Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:05 PM GMT

PDB ID	:	1N6F
Title	:	tricorn protease in complex with Z-Phe-diketo-Arg-Glu-Phe
Authors	:	Kim, J.-S.; Groll, M.; Huber, R.; Brandstetter, H.
Deposited on	:	2002-11-10
Resolution	:	2.70 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:

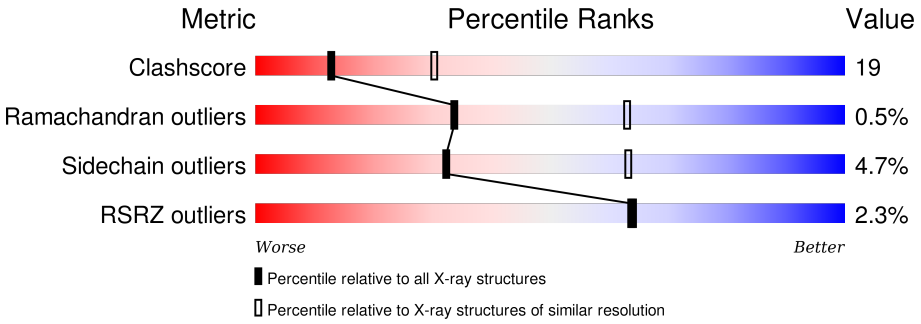
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	1071	% 65% 27%
1	B	1071	% 65% 28%
1	C	1071	4% 59% 33%
1	D	1071	% 62% 30%
1	E	1071	% 64% 29%
1	F	1071	4% 61% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DKT	A	1214	X	-	-	X
2	DKT	B	1214	X	-	-	X
2	DKT	C	1214	X	-	-	X
2	DKT	D	1214	X	-	-	X
2	DKT	E	1214	X	-	-	X
2	DKT	F	1214	X	-	-	X

2 Entry composition

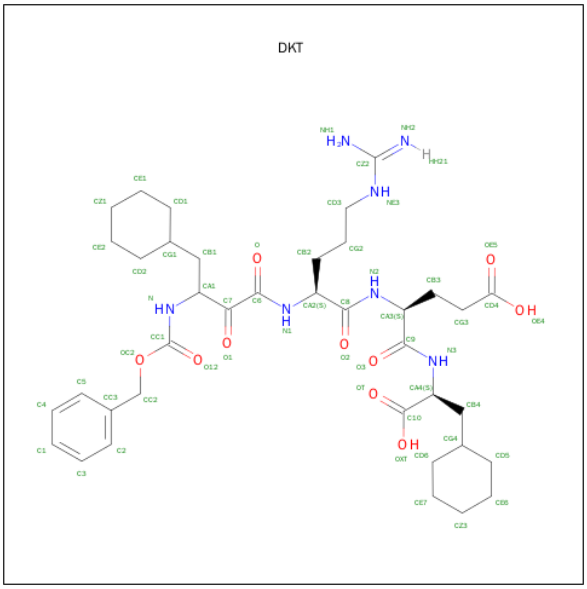
There are 3 unique types of molecules in this entry. The entry contains 50087 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 tricorn protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	B	1023	Total	C	N	O	S	94	0	0
			8176	5196	1402	1550	28			
1	C	1023	Total	C	N	O	S	94	0	0
			8176	5196	1402	1550	28			
1	D	1023	Total	C	N	O	S	94	0	0
			8176	5196	1402	1550	28			
1	E	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	F	1023	Total	C	N	O	S	94	0	0
			8176	5196	1402	1550	28			

- Molecule 2 is 4-[2-(3-BENZYLOXYCARBONYLAMINO-4-CYCLOHEXYL-1-HYDROXY-2-OXO-BUTYLAMINO)-5-GUANIDINO-PENTANOYLAMINO]-4-(1-CARBOXY-2-CYCLOHEXYL-ETHYLCARBAMOYL)-BUTYRIC ACID (three-letter code: DKT) (formula: $C_{38}H_{57}N_7O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			55	38	7	10		
2	B	1	Total	C	N	O	0	0
			55	38	7	10		
2	C	1	Total	C	N	O	0	0
			55	38	7	10		
2	D	1	Total	C	N	O	0	0
			55	38	7	10		
2	E	1	Total	C	N	O	0	0
			55	38	7	10		
2	F	1	Total	C	N	O	0	0
			55	38	7	10		

- Molecule 3 is water.

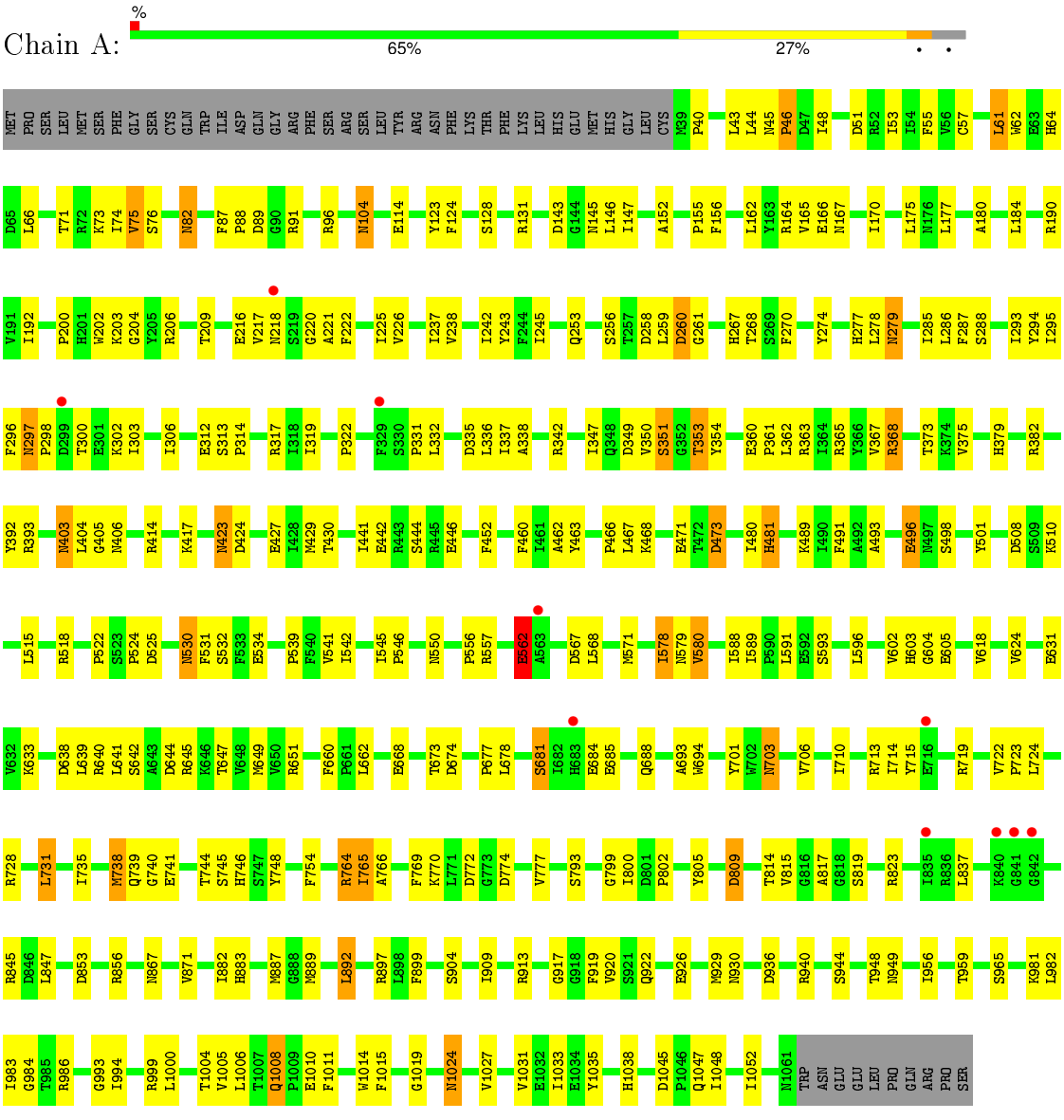
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total	O	0	0
			114	114		
3	B	108	Total	O	0	0
			108	108		
3	C	136	Total	O	0	0
			136	136		
3	D	132	Total	O	0	0
			132	132		
3	E	105	Total	O	0	0
			105	105		
3	F	104	Total	O	0	0
			104	104		

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.

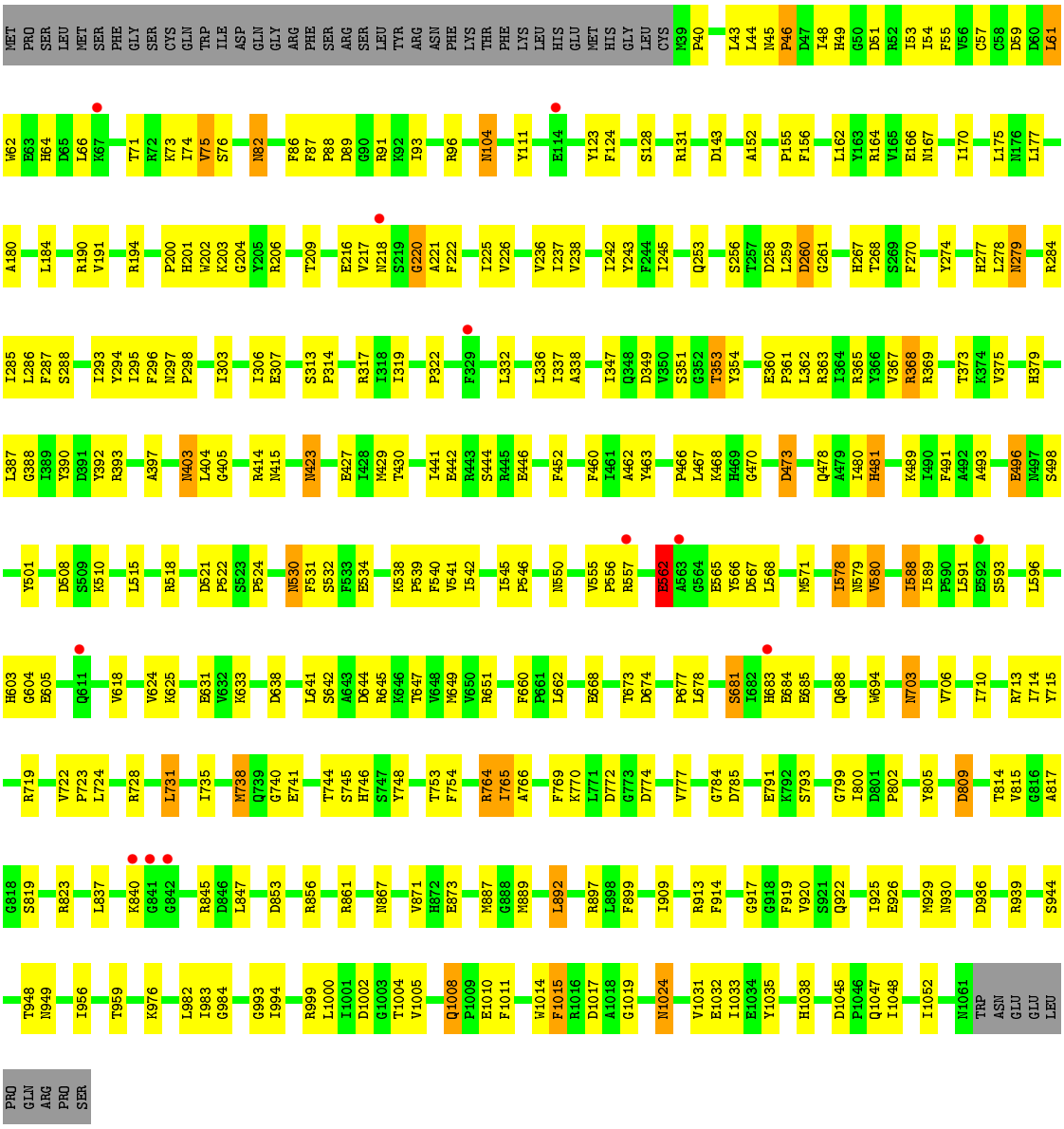
- Molecule 1: tricorn protease

Chain A:



