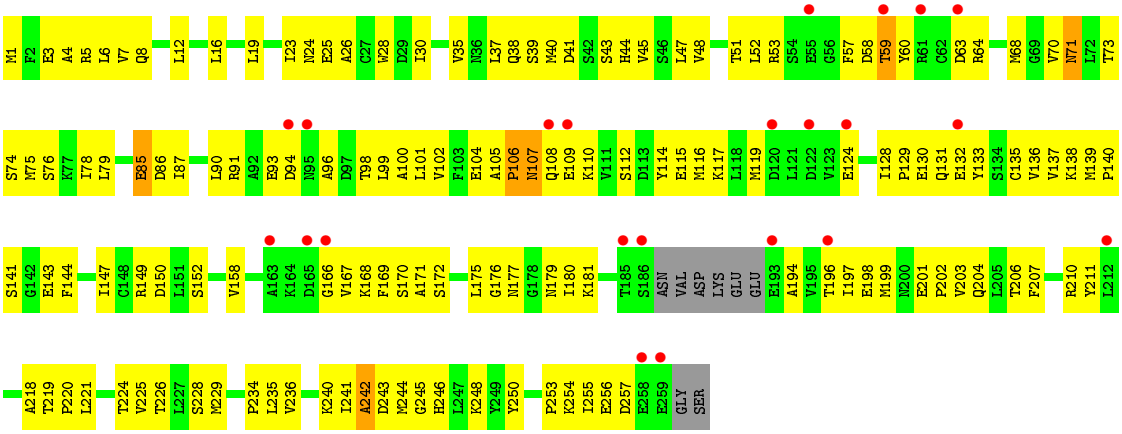
- Molecule 1: Proliferating cell nuclear antigen

Chain C:



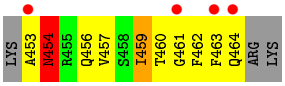
- Molecule 1: Proliferating cell nuclear antigen

Chain E:



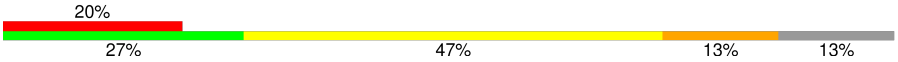
- Molecule 2: KANRQVSITGFFQRK peptide from DNA polymerase delta subunit 3

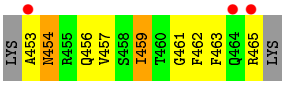
Chain B:



- Molecule 2: KANRQVSITGFFQRK peptide from DNA polymerase delta subunit 3

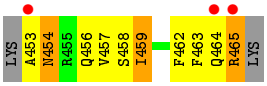
Chain D:





- Molecule 2: KANRQVSITGFFQRK peptide from DNA polymerase delta subunit 3

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	82.48Å 82.48Å 203.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.60 29.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.0 (10.00-2.60) 95.5 (29.25-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.278 0.241 , 0.278	Depositor DCC
R_{free} test set	1150 reflections (4.89%)	DCC
Wilson B-factor (Å^2)	58.0	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 71.9	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	8 of 24471 reflections (0.033%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6701	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.58 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.0861e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.38	0/1959	0.63	0/2646
1	C	0.39	0/1947	0.62	0/2628
1	E	0.38	0/1958	0.64	0/2645
2	B	0.51	0/97	0.61	0/129
2	D	0.47	0/108	0.58	0/143
2	F	0.50	0/108	0.62	0/143
All	All	0.39	0/6177	0.63	0/8334

There are no bond length outliers.

There are no bond angle outliers.

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	1934	0	1934	265	0
1	C	1923	0	1926	270	0
1	E	1933	0	1936	269	1
2	B	96	0	92	23	0
2	D	107	0	105	29	0
2	F	107	0	105	24	0
3	A	181	0	0	166	0
3	B	10	0	0	11	0
3	C	197	0	0	204	0
3	D	11	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	187	0	0	199	1
3	F	15	0	0	10	0
All	All	6701	0	6098	844	2

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 69.