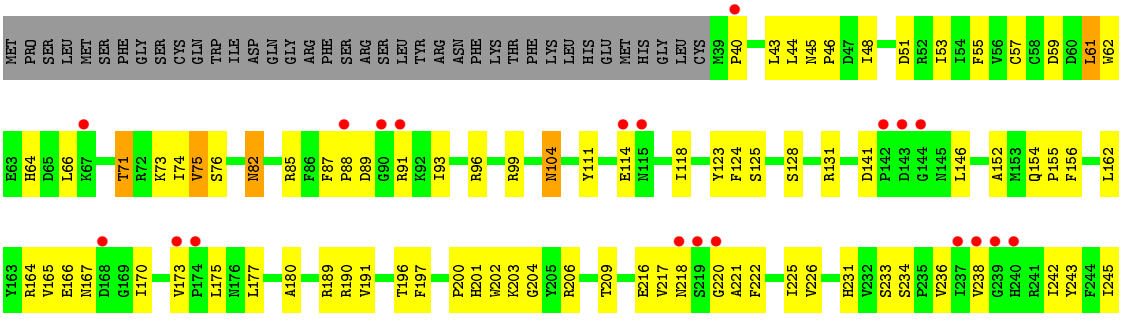
- Molecule 1: tricorn protease

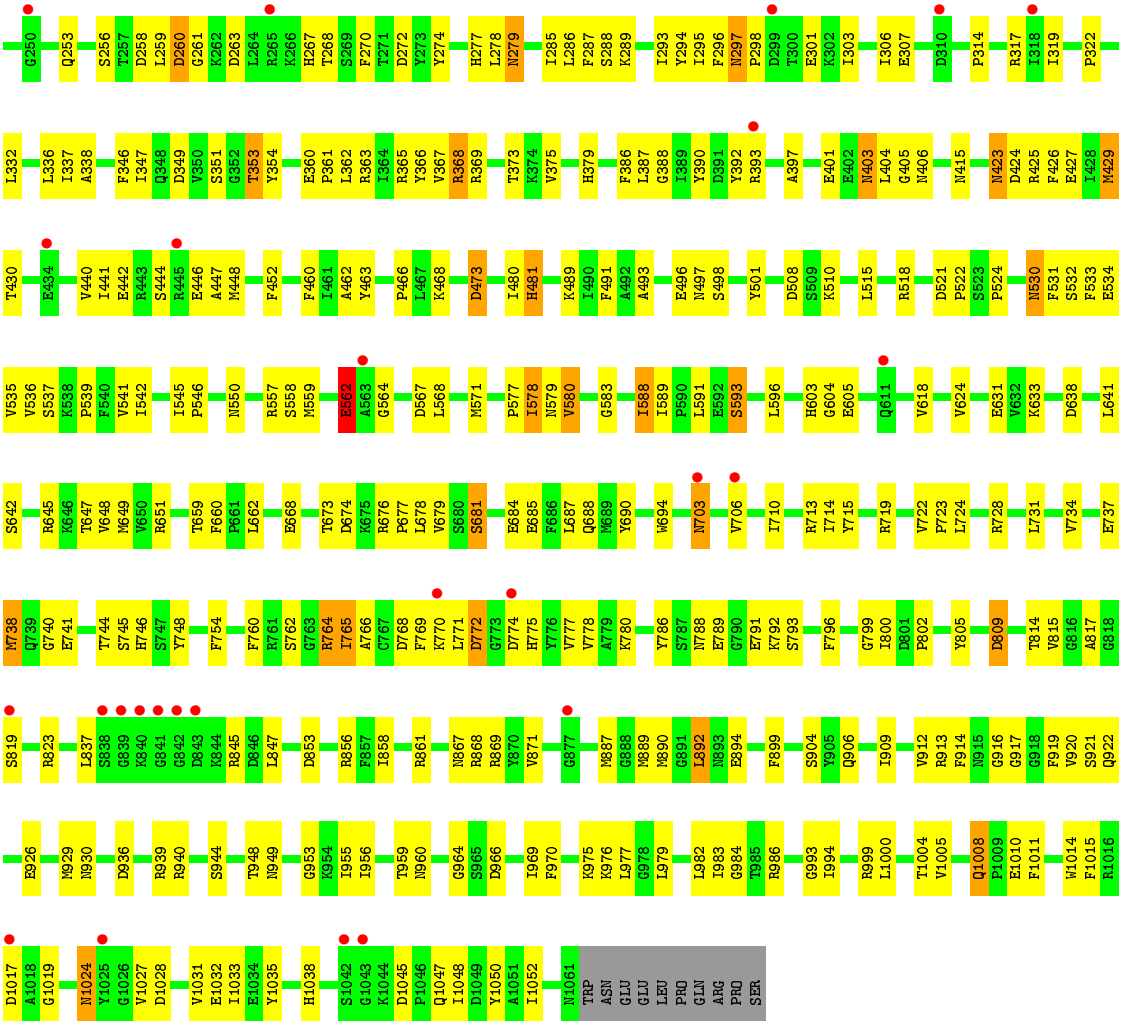
Chain B:



• Molecule 1: tricorn protease

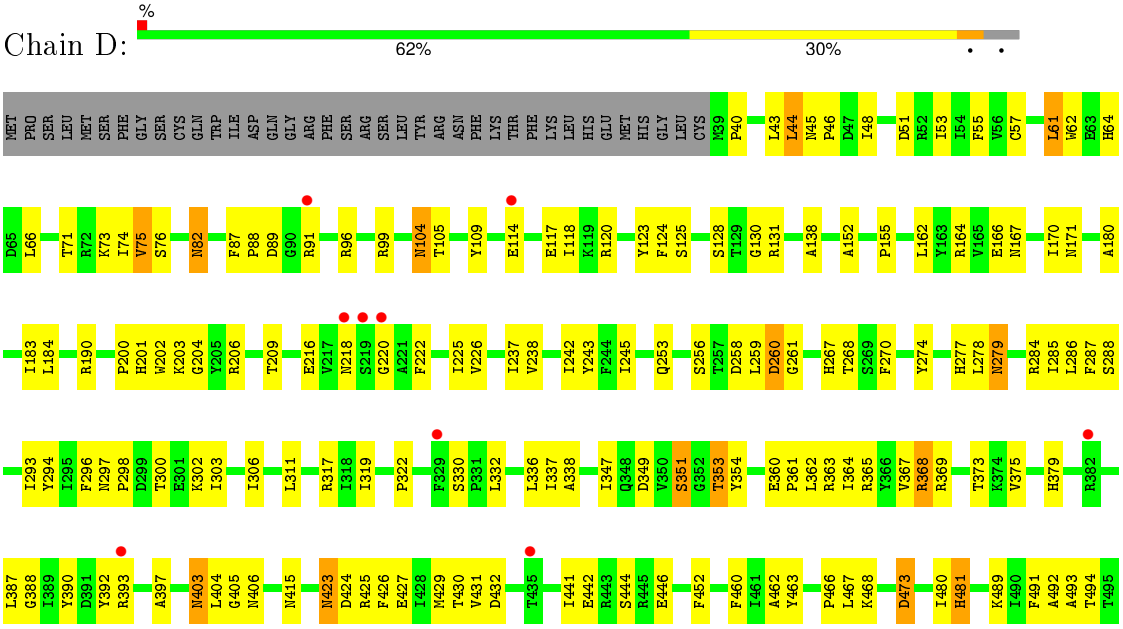
Chain C:

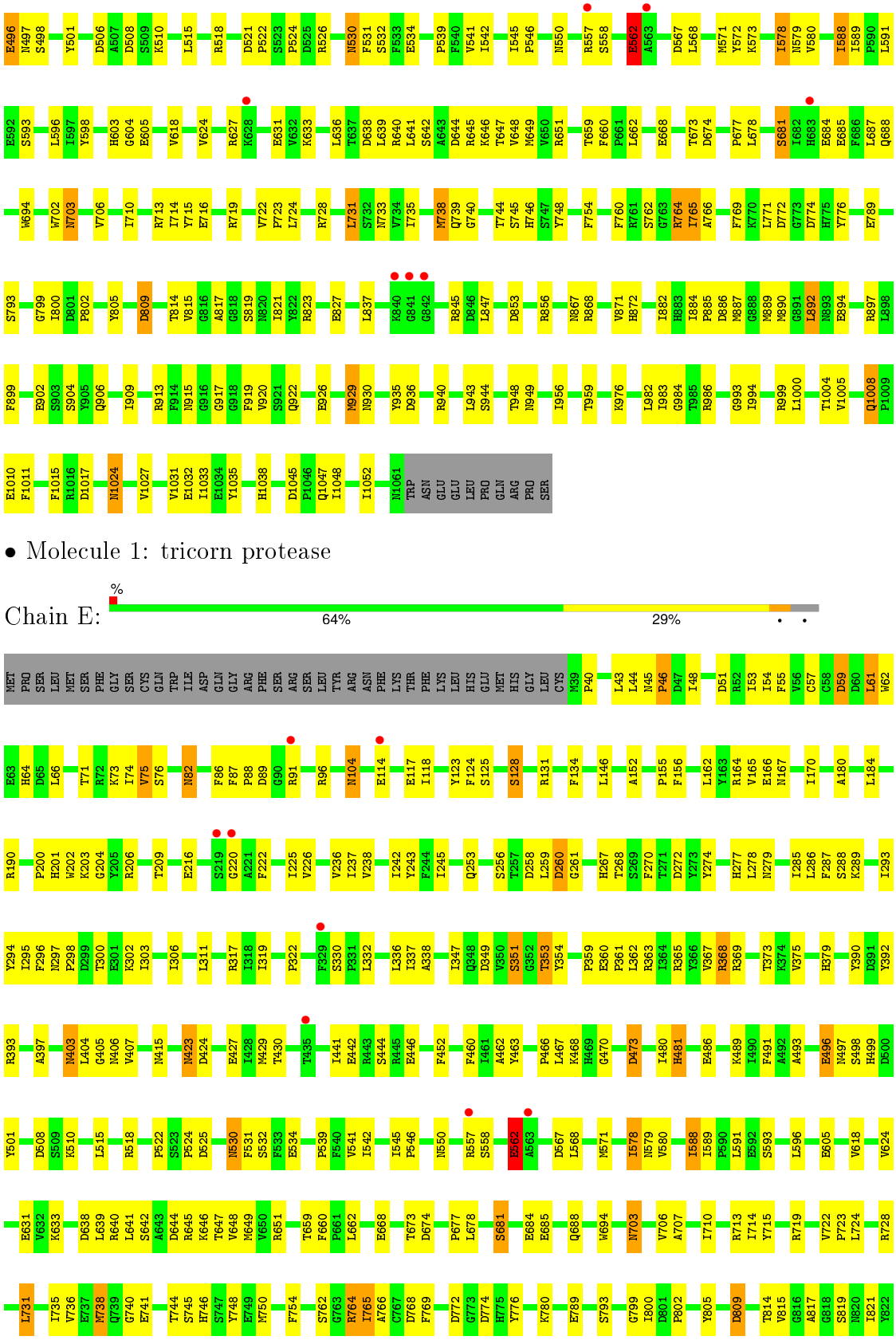




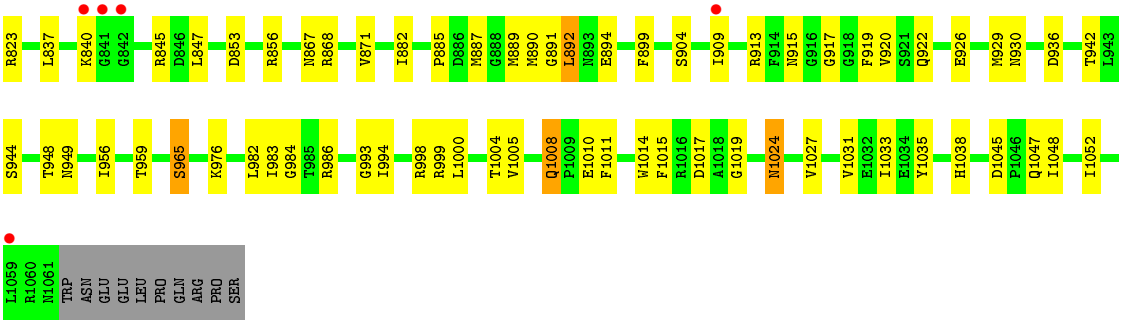
• Molecule 1: tricorn protease

Chain D:



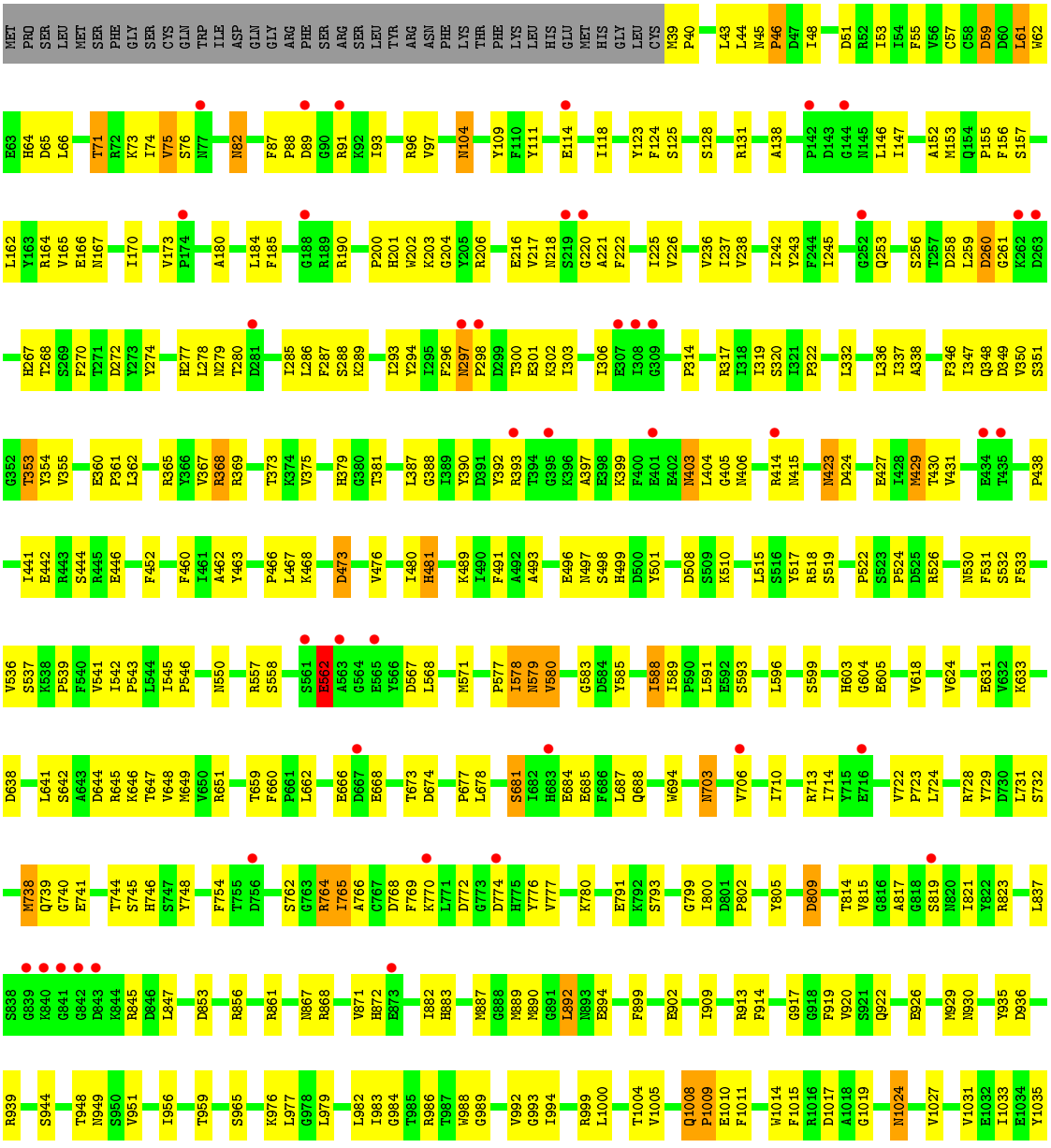


• Molecule 1: tricorn protease



- Molecule 1: tricorn protease

Chain F:




A1036
P1037
H1038
D1039
S1042
D1045
P1046
Q1047
I1048
I1052
N1061
TRP
ASN
GLU
GLU
LEU
PRO
GLN
ARG
PRO
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.67Å 244.55Å 158.32Å 90.00° 104.59° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 19.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	85.8 (6.00-2.70) 86.0 (19.99-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.280 0.251 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.2	EDS
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 178807 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	50087	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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

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	0.52	0/8367	0.65	0/11311
1	B	0.53	0/8366	0.66	0/11310
1	C	0.54	0/8366	0.66	0/11310
1	D	0.51	0/8366	0.65	0/11310
1	E	0.52	0/8367	0.66	0/11311
1	F	0.52	0/8366	0.65	0/11310
All	All	0.53	0/50198	0.66	0/67862