All (844) 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:E:64:ARG:HA	3:E:444:HOH:O	1.33	1.27
1:E:236:VAL:HA	3:E:420:HOH:O	1.35	1.26
1:A:40:MET:HB3	3:A:351:HOH:O	1.37	1.24
1:E:73:THR:HB	3:E:395:HOH:O	1.30	1.23
2:F:456:GLN:HG3	3:F:540:HOH:O	1.38	1.21
1:C:194:ALA:HB1	3:C:343:HOH:O	1.45	1.14
2:B:460:THR:HA	3:B:525:HOH:O	1.48	1.13
1:A:126:LEU:HB3	3:A:366:HOH:O	1.47	1.12
1:E:152:SER:HA	3:E:443:HOH:O	1.49	1.11
1:E:133:TYR:HA	3:E:448:HOH:O	1.47	1.11
1:E:171:ALA:HB2	3:E:349:HOH:O	1.48	1.11
1:A:23:ILE:HA	3:A:343:HOH:O	1.49	1.11
1:C:102:VAL:HG23	3:C:368:HOH:O	1.50	1.10
1:A:217:LYS:HG3	3:A:339:HOH:O	1.51	1.09
1:E:45:VAL:HB	3:E:376:HOH:O	1.53	1.09
1:A:73:THR:HA	3:A:402:HOH:O	1.53	1.08
1:A:203:VAL:HA	3:A:422:HOH:O	1.51	1.08
1:A:49:GLN:HB2	3:A:439:HOH:O	1.54	1.07
1:E:105:ALA:HB3	3:E:348:HOH:O	1.53	1.07
3:C:385:HOH:O	2:D:454:ASN:HB3	1.53	1.06
1:A:36:ASN:HB2	3:A:334:HOH:O	1.55	1.06
1:C:131:GLN:HB2	3:C:426:HOH:O	1.56	1.04
1:E:108:GLN:HA	3:E:383:HOH:O	1.57	1.04
1:A:16:LEU:HD22	1:A:79:LEU:HD12	1.38	1.04
1:A:203:VAL:HB	3:A:348:HOH:O	1.57	1.04
1:A:58:ASP:HB3	3:A:338:HOH:O	1.57	1.03
1:A:248:LYS:HD3	3:A:409:HOH:O	1.57	1.03
1:E:16:LEU:HD22	1:E:79:LEU:HD12	1.41	1.01
1:E:242:ALA:HB2	3:E:417:HOH:O	1.59	1.01
1:C:24:ASN:HB3	3:C:374:HOH:O	1.58	1.01
1:E:35:VAL:HB	3:E:398:HOH:O	1.56	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HA	3:A:357:HOH:O	1.61	1.00
1:E:114:TYR:HA	3:E:340:HOH:O	1.60	0.99
1:C:243:ASP:HB2	3:C:401:HOH:O	1.64	0.97
1:E:73:THR:HA	3:E:406:HOH:O	1.63	0.97
1:A:239:TYR:HB3	3:A:427:HOH:O	1.64	0.97
1:A:252:ALA:HB3	3:A:346:HOH:O	1.63	0.97
1:C:131:GLN:HB3	3:C:373:HOH:O	1.64	0.97
1:C:194:ALA:HB3	3:C:377:HOH:O	1.65	0.97
1:A:169:PHE:HB2	3:A:425:HOH:O	1.62	0.96
1:A:101:LEU:HG	3:A:405:HOH:O	1.63	0.96
1:E:23:ILE:HA	3:E:425:HOH:O	1.65	0.96
1:C:124:GLU:HG3	2:D:465:ARG:HH21	1.28	0.96
1:A:247:LEU:HD12	3:A:404:HOH:O	1.65	0.95
1:E:85:GLU:HG2	3:E:360:HOH:O	1.66	0.95
1:E:206:THR:OG1	2:F:453:ALA:HB2	1.65	0.95
1:E:48:VAL:HG23	3:E:401:HOH:O	1.66	0.95
1:A:103:PHE:HE2	3:A:377:HOH:O	1.50	0.94
2:D:457:VAL:HA	3:D:272:HOH:O	1.65	0.93
1:E:102:VAL:HG12	3:E:346:HOH:O	1.66	0.93
1:C:170:SER:HB3	1:C:179:ASN:HB3	1.51	0.93
1:A:44:HIS:HA	3:A:351:HOH:O	1.67	0.93
1:A:103:PHE:CE2	3:A:377:HOH:O	2.21	0.93
1:E:96:ALA:HB3	3:E:338:HOH:O	1.67	0.93
1:C:70:VAL:HG11	3:C:405:HOH:O	1.68	0.92
1:C:130:GLU:HG3	3:C:389:HOH:O	1.69	0.92
1:A:153:HIS:HE1	3:A:431:HOH:O	1.54	0.91
1:E:225:VAL:HG22	3:E:385:HOH:O	1.67	0.91
1:A:76:SER:HB3	3:A:402:HOH:O	1.72	0.90
1:E:170:SER:HB3	1:E:179:ASN:HB3	1.54	0.88
1:C:240:LYS:HE2	3:C:439:HOH:O	1.71	0.88
1:E:25:GLU:HG2	3:E:370:HOH:O	1.74	0.88
1:A:94:ASP:HB3	3:A:365:HOH:O	1.73	0.87
1:E:52:LEU:HB2	3:E:398:HOH:O	1.72	0.87
1:C:117:LYS:HB3	3:C:421:HOH:O	1.73	0.87
1:A:170:SER:HB3	1:A:179:ASN:HB3	1.55	0.87
1:E:76:SER:HB3	3:E:406:HOH:O	1.74	0.87
1:C:153:HIS:CB	3:C:347:HOH:O	2.21	0.86
1:A:48:VAL:HG12	3:A:404:HOH:O	1.75	0.86
1:A:151:LEU:HB2	3:A:437:HOH:O	1.75	0.85
1:E:167:VAL:HG22	3:E:367:HOH:O	1.76	0.85
1:C:16:LEU:HD22	1:C:79:LEU:HD12	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:HG22	3:A:396:HOH:O	1.76	0.84
1:C:160:ILE:HG22	3:C:408:HOH:O	1.76	0.84
1:A:167:VAL:HG22	3:A:378:HOH:O	1.78	0.84
1:A:18:ALA:C	3:A:435:HOH:O	2.16	0.84
1:C:91:ARG:HB2	3:C:397:HOH:O	1.76	0.83
1:C:224:THR:HB	3:C:386:HOH:O	1.76	0.83
1:E:139:MET:HG2	3:E:426:HOH:O	1.78	0.83
1:A:199:MET:HB2	3:A:396:HOH:O	1.77	0.82
1:E:150:ASP:N	3:E:433:HOH:O	2.11	0.82
1:A:203:VAL:CA	3:A:422:HOH:O	2.17	0.82
1:A:219:THR:HA	3:A:354:HOH:O	1.79	0.82
1:C:181:LYS:HG3	3:C:348:HOH:O	1.78	0.82
1:A:169:PHE:HD1	3:A:425:HOH:O	1.62	0.82
1:E:107:ASN:HB2	3:E:342:HOH:O	1.79	0.81
1:C:75:MET:SD	3:C:405:HOH:O	2.36	0.81
1:C:214:PHE:HA	3:C:330:HOH:O	1.79	0.81
1:E:225:VAL:HG13	3:E:385:HOH:O	1.81	0.81
1:E:149:ARG:HB3	3:E:433:HOH:O	1.81	0.81
1:E:5:ARG:HB3	1:E:59:THR:HB	1.63	0.81
1:E:43:SER:HB3	3:E:364:HOH:O	1.80	0.80
1:E:94:ASP:N	3:E:439:HOH:O	2.15	0.80
1:E:48:VAL:N	3:E:401:HOH:O	2.14	0.80
1:A:103:PHE:CB	3:A:412:HOH:O	2.29	0.80
1:C:91:ARG:HD3	3:C:397:HOH:O	1.81	0.80
1:C:148:CYS:SG	3:C:444:HOH:O	2.40	0.80
1:A:254:LYS:HE2	3:B:271:HOH:O	1.82	0.80
1:C:57:PHE:HB3	3:C:455:HOH:O	1.82	0.79
1:E:201:GLU:HA	3:E:388:HOH:O	1.83	0.79
1:C:61:ARG:HG2	3:C:396:HOH:O	1.81	0.79
1:A:169:PHE:CD1	3:A:425:HOH:O	2.33	0.79
1:C:58:ASP:HA	3:C:356:HOH:O	1.84	0.78
1:A:156:ASP:HB3	3:A:423:HOH:O	1.82	0.78
1:A:239:TYR:C	3:A:427:HOH:O	2.21	0.78
2:B:464:GLN:NE2	2:B:464:GLN:H	1.80	0.78
1:E:106:PRO:HB2	3:E:350:HOH:O	1.84	0.78
1:A:213:ASN:C	3:A:434:HOH:O	2.21	0.78
1:A:182:LEU:N	3:A:393:HOH:O	2.16	0.78
1:E:211:TYR:CE1	3:F:449:HOH:O	2.35	0.78
1:A:5:ARG:HB3	1:A:59:THR:HB	1.64	0.77
1:C:194:ALA:HA	3:C:403:HOH:O	1.83	0.77
1:C:5:ARG:HB3	1:C:59:THR:HB	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:LYS:HG3	3:E:358:HOH:O	1.84	0.77
1:C:194:ALA:C	3:C:403:HOH:O	2.23	0.77
1:E:201:GLU:CA	3:E:388:HOH:O	2.33	0.77
1:A:110:LYS:HE2	3:A:420:HOH:O	1.84	0.77
1:E:90:LEU:HA	3:E:405:HOH:O	1.83	0.76
1:A:203:VAL:CB	3:A:348:HOH:O	2.21	0.76
1:E:196:THR:HG23	3:E:434:HOH:O	1.85	0.76
1:E:256:GLU:HA	3:E:374:HOH:O	1.85	0.76
1:C:50:LEU:HA	3:C:431:HOH:O	1.85	0.76
1:C:5:ARG:N	3:C:455:HOH:O	2.17	0.76
1:C:42:SER:HA	3:C:355:HOH:O	1.87	0.75
1:C:192:GLU:HB2	3:C:338:HOH:O	1.85	0.75
1:C:242:ALA:O	3:C:401:HOH:O	2.04	0.75
1:C:94:ASP:N	3:C:415:HOH:O	2.19	0.75
1:A:156:ASP:N	3:A:423:HOH:O	2.20	0.75
1:C:146:ARG:CZ	3:C:400:HOH:O	2.35	0.75
1:A:225:VAL:CA	3:A:358:HOH:O	2.34	0.74
1:A:167:VAL:C	3:A:378:HOH:O	2.26	0.74
1:C:6:LEU:C	3:C:422:HOH:O	2.25	0.74
1:A:207:PHE:HA	3:A:428:HOH:O	1.88	0.74
1:A:147:ILE:HG23	1:A:180:ILE:HD12	1.69	0.74
1:A:92:ALA:HA	3:A:357:HOH:O	1.87	0.74
1:E:139:MET:N	3:E:426:HOH:O	2.19	0.74
1:E:5:ARG:HB2	3:E:422:HOH:O	1.87	0.74
1:A:203:VAL:HG13	3:A:422:HOH:O	1.88	0.73
1:E:114:TYR:CA	3:E:340:HOH:O	2.24	0.73
1:C:124:GLU:HG3	2:D:465:ARG:NH2	2.02	0.73
1:C:175:LEU:HG	3:C:360:HOH:O	1.89	0.73
3:C:372:HOH:O	2:D:456:GLN:NE2	2.20	0.73
1:E:137:VAL:HG23	3:E:347:HOH:O	1.88	0.73
1:E:255:ILE:HD13	2:F:457:VAL:HG21	1.69	0.73
1:E:59:THR:C	3:E:381:HOH:O	2.27	0.73
1:A:254:LYS:HB3	3:B:271:HOH:O	1.89	0.73
1:E:5:ARG:CG	3:E:422:HOH:O	2.36	0.72
2:D:454:ASN:N	3:D:393:HOH:O	2.20	0.72
1:E:199:MET:HG2	3:E:396:HOH:O	1.89	0.72
1:A:123:VAL:HG12	3:A:370:HOH:O	1.88	0.72
2:F:456:GLN:C	3:F:540:HOH:O	2.26	0.72
1:A:49:GLN:HG2	3:A:386:HOH:O	1.87	0.72
1:E:202:PRO:HD2	3:E:388:HOH:O	1.88	0.72
1:C:64:ARG:HG2	3:C:351:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:ASP:HB3	3:E:375:HOH:O	1.90	0.72
1:C:58:ASP:HB2	3:C:328:HOH:O	1.89	0.72
1:A:203:VAL:N	3:A:348:HOH:O	2.22	0.71
1:A:225:VAL:C	3:A:406:HOH:O	2.28	0.71
1:A:180:ILE:HD11	3:E:421:HOH:O	1.89	0.71
1:E:3:GLU:HG2	3:E:368:HOH:O	1.90	0.71
1:A:18:ALA:HB3	3:A:435:HOH:O	1.90	0.71
1:C:6:LEU:N	3:C:422:HOH:O	2.22	0.71
1:A:22:LEU:HD21	3:A:356:HOH:O	1.90	0.71
2:F:464:GLN:HG2	3:F:303:HOH:O	1.90	0.71
1:C:194:ALA:CA	3:C:403:HOH:O	2.38	0.71
1:C:224:THR:CB	3:C:386:HOH:O	2.34	0.71
1:E:130:GLU:HA	3:E:399:HOH:O	1.89	0.71
1:A:112:SER:HB3	3:C:458:HOH:O	1.91	0.71