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	8177	0	8003	290	0
1	B	8176	0	8000	286	0
1	C	8176	0	8000	381	0
1	D	8176	0	8000	315	0
1	E	8177	0	8003	296	0
1	F	8176	0	8000	346	0
2	A	55	0	46	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	55	0	46	5	0
2	C	55	0	46	6	0
2	D	55	0	46	6	0
2	E	55	0	46	13	0
2	F	55	0	46	7	0
3	A	114	0	0	36	0
3	B	108	0	0	38	0
3	C	136	0	0	93	0
3	D	132	0	0	53	0
3	E	105	0	0	24	0
3	F	104	0	0	82	0
All	All	50087	0	48282	1824	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1824) 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:A:965:SER:HB3	2:A:1214:DKT:C7	1.23	1.62
1:E:965:SER:HB3	2:E:1214:DKT:C7	1.52	1.36
1:D:171:ASN:HB3	3:D:1215:HOH:O	1.25	1.28
1:F:476:VAL:HG13	3:F:1283:HOH:O	1.41	1.20
2:A:1214:DKT:HE61	3:A:1276:HOH:O	1.51	1.08
1:F:97:VAL:HG12	3:F:1217:HOH:O	1.55	1.06
3:C:1231:HOH:O	1:D:702:TRP:HA	1.53	1.06
1:C:741:GLU:HB3	3:C:1322:HOH:O	1.54	1.05
1:C:771:LEU:HD22	3:C:1234:HOH:O	1.56	1.05
1:A:143:ASP:HA	3:A:1291:HOH:O	1.57	1.04
1:E:965:SER:HB3	2:E:1214:DKT:C6	1.89	1.02
1:B:220:GLY:HA2	3:B:1278:HOH:O	1.60	1.02
1:E:965:SER:HB3	2:E:1214:DKT:O1	0.82	0.98
1:E:965:SER:CB	2:E:1214:DKT:C6	2.43	0.96
1:A:965:SER:HB3	2:A:1214:DKT:C6	1.94	0.96
1:A:192:ILE:HG13	3:A:1266:HOH:O	1.65	0.95
1:A:965:SER:CB	2:A:1214:DKT:C6	2.45	0.94
1:F:965:SER:CB	2:F:1214:DKT:C6	2.44	0.94
1:C:124:PHE:HB2	3:C:1232:HOH:O	1.68	0.93
1:B:625:LYS:HG3	3:B:1268:HOH:O	1.69	0.92
1:F:173:VAL:HB	3:F:1250:HOH:O	1.69	0.91
1:B:1015:PHE:HB3	3:B:1283:HOH:O	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:948:THR:H	1:F:922:GLN:HE22	1.17	0.90
1:A:297:ASN:HB2	3:A:1319:HOH:O	1.70	0.90
1:C:446:GLU:N	3:C:1263:HOH:O	2.03	0.90
1:D:494:THR:HA	3:D:1240:HOH:O	1.71	0.90
1:C:82:ASN:HA	3:C:1216:HOH:O	1.71	0.89
1:A:965:SER:HB3	2:A:1214:DKT:O1	0.71	0.89
1:C:557:ARG:HH22	1:C:562:GLU:H	1.23	0.87
1:D:557:ARG:HH22	1:D:562:GLU:H	1.23	0.86
1:D:99:ARG:HB2	3:D:1297:HOH:O	1.75	0.86
1:F:557:ARG:HH22	1:F:562:GLU:H	1.22	0.86
1:E:557:ARG:HH22	1:E:562:GLU:H	1.24	0.85
1:A:525:ASP:HA	3:B:1262:HOH:O	1.75	0.85
1:A:557:ARG:HH22	1:A:562:GLU:H	1.23	0.85
1:B:206:ARG:H	1:B:1024:ASN:HD21	1.24	0.84
1:C:245:ILE:HB	3:C:1223:HOH:O	1.78	0.83
1:F:164:ARG:HB3	3:F:1250:HOH:O	1.78	0.83
1:A:253:GLN:HE22	1:A:270:PHE:H	1.27	0.83
1:C:401:GLU:HB2	3:C:1243:HOH:O	1.79	0.83
1:F:206:ARG:H	1:F:1024:ASN:HD21	1.25	0.83
1:D:760:PHE:HD2	3:D:1297:HOH:O	1.61	0.82
1:A:40:PRO:HG2	1:A:724:LEU:HD22	1.62	0.82
1:C:206:ARG:H	1:C:1024:ASN:HD21	1.27	0.82
1:B:784:GLY:HA3	3:B:1236:HOH:O	1.78	0.82
1:F:253:GLN:HE22	1:F:270:PHE:H	1.26	0.82
1:F:526:ARG:HD3	3:F:1225:HOH:O	1.80	0.82
1:B:557:ARG:HH22	1:B:562:GLU:H	1.22	0.81
1:E:134:PHE:HB2	3:E:1286:HOH:O	1.80	0.81
1:A:948:THR:H	1:B:922:GLN:HE22	1.29	0.81
1:E:922:GLN:HE22	1:F:948:THR:H	1.25	0.81
1:E:253:GLN:HE22	1:E:270:PHE:H	1.27	0.81
1:C:253:GLN:HE22	1:C:270:PHE:H	1.26	0.81
1:B:317:ARG:HD3	1:E:823:ARG:HD2	1.60	0.81
1:D:253:GLN:HE22	1:D:270:PHE:H	1.27	0.81
1:C:775:HIS:O	3:C:1234:HOH:O	1.98	0.81
1:D:871:VAL:HG22	1:D:1052:ILE:HD11	1.62	0.80
1:A:206:ARG:H	1:A:1024:ASN:ND2	1.80	0.80
1:A:317:ARG:HD3	1:D:823:ARG:HD2	1.63	0.80
1:B:143:ASP:HA	3:B:1287:HOH:O	1.80	0.80
1:C:337:ILE:HD12	1:C:649:MET:CE	2.12	0.80
1:B:871:VAL:HG22	1:B:1052:ILE:HD11	1.64	0.80
1:F:1036:ALA:HB3	3:F:1267:HOH:O	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:PRO:HG2	1:B:724:LEU:HD22	1.62	0.79
1:E:40:PRO:HG2	1:E:724:LEU:HD22	1.65	0.79
1:B:284:ARG:HD3	3:B:1222:HOH:O	1.82	0.79
1:B:295:ILE:HD13	3:B:1320:HOH:O	1.81	0.79
1:A:206:ARG:H	1:A:1024:ASN:HD21	1.26	0.79
1:D:206:ARG:H	1:D:1024:ASN:HD21	1.29	0.79
1:B:253:GLN:HE22	1:B:270:PHE:H	1.31	0.79
1:A:897:ARG:NE	3:A:1217:HOH:O	2.15	0.79
1:F:992:VAL:HB	3:F:1257:HOH:O	1.81	0.79
1:C:173:VAL:HB	3:C:1219:HOH:O	1.82	0.79
1:F:337:ILE:HD12	1:F:649:MET:CE	2.12	0.78
1:C:403:ASN:ND2	1:C:405:GLY:H	1.81	0.78
1:C:871:VAL:HG22	1:C:1052:ILE:HD11	1.64	0.78
1:B:337:ILE:HD12	1:B:649:MET:CE	2.12	0.78
1:D:636:LEU:HB3	3:D:1310:HOH:O	1.82	0.78
1:A:815:VAL:HA	1:A:819:SER:HB3	1.64	0.78
1:C:40:PRO:HG2	1:C:724:LEU:HD22	1.66	0.78
1:D:530:ASN:ND2	1:D:531:PHE:H	1.82	0.78
1:F:815:VAL:HA	1:F:819:SER:HB3	1.65	0.78
1:E:206:ARG:H	1:E:1024:ASN:HD21	1.31	0.78
1:D:218:ASN:HB2	3:D:1258:HOH:O	1.84	0.78
1:E:337:ILE:HD12	1:E:649:MET:CE	2.14	0.78
1:D:349:ASP:OD2	1:D:351:SER:HB3	1.84	0.78
1:E:88:PRO:HB3	3:E:1234:HOH:O	1.81	0.78
1:F:871:VAL:HG22	1:F:1052:ILE:HD11	1.64	0.77
1:A:871:VAL:HG22	1:A:1052:ILE:HD11	1.65	0.77
1:F:203:LYS:HA	3:F:1226:HOH:O	1.84	0.77
1:E:337:ILE:HD12	1:E:649:MET:HE1	1.67	0.77
1:E:349:ASP:OD2	1:E:351:SER:HB3	1.84	0.77
1:B:206:ARG:H	1:B:1024:ASN:ND2	1.81	0.77
1:F:40:PRO:HG2	1:F:724:LEU:HD22	1.65	0.77
1:C:263:ASP:HB2	3:C:1284:HOH:O	1.83	0.77
1:E:530:ASN:ND2	1:E:531:PHE:H	1.82	0.77
1:B:268:THR:HG22	1:B:303:ILE:HD11	1.66	0.77
1:C:922:GLN:HE22	1:D:948:THR:H	1.29	0.77
1:A:403:ASN:ND2	1:A:405:GLY:H	1.83	0.77
1:B:815:VAL:HA	1:B:819:SER:HB3	1.67	0.77
1:A:73:LYS:HD3	1:A:76:SER:HB3	1.68	0.76
1:A:337:ILE:HD12	1:A:649:MET:CE	2.15	0.76
1:A:53:ILE:HG23	1:A:286:LEU:HD21	1.67	0.76
1:E:403:ASN:ND2	1:E:405:GLY:H	1.83	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:518:ARG:NH1	3:E:1278:HOH:O	2.19	0.76
1:C:970:PHE:HA	3:C:1252:HOH:O	1.83	0.76
1:B:73:LYS:HD3	1:B:76:SER:HB3	1.67	0.76
1:D:268:THR:HG22	1:D:303:ILE:HD11	1.66	0.76
1:E:871:VAL:HG22	1:E:1052:ILE:HD11	1.65	0.76
1:D:337:ILE:HD12	1:D:649:MET:CE	2.14	0.76
1:B:87:PHE:HB3	1:B:88:PRO:HD2	1.68	0.76
1:C:948:THR:H	1:D:922:GLN:HE22	1.33	0.76
1:A:530:ASN:ND2	1:A:531:PHE:H	1.84	0.75
1:E:53:ILE:HG23	1:E:286:LEU:HD21	1.66	0.75
1:D:40:PRO:HG2	1:D:724:LEU:HD22	1.65	0.75
1:E:578:ILE:HD11	1:E:580:VAL:HG23	1.68	0.75
1:D:815:VAL:HA	1:D:819:SER:HB3	1.67	0.75
1:A:596:LEU:HD11	1:A:662:LEU:HD11	1.68	0.75
1:F:403:ASN:ND2	1:F:405:GLY:H	1.83	0.75
1:F:939:ARG:NH2	3:F:1216:HOH:O	2.20	0.75
1:E:268:THR:HG22	1:E:303:ILE:HD11	1.69	0.75
1:D:53:ILE:HG23	1:D:286:LEU:HD21	1.69	0.75
1:C:206:ARG:H	1:C:1024:ASN:ND2	1.83	0.75
1:E:815:VAL:HA	1:E:819:SER:HB3	1.69	0.75
1:F:162:LEU:HD22	3:F:1293:HOH:O	1.86	0.75
1:D:578:ILE:HD11	1:D:580:VAL:HG23	1.69	0.75
1:F:206:ARG:H	1:F:1024:ASN:ND2	1.83	0.74
1:D:351:SER:OG	1:D:353:THR:HG22	1.87	0.74
1:C:578:ILE:HD11	1:C:580:VAL:HG23	1.68	0.74
1:D:760:PHE:CD2	3:D:1297:HOH:O	2.36	0.74
1:C:979:LEU:HB3	3:C:1316:HOH:O	1.85	0.74
1:F:73:LYS:HD3	1:F:76:SER:HB3	1.68	0.74
1:D:403:ASN:ND2	1:D:405:GLY:H	1.84	0.74
1:D:206:ARG:H	1:D:1024:ASN:ND2	1.84	0.74
1:E:351:SER:OG	1:E:353:THR:HG22	1.88	0.74
1:C:955:ILE:HD12	3:C:1316:HOH:O	1.86	0.74
1:B:578:ILE:HD11	1:B:580:VAL:HG23	1.70	0.74
1:D:260:ASP:OD1	3:D:1326:HOH:O	2.05	0.74
1:C:815:VAL:HA	1:C:819:SER:HB3	1.66	0.74
1:F:596:LEU:HD11	1:F:662:LEU:HD11	1.68	0.74
1:C:994:ILE:HG22	1:C:1008:GLN:O	1.87	0.74
1:A:268:THR:HG22	1:A:303:ILE:HD11	1.69	0.74
1:F:53:ILE:HG23	1:F:286:LEU:HD21	1.70	0.74
1:C:796:PHE:HA	3:C:1269:HOH:O	1.87	0.74
1:A:965:SER:OG	2:A:1214:DKT:C7	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:LEU:HD11	1:D:662:LEU:HD11	1.70	0.73
1:E:167:ASN:HB2	1:E:170:ILE:HB	1.70	0.73
1:C:366:TYR:HB3	3:C:1251:HOH:O	1.89	0.73
1:D:403:ASN:HD22	1:D:404:LEU:N	1.86	0.73
1:F:337:ILE:HD12	1:F:649:MET:HE1	1.70	0.73
1:F:167:ASN:HB2	1:F:170:ILE:HB	1.69	0.73
1:F:355:VAL:HG13	3:F:1299:HOH:O	1.88	0.73
1:C:823:ARG:HD2	1:F:317:ARG:HD3	1.70	0.73
1:C:351:SER:OG	1:C:353:THR:HG22	1.88	0.73
1:B:873:GLU:OE2	3:B:1244:HOH:O	2.07	0.73
2:C:1214:DKT:HB12	3:C:1276:HOH:O	1.86	0.72
1:E:87:PHE:HB3	1:E:88:PRO:HD2	1.70	0.72
1:C:268:THR:HG22	1:C:303:ILE:HD11	1.71	0.72
1:E:596:LEU:HD11	1:E:662:LEU:HD11	1.71	0.72
1:F:578:ILE:HD11	1:F:580:VAL:HG23	1.69	0.72
1:C:167:ASN:HB2	1:C:170:ILE:HB	1.72	0.72
1:C:403:ASN:HD22	1:C:404:LEU:N	1.87	0.72
1:C:349:ASP:OD2	1:C:351:SER:HB3	1.88	0.72
1:B:349:ASP:OD2	1:B:351:SER:HB3	1.89	0.72
1:C:164:ARG:HB3	3:C:1219:HOH:O	1.90	0.72
1:E:206:ARG:H	1:E:1024:ASN:ND2	1.86	0.72
1:D:73:LYS:HD3	1:D:76:SER:HB3	1.71	0.72
1:A:922:GLN:HE22	1:B:948:THR:H	1.37	0.72
1:C:393:ARG:CZ	1:E:558:SER:HA	2.20	0.71
1:C:337:ILE:HD12	1:C:649:MET:HE1	1.70	0.71
1:B:351:SER:OG	1:B:353:THR:HG22	1.89	0.71
1:F:349:ASP:OD2	1:F:351:SER:HB3	1.89	0.71
1:E:948:THR:H	1:F:922:GLN:NE2	1.86	0.71
1:C:53:ILE:HG23	1:C:286:LEU:HD21	1.72	0.71
1:A:351:SER:OG	1:A:353:THR:HG22	1.90	0.71
1:C:530:ASN:ND2	1:C:531:PHE:H	1.88	0.71
1:C:596:LEU:HD11	1:C:662:LEU:HD11	1.72	0.71
1:A:578:ILE:HD11	1:A:580:VAL:HG23	1.72	0.71
1:B:53:ILE:HG23	1:B:286:LEU:HD21	1.72	0.71
1:D:994:ILE:HG22	1:D:1008:GLN:O	1.91	0.71
1:A:746:HIS:NE2	1:A:965:SER:OG	2.24	0.71
1:E:922:GLN:NE2	1:F:948:THR:H	1.89	0.71
1:B:403:ASN:ND2	1:B:405:GLY:H	1.87	0.71
1:E:403:ASN:HD22	1:E:404:LEU:N	1.88	0.71
1:F:530:ASN:ND2	1:F:531:PHE:H	1.89	0.71
1:D:571:MET:HB3	3:D:1256:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:LEU:HD11	1:D:338:ALA:HB2	1.72	0.71
1:C:191:VAL:HG23	3:C:1215:HOH:O	1.91	0.71
1:A:403:ASN:HD22	1:A:404:LEU:N	1.89	0.71
1:C:203:LYS:NZ	3:C:1237:HOH:O	2.23	0.71
1:B:596:LEU:HD11	1:B:662:LEU:HD11	1.72	0.71
1:A:104:ASN:HB2	3:A:1271:HOH:O	1.91	0.71
1:C:73:LYS:HD3	1:C:76:SER:HB3	1.72	0.70
1:B:61:LEU:HB3	1:B:75:VAL:HG13	1.71	0.70
1:A:61:LEU:HB3	1:A:75:VAL:HG13	1.73	0.70
1:D:167:ASN:HB2	1:D:170:ILE:HB	1.72	0.70
1:F:468:LYS:HD2	1:F:473:ASP:HB3	1.72	0.70
1:F:1024:ASN:HA	3:F:1244:HOH:O	1.90	0.70
1:D:468:LYS:HD2	1:D:473:ASP:HB3	1.73	0.70
1:C:222:PHE:N	3:C:1327:HOH:O	2.25	0.70
1:A:167:ASN:HB2	1:A:170:ILE:HB	1.73	0.70
1:D:935:TYR:HB3	3:D:1269:HOH:O	1.89	0.70
1:B:337:ILE:HD12	1:B:649:MET:HE2	1.72	0.70
1:E:73:LYS:HD3	1:E:76:SER:HB3	1.72	0.70
1:E:994:ILE:HG22	1:E:1008:GLN:O	1.92	0.70
1:C:87:PHE:HB3	1:C:88:PRO:HD2	1.74	0.70
1:B:994:ILE:HG22	1:B:1008:GLN:O	1.92	0.69
1:F:87:PHE:HB3	1:F:88:PRO:HD2	1.74	0.69
2:D:1214:DKT:OT	3:D:1282:HOH:O	2.10	0.69
1:E:61:LEU:HB3	1:E:75:VAL:HG13	1.74	0.69
1:C:82:ASN:H	1:C:82:ASN:HD22	1.38	0.69
1:F:403:ASN:HD22	1:F:404:LEU:N	1.90	0.69
1:F:153:MET:HB3	3:F:1294:HOH:O	1.91	0.69
1:F:332:LEU:HD11	1:F:338:ALA:HB2	1.74	0.69
1:D:61:LEU:HD13	1:D:74:ILE:HD11	1.74	0.69
1:C:317:ARG:HD3	1:F:823:ARG:HD2	1.73	0.69
1:F:994:ILE:HG22	1:F:1008:GLN:O	1.92	0.69
1:F:51:ASP:O	3:F:1222:HOH:O	2.09	0.69
1:F:268:THR:HG22	1:F:303:ILE:HD11	1.73	0.69
1:C:307:GLU:HG2	3:C:1304:HOH:O	1.92	0.69
1:D:446:GLU:OE1	1:D:468:LYS:HE2	1.93	0.69
1:E:322:PRO:HA	1:E:678:LEU:HD22	1.75	0.69
1:C:678:LEU:HG	3:C:1291:HOH:O	1.92	0.69
1:D:87:PHE:HB3	1:D:88:PRO:HD2	1.73	0.69
1:D:530:ASN:HD22	1:D:531:PHE:H	1.41	0.69
1:D:432:ASP:N	3:D:1262:HOH:O	2.26	0.69
1:A:87:PHE:HB3	1:A:88:PRO:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ARG:NH2	3:C:1251:HOH:O	2.25	0.68
1:A:994:ILE:HG22	1:A:1008:GLN:O	1.94	0.68
1:D:322:PRO:HA	1:D:678:LEU:HD22	1.75	0.68
1:F:603:HIS:NE2	3:F:1235:HOH:O	2.25	0.68
1:C:279:ASN:ND2	3:C:1245:HOH:O	2.06	0.68
1:E:530:ASN:HD22	1:E:531:PHE:H	1.40	0.68
1:B:403:ASN:HD22	1:B:404:LEU:N	1.92	0.68
1:C:737:GLU:HA	3:C:1237:HOH:O	1.92	0.68
1:A:61:LEU:HD13	1:A:74:ILE:HD11	1.75	0.68
1:E:332:LEU:HD11	1:E:338:ALA:HB2	1.74	0.68
1:A:167:ASN:HB3	3:A:1301:HOH:O	1.93	0.68
1:B:322:PRO:HA	1:B:678:LEU:HD22	1.75	0.68
1:E:486:GLU:HB2	3:E:1231:HOH:O	1.93	0.68
1:A:349:ASP:OD2	1:A:351:SER:HB3	1.94	0.68
1:E:468:LYS:HD2	1:E:473:ASP:HB3	1.75	0.68
1:E:61:LEU:HD13	1:E:74:ILE:HD11	1.75	0.68
1:C:939:ARG:N	3:C:1231:HOH:O	2.27	0.68
1:C:1027:VAL:HA	3:C:1217:HOH:O	1.94	0.68
1:C:766:ALA:HB3	1:C:793:SER:HA	1.76	0.68
1:C:332:LEU:HD11	1:C:338:ALA:HB2	1.76	0.68
1:C:446:GLU:OE1	1:C:468:LYS:HE2	1.94	0.67
1:A:948:THR:H	1:B:922:GLN:NE2	1.91	0.67
1:D:190:ARG:HG3	1:D:216:GLU:OE2	1.93	0.67
1:B:530:ASN:ND2	1:B:531:PHE:H	1.92	0.67
1:F:322:PRO:HA	1:F:678:LEU:HD22	1.76	0.67
1:F:913:ARG:HH21	1:F:1047:GLN:HE21	1.41	0.67
1:B:468:LYS:HD2	1:B:473:ASP:HB3	1.77	0.67
1:D:337:ILE:HD12	1:D:649:MET:HE1	1.75	0.67
1:C:123:TYR:OH	1:C:823:ARG:HD3	1.95	0.67
1:C:61:LEU:HB3	1:C:75:VAL:HG13	1.74	0.67
1:D:558:SER:HA	1:F:393:ARG:CZ	2.24	0.67
1:A:206:ARG:N	1:A:1024:ASN:HD21	1.93	0.67
1:B:167:ASN:HB2	1:B:170:ILE:HB	1.75	0.67
1:E:499:HIS:HD2	3:E:1221:HOH:O	1.77	0.67
1:D:913:ARG:HH21	1:D:1047:GLN:HE21	1.41	0.67
1:F:61:LEU:HB3	1:F:75:VAL:HG13	1.75	0.67
1:C:164:ARG:O	3:C:1219:HOH:O	2.12	0.66
1:C:724:LEU:O	3:C:1289:HOH:O	2.13	0.66
1:E:190:ARG:HG3	1:E:216:GLU:OE2	1.95	0.66
1:C:430:THR:C	3:C:1227:HOH:O	2.34	0.66
1:D:639:LEU:HG	3:D:1218:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:ASN:HD22	1:A:531:PHE:H	1.42	0.66
1:F:65:ASP:OD1	3:F:1222:HOH:O	2.13	0.66
1:C:322:PRO:HA	1:C:678:LEU:HD22	1.77	0.66
1:D:897:ARG:NE	3:D:1267:HOH:O	2.28	0.66
1:F:585:TYR:CD2	3:F:1302:HOH:O	2.46	0.66
1:B:791:GLU:OE1	3:B:1236:HOH:O	2.12	0.66
1:C:51:ASP:HA	1:C:66:LEU:HD12	1.76	0.66
1:B:766:ALA:HB3	1:B:793:SER:HA	1.78	0.66
1:C:346:PHE:HD1	3:C:1298:HOH:O	1.77	0.66
1:A:468:LYS:HD2	1:A:473:ASP:HB3	1.76	0.66
1:C:231:HIS:CE1	3:C:1274:HOH:O	2.47	0.66
1:D:364:ILE:O	3:D:1325:HOH:O	2.12	0.66
1:B:51:ASP:HA	1:B:66:LEU:HD12	1.77	0.66
1:A:337:ILE:HD12	1:A:649:MET:HE2	1.78	0.66
1:A:322:PRO:HA	1:A:678:LEU:HD22	1.77	0.66
1:C:447:ALA:N	3:C:1263:HOH:O	2.29	0.66
1:C:468:LYS:HD2	1:C:473:ASP:HB3	1.78	0.66
1:B:61:LEU:HD13	1:B:74:ILE:HD11	1.78	0.66
1:E:446:GLU:OE1	1:E:468:LYS:HE2	1.96	0.66
1:C:233:SER:OG	3:C:1223:HOH:O	2.13	0.65
1:A:589:ILE:HD13	1:A:641:LEU:HD22	1.79	0.65
1:F:286:LEU:HD12	1:F:294:TYR:O	1.95	0.65
1:F:280:THR:HA	3:F:1265:HOH:O	1.96	0.65
1:F:82:ASN:H	1:F:82:ASN:HD22	1.44	0.65
1:B:225:ILE:HG13	1:B:226:VAL:HG23	1.77	0.65
1:E:913:ARG:HH21	1:E:1047:GLN:HE21	1.45	0.65
1:C:913:ARG:HH21	1:C:1047:GLN:HE21	1.43	0.65
1:C:225:ILE:HG13	1:C:226:VAL:HG23	1.79	0.65
1:C:921:SER:HB2	3:C:1252:HOH:O	1.96	0.65
1:F:766:ALA:HB3	1:F:793:SER:HA	1.78	0.65
1:A:82:ASN:H	1:A:82:ASN:HD22	1.44	0.65
1:F:965:SER:CA	2:F:1214:DKT:O1	2.44	0.65
1:E:766:ALA:HB3	1:E:793:SER:HA	1.79	0.65
1:A:382:ARG:HA	3:A:1224:HOH:O	1.96	0.65
1:F:446:GLU:OE1	1:F:468:LYS:HE2	1.96	0.65
1:F:367:VAL:O	1:F:368:ARG:HD3	1.96	0.65
1:D:61:LEU:HB3	1:D:75:VAL:HG13	1.78	0.65
1:A:892:LEU:HD13	1:A:920:VAL:HG21	1.79	0.65
1:E:202:TRP:CH2	1:E:745:SER:HB3	2.32	0.65
1:D:268:THR:HG22	1:D:303:ILE:CD1	2.26	0.64
1:F:351:SER:OG	1:F:353:THR:HG22	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ARG:HG3	1:B:216:GLU:OE2	1.96	0.64
1:B:1000:LEU:HD12	1:B:1004:THR:HB	1.79	0.64
1:A:766:ALA:HB3	1:A:793:SER:HA	1.77	0.64
1:B:897:ARG:NE	3:B:1216:HOH:O	2.29	0.64
1:D:766:ALA:HB3	1:D:793:SER:HA	1.79	0.64
1:C:969:ILE:HG13	3:C:1276:HOH:O	1.97	0.64
1:A:913:ARG:HH21	1:A:1047:GLN:HE21	1.45	0.64
1:F:430:THR:HG23	1:F:441:ILE:HD11	1.79	0.64
1:A:202:TRP:CH2	1:A:745:SER:HB3	2.33	0.64
1:B:268:THR:HG22	1:B:303:ILE:CD1	2.28	0.64
1:C:589:ILE:HD13	1:C:641:LEU:HD22	1.79	0.64
1:F:225:ILE:HG13	1:F:226:VAL:HG23	1.79	0.64
1:F:713:ARG:NH1	3:F:1231:HOH:O	2.29	0.64
1:A:268:THR:HG22	1:A:303:ILE:CD1	2.27	0.64
1:D:892:LEU:HB3	3:D:1321:HOH:O	1.96	0.64
1:F:710:ILE:O	1:F:714:ILE:HG12	1.98	0.64
1:E:530:ASN:ND2	1:E:531:PHE:N	2.45	0.64
1:F:892:LEU:HD13	1:F:920:VAL:HG21	1.78	0.64
2:A:1214:DKT:C8	3:A:1308:HOH:O	2.45	0.64
1:F:51:ASP:HA	1:F:66:LEU:HD12	1.79	0.64
1:E:710:ILE:O	1:E:714:ILE:HG12	1.97	0.64
1:E:268:THR:HG22	1:E:303:ILE:CD1	2.27	0.64
1:E:430:THR:HG23	1:E:441:ILE:HD11	1.80	0.64
1:A:190:ARG:HG3	1:A:216:GLU:OE2	1.98	0.64
1:C:892:LEU:HD13	1:C:920:VAL:HG21	1.80	0.64
1:B:155:PRO:O	1:B:856:ARG:HD2	1.98	0.64
1:B:710:ILE:O	1:B:714:ILE:HG12	1.98	0.64
1:E:930:ASN:HD21	1:F:926:GLU:HG3	1.63	0.64
1:C:155:PRO:O	1:C:856:ARG:HD2	1.98	0.63
1:C:530:ASN:HD22	1:C:531:PHE:H	1.46	0.63