1:C:118:LEU:HB3	3:C:345:HOH:O	1.90	0.71
1:E:175:LEU:HG	3:E:294:HOH:O	1.91	0.70
1:E:58:ASP:HB2	3:E:341:HOH:O	1.90	0.70
1:A:18:ALA:CB	3:A:435:HOH:O	2.39	0.70
1:E:35:VAL:CB	3:E:398:HOH:O	2.25	0.70
1:A:200:ASN:N	3:A:436:HOH:O	2.23	0.70
1:E:101:LEU:HD12	3:E:392:HOH:O	1.90	0.70
1:C:151:LEU:HD21	3:C:362:HOH:O	1.91	0.70
1:E:119:MET:SD	3:E:370:HOH:O	2.49	0.70
1:A:214:PHE:N	3:A:434:HOH:O	2.24	0.70
1:E:199:MET:CG	3:E:396:HOH:O	2.39	0.70
1:E:78:ILE:CG2	3:E:442:HOH:O	2.39	0.70
1:C:153:HIS:ND1	3:C:347:HOH:O	2.23	0.70
1:E:3:GLU:OE2	1:E:91:ARG:HD3	1.92	0.70
1:C:253:PRO:C	3:C:372:HOH:O	2.31	0.69
1:A:214:PHE:HA	3:A:434:HOH:O	1.91	0.69
1:A:66:LEU:HD23	3:A:400:HOH:O	1.92	0.69
1:A:244:MET:C	3:A:382:HOH:O	2.30	0.69
1:A:225:VAL:HA	3:A:358:HOH:O	1.90	0.69
1:C:119:MET:HE1	3:C:337:HOH:O	1.91	0.69
1:A:63:ASP:C	3:A:359:HOH:O	2.31	0.69
1:C:50:LEU:CA	3:C:431:HOH:O	2.39	0.69
1:E:255:ILE:HD12	3:E:296:HOH:O	1.90	0.69
1:A:180:ILE:HG13	3:E:421:HOH:O	1.92	0.69
1:C:70:VAL:C	3:C:381:HOH:O	2.30	0.69
1:A:126:LEU:HD21	3:B:525:HOH:O	1.93	0.69
1:E:60:TYR:C	3:E:381:HOH:O	2.31	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:LYS:C	3:E:426:HOH:O	2.31	0.69
1:A:168:LYS:N	3:A:378:HOH:O	2.25	0.69
1:E:135:CYS:SG	3:E:396:HOH:O	2.50	0.69
2:F:465:ARG:HH11	2:F:465:ARG:HG2	1.56	0.69
1:E:53:ARG:NE	3:E:365:HOH:O	2.25	0.69
1:E:254:LYS:HG2	2:F:456:GLN:HA	1.74	0.69
1:C:255:ILE:HD13	2:D:457:VAL:HG21	1.75	0.69
1:C:144:PHE:CD1	3:C:444:HOH:O	2.46	0.68
1:C:138:LYS:HG3	3:C:369:HOH:O	1.92	0.68
1:E:58:ASP:C	3:E:341:HOH:O	2.32	0.68
1:E:37:LEU:HD23	3:E:404:HOH:O	1.93	0.68
3:C:385:HOH:O	2:D:454:ASN:CB	2.26	0.68
1:A:66:LEU:HA	3:A:400:HOH:O	1.93	0.68
1:E:3:GLU:CG	3:E:368:HOH:O	2.41	0.68
1:C:41:ASP:O	3:C:355:HOH:O	2.12	0.68
1:E:133:TYR:CD1	3:E:371:HOH:O	2.46	0.67
1:E:158:VAL:HA	3:E:349:HOH:O	1.95	0.67
1:E:60:TYR:CA	3:E:381:HOH:O	2.42	0.67
1:A:3:GLU:OE2	1:A:91:ARG:HD3	1.95	0.67
1:A:180:ILE:CG1	3:E:421:HOH:O	2.42	0.67
1:A:180:ILE:HB	3:A:425:HOH:O	1.94	0.67
1:A:103:PHE:HB3	3:A:412:HOH:O	1.92	0.67
1:A:64:ARG:HD2	3:A:365:HOH:O	1.93	0.67
1:E:202:PRO:HG3	3:E:366:HOH:O	1.95	0.67
1:A:181:LYS:C	3:A:393:HOH:O	2.33	0.67
1:C:30:ILE:HD12	1:C:35:VAL:HG22	1.76	0.67
1:E:253:PRO:HB2	3:E:296:HOH:O	1.94	0.67
1:E:30:ILE:HD12	1:E:35:VAL:HG22	1.76	0.67
1:E:5:ARG:CB	3:E:422:HOH:O	2.42	0.67
1:E:7:VAL:O	3:E:354:HOH:O	2.13	0.67
2:B:461:GLY:N	3:B:471:HOH:O	2.19	0.67
1:C:254:LYS:HE2	3:D:393:HOH:O	1.92	0.67
1:A:225:VAL:HG22	3:A:406:HOH:O	1.95	0.67
1:A:169:PHE:CB	3:A:425:HOH:O	2.30	0.67
1:E:139:MET:SD	3:E:427:HOH:O	2.53	0.67
1:A:87:ILE:CG1	3:A:417:HOH:O	2.43	0.67
1:C:254:LYS:HG2	2:D:456:GLN:HA	1.77	0.66
1:E:5:ARG:HG3	3:E:422:HOH:O	1.94	0.66
1:C:195:VAL:HG23	3:C:403:HOH:O	1.93	0.66
3:C:359:HOH:O	2:D:463:PHE:HA	1.95	0.66
1:E:117:LYS:NZ	3:E:384:HOH:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:ASP:CB	3:E:439:HOH:O	2.42	0.66
1:A:172:SER:HB3	1:A:177:ASN:HB3	1.78	0.66
1:E:168:LYS:C	3:E:367:HOH:O	2.33	0.66
1:E:207:PHE:HA	3:E:358:HOH:O	1.95	0.66
1:C:238:GLU:CD	3:C:439:HOH:O	2.34	0.66
1:E:138:LYS:HE3	3:E:434:HOH:O	1.95	0.66
1:A:182:LEU:HG	3:A:393:HOH:O	1.96	0.66
1:A:180:ILE:CD1	3:E:421:HOH:O	2.43	0.66
1:E:59:THR:HG22	3:E:381:HOH:O	1.95	0.66
1:C:144:PHE:CE1	3:C:444:HOH:O	2.48	0.66
1:C:103:PHE:O	3:C:380:HOH:O	2.14	0.66
1:C:40:MET:HE3	2:D:459:ILE:HD13	1.78	0.66
1:E:201:GLU:CB	3:E:388:HOH:O	2.44	0.65
1:A:10:SER:N	3:A:362:HOH:O	2.28	0.65
1:A:108:GLN:CB	3:A:341:HOH:O	2.44	0.65
1:E:41:ASP:OD2	1:E:43:SER:HB2	1.97	0.65
1:C:6:LEU:HG	3:C:414:HOH:O	1.96	0.65
1:C:11:ILE:HG13	3:C:388:HOH:O	1.97	0.65
1:A:226:THR:N	3:A:406:HOH:O	2.29	0.65
1:C:165:ASP:HA	3:C:402:HOH:O	1.96	0.65
1:E:133:TYR:CE1	3:E:371:HOH:O	2.48	0.65
1:E:5:ARG:HB3	3:E:341:HOH:O	1.96	0.65
1:A:24:ASN:N	3:A:343:HOH:O	2.29	0.65
1:A:214:PHE:CA	3:A:434:HOH:O	2.45	0.65
1:C:250:TYR:N	3:C:429:HOH:O	2.23	0.65
1:E:229:MET:N	3:E:409:HOH:O	2.23	0.65
1:C:102:VAL:N	3:C:368:HOH:O	2.29	0.65
1:A:252:ALA:N	3:A:346:HOH:O	2.29	0.65
1:C:214:PHE:CD1	3:C:330:HOH:O	2.50	0.65
1:C:121:LEU:HA	3:C:437:HOH:O	1.95	0.65
1:C:229:MET:HA	3:C:315:HOH:O	1.97	0.64
1:A:26:ALA:HA	3:A:394:HOH:O	1.97	0.64
1:C:153:HIS:CG	3:C:347:HOH:O	2.47	0.64
1:C:51:THR:N	3:C:431:HOH:O	2.31	0.64
1:C:5:ARG:HD3	3:C:328:HOH:O	1.96	0.64
1:E:39:SER:N	3:E:404:HOH:O	2.30	0.64
1:E:172:SER:HB3	1:E:177:ASN:HB3	1.78	0.64
1:E:47:LEU:C	3:E:401:HOH:O	2.36	0.64
1:E:170:SER:CB	1:E:179:ASN:HB3	2.28	0.64
1:C:8:GLN:N	3:C:414:HOH:O	2.30	0.64
1:A:243:ASP:C	3:A:382:HOH:O	2.35	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ILE:CG1	3:C:388:HOH:O	2.45	0.64
1:A:53:ARG:HB2	3:A:408:HOH:O	1.97	0.64
1:A:19:LEU:HG	3:A:435:HOH:O	1.96	0.64
1:A:64:ARG:N	3:A:359:HOH:O	2.30	0.64
1:A:252:ALA:CB	3:A:346:HOH:O	2.33	0.64
1:A:151:LEU:N	3:A:437:HOH:O	2.31	0.64
1:E:43:SER:CB	3:E:364:HOH:O	2.44	0.64
1:C:216:THR:HB	3:C:413:HOH:O	1.96	0.63
1:E:94:ASP:CA	3:E:375:HOH:O	2.46	0.63
1:A:170:SER:CB	1:A:179:ASN:HB3	2.27	0.63
1:C:47:LEU:O	3:C:429:HOH:O	2.16	0.63
1:C:77:LYS:HE3	3:C:353:HOH:O	1.98	0.63
1:E:140:PRO:HB3	3:E:429:HOH:O	1.98	0.63
1:C:126:LEU:CA	3:C:412:HOH:O	2.45	0.63
1:A:44:HIS:ND1	3:A:345:HOH:O	2.31	0.63
1:A:124:GLU:HB3	3:A:332:HOH:O	1.97	0.63
1:C:172:SER:HB3	1:C:177:ASN:HB3	1.80	0.62
1:C:110:LYS:CE	3:C:354:HOH:O	2.47	0.62
1:A:30:ILE:HD12	1:A:35:VAL:HG22	1.80	0.62
1:E:87:ILE:HG12	3:E:354:HOH:O	1.99	0.62
1:C:126:LEU:C	3:C:412:HOH:O	2.37	0.62
1:C:149:ARG:NH1	3:C:371:HOH:O	2.32	0.62
1:E:210:ARG:NH1	3:E:382:HOH:O	2.32	0.62
1:E:175:LEU:C	3:E:379:HOH:O	2.38	0.62
1:E:168:LYS:CD	3:E:430:HOH:O	2.47	0.62
1:A:204:GLN:N	3:A:422:HOH:O	2.30	0.62
1:E:257:ASP:N	3:E:374:HOH:O	2.33	0.62
1:E:78:ILE:HG22	3:E:442:HOH:O	1.96	0.62
1:C:164:LYS:O	3:C:402:HOH:O	2.16	0.62
1:C:216:THR:CB	3:C:413:HOH:O	2.46	0.62
1:A:40:MET:HG3	3:A:383:HOH:O	1.98	0.62
2:D:461:GLY:C	3:D:254:HOH:O	2.38	0.61
1:E:35:VAL:C	3:E:398:HOH:O	2.38	0.61
1:A:87:ILE:HG12	3:A:417:HOH:O	1.99	0.61
1:C:207:PHE:HA	3:C:288:HOH:O	1.99	0.61
1:E:181:LYS:HE2	3:E:430:HOH:O	2.00	0.61
2:D:465:ARG:N	3:D:246:HOH:O	2.33	0.61
1:E:171:ALA:O	1:E:177:ASN:HB2	2.01	0.61
2:D:459:ILE:N	2:D:459:ILE:HD12	2.15	0.61
2:D:456:GLN:O	3:D:272:HOH:O	2.16	0.61
1:E:202:PRO:CD	3:E:403:HOH:O	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LYS:HD3	3:C:441:HOH:O	2.00	0.61
1:C:103:PHE:CE2	3:C:432:HOH:O	2.51	0.61
1:E:229:MET:CA	3:E:409:HOH:O	2.49	0.61
1:C:180:ILE:HG13	3:C:362:HOH:O	2.01	0.61
1:A:234:PRO:HD3	2:B:462:PHE:CD2	2.36	0.61
1:A:246:HIS:NE2	3:A:407:HOH:O	2.31	0.61
1:A:168:LYS:CA	3:A:378:HOH:O	2.49	0.60
1:E:131:GLN:HB3	3:E:264:HOH:O	2.00	0.60
1:A:171:ALA:O	1:A:177:ASN:HB2	2.02	0.60
1:E:52:LEU:HB3	1:E:244:MET:HE1	1.83	0.60
1:C:174:GLU:N	3:C:433:HOH:O	2.33	0.60
1:C:57:PHE:HD2	3:C:455:HOH:O	1.84	0.60
1:E:94:ASP:CA	3:E:439:HOH:O	2.50	0.60
1:C:58:ASP:CA	3:C:356:HOH:O	2.46	0.60
1:A:245:GLY:N	3:A:382:HOH:O	2.34	0.60
1:A:178:GLY:HA2	3:E:340:HOH:O	2.01	0.60
1:C:214:PHE:CA	3:C:330:HOH:O	2.42	0.60
1:A:53:ARG:NH2	3:A:270:HOH:O	2.29	0.60
1:C:170:SER:CB	1:C:179:ASN:HB3	2.28	0.60
1:C:226:THR:HG22	3:C:369:HOH:O	2.01	0.60