1:D:82:ASN:H	1:D:82:ASN:HD22	1.45	0.63
1:A:965:SER:CA	2:A:1214:DKT:O1	2.45	0.63
1:C:286:LEU:HD12	1:C:294:TYR:O	1.97	0.63
1:A:1000:LEU:HD12	1:A:1004:THR:HB	1.79	0.63
1:A:922:GLN:NE2	1:B:948:THR:H	1.96	0.63
1:A:332:LEU:HD11	1:A:338:ALA:HB2	1.79	0.63
1:A:522:PRO:HG2	1:B:889:MET:SD	2.38	0.63
1:C:430:THR:HG23	1:C:441:ILE:HD11	1.79	0.63
1:C:1045:ASP:HB3	1:C:1048:ILE:HG22	1.81	0.63
1:F:123:TYR:OH	1:F:823:ARG:HD3	1.99	0.63
1:E:1000:LEU:HD12	1:E:1004:THR:HB	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:739:GLN:NE2	3:F:1255:HOH:O	2.32	0.63
1:F:467:LEU:O	3:F:1283:HOH:O	2.16	0.63
1:E:589:ILE:HB	1:E:596:LEU:HB2	1.81	0.63
1:D:104:ASN:H	1:D:104:ASN:HD22	1.47	0.63
1:A:710:ILE:O	1:A:714:ILE:HG12	1.99	0.63
1:C:361:PRO:HG2	1:C:379:HIS:NE2	2.14	0.63
1:F:65:ASP:HA	3:F:1222:HOH:O	1.98	0.63
1:A:446:GLU:OE1	1:A:468:LYS:HE2	1.99	0.63
1:D:1000:LEU:HD12	1:D:1004:THR:HB	1.80	0.63
1:D:681:SER:HB3	1:D:684:GLU:HG2	1.81	0.63
1:C:1000:LEU:HD12	1:C:1004:THR:HB	1.80	0.62
1:D:892:LEU:HD13	1:D:920:VAL:HG21	1.80	0.62
1:D:508:ASP:HB3	1:D:510:LYS:HE2	1.81	0.62
1:A:51:ASP:HA	1:A:66:LEU:HD12	1.81	0.62
1:D:367:VAL:O	1:D:368:ARG:HD3	1.99	0.62
1:E:361:PRO:HG2	1:E:379:HIS:NE2	2.13	0.62
1:F:951:VAL:O	3:F:1281:HOH:O	2.16	0.62
1:E:508:ASP:HB3	1:E:510:LYS:HE2	1.82	0.62
1:C:939:ARG:HB2	3:C:1231:HOH:O	1.99	0.62
1:F:890:MET:HB3	3:F:1304:HOH:O	2.00	0.62
1:F:39:MET:N	3:F:1260:HOH:O	2.32	0.62
1:F:446:GLU:HG3	3:F:1283:HOH:O	1.99	0.62
1:C:373:THR:HG21	1:C:393:ARG:HD2	1.81	0.62
1:C:403:ASN:C	1:C:403:ASN:HD22	2.02	0.62
1:F:868:ARG:NH2	3:F:1315:HOH:O	2.33	0.62
1:C:522:PRO:HG2	1:D:889:MET:SD	2.40	0.62
1:B:332:LEU:HD11	1:B:338:ALA:HB2	1.81	0.62
1:A:940:ARG:HD2	3:A:1290:HOH:O	1.99	0.62
1:C:202:TRP:CH2	1:C:745:SER:HB3	2.35	0.62
1:B:589:ILE:HD13	1:B:641:LEU:HD22	1.81	0.62
1:F:403:ASN:C	1:F:403:ASN:HD22	2.02	0.62
1:C:61:LEU:HD13	1:C:74:ILE:HD11	1.81	0.62
1:F:361:PRO:HG2	1:F:379:HIS:NE2	2.15	0.62
1:F:399:LYS:HB2	3:F:1258:HOH:O	2.00	0.62
1:D:286:LEU:HD12	1:D:294:TYR:O	1.99	0.62
1:F:147:ILE:HG22	3:F:1293:HOH:O	1.99	0.62
1:F:589:ILE:HD13	1:F:641:LEU:HD22	1.81	0.62
1:D:681:SER:CB	1:D:684:GLU:HG2	2.30	0.62
1:E:976:LYS:HZ3	1:E:1017:ASP:HB2	1.64	0.62
1:E:891:GLY:HA3	3:E:1244:HOH:O	1.98	0.62
1:F:190:ARG:HG3	1:F:216:GLU:OE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:THR:HG23	1:B:441:ILE:HD11	1.82	0.62
1:B:49:HIS:CG	3:B:1225:HOH:O	2.52	0.62
1:A:596:LEU:HD11	1:A:662:LEU:CD1	2.29	0.61
1:F:1008:GLN:NE2	3:F:1317:HOH:O	2.32	0.61
1:E:104:ASN:H	1:E:104:ASN:HD22	1.48	0.61
1:F:1000:LEU:HD12	1:F:1004:THR:HB	1.81	0.61
1:D:982:LEU:C	1:D:983:ILE:HD12	2.19	0.61
1:A:403:ASN:HD22	1:A:405:GLY:H	1.48	0.61
1:A:367:VAL:O	1:A:368:ARG:HD3	1.99	0.61
1:F:599:SER:CB	3:F:1302:HOH:O	2.48	0.61
1:B:82:ASN:HD22	1:B:82:ASN:H	1.47	0.61
1:A:593:SER:O	1:A:624:VAL:HG22	2.01	0.61
1:F:944:SER:N	3:F:1254:HOH:O	2.22	0.61
1:A:286:LEU:HD12	1:A:294:TYR:O	1.99	0.61
1:C:367:VAL:O	1:C:368:ARG:HD3	2.01	0.61
1:F:61:LEU:HD13	1:F:74:ILE:HD11	1.81	0.61
1:D:104:ASN:H	1:D:104:ASN:ND2	1.99	0.61
1:E:82:ASN:HD22	1:E:82:ASN:H	1.48	0.61
1:B:892:LEU:HD13	1:B:920:VAL:HG21	1.82	0.61
1:E:330:SER:HB3	3:E:1260:HOH:O	1.98	0.61
1:A:530:ASN:ND2	1:A:531:PHE:N	2.49	0.61
1:E:286:LEU:HD12	1:E:294:TYR:O	2.01	0.61
1:B:982:LEU:C	1:B:983:ILE:HD12	2.21	0.61
1:F:681:SER:CB	1:F:684:GLU:HG2	2.31	0.61
1:F:681:SER:HB3	1:F:684:GLU:HG2	1.83	0.61
1:B:556:PRO:HD3	1:D:354:TYR:CD1	2.35	0.61
1:A:48:ILE:HB	1:A:286:LEU:HD22	1.83	0.61
1:E:74:ILE:HG13	1:E:75:VAL:HG12	1.81	0.61
1:A:225:ILE:HG13	1:A:226:VAL:HG23	1.83	0.61
1:F:373:THR:HG21	1:F:393:ARG:HD2	1.83	0.61
1:B:367:VAL:O	1:B:368:ARG:HD3	2.01	0.61
1:E:892:LEU:HD13	1:E:920:VAL:HG21	1.83	0.61
1:D:330:SER:HB3	3:D:1273:HOH:O	2.01	0.61
1:B:1048:ILE:O	1:B:1052:ILE:HG12	2.01	0.60
1:D:589:ILE:HD13	1:D:641:LEU:HD22	1.84	0.60
1:C:196:THR:C	3:C:1274:HOH:O	2.38	0.60
1:A:524:PRO:HD3	1:B:605:GLU:CG	2.30	0.60
1:D:361:PRO:HG2	1:D:379:HIS:NE2	2.17	0.60
1:A:74:ILE:HG13	1:A:75:VAL:HG12	1.83	0.60
1:A:361:PRO:HG2	1:A:379:HIS:NE2	2.16	0.60
1:B:202:TRP:CH2	1:B:745:SER:HB3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:710:ILE:O	1:C:714:ILE:HG12	2.00	0.60
1:D:206:ARG:N	1:D:1024:ASN:HD21	1.98	0.60
1:A:589:ILE:HB	1:A:596:LEU:HB2	1.82	0.60
1:D:403:ASN:HD22	1:D:403:ASN:C	2.03	0.60
1:F:596:LEU:HD11	1:F:662:LEU:CD1	2.32	0.60
1:C:221:ALA:HB1	3:C:1327:HOH:O	2.00	0.60
1:A:605:GLU:CG	1:B:524:PRO:HD3	2.31	0.60
1:C:423:ASN:ND2	1:C:427:GLU:H	2.00	0.60
1:D:171:ASN:CB	3:D:1215:HOH:O	2.08	0.60
1:C:245:ILE:HD11	1:C:278:LEU:HG	1.84	0.60
1:C:403:ASN:HD22	1:C:405:GLY:H	1.47	0.60
1:A:167:ASN:CB	3:A:1301:HOH:O	2.50	0.60
1:C:558:SER:C	3:C:1220:HOH:O	2.40	0.60
1:D:51:ASP:HA	1:D:66:LEU:HD12	1.83	0.60
1:C:964:GLY:O	3:C:1224:HOH:O	2.17	0.60
1:F:202:TRP:CH2	1:F:745:SER:HB3	2.37	0.60
1:C:772:ASP:N	3:C:1234:HOH:O	2.35	0.60
1:C:982:LEU:C	1:C:983:ILE:HD12	2.22	0.60
1:B:337:ILE:HD12	1:B:649:MET:HE1	1.83	0.60
1:E:403:ASN:HD22	1:E:403:ASN:C	2.03	0.60
1:E:403:ASN:HD22	1:E:405:GLY:H	1.50	0.60
1:D:589:ILE:HB	1:D:596:LEU:HB2	1.82	0.60
1:C:959:THR:HG23	3:C:1247:HOH:O	2.01	0.60
1:A:403:ASN:C	1:A:403:ASN:HD22	2.05	0.60
1:C:189:ARG:O	3:C:1215:HOH:O	2.16	0.60
1:F:603:HIS:CD2	3:F:1235:HOH:O	2.54	0.60
1:B:446:GLU:OE1	1:B:468:LYS:HE2	2.02	0.60
1:C:765:ILE:H	1:C:765:ILE:HD13	1.67	0.60
1:F:536:VAL:HB	3:F:1221:HOH:O	2.02	0.60
1:C:497:ASN:ND2	1:D:868:ARG:HH12	2.00	0.60
1:E:225:ILE:HG13	1:E:226:VAL:HG23	1.83	0.60
1:B:478:GLN:HB3	3:B:1270:HOH:O	2.01	0.60
1:D:596:LEU:HD11	1:D:662:LEU:CD1	2.32	0.60
1:E:367:VAL:O	1:E:368:ARG:HD3	2.00	0.60
1:A:982:LEU:C	1:A:983:ILE:HD12	2.21	0.60
1:C:206:ARG:N	1:C:1024:ASN:HD21	1.97	0.59
1:D:123:TYR:OH	1:D:823:ARG:HD3	2.02	0.59
1:C:1048:ILE:O	1:C:1052:ILE:HG12	2.01	0.59
1:A:337:ILE:HD12	1:A:649:MET:HE1	1.82	0.59
1:F:982:LEU:C	1:F:983:ILE:HD12	2.23	0.59
1:F:666:GLU:HB3	3:F:1312:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ARG:N	1:B:1024:ASN:HD21	1.95	0.59
1:F:206:ARG:N	1:F:1024:ASN:HD21	1.96	0.59
1:B:1045:ASP:HB3	1:B:1048:ILE:HG22	1.83	0.59
1:C:589:ILE:HB	1:C:596:LEU:HB2	1.83	0.59
1:F:268:THR:HG22	1:F:303:ILE:CD1	2.32	0.59
1:C:522:PRO:HD3	3:D:1321:HOH:O	2.01	0.59
1:A:930:ASN:HD21	1:B:926:GLU:HG3	1.66	0.59
1:B:286:LEU:HD12	1:B:294:TYR:O	2.02	0.59
1:A:446:GLU:HA	3:A:1296:HOH:O	2.01	0.59
1:C:1027:VAL:CA	3:C:1217:HOH:O	2.49	0.59
1:D:104:ASN:ND2	3:D:1251:HOH:O	2.33	0.59
1:E:104:ASN:H	1:E:104:ASN:ND2	2.00	0.59
1:A:889:MET:SD	1:B:522:PRO:HG2	2.43	0.59
1:A:508:ASP:HB3	1:A:510:LYS:HE2	1.85	0.59
1:C:190:ARG:HG3	1:C:216:GLU:OE2	2.01	0.59
1:E:51:ASP:HA	1:E:66:LEU:HD12	1.84	0.59
1:E:681:SER:HB3	1:E:684:GLU:HG2	1.84	0.59
1:D:430:THR:HG23	1:D:441:ILE:HD11	1.83	0.59
1:A:155:PRO:O	1:A:856:ARG:HD2	2.01	0.59
1:A:430:THR:HG23	1:A:441:ILE:HD11	1.84	0.59
1:D:337:ILE:HD12	1:D:649:MET:HE2	1.84	0.59
1:A:744:THR:HG22	1:A:745:SER:N	2.17	0.59
1:A:681:SER:HB3	1:A:684:GLU:HG2	1.85	0.59
1:C:618:VAL:HG23	1:C:633:LYS:O	2.03	0.59
1:E:746:HIS:NE2	1:E:965:SER:OG	2.33	0.59
1:C:771:LEU:HA	3:C:1234:HOH:O	2.01	0.59
1:A:1045:ASP:HB3	1:A:1048:ILE:HG22	1.85	0.59
1:E:596:LEU:HD11	1:E:662:LEU:CD1	2.32	0.59
1:B:530:ASN:HD22	1:B:531:PHE:H	1.51	0.59
1:F:423:ASN:ND2	1:F:427:GLU:H	2.00	0.59
1:E:184:LEU:HD21	3:E:1291:HOH:O	2.02	0.59
1:D:202:TRP:CH2	1:D:745:SER:HB3	2.38	0.59
1:B:508:ASP:HB3	1:B:510:LYS:HE2	1.84	0.59
1:B:596:LEU:HD11	1:B:662:LEU:CD1	2.33	0.59
1:D:74:ILE:HG13	1:D:75:VAL:HG12	1.84	0.59
1:C:423:ASN:HD21	1:C:427:GLU:H	1.51	0.59
1:B:74:ILE:HG13	1:B:75:VAL:HG12	1.84	0.59
1:F:722:VAL:N	1:F:723:PRO:HD2	2.18	0.59
1:E:373:THR:HG21	1:E:393:ARG:HD2	1.84	0.59
1:E:965:SER:CA	2:E:1214:DKT:O1	2.45	0.58
1:D:640:ARG:O	3:D:1218:HOH:O	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:593:SER:O	1:F:624:VAL:HG22	2.04	0.58