1:C:195:VAL:N	3:C:403:HOH:O	2.33	0.59
1:C:42:SER:CA	3:C:355:HOH:O	2.49	0.59
1:E:202:PRO:N	3:E:403:HOH:O	2.34	0.59
1:E:250:TYR:HA	3:E:420:HOH:O	2.01	0.59
1:C:161:SER:N	3:C:408:HOH:O	2.35	0.59
1:E:64:ARG:HD2	1:E:94:ASP:HB3	1.84	0.59
1:C:254:LYS:HG3	3:C:288:HOH:O	2.01	0.59
1:C:135:CYS:SG	1:C:199:MET:HG2	2.42	0.59
1:E:115:GLU:HG3	3:E:304:HOH:O	2.02	0.59
1:E:115:GLU:N	3:E:340:HOH:O	2.36	0.59
1:A:252:ALA:CA	3:A:346:HOH:O	2.50	0.59
2:B:464:GLN:CD	2:B:464:GLN:H	2.05	0.59
1:C:224:THR:CG2	3:C:386:HOH:O	2.51	0.59
1:C:87:ILE:HG23	3:C:422:HOH:O	2.02	0.58
1:A:52:LEU:HB3	1:A:244:MET:HE1	1.84	0.58
1:A:226:THR:C	3:A:406:HOH:O	2.40	0.58
1:A:70:VAL:HB	3:A:399:HOH:O	2.02	0.58
1:E:225:VAL:C	3:E:385:HOH:O	2.40	0.58
1:E:202:PRO:HD2	3:E:403:HOH:O	2.02	0.58
1:E:70:VAL:HB	3:E:353:HOH:O	2.04	0.58
1:A:255:ILE:HD13	2:B:457:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:462:PHE:N	3:D:254:HOH:O	2.36	0.58
1:C:58:ASP:C	3:C:328:HOH:O	2.40	0.58
1:C:30:ILE:HG13	1:C:68:MET:CE	2.33	0.58
1:E:254:LYS:HE3	3:F:132:HOH:O	2.04	0.58
1:E:12:LEU:CA	3:E:344:HOH:O	2.52	0.58
1:C:3:GLU:OE2	1:C:91:ARG:HD3	2.03	0.58
1:E:78:ILE:HG23	3:E:442:HOH:O	2.03	0.58
1:E:4:ALA:HB1	1:E:57:PHE:CD2	2.38	0.58
1:C:105:ALA:N	3:C:380:HOH:O	2.37	0.58
1:C:101:LEU:C	3:C:368:HOH:O	2.41	0.58
1:C:149:ARG:HG2	1:C:149:ARG:HH11	1.68	0.57
1:A:141:SER:HB2	1:A:219:THR:HG23	1.86	0.57
1:C:61:ARG:NH2	3:C:451:HOH:O	2.37	0.57
1:A:175:LEU:HG	3:A:316:HOH:O	2.04	0.57
1:E:202:PRO:CD	3:E:388:HOH:O	2.50	0.57
1:E:176:GLY:HA3	3:E:379:HOH:O	2.04	0.57
1:E:28:TRP:HE3	1:E:35:VAL:HG11	1.70	0.57
1:C:124:GLU:HB2	3:C:435:HOH:O	2.03	0.57
1:C:51:THR:O	1:C:245:GLY:HA3	2.03	0.57
1:A:113:ASP:N	3:C:458:HOH:O	2.37	0.57
1:A:244:MET:N	3:A:382:HOH:O	2.37	0.57
1:E:86:ASP:OD1	1:E:105:ALA:HA	2.04	0.57
2:B:459:ILE:N	2:B:459:ILE:HD12	2.20	0.57
1:A:49:GLN:N	3:A:439:HOH:O	2.37	0.57
1:E:94:ASP:HB2	3:E:439:HOH:O	2.03	0.57
1:C:153:HIS:HB2	3:C:347:HOH:O	1.93	0.57
1:E:40:MET:HE1	1:E:44:HIS:ND1	2.19	0.57
1:A:40:MET:HE3	2:B:459:ILE:HD13	1.87	0.57
1:A:48:VAL:C	3:A:439:HOH:O	2.43	0.57
1:E:51:THR:O	1:E:245:GLY:HA3	2.05	0.57
1:C:144:PHE:CG	3:C:444:HOH:O	2.57	0.56
1:A:226:THR:CA	3:A:406:HOH:O	2.53	0.56
1:A:156:ASP:CB	3:A:423:HOH:O	2.46	0.56
1:A:37:LEU:O	3:A:386:HOH:O	2.18	0.56
1:C:144:PHE:CZ	3:C:444:HOH:O	2.58	0.56
2:F:464:GLN:N	3:F:303:HOH:O	2.38	0.56
1:E:53:ARG:NH2	3:E:278:HOH:O	2.36	0.56
1:A:91:ARG:NH1	3:A:432:HOH:O	2.37	0.56
2:B:460:THR:HG22	3:B:525:HOH:O	2.05	0.56
1:E:107:ASN:O	1:E:109:GLU:OE1	2.23	0.56
1:C:16:LEU:HD13	1:C:79:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:TYR:N	3:E:381:HOH:O	2.39	0.56
1:E:168:LYS:CA	3:E:367:HOH:O	2.53	0.56
1:E:107:ASN:C	3:E:342:HOH:O	2.42	0.56
1:E:43:SER:CA	3:E:364:HOH:O	2.52	0.56
1:C:210:ARG:HB3	3:C:367:HOH:O	2.05	0.56
1:C:129:PRO:HD3	3:C:359:HOH:O	2.05	0.56
2:F:457:VAL:N	3:F:540:HOH:O	2.37	0.56
1:A:208:ALA:HB2	3:B:50:HOH:O	2.05	0.56
1:C:64:ARG:HD2	1:C:94:ASP:HB3	1.88	0.56
1:C:171:ALA:O	1:C:177:ASN:HB2	2.05	0.56
1:C:194:ALA:CB	3:C:377:HOH:O	2.39	0.56
1:E:87:ILE:HG22	3:E:292:HOH:O	2.04	0.56
1:A:211:TYR:HB3	3:A:289:HOH:O	2.05	0.56
1:E:90:LEU:HD22	3:E:405:HOH:O	2.07	0.55
1:C:52:LEU:HB3	1:C:244:MET:HE1	1.88	0.55
1:A:49:GLN:CA	3:A:439:HOH:O	2.54	0.55
1:A:16:LEU:HD21	1:A:75:MET:CG	2.37	0.55
1:A:240:LYS:N	3:A:427:HOH:O	2.38	0.55
1:C:8:GLN:CA	3:C:414:HOH:O	2.55	0.55
1:E:100:ALA:HA	3:E:392:HOH:O	2.06	0.55
1:C:19:LEU:CD2	1:C:48:VAL:HG11	2.37	0.55
1:E:132:GLU:O	3:E:448:HOH:O	2.18	0.55
1:E:3:GLU:CD	3:E:368:HOH:O	2.45	0.55
1:C:141:SER:HB2	1:C:219:THR:HG23	1.89	0.55
2:B:464:GLN:CD	2:B:464:GLN:N	2.61	0.55
1:C:167:VAL:HG23	3:C:408:HOH:O	2.07	0.55
1:A:112:SER:CA	3:C:458:HOH:O	2.54	0.55
1:C:93:GLU:HB2	1:C:96:ALA:HB3	1.89	0.55
1:A:86:ASP:OD1	1:A:105:ALA:HA	2.07	0.55
1:C:53:ARG:NH2	3:C:266:HOH:O	2.37	0.55
1:A:254:LYS:HG2	2:B:456:GLN:HA	1.89	0.55
1:A:151:LEU:HD21	3:E:421:HOH:O	2.06	0.55
1:A:135:CYS:SG	1:A:199:MET:HG2	2.46	0.55
1:C:174:GLU:CG	3:C:433:HOH:O	2.55	0.55
1:A:93:GLU:HB2	1:A:96:ALA:HB3	1.89	0.55
1:E:139:MET:HG3	3:E:427:HOH:O	2.05	0.54
1:A:135:CYS:HG	1:A:162:CYS:HG	1.55	0.54
1:C:194:ALA:CA	3:C:377:HOH:O	2.54	0.54
1:E:19:LEU:CD2	1:E:48:VAL:HG11	2.38	0.54
1:E:135:CYS:HB3	3:E:347:HOH:O	2.05	0.54
1:E:99:LEU:O	3:E:392:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:GLU:N	3:C:426:HOH:O	2.40	0.54
1:A:219:THR:CA	3:A:354:HOH:O	2.44	0.54
1:C:30:ILE:CD1	1:C:35:VAL:HG22	2.37	0.54
1:A:51:THR:O	1:A:245:GLY:HA3	2.07	0.54
1:A:26:ALA:CA	3:A:394:HOH:O	2.54	0.54
1:A:49:GLN:CB	3:A:439:HOH:O	2.30	0.54
2:B:461:GLY:CA	3:B:471:HOH:O	2.56	0.54
1:E:6:LEU:HD12	3:E:378:HOH:O	2.07	0.54
2:D:463:PHE:N	3:D:254:HOH:O	2.40	0.54
1:E:139:MET:CG	3:E:427:HOH:O	2.56	0.54
1:E:229:MET:C	3:E:409:HOH:O	2.46	0.54
1:A:28:TRP:HE3	1:A:35:VAL:HG11	1.73	0.54
1:A:40:MET:HE1	1:A:44:HIS:ND1	2.23	0.54
1:E:236:VAL:HG22	3:E:420:HOH:O	2.07	0.53
1:E:229:MET:O	3:E:409:HOH:O	2.18	0.53
1:C:135:CYS:HG	1:C:162:CYS:HG	1.56	0.53
1:C:224:THR:HG21	3:C:386:HOH:O	2.08	0.53
1:C:65:ASN:N	3:C:351:HOH:O	2.38	0.53
1:E:40:MET:HE3	2:F:459:ILE:HD13	1.90	0.53
1:A:25:GLU:O	3:A:394:HOH:O	2.19	0.53
1:A:203:VAL:CG1	3:A:422:HOH:O	2.52	0.53
1:A:239:TYR:CB	3:A:427:HOH:O	2.37	0.53
1:A:1:MET:H3	1:A:63:ASP:HB2	1.72	0.53
1:E:37:LEU:CD2	3:E:404:HOH:O	2.54	0.53
1:C:82:ALA:HA	3:C:430:HOH:O	2.07	0.53
2:B:454:ASN:N	3:B:271:HOH:O	2.41	0.53
1:E:147:ILE:HG23	1:E:180:ILE:HD12	1.91	0.53
1:C:77:LYS:CD	3:C:441:HOH:O	2.55	0.53
1:E:199:MET:HG3	3:E:396:HOH:O	2.06	0.53
2:B:461:GLY:HA3	3:B:471:HOH:O	2.09	0.53
1:A:30:ILE:HG13	1:A:68:MET:CE	2.39	0.53
2:F:459:ILE:N	2:F:459:ILE:HD12	2.23	0.53
1:E:1:MET:H3	1:E:63:ASP:HB2	1.73	0.53
1:A:45:VAL:HG13	3:A:346:HOH:O	2.08	0.53
1:E:143:GLU:HB3	3:E:427:HOH:O	2.08	0.53
1:C:98:THR:HG22	3:C:276:HOH:O	2.09	0.53
1:E:108:GLN:N	3:E:342:HOH:O	2.42	0.53
1:C:40:MET:HE1	1:C:44:HIS:ND1	2.24	0.53
1:C:40:MET:HE3	2:D:459:ILE:CD1	2.39	0.53
2:D:454:ASN:CA	3:D:393:HOH:O	2.57	0.53
1:A:151:LEU:CA	3:A:437:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ASN:HA	3:C:362:HOH:O	2.09	0.53
1:A:94:ASP:CA	3:A:365:HOH:O	2.56	0.53
1:A:246:HIS:CD2	3:A:407:HOH:O	2.61	0.53
1:C:8:GLN:C	3:C:414:HOH:O	2.46	0.53
1:E:30:ILE:HG13	1:E:68:MET:CE	2.39	0.52
1:C:205:LEU:HD23	3:C:268:HOH:O	2.09	0.52
1:C:204:GLN:HG2	3:C:285:HOH:O	2.09	0.52
1:C:140:PRO:HD3	3:C:457:HOH:O	2.10	0.52
1:E:16:LEU:HD13	1:E:79:LEU:CD1	2.40	0.52
1:C:174:GLU:HG2	3:C:433:HOH:O	2.10	0.52
1:C:254:LYS:HG3	3:C:372:HOH:O	2.08	0.52
1:A:16:LEU:HD21	1:A:75:MET:HG2	1.90	0.52
1:A:170:SER:HB3	1:A:179:ASN:CB	2.34	0.52
1:C:50:LEU:C	3:C:431:HOH:O	2.48	0.52
1:E:135:CYS:HA	1:E:198:GLU:O	2.09	0.52
1:E:194:ALA:HA	3:E:318:HOH:O	2.09	0.52
1:E:168:LYS:NZ	3:E:430:HOH:O	2.43	0.52
1:C:217:LYS:HG3	3:C:387:HOH:O	2.09	0.52
1:E:94:ASP:CB	3:E:375:HOH:O	2.54	0.52
1:C:248:LYS:HE3	3:C:341:HOH:O	2.08	0.52
1:E:256:GLU:CA	3:E:374:HOH:O	2.51	0.52
1:A:196:THR:C	3:A:397:HOH:O	2.48	0.52
1:E:104:GLU:HG3	3:E:346:HOH:O	2.09	0.52
1:C:147:ILE:HG23	1:C:180:ILE:HD12	1.92	0.51
1:A:4:ALA:HB1	1:A:57:PHE:CD2	2.44	0.51
1:E:45:VAL:HG13	2:F:456:GLN:NE2	2.25	0.51
1:C:16:LEU:HD21	1:C:75:MET:CG	2.40	0.51
1:C:126:LEU:N	3:C:412:HOH:O	2.44	0.51
1:C:21:ASP:HA	3:C:322:HOH:O	2.10	0.51
1:E:107:ASN:CB	3:E:342:HOH:O	2.50	0.51
1:A:16:LEU:HD13	1:A:79:LEU:CD1	2.41	0.51
1:A:92:ALA:HA	3:A:323:HOH:O	2.10	0.51
1:A:254:LYS:NZ	3:A:315:HOH:O	2.41	0.51
1:E:85:GLU:CG	3:E:360:HOH:O	2.38	0.51
1:C:28:TRP:HE3	1:C:35:VAL:HG11	1.75	0.51
1:E:107:ASN:CA	3:E:342:HOH:O	2.58	0.51
3:C:350:HOH:O	2:D:462:PHE:CE2	2.64	0.51
1:E:16:LEU:HD21	1:E:75:MET:CG	2.41	0.51
1:C:214:PHE:N	3:C:330:HOH:O	2.43	0.51
1:E:59:THR:O	3:E:381:HOH:O	2.18	0.51
1:C:1:MET:H3	1:C:63:ASP:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:374:HOH:O	2:F:454:ASN:CB	2.59	0.51
2:D:462:PHE:C	3:D:254:HOH:O	2.49	0.51
1:A:19:LEU:CD2	1:A:48:VAL:HG11	2.41	0.51
1:E:110:LYS:HB3	3:E:348:HOH:O	2.10	0.51
1:A:200:ASN:CG	3:A:436:HOH:O	2.49	0.51
1:C:255:ILE:HD11	3:C:350:HOH:O	2.11	0.51
1:E:93:GLU:HB2	1:E:96:ALA:HB3	1.92	0.51
1:C:110:LYS:HE3	3:C:354:HOH:O	2.10	0.50
1:C:172:SER:HB3	1:C:177:ASN:CB	2.41	0.50
1:E:24:ASN:OD1	3:E:397:HOH:O	2.19	0.50
1:C:146:ARG:NE	3:C:400:HOH:O	2.44	0.50
1:E:136:VAL:N	3:E:347:HOH:O	2.44	0.50
1:A:112:SER:CB	3:C:458:HOH:O	2.56	0.50
1:C:174:GLU:CA	3:C:433:HOH:O	2.58	0.50
1:A:95:ASN:OD1	3:A:387:HOH:O	2.19	0.50
1:C:194:ALA:O	3:C:457:HOH:O	2.20	0.50
1:A:151:LEU:CD2	3:E:421:HOH:O	2.59	0.50
1:E:47:LEU:CA	3:E:401:HOH:O	2.58	0.50
1:A:107:ASN:CB	3:A:372:HOH:O	2.59	0.50
1:C:135:CYS:HA	1:C:198:GLU:O	2.10	0.50
1:A:254:LYS:HG3	3:A:428:HOH:O	2.11	0.50
1:C:226:THR:CG2	3:C:369:HOH:O	2.58	0.50
1:A:72:LEU:HD21	3:A:399:HOH:O	2.10	0.50
1:C:180:ILE:N	3:C:362:HOH:O	2.43	0.50
1:A:40:MET:HE2	1:A:44:HIS:CG	2.47	0.50
1:E:168:LYS:N	3:E:367:HOH:O	2.45	0.50
1:C:161:SER:C	3:C:408:HOH:O	2.49	0.50
1:C:86:ASP:OD1	1:C:105:ALA:HA	2.11	0.50
1:E:170:SER:HB3	1:E:179:ASN:CB	2.33	0.50
1:A:149:ARG:HH11	1:A:149:ARG:HG2	1.76	0.50
1:C:45:VAL:HG13	2:D:456:GLN:NE2	2.26	0.49
1:A:45:VAL:CG1	3:A:346:HOH:O	2.59	0.49
1:C:8:GLN:HB2	3:C:414:HOH:O	2.11	0.49
1:C:119:MET:CE	3:C:337:HOH:O	2.56	0.49
1:A:49:GLN:HA	3:A:386:HOH:O	2.12	0.49
1:E:143:GLU:O	1:E:147:ILE:HG13	2.12	0.49
2:F:462:PHE:C	2:F:463:PHE:HD2	2.16	0.49
1:E:52:LEU:HB3	1:E:244:MET:CE	2.42	0.49
1:C:70:VAL:CG1	3:C:405:HOH:O	2.41	0.49
1:E:228:SER:HB2	1:E:236:VAL:HB	1.94	0.49
1:A:207:PHE:CA	3:A:428:HOH:O	2.54	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:VAL:CG2	3:E:385:HOH:O	2.43	0.49
1:A:28:TRP:CE3	1:A:35:VAL:HG11	2.47	0.49
1:E:141:SER:HB2	1:E:219:THR:HG23	1.93	0.49
1:C:143:GLU:O	1:C:147:ILE:HG13	2.12	0.49
1:A:40:MET:CG	3:A:383:HOH:O	2.59	0.49
1:C:139:MET:HA	3:C:457:HOH:O	2.11	0.49
1:E:131:GLN:N	3:E:399:HOH:O	2.44	0.49
1:E:94:ASP:HA	3:E:375:HOH:O	2.10	0.49
1:C:40:MET:HE2	1:C:44:HIS:CG	2.48	0.49
1:C:5:ARG:HB3	3:C:328:HOH:O	2.11	0.49
1:E:12:LEU:HA	3:E:344:HOH:O	2.13	0.49
1:A:77:LYS:NZ	3:A:350:HOH:O	2.45	0.48
3:A:366:HOH:O	2:B:463:PHE:HD1	1.96	0.48
1:E:166:GLY:HA2	1:E:197:ILE:CD1	2.43	0.48
1:A:40:MET:HE3	2:B:459:ILE:CD1	2.43	0.48
1:A:103:PHE:CG	3:A:412:HOH:O	2.61	0.48
1:E:172:SER:HB3	1:E:177:ASN:CB	2.43	0.48
1:C:107:ASN:O	1:C:109:GLU:OE1	2.32	0.48
1:E:30:ILE:CD1	1:E:35:VAL:HG22	2.43	0.48
1:C:38:GLN:HA	1:C:48:VAL:O	2.14	0.48
1:E:149:ARG:HG2	1:E:149:ARG:HH11	1.79	0.48
1:C:255:ILE:HG23	3:C:286:HOH:O	2.13	0.48
1:E:28:TRP:CE3	1:E:35:VAL:HG11	2.46	0.48
1:E:225:VAL:CG1	3:E:385:HOH:O	2.52	0.48
1:A:172:SER:HB3	1:A:177:ASN:CB	2.42	0.48
1:A:87:ILE:HG13	3:A:417:HOH:O	2.13	0.48
1:C:153:HIS:CD2	3:C:298:HOH:O	2.66	0.48
1:A:30:ILE:CD1	1:A:35:VAL:HG22	2.43	0.48
1:C:21:ASP:HB2	3:C:277:HOH:O	2.13	0.48
1:C:166:GLY:HA2	1:C:197:ILE:HD12	1.96	0.48
1:C:7:VAL:HG13	3:C:420:HOH:O	2.14	0.48
1:C:144:PHE:CD2	3:C:444:HOH:O	2.66	0.47
1:C:28:TRP:CE3	1:C:35:VAL:HG11	2.49	0.47
2:B:457:VAL:HG11	2:B:462:PHE:HE1	1.79	0.47
1:C:124:GLU:N	3:C:435:HOH:O	2.33	0.47
1:E:168:LYS:HD3	3:E:430:HOH:O	2.11	0.47
1:A:68:MET:O	1:A:70:VAL:HG23	2.14	0.47
1:E:203:VAL:HG12	1:E:204:GLN:N	2.28	0.47
1:E:63:ASP:O	3:E:444:HOH:O	2.20	0.47
1:E:254:LYS:HG2	2:F:456:GLN:CA	2.44	0.47
1:A:23:ILE:HG21	3:A:394:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:LEU:HD21	1:C:75:MET:HG2	1.97	0.47
1:A:225:VAL:C	3:A:358:HOH:O	2.51	0.47
1:E:207:PHE:CZ	1:E:235:LEU:HB2	2.49	0.47
1:A:135:CYS:HA	1:A:198:GLU:O	2.14	0.47
1:C:64:ARG:HB3	1:C:94:ASP:OD1	2.15	0.47
1:C:241:ILE:O	1:C:244:MET:HB2	2.15	0.47
1:A:73:THR:CA	3:A:402:HOH:O	2.34	0.47
1:E:16:LEU:HD21	1:E:75:MET:HG2	1.97	0.47
1:E:196:THR:HA	3:E:355:HOH:O	2.14	0.47
1:E:234:PRO:HD3	2:F:462:PHE:CD2	2.50	0.47
1:E:124:GLU:OE2	2:F:465:ARG:NH1	2.48	0.47
1:C:172:SER:CB	1:C:177:ASN:HB3	2.44	0.47
1:A:129:PRO:HD3	2:B:463:PHE:CG	2.49	0.47
1:C:24:ASN:CA	3:C:374:HOH:O	2.61	0.47
1:C:24:ASN:C	3:C:374:HOH:O	2.53	0.47
1:C:4:ALA:HB1	1:C:57:PHE:CD2	2.50	0.47
1:E:240:LYS:NZ	3:E:278:HOH:O	2.45	0.47
1:E:236:VAL:CA	3:E:420:HOH:O	2.20	0.47
1:A:95:ASN:HB2	3:A:297:HOH:O	2.13	0.47
1:E:175:LEU:O	1:E:175:LEU:HD12	2.15	0.47
2:F:457:VAL:C	3:F:540:HOH:O	2.54	0.46
1:C:44:HIS:C	2:D:459:ILE:HD11	2.35	0.46
1:C:110:LYS:HE3	1:E:180:ILE:HG21	1.96	0.46
1:C:144:PHE:CE2	3:C:444:HOH:O	2.67	0.46
1:A:64:ARG:C	3:A:359:HOH:O	2.54	0.46
1:A:152:SER:N	3:A:437:HOH:O	2.44	0.46
1:A:166:GLY:HA2	1:A:197:ILE:CD1	2.45	0.46
1:E:166:GLY:HA2	1:E:197:ILE:HD12	1.97	0.46
1:A:26:ALA:HB2	3:A:394:HOH:O	2.15	0.46
1:E:110:LYS:HG2	3:E:314:HOH:O	2.15	0.46
1:C:24:ASN:CB	3:C:374:HOH:O	2.36	0.46
1:E:5:ARG:HD3	3:E:341:HOH:O	2.15	0.46
1:C:27:CYS:SG	3:C:449:HOH:O	2.61	0.46
1:C:153:HIS:HB3	3:C:347:HOH:O	2.03	0.46
1:C:41:ASP:OD2	1:C:43:SER:HB2	2.15	0.46
1:A:211:TYR:HD2	3:A:289:HOH:O	1.97	0.46
1:C:104:GLU:CA	3:C:380:HOH:O	2.64	0.46
1:E:248:LYS:NZ	3:E:408:HOH:O	2.46	0.46
1:E:74:SER:N	3:E:395:HOH:O	2.48	0.46
1:C:200:ASN:HB2	3:C:274:HOH:O	2.16	0.46
1:C:207:PHE:CZ	1:C:235:LEU:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:LYS:NZ	3:C:335:HOH:O	2.44	0.46
1:C:170:SER:HB3	1:C:179:ASN:CB	2.34	0.46
1:A:110:LYS:HE3	1:C:180:ILE:HG21	1.97	0.45
1:A:166:GLY:HA2	1:A:197:ILE:HD12	1.98	0.45
2:F:465:ARG:HG2	2:F:465:ARG:NH1	2.28	0.45
1:E:40:MET:HE3	2:F:459:ILE:CD1	2.46	0.45
1:E:40:MET:HE2	1:E:44:HIS:CG	2.51	0.45
1:A:19:LEU:N	3:A:435:HOH:O	2.45	0.45
1:C:128:ILE:HA	1:C:129:PRO:HD3	1.85	0.45
1:A:82:ALA:HA	3:A:412:HOH:O	2.17	0.45
1:A:206:THR:OG1	2:B:453:ALA:HB2	2.16	0.45
1:E:149:ARG:O	1:E:152:SER:HB2	2.16	0.45
1:E:38:GLN:HA	1:E:48:VAL:O	2.17	0.45
1:E:170:SER:CB	3:E:387:HOH:O	2.64	0.45
1:A:127:GLY:N	3:A:366:HOH:O	2.49	0.45
1:E:241:ILE:HG22	1:E:244:MET:HB2	1.99	0.45
1:A:52:LEU:HB3	1:A:244:MET:CE	2.46	0.45
1:C:125:GLN:C	3:C:412:HOH:O	2.55	0.45
1:C:166:GLY:HA2	1:C:197:ILE:CD1	2.46	0.45
1:C:149:ARG:NH1	3:C:456:HOH:O	2.48	0.45
1:E:246:HIS:HD2	1:E:248:LYS:HG3	1.81	0.45
1:A:64:ARG:HD2	1:A:94:ASP:HB3	1.99	0.45
1:C:135:CYS:HB3	1:C:162:CYS:HG	1.81	0.45
1:A:45:VAL:HG13	2:B:456:GLN:NE2	2.32	0.45
1:E:138:LYS:CA	3:E:426:HOH:O	2.63	0.45
1:C:61:ARG:NH1	3:C:396:HOH:O	2.49	0.45
1:C:244:MET:HE2	1:C:244:MET:HB3	1.52	0.45
1:E:71:ASN:ND2	3:E:395:HOH:O	2.50	0.45
1:E:73:THR:CA	3:E:406:HOH:O	2.39	0.45