1:F:245:ILE:HD11	1:F:278:LEU:HG	1.85	0.58
1:F:765:ILE:HD13	1:F:765:ILE:H	1.68	0.58
1:F:1045:ASP:HB3	1:F:1048:ILE:HG22	1.84	0.58
1:C:530:ASN:ND2	1:C:531:PHE:N	2.51	0.58
1:B:403:ASN:HD22	1:B:405:GLY:H	1.51	0.58
1:C:74:ILE:HG13	1:C:75:VAL:HG12	1.84	0.58
1:E:681:SER:CB	1:E:684:GLU:HG2	2.33	0.58
1:D:999:ARG:HG2	1:D:1005:VAL:HG22	1.85	0.58
1:B:593:SER:O	1:B:624:VAL:HG22	2.03	0.58
1:D:530:ASN:ND2	1:D:531:PHE:N	2.48	0.58
1:F:403:ASN:HD22	1:F:405:GLY:H	1.49	0.58
1:C:268:THR:HG22	1:C:303:ILE:CD1	2.32	0.58
1:E:589:ILE:HD13	1:E:641:LEU:HD22	1.85	0.58
1:F:618:VAL:HG23	1:F:633:LYS:O	2.04	0.58
1:C:868:ARG:HH12	1:D:497:ASN:ND2	2.01	0.58
1:E:899:PHE:HE2	1:E:949:ASN:HD22	1.51	0.58
1:F:917:GLY:HA3	2:F:1214:DKT:O	2.03	0.58
1:C:197:PHE:N	3:C:1274:HOH:O	2.36	0.58
1:A:256:SER:OG	1:A:267:HIS:HE1	1.87	0.58
1:E:245:ILE:HD11	1:E:278:LEU:HG	1.86	0.58
1:E:660:PHE:HB3	1:E:668:GLU:HB3	1.85	0.58
1:D:423:ASN:ND2	1:D:427:GLU:H	2.02	0.58
1:C:203:LYS:HG2	3:C:1337:HOH:O	2.02	0.58
1:B:1002:ASP:HB2	3:B:1319:HOH:O	2.04	0.58
1:B:589:ILE:HB	1:B:596:LEU:HB2	1.84	0.58
1:F:74:ILE:HG13	1:F:75:VAL:HG12	1.84	0.58
1:C:196:THR:HA	3:C:1274:HOH:O	2.04	0.58
1:F:430:THR:C	3:F:1276:HOH:O	2.42	0.58
1:E:917:GLY:HA3	2:E:1214:DKT:O	2.04	0.58
1:E:423:ASN:ND2	1:E:427:GLU:H	2.02	0.58
1:D:203:LYS:HD3	1:D:274:TYR:CZ	2.38	0.58
1:F:1039:ASP:N	3:F:1267:HOH:O	2.31	0.58
1:E:999:ARG:HG2	1:E:1005:VAL:HG22	1.85	0.58
1:B:284:ARG:CZ	3:B:1320:HOH:O	2.52	0.58
1:F:337:ILE:HD12	1:F:649:MET:HE2	1.85	0.58
1:F:530:ASN:HD22	1:F:531:PHE:H	1.50	0.58
1:F:61:LEU:CB	1:F:75:VAL:HG13	2.34	0.58
1:C:681:SER:CB	1:C:684:GLU:HG2	2.34	0.58
1:C:508:ASP:HB3	1:C:510:LYS:HE2	1.86	0.58
1:F:660:PHE:HB3	1:F:668:GLU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:LEU:C	3:F:1283:HOH:O	2.41	0.57
1:C:917:GLY:HA3	2:C:1214:DKT:O	2.04	0.57
1:F:710:ILE:HD13	1:F:713:ARG:HH22	1.69	0.57
1:D:203:LYS:HD3	1:D:274:TYR:CE1	2.40	0.57
1:E:982:LEU:C	1:E:983:ILE:HD12	2.24	0.57
1:D:1048:ILE:O	1:D:1052:ILE:HG12	2.04	0.57
1:F:155:PRO:O	1:F:856:ARG:HD2	2.03	0.57
1:B:618:VAL:HG23	1:B:633:LYS:O	2.04	0.57
1:B:361:PRO:HG2	1:B:379:HIS:NE2	2.19	0.57
1:A:373:THR:HG21	1:A:393:ARG:HD2	1.86	0.57
1:B:917:GLY:HA3	2:B:1214:DKT:O	2.04	0.57
1:D:944:SER:N	3:D:1269:HOH:O	2.37	0.57
1:E:123:TYR:OH	1:E:823:ARG:HD3	2.03	0.57
1:E:48:ILE:HB	1:E:286:LEU:HD22	1.86	0.57
1:B:423:ASN:ND2	1:B:427:GLU:H	2.03	0.57
1:B:373:THR:HG21	1:B:393:ARG:HD2	1.85	0.57
1:A:1048:ILE:O	1:A:1052:ILE:HG12	2.04	0.57
1:A:423:ASN:ND2	1:A:427:GLU:H	2.02	0.57
1:D:373:THR:HG21	1:D:393:ARG:HD2	1.84	0.57
1:C:596:LEU:HD11	1:C:662:LEU:CD1	2.33	0.57
1:C:922:GLN:NE2	1:D:948:THR:H	2.00	0.57
1:E:578:ILE:HD11	1:E:580:VAL:CG2	2.35	0.57
1:C:578:ILE:HD11	1:C:580:VAL:CG2	2.35	0.57
1:B:403:ASN:HD22	1:B:403:ASN:C	2.07	0.57
1:C:346:PHE:HB2	3:C:1298:HOH:O	2.04	0.57
1:D:225:ILE:HG13	1:D:226:VAL:HG23	1.87	0.57
1:D:710:ILE:O	1:D:714:ILE:HG12	2.04	0.57
1:A:40:PRO:HG2	1:A:724:LEU:CD2	2.34	0.57
1:F:589:ILE:HB	1:F:596:LEU:HB2	1.85	0.57
1:A:61:LEU:CB	1:A:75:VAL:HG13	2.34	0.57
1:B:48:ILE:HB	1:B:286:LEU:HD22	1.87	0.57
1:F:939:ARG:CZ	3:F:1216:HOH:O	2.50	0.57
1:B:994:ILE:HD12	1:B:994:ILE:O	2.05	0.57
1:B:104:ASN:ND2	1:B:104:ASN:H	2.03	0.57
1:C:104:ASN:H	1:C:104:ASN:ND2	2.03	0.57
1:F:508:ASP:HB3	1:F:510:LYS:HE2	1.87	0.57
1:F:203:LYS:HD3	1:F:274:TYR:CE1	2.40	0.57
1:A:556:PRO:HD3	1:E:354:TYR:CD1	2.39	0.57
1:B:681:SER:CB	1:B:684:GLU:HG2	2.35	0.57
1:D:593:SER:O	1:D:624:VAL:HG22	2.05	0.57
1:E:965:SER:C	2:E:1214:DKT:O1	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:917:GLY:HA3	2:D:1214:DKT:O	2.05	0.56
1:E:206:ARG:N	1:E:1024:ASN:HD21	2.02	0.56
1:C:85:ARG:NH2	3:C:1245:HOH:O	2.38	0.56
1:C:660:PHE:HB3	1:C:668:GLU:HB3	1.86	0.56
1:A:722:VAL:N	1:A:723:PRO:HD2	2.20	0.56
1:E:155:PRO:O	1:E:856:ARG:HD2	2.04	0.56
1:D:660:PHE:HB3	1:D:668:GLU:HB3	1.87	0.56
1:A:164:ARG:HG3	3:A:1264:HOH:O	2.05	0.56
1:C:970:PHE:CA	3:C:1252:HOH:O	2.50	0.56
1:D:403:ASN:HD22	1:D:405:GLY:H	1.50	0.56
1:C:367:VAL:N	3:C:1251:HOH:O	2.38	0.56
1:E:61:LEU:HD13	1:E:74:ILE:CD1	2.36	0.56
1:B:49:HIS:CE1	3:B:1225:HOH:O	2.59	0.56
1:E:423:ASN:HD21	1:E:427:GLU:H	1.52	0.56
1:F:242:ILE:O	1:F:256:SER:HA	2.05	0.56
1:B:307:GLU:HA	3:B:1259:HOH:O	2.04	0.56
1:C:792:LYS:NZ	3:D:1252:HOH:O	2.37	0.56
1:A:618:VAL:HG23	1:A:633:LYS:O	2.05	0.56
1:B:489:LYS:HG3	1:B:491:PHE:CE1	2.40	0.56
1:A:471:GLU:HG2	3:B:1256:HOH:O	2.04	0.56
1:F:423:ASN:HD21	1:F:427:GLU:H	1.51	0.56
1:C:786:TYR:HB3	3:D:1252:HOH:O	2.06	0.56
1:B:314:PRO:HA	1:E:118:ILE:HG22	1.86	0.56
1:D:722:VAL:N	1:D:723:PRO:HD2	2.20	0.56
1:F:1048:ILE:O	1:F:1052:ILE:HG12	2.06	0.56
1:B:744:THR:HG22	1:B:745:SER:N	2.21	0.56
1:C:690:TYR:HD1	3:C:1306:HOH:O	1.87	0.56
1:F:203:LYS:HD3	1:F:274:TYR:CZ	2.41	0.56
1:A:578:ILE:O	1:A:578:ILE:HG13	2.04	0.56
1:A:681:SER:CB	1:A:684:GLU:HG2	2.35	0.56
1:B:899:PHE:HE2	1:B:949:ASN:HD22	1.54	0.56
1:B:256:SER:OG	1:B:267:HIS:HE1	1.88	0.56
3:C:1233:HOH:O	1:D:976:LYS:HE2	2.05	0.56
1:A:899:PHE:HE2	1:A:949:ASN:HD22	1.53	0.56
1:C:365:ARG:HG2	1:C:365:ARG:HH21	1.71	0.56
1:A:917:GLY:HA3	2:A:1214:DKT:O	2.05	0.56
1:F:530:ASN:ND2	1:F:531:PHE:N	2.53	0.56
1:B:710:ILE:HD13	1:B:713:ARG:HH22	1.71	0.56
1:C:899:PHE:HE2	1:C:949:ASN:HD22	1.54	0.56
1:B:999:ARG:HG2	1:B:1005:VAL:HG22	1.88	0.56
1:C:337:ILE:HD12	1:C:649:MET:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD13	1:A:74:ILE:CD1	2.36	0.56
1:C:61:LEU:CB	1:C:75:VAL:HG13	2.36	0.56
1:C:429:MET:HG3	3:C:1227:HOH:O	2.05	0.56
1:F:744:THR:HG22	1:F:745:SER:N	2.20	0.56
1:D:568:LEU:C	3:D:1256:HOH:O	2.45	0.56
1:D:423:ASN:HD21	1:D:427:GLU:H	1.54	0.56
1:C:681:SER:HB3	1:C:684:GLU:HG2	1.88	0.56
1:F:999:ARG:HG2	1:F:1005:VAL:HG22	1.88	0.56
1:C:722:VAL:N	1:C:723:PRO:HD2	2.21	0.56
1:C:242:ILE:O	1:C:256:SER:HA	2.05	0.56
1:F:346:PHE:HB3	3:F:1299:HOH:O	2.06	0.56
1:B:104:ASN:HD22	1:B:104:ASN:H	1.54	0.56
1:E:242:ILE:O	1:E:256:SER:HA	2.06	0.56
1:E:645:ARG:HG3	1:E:645:ARG:HH21	1.70	0.56
1:B:203:LYS:HD3	1:B:274:TYR:CZ	2.41	0.56
1:C:710:ILE:HD13	1:C:713:ARG:HH22	1.70	0.55
1:E:578:ILE:HG13	1:E:578:ILE:O	2.06	0.55
1:B:722:VAL:N	1:B:723:PRO:HD2	2.22	0.55
1:B:123:TYR:OH	1:B:823:ARG:HD3	2.06	0.55
1:B:765:ILE:H	1:B:765:ILE:HD13	1.70	0.55
1:A:417:LYS:HD2	3:A:1222:HOH:O	2.06	0.55
1:E:965:SER:HG	2:E:1214:DKT:C7	2.11	0.55
1:D:218:ASN:HA	3:D:1340:HOH:O	2.07	0.55
1:D:765:ILE:HD11	1:D:769:PHE:HZ	1.72	0.55
1:A:203:LYS:HD3	1:A:274:TYR:CZ	2.42	0.55
1:D:61:LEU:HD13	1:D:74:ILE:CD1	2.36	0.55
1:F:104:ASN:H	1:F:104:ASN:ND2	2.03	0.55
1:C:104:ASN:HD22	1:C:104:ASN:H	1.53	0.55
1:B:681:SER:HB3	1:B:684:GLU:HG2	1.86	0.55
1:E:442:GLU:HG3	3:E:1242:HOH:O	2.06	0.55
1:E:203:LYS:HD3	1:E:274:TYR:CE1	2.41	0.55
1:D:774:ASP:HA	1:D:817:ALA:HB2	1.89	0.55
1:D:943:LEU:HB3	3:D:1269:HOH:O	2.07	0.55
1:F:360:GLU:OE2	1:F:361:PRO:HD2	2.07	0.55
1:A:965:SER:C	2:A:1214:DKT:O1	2.44	0.55
1:B:61:LEU:CB	1:B:75:VAL:HG13	2.34	0.55
1:A:164:ARG:CD	3:A:1264:HOH:O	2.54	0.55
1:E:765:ILE:HD13	3:E:1227:HOH:O	2.05	0.55
1:B:40:PRO:HG2	1:B:724:LEU:CD2	2.35	0.55
1:D:155:PRO:O	1:D:856:ARG:HD2	2.07	0.55
1:A:123:TYR:OH	1:A:823:ARG:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:VAL:N	3:C:1312:HOH:O	2.32	0.55
1:C:452:PHE:HB3	1:C:463:TYR:HB3	1.89	0.55
1:C:939:ARG:CA	3:C:1231:HOH:O	2.55	0.55
1:C:578:ILE:HG13	1:C:578:ILE:O	2.05	0.55
1:C:203:LYS:HD3	1:C:274:TYR:CZ	2.41	0.55
1:A:104:ASN:ND2	1:A:104:ASN:H	2.05	0.55
1:F:519:SER:N	3:F:1221:HOH:O	2.39	0.55
1:B:245:ILE:HD11	1:B:278:LEU:HG	1.89	0.55
1:F:517:TYR:C	3:F:1221:HOH:O	2.44	0.55
1:E:203:LYS:HD3	1:E:274:TYR:CZ	2.42	0.55
1:F:452:PHE:HB3	1:F:463:TYR:HB3	1.88	0.55
1:C:999:ARG:HG2	1:C:1005:VAL:HG22	1.88	0.55
1:F:104:ASN:H	1:F:104:ASN:HD22	1.55	0.54
1:F:201:HIS:CE1	3:F:1282:HOH:O	2.60	0.54