1:C:255:ILE:HD13	2:D:457:VAL:CG2	2.45	0.45
1:C:217:LYS:CG	3:C:387:HOH:O	2.64	0.45
1:C:67:ALA:HA	3:C:449:HOH:O	2.16	0.45
1:C:235:LEU:HA	3:C:315:HOH:O	2.17	0.44
1:E:26:ALA:HB3	3:E:353:HOH:O	2.16	0.44
1:C:91:ARG:CD	3:C:397:HOH:O	2.52	0.44
1:C:213:ASN:C	3:C:330:HOH:O	2.55	0.44
1:E:176:GLY:CA	3:E:379:HOH:O	2.64	0.44
1:E:12:LEU:CB	3:E:344:HOH:O	2.66	0.44
1:C:52:LEU:HD22	1:C:244:MET:HE1	1.99	0.44
1:C:217:LYS:CD	3:C:387:HOH:O	2.65	0.44
1:A:246:HIS:HD2	1:A:248:LYS:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASP:OD2	1:A:43:SER:HB2	2.17	0.44
1:E:105:ALA:O	3:E:383:HOH:O	2.21	0.44
1:A:205:LEU:HD11	1:A:230:SER:O	2.18	0.44
1:C:158:VAL:HB	1:C:209:LEU:HD21	1.99	0.44
1:E:255:ILE:HD13	2:F:457:VAL:CG2	2.44	0.44
1:C:64:ARG:CG	3:C:351:HOH:O	2.54	0.44
1:A:16:LEU:CD2	1:A:75:MET:HG2	2.48	0.44
1:A:226:THR:HG21	3:A:410:HOH:O	2.17	0.44
1:E:7:VAL:HG13	3:E:354:HOH:O	2.16	0.44
1:C:254:LYS:HB3	3:D:393:HOH:O	2.17	0.44
1:E:246:HIS:CD2	1:E:248:LYS:HG3	2.53	0.44
1:A:140:PRO:HG3	1:A:192:GLU:O	2.17	0.44
1:C:45:VAL:HG12	1:C:251:LEU:HD12	2.00	0.44
1:C:135:CYS:CB	1:C:162:CYS:HG	2.30	0.44
1:A:46:SER:HB2	1:A:250:TYR:O	2.18	0.44
1:C:140:PRO:CD	3:C:457:HOH:O	2.65	0.44
1:A:26:ALA:CB	3:A:394:HOH:O	2.66	0.44
1:A:228:SER:HB2	1:A:236:VAL:HB	1.98	0.44
1:C:84:ASN:ND2	3:C:269:HOH:O	2.50	0.44
1:C:25:GLU:HG3	3:C:361:HOH:O	2.17	0.43
1:E:176:GLY:N	3:E:379:HOH:O	2.49	0.43
1:A:72:LEU:CD2	3:A:399:HOH:O	2.65	0.43
1:A:21:ASP:HB2	3:A:388:HOH:O	2.17	0.43
1:A:158:VAL:HB	1:A:209:LEU:HD21	1.99	0.43
1:C:63:ASP:CG	3:C:396:HOH:O	2.56	0.43
1:A:65:ASN:HB3	3:A:426:HOH:O	2.18	0.43
1:C:115:GLU:HG2	3:C:376:HOH:O	2.18	0.43
1:A:38:GLN:HA	1:A:48:VAL:O	2.18	0.43
1:C:128:ILE:HG22	2:D:463:PHE:CE2	2.53	0.43
2:D:453:ALA:C	3:D:393:HOH:O	2.53	0.43
1:A:16:LEU:HD21	1:A:75:MET:SD	2.59	0.43
1:A:197:ILE:CG2	3:A:396:HOH:O	2.47	0.43
1:A:48:VAL:CG1	3:A:404:HOH:O	2.50	0.43
1:A:146:ARG:HD3	1:A:149:ARG:NH2	2.33	0.43
1:A:246:HIS:CD2	1:A:248:LYS:HG3	2.53	0.43
1:A:172:SER:CB	1:A:177:ASN:HB3	2.48	0.43
1:E:108:GLN:HG3	1:E:108:GLN:O	2.18	0.43
1:C:16:LEU:HD21	1:C:75:MET:SD	2.59	0.43
1:E:99:LEU:HD12	1:E:100:ALA:H	1.83	0.43
1:C:52:LEU:HB3	1:C:244:MET:CE	2.48	0.43
1:E:203:VAL:CG1	1:E:204:GLN:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:CA	3:A:343:HOH:O	2.28	0.43
1:E:105:ALA:O	1:E:106:PRO:C	2.57	0.43
1:A:16:LEU:CD2	1:A:79:LEU:HD12	2.28	0.43
1:E:244:MET:HE2	1:E:244:MET:HB3	1.48	0.43
1:C:60:TYR:O	1:C:61:ARG:HB2	2.19	0.43
1:A:225:VAL:HG13	3:A:406:HOH:O	2.19	0.43
1:C:131:GLN:CB	3:C:426:HOH:O	2.35	0.43
1:A:110:LYS:HA	1:C:181:LYS:O	2.18	0.43
1:C:11:ILE:HG12	3:C:388:HOH:O	2.12	0.43
1:E:229:MET:HB2	3:E:409:HOH:O	2.18	0.43
1:A:115:GLU:HG3	3:C:390:HOH:O	2.19	0.43
1:E:1:MET:N	1:E:94:ASP:OD2	2.50	0.43
1:A:207:PHE:CZ	1:A:235:LEU:HB2	2.54	0.43
1:C:160:ILE:CG2	3:C:408:HOH:O	2.51	0.43
1:A:219:THR:N	1:A:220:PRO:HD2	2.33	0.43
1:C:47:LEU:N	3:C:429:HOH:O	2.42	0.43
1:A:181:LYS:CA	3:A:393:HOH:O	2.67	0.42
1:C:210:ARG:CB	3:C:367:HOH:O	2.65	0.42
1:E:64:ARG:HD2	3:E:375:HOH:O	2.18	0.42
1:C:253:PRO:O	3:C:372:HOH:O	2.20	0.42
1:E:135:CYS:SG	1:E:199:MET:HG2	2.59	0.42
1:A:112:SER:HA	3:C:458:HOH:O	2.19	0.42
1:C:219:THR:N	1:C:220:PRO:HD2	2.34	0.42
1:C:129:PRO:HD2	3:C:309:HOH:O	2.18	0.42
1:A:5:ARG:CB	1:A:59:THR:HB	2.42	0.42
1:A:137:VAL:O	1:A:226:THR:HA	2.18	0.42
1:A:241:ILE:O	1:A:244:MET:HB2	2.19	0.42
1:A:107:ASN:O	1:A:108:GLN:CB	2.66	0.42
1:E:64:ARG:HB3	1:E:94:ASP:OD1	2.19	0.42
1:C:223:SER:HB3	3:C:338:HOH:O	2.19	0.42
1:C:228:SER:HB2	1:C:236:VAL:HB	2.00	0.42
1:A:208:ALA:N	3:A:428:HOH:O	2.53	0.42
1:E:5:ARG:CB	1:E:59:THR:HB	2.42	0.42
1:C:246:HIS:CD2	1:C:248:LYS:HG3	2.55	0.42
1:C:24:ASN:HB3	3:C:361:HOH:O	2.19	0.42
1:A:199:MET:CE	1:A:202:PRO:HG3	2.50	0.42
1:C:203:VAL:HG12	1:C:204:GLN:N	2.33	0.42
1:E:116:MET:HG3	3:E:290:HOH:O	2.18	0.42
1:A:125:GLN:NE2	3:A:331:HOH:O	2.53	0.42
1:E:172:SER:CB	1:E:177:ASN:HB3	2.47	0.42
1:C:110:LYS:HA	1:E:181:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:PHE:CB	3:C:430:HOH:O	2.67	0.42
1:C:217:LYS:HD2	3:C:387:HOH:O	2.20	0.42
1:A:25:GLU:HG3	3:A:352:HOH:O	2.19	0.42
1:E:201:GLU:HG2	3:E:388:HOH:O	2.18	0.42
1:A:12:LEU:HD12	1:A:12:LEU:HA	1.83	0.42
1:A:64:ARG:HB3	1:A:94:ASP:OD1	2.19	0.42
1:C:160:ILE:C	3:C:408:HOH:O	2.58	0.42
1:A:203:VAL:CG1	1:A:204:GLN:N	2.83	0.42
1:E:106:PRO:HD2	3:E:350:HOH:O	2.19	0.42
2:D:454:ASN:HD22	2:D:454:ASN:C	2.22	0.42
1:A:248:LYS:HB3	3:A:409:HOH:O	2.20	0.42
1:A:1:MET:N	1:A:94:ASP:OD2	2.49	0.42
1:C:149:ARG:HD3	3:C:427:HOH:O	2.19	0.42
1:A:96:ALA:HB1	1:A:98:THR:HG23	2.02	0.42
1:E:106:PRO:CB	3:E:350:HOH:O	2.57	0.41
1:E:112:SER:HB3	1:E:114:TYR:HE1	1.86	0.41
1:E:168:LYS:HD2	3:E:430:HOH:O	2.17	0.41
1:A:17:GLU:HA	1:A:17:GLU:OE1	2.19	0.41
1:C:194:ALA:C	3:C:377:HOH:O	2.59	0.41
1:E:169:PHE:CE1	3:E:367:HOH:O	2.73	0.41
1:A:87:ILE:HG22	3:A:330:HOH:O	2.19	0.41
2:F:458:SER:HB3	3:F:517:HOH:O	2.20	0.41
1:A:11:ILE:O	1:A:15:VAL:HG23	2.21	0.41
1:A:40:MET:N	3:A:383:HOH:O	2.38	0.41
1:E:114:TYR:C	3:E:340:HOH:O	2.54	0.41
1:A:219:THR:C	3:A:354:HOH:O	2.59	0.41
1:C:46:SER:HB2	3:C:429:HOH:O	2.20	0.41
1:E:12:LEU:HD13	3:E:344:HOH:O	2.19	0.41
1:E:68:MET:O	1:E:70:VAL:HG23	2.21	0.41
1:A:254:LYS:CB	3:B:271:HOH:O	2.61	0.41
1:E:144:PHE:N	3:E:427:HOH:O	2.53	0.41
1:C:103:PHE:CD2	3:C:430:HOH:O	2.57	0.41
1:E:128:ILE:HA	1:E:129:PRO:HD3	1.83	0.41
1:A:164:LYS:HG2	3:A:328:HOH:O	2.21	0.41
1:A:203:VAL:HG12	1:A:204:GLN:N	2.36	0.41
1:C:131:GLN:CG	3:C:426:HOH:O	2.68	0.41
1:C:16:LEU:CD2	1:C:75:MET:HG2	2.50	0.41
1:C:17:GLU:HA	1:C:17:GLU:OE1	2.20	0.41
1:E:1:MET:HB3	1:E:63:ASP:OD2	2.21	0.41
2:D:459:ILE:H	2:D:459:ILE:HD12	1.85	0.41
1:A:64:ARG:NH1	3:A:365:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:C	2:B:459:ILE:HD11	2.40	0.41
1:A:23:ILE:CG2	3:A:394:HOH:O	2.69	0.41
1:C:131:GLN:CB	3:C:373:HOH:O	2.43	0.41
1:E:115:GLU:HG2	3:E:340:HOH:O	2.21	0.41
1:A:62:CYS:C	3:A:359:HOH:O	2.58	0.41
1:E:169:PHE:CD1	3:E:367:HOH:O	2.57	0.41
1:C:3:GLU:HB2	3:C:399:HOH:O	2.21	0.41
1:A:244:MET:HE2	1:A:244:MET:HB3	1.53	0.41
1:C:52:LEU:HD22	1:C:244:MET:CE	2.51	0.41
1:C:248:LYS:CE	3:C:341:HOH:O	2.68	0.41
1:C:203:VAL:HA	3:C:384:HOH:O	2.21	0.41
1:E:218:ALA:O	1:E:221:LEU:HB2	2.21	0.41
1:C:256:GLU:HA	3:C:385:HOH:O	2.20	0.40
1:C:45:VAL:C	2:D:459:ILE:HG13	2.41	0.40
1:E:226:THR:N	3:E:385:HOH:O	2.54	0.40
1:E:196:THR:N	3:E:434:HOH:O	2.54	0.40
2:F:463:PHE:C	3:F:303:HOH:O	2.60	0.40
1:C:205:LEU:CD2	3:C:391:HOH:O	2.68	0.40
1:A:129:PRO:CG	2:B:463:PHE:HB3	2.51	0.40
1:E:12:LEU:HB2	3:E:344:HOH:O	2.21	0.40
1:E:219:THR:N	1:E:220:PRO:HD2	2.35	0.40
1:A:126:LEU:CD2	2:B:464:GLN:HA	2.52	0.40
1:E:149:ARG:C	3:E:433:HOH:O	2.56	0.40
1:E:112:SER:HB3	1:E:114:TYR:CE1	2.56	0.40
1:E:202:PRO:CG	3:E:366:HOH:O	2.63	0.40
1:A:255:ILE:CG2	1:A:256:GLU:N	2.84	0.40
1:A:185:THR:OG1	1:A:194:ALA:HB1	2.21	0.40
1:E:23:ILE:C	3:E:397:HOH:O	2.60	0.40
1:C:49:GLN:O	3:C:431:HOH:O	2.22	0.40
1:E:71:ASN:C	1:E:71:ASN:HD22	2.23	0.40
1:C:254:LYS:N	3:C:372:HOH:O	2.53	0.40
1:A:207:PHE:C	3:A:428:HOH:O	2.59	0.40
2:F:465:ARG:NH1	2:F:465:ARG:CG	2.85	0.40
1:A:164:LYS:CG	3:A:328:HOH:O	2.69	0.40

All (2) 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:8:GLN:NE2	1:E:8:GLN:NE2[5_674]	1.61	0.59
3:E:315:HOH:O	3:E:360:HOH:O[5_674]	2.17	0.03

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	249/261 (95%)	226 (91%)	21 (8%)	2 (1%)	24 46
1	C	245/261 (94%)	226 (92%)	15 (6%)	4 (2%)	12 24
1	E	249/261 (95%)	228 (92%)	17 (7%)	4 (2%)	12 24
2	B	10/15 (67%)	9 (90%)	0	1 (10%)	1 0
2	D	11/15 (73%)	10 (91%)	1 (9%)	0	100 100
2	F	11/15 (73%)	10 (91%)	0	1 (9%)	1 1
All	All	775/828 (94%)	709 (92%)	54 (7%)	12 (2%)	13 26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	ALA
1	C	242	ALA
1	E	242	ALA
2	F	454	ASN
1	A	59	THR
1	C	59	THR
1	C	61	ARG
2	B	454	ASN
1	E	106	PRO
1	C	243	ASP
1	E	59	THR
1	E	243	ASP

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	217/228 (95%)	211 (97%)	6 (3%)	51 78
1	C	216/228 (95%)	211 (98%)	5 (2%)	58 83
1	E	217/228 (95%)	212 (98%)	5 (2%)	58 83
2	B	10/13 (77%)	8 (80%)	2 (20%)	1 2
2	D	11/13 (85%)	9 (82%)	2 (18%)	2 3
2	F	11/13 (85%)	9 (82%)	2 (18%)	2 3
All	All	682/723 (94%)	660 (97%)	22 (3%)	46 74