1:D:82:ASN:HD21	1:D:96:ARG:HH21	1.55	0.54
1:C:558:SER:CB	3:C:1220:HOH:O	2.55	0.54
1:A:245:ILE:HD11	1:A:278:LEU:HG	1.88	0.54
1:B:452:PHE:HB3	1:B:463:TYR:HB3	1.89	0.54
1:C:948:THR:H	1:D:922:GLN:NE2	2.01	0.54
1:C:197:PHE:O	3:C:1274:HOH:O	2.17	0.54
1:D:492:ALA:C	3:D:1221:HOH:O	2.44	0.54
1:D:572:TYR:O	3:D:1252:HOH:O	2.18	0.54
1:E:568:LEU:HB3	1:E:571:MET:CE	2.38	0.54
1:E:707:ALA:CB	3:F:1216:HOH:O	2.54	0.54
1:B:61:LEU:HD13	1:B:74:ILE:CD1	2.37	0.54
1:C:238:VAL:HG11	1:C:298:PRO:HG2	1.89	0.54
1:C:203:LYS:HD3	1:C:274:TYR:CE1	2.42	0.54
1:E:722:VAL:N	1:E:723:PRO:HD2	2.23	0.54
1:C:498:SER:OG	1:C:518:ARG:HG2	2.08	0.54
1:A:660:PHE:HB3	1:A:668:GLU:HB3	1.88	0.54
1:A:765:ILE:HD13	1:A:765:ILE:H	1.71	0.54
1:E:40:PRO:HG2	1:E:724:LEU:CD2	2.37	0.54
1:A:430:THR:C	3:A:1249:HOH:O	2.45	0.54
1:D:765:ILE:HD11	1:D:769:PHE:CZ	2.42	0.54
1:C:480:ILE:HB	1:C:493:ALA:HB3	1.89	0.54
1:C:162:LEU:HD21	1:C:180:ALA:HB3	1.89	0.54
1:C:360:GLU:OE2	1:C:361:PRO:HD2	2.07	0.54
1:B:203:LYS:HD3	1:B:274:TYR:CE1	2.43	0.54
1:D:105:THR:OG1	3:D:1297:HOH:O	2.18	0.54
1:D:218:ASN:CB	3:D:1258:HOH:O	2.49	0.54
1:E:765:ILE:HD11	1:E:769:PHE:HZ	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:PHE:HB3	1:B:668:GLU:HB3	1.89	0.54
1:E:618:VAL:HG23	1:E:633:LYS:O	2.08	0.54
1:A:999:ARG:HG2	1:A:1005:VAL:HG22	1.90	0.54
1:D:164:ARG:NH2	1:D:166:GLU:OE1	2.39	0.54
1:F:965:SER:C	2:F:1214:DKT:O1	2.46	0.54
1:F:48:ILE:HB	1:F:286:LEU:HD22	1.90	0.54
1:E:164:ARG:NH2	1:E:166:GLU:OE1	2.41	0.54
1:D:618:VAL:HG23	1:D:633:LYS:O	2.08	0.54
1:F:645:ARG:HG3	1:F:645:ARG:HH21	1.73	0.54
1:D:1045:ASP:HB3	1:D:1048:ILE:HG22	1.89	0.53
1:C:994:ILE:HD12	1:C:994:ILE:O	2.08	0.53
1:A:82:ASN:HD21	1:A:96:ARG:HG2	1.73	0.53
1:A:242:ILE:O	1:A:256:SER:HA	2.07	0.53
1:E:593:SER:O	1:E:624:VAL:HG22	2.09	0.53
1:F:988:TRP:C	3:F:1256:HOH:O	2.46	0.53
1:C:593:SER:O	1:C:624:VAL:HG22	2.07	0.53
1:C:473:ASP:HA	1:D:904:SER:OG	2.07	0.53
2:A:1214:DKT:CE6	3:A:1276:HOH:O	2.29	0.53
1:C:744:THR:HG22	1:C:745:SER:N	2.23	0.53
1:E:765:ILE:H	1:E:765:ILE:HD13	1.73	0.53
1:D:284:ARG:HD3	3:D:1227:HOH:O	2.07	0.53
1:E:868:ARG:HH12	1:F:497:ASN:ND2	2.06	0.53
1:F:365:ARG:HG2	1:F:365:ARG:HH21	1.72	0.53
1:D:61:LEU:CB	1:D:75:VAL:HG13	2.38	0.53
1:E:499:HIS:CD2	3:E:1221:HOH:O	2.58	0.53
1:A:774:ASP:HA	1:A:817:ALA:HB2	1.90	0.53
1:D:48:ILE:HB	1:D:286:LEU:HD22	1.90	0.53
1:D:744:THR:HG22	1:D:745:SER:N	2.23	0.53
1:A:145:ASN:HB2	3:A:1264:HOH:O	2.07	0.53
1:D:645:ARG:HH21	1:D:645:ARG:HG3	1.73	0.53
1:B:1031:VAL:HG12	1:B:1033:ILE:CD1	2.39	0.53
1:F:238:VAL:HG11	1:F:298:PRO:HG2	1.89	0.53
1:E:1045:ASP:HB3	1:E:1048:ILE:HG22	1.91	0.53
1:B:87:PHE:CB	1:B:88:PRO:HD2	2.38	0.53
1:C:85:ARG:CZ	3:C:1245:HOH:O	2.56	0.53
1:E:1048:ILE:O	1:E:1052:ILE:HG12	2.09	0.53
1:F:138:ALA:CB	3:F:1293:HOH:O	2.57	0.53
1:D:765:ILE:H	1:D:765:ILE:HD13	1.73	0.53
1:C:837:LEU:HB2	1:C:845:ARG:HB2	1.90	0.53
1:D:986:ARG:HA	1:D:1027:VAL:O	2.09	0.53
1:E:61:LEU:CB	1:E:75:VAL:HG13	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:HD13	1:C:74:ILE:CD1	2.39	0.53
1:B:423:ASN:HD21	1:B:427:GLU:H	1.54	0.53
1:E:645:ARG:NH2	1:E:645:ARG:HG3	2.23	0.53
1:B:913:ARG:HH21	1:B:1047:GLN:HE21	1.56	0.53
1:A:746:HIS:CE1	1:A:965:SER:OG	2.62	0.53
1:A:104:ASN:HD22	1:A:104:ASN:H	1.57	0.53
1:E:360:GLU:OE2	1:E:361:PRO:HD2	2.08	0.53
1:E:82:ASN:HD21	1:E:96:ARG:HH21	1.57	0.53
1:A:524:PRO:HD3	1:B:605:GLU:HG3	1.89	0.53
1:E:1031:VAL:HG12	1:E:1033:ILE:CD1	2.39	0.53
1:E:994:ILE:O	1:E:994:ILE:HD12	2.08	0.53
1:A:605:GLU:HG3	1:B:524:PRO:HD3	1.90	0.53
1:D:572:TYR:HB3	3:D:1221:HOH:O	2.08	0.52
1:B:242:ILE:O	1:B:256:SER:HA	2.08	0.52
1:A:823:ARG:HD2	1:D:317:ARG:HD3	1.92	0.52
1:E:222:PHE:H	1:E:1038:HIS:CD2	2.28	0.52
1:C:164:ARG:NH2	1:C:166:GLU:OE1	2.42	0.52
1:C:498:SER:HB2	3:C:1320:HOH:O	2.09	0.52
1:A:279:ASN:ND2	3:A:1273:HOH:O	2.42	0.52
1:F:837:LEU:HB2	1:F:845:ARG:HB2	1.92	0.52
1:B:365:ARG:HH21	1:B:365:ARG:HG2	1.75	0.52
1:D:245:ILE:HD11	1:D:278:LEU:HG	1.91	0.52
1:C:959:THR:O	1:C:984:GLY:HA3	2.09	0.52
1:B:530:ASN:ND2	1:B:531:PHE:N	2.56	0.52
1:A:203:LYS:HD3	1:A:274:TYR:CE1	2.44	0.52
1:E:765:ILE:HD11	1:E:769:PHE:CZ	2.44	0.52
1:A:452:PHE:HB3	1:A:463:TYR:HB3	1.91	0.52
1:A:489:LYS:HG3	1:A:491:PHE:CE1	2.44	0.52
1:D:336:LEU:O	1:D:337:ILE:HD13	2.10	0.52
1:E:591:LEU:HD11	1:E:662:LEU:HD21	1.91	0.52
1:E:703:ASN:OD1	1:E:706:VAL:HG23	2.09	0.52
1:F:157:SER:HB2	3:F:1314:HOH:O	2.08	0.52
1:F:899:PHE:HE2	1:F:949:ASN:HD22	1.58	0.52
1:C:124:PHE:HB3	1:C:152:ALA:CB	2.39	0.52
1:B:278:LEU:HD23	1:B:287:PHE:HB3	1.91	0.52
1:F:599:SER:HA	3:F:1302:HOH:O	2.08	0.52
1:E:744:THR:HG22	1:E:745:SER:N	2.25	0.52
1:F:642:SER:HB3	1:F:647:THR:HB	1.92	0.52
1:A:926:GLU:HG3	1:B:930:ASN:HD21	1.74	0.52
1:F:256:SER:OG	1:F:267:HIS:HE1	1.93	0.52
1:A:314:PRO:HA	1:D:118:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:541:VAL:HG22	1:F:542:ILE:N	2.25	0.52
1:E:926:GLU:HG3	1:F:930:ASN:HD21	1.74	0.52
1:C:774:ASP:HA	1:C:817:ALA:HB2	1.92	0.52
1:C:278:LEU:HD23	1:C:287:PHE:HB3	1.92	0.52
1:D:703:ASN:OD1	1:D:706:VAL:HG23	2.10	0.52
1:A:471:GLU:CG	3:B:1256:HOH:O	2.57	0.52
1:C:442:GLU:C	3:C:1267:HOH:O	2.48	0.52
1:F:645:ARG:HG3	1:F:645:ARG:NH2	2.25	0.52
1:D:452:PHE:HB3	1:D:463:TYR:HB3	1.92	0.52
1:E:452:PHE:HB3	1:E:463:TYR:HB3	1.91	0.52
1:F:728:ARG:HG3	1:F:754:PHE:CE1	2.45	0.52
1:E:887:MET:O	1:E:920:VAL:HG22	2.09	0.52
1:F:278:LEU:HD23	1:F:287:PHE:HB3	1.91	0.52
1:A:604:GLY:HA3	1:B:521:ASP:OD1	2.10	0.52
1:A:360:GLU:OE2	1:A:361:PRO:HD2	2.10	0.52
1:A:959:THR:O	1:A:984:GLY:HA3	2.10	0.52
1:C:541:VAL:HG22	1:C:542:ILE:N	2.25	0.52
1:A:524:PRO:HD3	1:B:605:GLU:HG2	1.92	0.51
1:A:423:ASN:HD21	1:A:427:GLU:H	1.55	0.51
1:B:774:ASP:HA	1:B:817:ALA:HB2	1.92	0.51
1:B:959:THR:O	1:B:984:GLY:HA3	2.10	0.51
1:E:774:ASP:HA	1:E:817:ALA:HB2	1.90	0.51
1:D:899:PHE:HE2	1:D:949:ASN:HD22	1.58	0.51
1:D:242:ILE:O	1:D:256:SER:HA	2.10	0.51
1:E:353:THR:HG23	1:E:354:TYR:CD1	2.45	0.51
1:C:955:ILE:HB	3:C:1316:HOH:O	2.10	0.51
1:E:802:PRO:O	1:E:805:TYR:HB2	2.10	0.51
1:C:926:GLU:HG3	1:D:930:ASN:HD21	1.76	0.51
1:E:525:ASP:HB2	1:F:532:SER:HB2	1.92	0.51
1:A:936:ASP:HB2	3:A:1281:HOH:O	2.10	0.51
1:E:238:VAL:HG11	1:E:298:PRO:HG2	1.92	0.51
1:D:703:ASN:HD22	1:D:703:ASN:C	2.12	0.51
1:D:645:ARG:HB2	3:D:1342:HOH:O	2.10	0.51
1:F:480:ILE:HB	1:F:493:ALA:HB3	1.92	0.51
1:A:764:ARG:NH2	3:A:1289:HOH:O	2.44	0.51
1:A:677:PRO:HD2	1:D:827:GLU:O	2.10	0.51
1:E:986:ARG:HA	1:E:1027:VAL:O	2.10	0.51
1:A:278:LEU:HD23	1:A:287:PHE:HB3	1.91	0.51
1:C:645:ARG:HG3	1:C:645:ARG:HH21	1.76	0.51
1:A:867:ASN:HD22	1:A:867:ASN:N	2.08	0.51
1:E:336:LEU:O	1:E:337:ILE:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ILE:HG13	1:B:578:ILE:O	2.09	0.51
1:E:317:ARG:NH1	3:E:1226:HOH:O	2.42	0.51
1:A:238:VAL:HG11	1:A:298:PRO:HG2	1.92	0.51
1:A:1031:VAL:HG12	1:A:1033:ILE:CD1	2.41	0.51
1:A:258:ASP:C	1:A:260:ASP:H	2.14	0.51
1:E:124:PHE:HB3	1:E:152:ALA:CB	2.40	0.51
1:D:530:ASN:HD22	1:D:531:PHE:N	2.09	0.51
1:C:904:SER:OG	1:D:473:ASP:HA	2.10	0.51
1:A:994:ILE:O	1:A:994:ILE:HD12	2.10	0.51
1:D:959:THR:O	1:D:984:GLY:HA3	2.11	0.51
1:E:959:THR:O	1:E:984:GLY:HA3	2.11	0.51
1:C:373:THR:HG22	1:E:558:SER:HB2	1.93	0.51
1:D:431:VAL:C	3:D:1262:HOH:O	2.48	0.51
1:E:256:SER:OG	1:E:267:HIS:HE1	1.93	0.51
1:F:764:ARG:HG3	3:F:1247:HOH:O	2.10	0.51
1:D:578:ILE:HD11	1:D:580:VAL:CG2	2.38	0.51
1:F:61:LEU:HD13	1:F:74:ILE:CD1	2.41	0.51
1:B:683:HIS:HB2	3:B:1295:HOH:O	2.10	0.51
1:E:546:PRO:HG2	1:E:567:ASP:HB3	1.93	0.51
1:B:82:ASN:HD21	1:B:96:ARG:HH21	1.59	0.51
1:D:867:ASN:N	1:D:867:ASN:HD22	2.09	0.51
1:E:131:ARG:HH21	1:E:131:ARG:HG2	1.75	0.50
1:D:278:LEU:HD23	1:D:287:PHE:HB3	1.92	0.50
1:F:48:ILE:HG21	3:F:1265:HOH:O	2.11	0.50
1:F:703:ASN:HD22	1:F:703:ASN:C	2.14	0.50
1:B:802:PRO:O	1:B:805:TYR:HB2	2.11	0.50