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	85	GLU
1	A	98	THR
1	A	192	GLU
1	A	224	THR
1	A	235	LEU
2	B	454	ASN
2	B	459	ILE
1	C	71	ASN
1	C	85	GLU
1	C	98	THR
1	C	224	THR
1	C	235	LEU
2	D	454	ASN
2	D	459	ILE
1	E	71	ASN
1	E	85	GLU
1	E	98	THR
1	E	107	ASN
1	E	224	THR
2	F	459	ILE
2	F	465	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN

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Mol	Chain	Res	Type
1	A	65	ASN
1	A	71	ASN
2	B	454	ASN
2	B	464	GLN
1	C	38	GLN
1	C	65	ASN
1	C	71	ASN
1	C	184	GLN
2	D	454	ASN
1	E	38	GLN
1	E	65	ASN
1	E	71	ASN
1	E	107	ASN
1	E	184	GLN
2	F	464	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	253/261 (96%)	0.19	18 (7%) 19 13	33, 59, 100, 122	0
1	C	251/261 (96%)	0.19	15 (5%) 25 18	35, 58, 99, 124	0
1	E	253/261 (96%)	0.22	22 (8%) 13 8	35, 59, 100, 122	0
2	B	12/15 (80%)	1.10	4 (33%) 0 0	41, 66, 90, 99	0
2	D	13/15 (86%)	0.98	3 (23%) 1 0	40, 60, 101, 109	0
2	F	13/15 (86%)	1.06	3 (23%) 1 0	41, 58, 109, 118	0
All	All	795/828 (96%)	0.24	65 (8%) 14 10	33, 59, 100, 124	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	185	THR	7.8
2	F	464	GLN	5.8
1	A	191	GLU	5.7
1	C	191	GLU	5.4
2	B	453	ALA	5.4
2	F	453	ALA	5.0
2	D	465	ARG	5.0
1	A	95	ASN	4.9
1	E	186	SER	4.8
1	C	120	ASP	4.7
1	A	164	LYS	4.7
1	A	192	GLU	4.2
1	C	121	LEU	3.9
2	D	453	ALA	3.9
1	C	185	THR	3.7
1	C	194	ALA	3.6
2	F	465	ARG	3.5
1	E	259	GLU	3.5
2	B	464	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	95	ASN	3.3
1	E	122	ASP	3.2
1	C	174	GLU	3.1
1	C	122	ASP	3.1
1	E	196	THR	3.0
1	A	124	GLU	3.0
1	C	123	VAL	3.0
1	A	64	ARG	3.0
1	E	163	ALA	2.9
1	E	166	GLY	2.8
1	A	96	ALA	2.8
1	C	199	MET	2.8
1	A	97	ASP	2.8
1	E	120	ASP	2.8
1	E	193	GLU	2.8
2	D	464	GLN	2.8
1	A	165	ASP	2.7
1	E	109	GLU	2.7
1	E	55	GLU	2.6
1	A	186	SER	2.6
2	B	461	GLY	2.6
1	C	63	ASP	2.6
1	A	122	ASP	2.6
1	C	193	GLU	2.6
1	E	258	GLU	2.5
1	C	64	ARG	2.5
1	A	132	GLU	2.4
1	E	108	GLN	2.4
1	E	165	ASP	2.4
1	A	63	ASP	2.3
1	C	132	GLU	2.3
1	C	175	LEU	2.3
1	E	132	GLU	2.2
2	B	463	PHE	2.2
1	E	59	THR	2.2
1	A	173	GLY	2.2
1	E	124	GLU	2.2
1	A	120	ASP	2.2
1	A	94	ASP	2.2
1	A	121	LEU	2.2
1	A	193	GLU	2.2
1	E	212	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	61	ARG	2.1
1	C	255	ILE	2.1
1	E	63	ASP	2.1
1	E	94	ASP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.