1:C:802:PRO:O	1:C:805:TYR:HB2	2.10	0.50
1:C:444:SER:OG	1:C:466:PRO:HG2	2.11	0.50
1:C:1028:ASP:N	3:C:1217:HOH:O	2.43	0.50
1:D:558:SER:HB2	1:F:373:THR:HG22	1.92	0.50
1:E:703:ASN:C	1:E:703:ASN:HD22	2.14	0.50
1:F:124:PHE:HB3	1:F:152:ALA:CB	2.41	0.50
1:D:222:PHE:H	1:D:1038:HIS:CD2	2.28	0.50
1:B:317:ARG:CD	1:E:823:ARG:HD2	2.37	0.50
1:E:225:ILE:O	1:E:261:GLY:HA3	2.11	0.50
1:C:642:SER:HB3	1:C:647:THR:HB	1.94	0.50
1:E:362:LEU:HD13	1:E:688:GLN:HG3	1.93	0.50
1:F:222:PHE:H	1:F:1038:HIS:CD2	2.29	0.50
1:B:785:ASP:N	3:B:1236:HOH:O	2.43	0.50
1:D:353:THR:HG23	1:D:354:TYR:CD1	2.46	0.50
1:F:286:LEU:N	3:F:1265:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ILE:O	1:D:261:GLY:HA3	2.11	0.50
1:F:543:PRO:HB3	3:F:1318:HOH:O	2.10	0.50
1:F:994:ILE:O	1:F:994:ILE:HD12	2.12	0.50
1:B:360:GLU:OE2	1:B:361:PRO:HD2	2.12	0.50
1:D:645:ARG:NH2	1:D:645:ARG:HG3	2.26	0.50
1:E:642:SER:HB3	1:E:647:THR:HB	1.93	0.50
1:B:164:ARG:NH2	1:B:166:GLU:OE1	2.45	0.50
1:F:162:LEU:HD21	1:F:180:ALA:HB3	1.93	0.50
1:B:541:VAL:HG22	1:B:542:ILE:N	2.27	0.50
1:D:124:PHE:HB3	1:D:152:ALA:CB	2.41	0.50
1:B:983:ILE:N	1:B:983:ILE:HD12	2.27	0.50
1:C:959:THR:C	3:C:1247:HOH:O	2.49	0.50
1:E:278:LEU:HD23	1:E:287:PHE:HB3	1.93	0.50
1:F:258:ASP:C	1:F:260:ASP:H	2.15	0.50
1:B:258:ASP:C	1:B:260:ASP:H	2.15	0.50
1:B:867:ASN:HD22	1:B:867:ASN:N	2.09	0.50
1:C:82:ASN:HD22	1:C:82:ASN:N	2.08	0.50
1:C:48:ILE:HB	1:C:286:LEU:HD22	1.93	0.50
1:F:82:ASN:HD21	1:F:96:ARG:HG2	1.76	0.50
1:E:710:ILE:HD13	1:E:713:ARG:HH22	1.77	0.50
1:F:935:TYR:HB3	3:F:1254:HOH:O	2.11	0.50
1:F:558:SER:CB	3:F:1249:HOH:O	2.59	0.50
1:C:256:SER:OG	1:C:267:HIS:HE1	1.94	0.50
1:F:1031:VAL:HG12	1:F:1033:ILE:CD1	2.42	0.50
1:A:568:LEU:HB3	1:A:571:MET:CE	2.41	0.50
1:E:365:ARG:HG2	1:E:365:ARG:HH21	1.75	0.50
1:C:993:GLY:H	2:C:1214:DKT:HE11	1.77	0.50
1:B:87:PHE:HB3	1:B:88:PRO:CD	2.39	0.50
1:A:887:MET:O	1:A:920:VAL:HG22	2.12	0.50
1:C:930:ASN:HD21	1:D:926:GLU:HG3	1.77	0.50
1:B:480:ILE:HB	1:B:493:ALA:HB3	1.94	0.50
1:F:185:PHE:HD2	3:F:1280:HOH:O	1.94	0.50
1:F:774:ASP:HA	1:F:817:ALA:HB2	1.94	0.50
1:D:578:ILE:O	1:D:578:ILE:HG13	2.11	0.49
1:C:858:ILE:HG13	3:C:1275:HOH:O	2.11	0.49
1:D:489:LYS:HG3	1:D:491:PHE:CE1	2.47	0.49
1:D:480:ILE:HB	1:D:493:ALA:HB3	1.93	0.49
1:F:381:THR:HA	3:F:1251:HOH:O	2.12	0.49
1:E:489:LYS:HG3	1:E:491:PHE:CE1	2.47	0.49
1:F:578:ILE:HG13	1:F:578:ILE:O	2.11	0.49
1:A:430:THR:O	3:A:1249:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:HIS:HD2	1:A:604:GLY:O	1.95	0.49
1:D:906:GLN:HG3	3:D:1302:HOH:O	2.11	0.49
1:D:568:LEU:HB3	1:D:571:MET:CE	2.42	0.49
1:C:307:GLU:N	3:C:1304:HOH:O	2.29	0.49
1:F:82:ASN:HD21	1:F:96:ARG:HH21	1.60	0.49
1:C:645:ARG:HG3	1:C:645:ARG:NH2	2.27	0.49
1:E:541:VAL:HG22	1:E:542:ILE:N	2.27	0.49
1:A:498:SER:OG	1:A:518:ARG:HG2	2.12	0.49
1:E:444:SER:OG	1:E:466:PRO:HG2	2.12	0.49
1:F:460:PHE:CE2	1:F:568:LEU:HD11	2.47	0.49
1:B:175:LEU:O	1:B:177:LEU:HG	2.12	0.49
1:B:534:GLU:OE1	3:B:1262:HOH:O	2.20	0.49
1:C:204:GLY:O	1:C:206:ARG:HG3	2.11	0.49
1:E:87:PHE:CB	1:E:88:PRO:HD2	2.40	0.49
1:D:53:ILE:HG23	1:D:286:LEU:CD2	2.39	0.49
1:C:765:ILE:HD11	1:C:769:PHE:CZ	2.47	0.49
1:F:57:CYS:HB3	1:F:62:TRP:NE1	2.28	0.49
1:A:362:LEU:HD13	1:A:688:GLN:HG3	1.95	0.49
1:F:164:ARG:NH2	1:F:166:GLU:OE1	2.46	0.49
1:F:578:ILE:HD11	1:F:580:VAL:CG2	2.38	0.49
1:F:225:ILE:O	1:F:261:GLY:HA3	2.12	0.49
1:C:1031:VAL:HG12	1:C:1033:ILE:CD1	2.42	0.49
1:A:645:ARG:HG3	1:A:645:ARG:HH21	1.77	0.49
1:D:99:ARG:N	3:D:1297:HOH:O	2.45	0.49
1:D:591:LEU:HD11	1:D:662:LEU:HD21	1.94	0.49
1:D:360:GLU:OE2	1:D:361:PRO:HD2	2.12	0.49
1:D:238:VAL:HG11	1:D:298:PRO:HG2	1.93	0.49
1:F:499:HIS:HD2	3:F:1263:HOH:O	1.94	0.49
1:E:501:TYR:CD2	1:E:501:TYR:N	2.80	0.49
1:C:703:ASN:HD22	1:C:703:ASN:C	2.15	0.49
1:D:710:ILE:HD13	1:D:713:ARG:HH22	1.76	0.49
1:C:180:ALA:C	3:C:1311:HOH:O	2.51	0.49
1:F:802:PRO:O	1:F:805:TYR:HB2	2.13	0.49
1:E:736:VAL:HG13	3:E:1276:HOH:O	2.11	0.49
1:D:498:SER:OG	1:D:518:ARG:HG2	2.13	0.49
1:A:642:SER:HB3	1:A:647:THR:HB	1.94	0.49
1:A:365:ARG:HG2	1:A:365:ARG:HH21	1.78	0.49
1:C:222:PHE:H	1:C:1038:HIS:CD2	2.31	0.49
1:C:913:ARG:HH21	1:C:1047:GLN:NE2	2.11	0.49
1:E:104:ASN:ND2	3:E:1220:HOH:O	2.46	0.49
1:E:764:ARG:HG2	1:E:764:ARG:HH21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:GLY:H	2:A:1214:DKT:HE11	1.76	0.49
1:E:965:SER:HB3	2:E:1214:DKT:O	2.11	0.49
1:C:173:VAL:CB	3:C:1219:HOH:O	2.51	0.49
1:F:40:PRO:HG2	1:F:724:LEU:CD2	2.40	0.49
1:C:591:LEU:HD11	1:C:662:LEU:HD21	1.95	0.49
1:C:87:PHE:CB	1:C:88:PRO:HD2	2.43	0.49
1:D:184:LEU:HD13	1:D:237:ILE:HG13	1.94	0.49
1:B:993:GLY:H	2:B:1214:DKT:HE11	1.77	0.49
1:E:337:ILE:HD12	1:E:649:MET:HE2	1.94	0.49
1:B:555:VAL:HG22	1:D:354:TYR:OH	2.12	0.49
1:B:591:LEU:HD11	1:B:662:LEU:HD21	1.94	0.49
1:A:88:PRO:HG2	1:A:89:ASP:H	1.78	0.49
1:A:331:PRO:HD2	3:A:1226:HOH:O	2.12	0.49
1:C:258:ASP:C	1:C:260:ASP:H	2.16	0.49
1:A:480:ILE:HB	1:A:493:ALA:HB3	1.95	0.49
1:B:204:GLY:O	1:B:206:ARG:HG3	2.13	0.48
1:E:568:LEU:HB3	1:E:571:MET:HE2	1.95	0.48
1:B:498:SER:OG	1:B:518:ARG:HG2	2.13	0.48
1:E:837:LEU:HB2	1:E:845:ARG:HB2	1.95	0.48
1:E:480:ILE:HB	1:E:493:ALA:HB3	1.95	0.48
1:D:802:PRO:O	1:D:805:TYR:HB2	2.12	0.48
1:F:429:MET:HG3	3:F:1276:HOH:O	2.13	0.48
1:C:559:MET:HG3	3:C:1220:HOH:O	2.13	0.48
1:C:889:MET:SD	1:D:522:PRO:HG2	2.53	0.48
1:C:867:ASN:HD22	1:C:867:ASN:N	2.11	0.48
1:F:87:PHE:CB	1:F:88:PRO:HD2	2.42	0.48
1:D:541:VAL:HG22	1:D:542:ILE:N	2.28	0.48
1:F:913:ARG:HH21	1:F:1047:GLN:NE2	2.10	0.48
1:C:460:PHE:CE2	1:C:568:LEU:HD11	2.49	0.48
1:B:124:PHE:HB3	1:B:152:ALA:CB	2.42	0.48
1:C:940:ARG:HD3	1:D:424:ASP:O	2.13	0.48
1:B:909:ILE:HG12	1:B:956:ILE:CG2	2.44	0.48
1:B:645:ARG:HG3	1:B:645:ARG:NH2	2.28	0.48
1:D:322:PRO:HG3	1:D:673:THR:O	2.14	0.48
1:F:959:THR:O	1:F:984:GLY:HA3	2.13	0.48
1:E:57:CYS:HB3	1:E:62:TRP:NE1	2.27	0.48
1:F:489:LYS:HG3	1:F:491:PHE:CE1	2.48	0.48
1:B:501:TYR:N	1:B:501:TYR:CD2	2.81	0.48
1:D:258:ASP:C	1:D:260:ASP:H	2.15	0.48
1:F:498:SER:OG	1:F:518:ARG:HG2	2.13	0.48
1:A:645:ARG:NH2	1:A:645:ARG:HG3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:ARG:HG3	1:B:645:ARG:HH21	1.78	0.48
1:B:238:VAL:HG11	1:B:298:PRO:HG2	1.94	0.48
1:A:639:LEU:HD23	1:A:640:ARG:N	2.28	0.48
1:D:993:GLY:H	2:D:1214:DKT:HE11	1.78	0.48
1:F:431:VAL:HG22	3:F:1276:HOH:O	2.12	0.48
1:F:200:PRO:O	1:F:740:GLY:HA3	2.14	0.48
1:D:642:SER:HB3	1:D:647:THR:HB	1.95	0.48
1:C:728:ARG:HG3	1:C:754:PHE:CE1	2.49	0.48
1:C:319:ILE:HG23	1:C:677:PRO:HB3	1.96	0.48
1:D:1031:VAL:HG12	1:D:1033:ILE:CD1	2.44	0.48
1:B:568:LEU:HB3	1:B:571:MET:CE	2.44	0.48
1:B:293:ILE:HG22	1:B:306:ILE:HD12	1.95	0.48
1:F:336:LEU:O	1:F:337:ILE:HD13	2.14	0.48
1:D:887:MET:O	1:D:920:VAL:HG22	2.13	0.48
1:C:916:GLY:C	3:C:1224:HOH:O	2.52	0.48
1:C:975:LYS:HA	3:C:1265:HOH:O	2.14	0.48
1:C:154:GLN:HG2	3:C:1323:HOH:O	2.12	0.48
1:C:524:PRO:HD3	1:D:605:GLU:CG	2.43	0.48
1:F:362:LEU:HD13	1:F:688:GLN:HG3	1.96	0.48
1:A:965:SER:HB2	2:A:1214:DKT:C6	2.38	0.48
1:C:1011:PHE:HB3	1:D:936:ASP:OD2	2.12	0.48
1:B:336:LEU:O	1:B:337:ILE:HD13	2.13	0.48
1:A:710:ILE:HD13	1:A:713:ARG:HH22	1.78	0.48
1:A:605:GLU:HG2	1:B:524:PRO:HD3	1.94	0.48
1:B:837:LEU:HB2	1:B:845:ARG:HB2	1.96	0.48
1:F:993:GLY:H	2:F:1214:DKT:HE11	1.78	0.48
1:C:703:ASN:OD1	1:C:706:VAL:HG23	2.14	0.48
1:E:498:SER:OG	1:E:518:ARG:HG2	2.14	0.48
1:C:87:PHE:HB3	1:C:88:PRO:CD	2.43	0.48
1:F:87:PHE:HB3	1:F:88:PRO:CD	2.43	0.48
1:E:524:PRO:HD3	1:F:605:GLU:CG	2.44	0.48
1:F:913:ARG:O	1:F:914:PHE:HB2	2.13	0.48
1:E:184:LEU:HD13	1:E:237:ILE:HG13	1.96	0.48
1:C:64:HIS:HB2	1:C:71:THR:HG23	1.96	0.48
1:E:285:ILE:HD12	1:E:296:PHE:HD2	1.79	0.48
1:E:347:ILE:HG12	1:E:392:TYR:CD2	2.49	0.48
1:D:546:PRO:HG2	1:D:567:ASP:HB3	1.95	0.48
1:D:545:ILE:N	1:D:545:ILE:HD12	2.28	0.48
1:C:82:ASN:HD21	1:C:96:ARG:HG2	1.79	0.47
1:C:225:ILE:O	1:C:261:GLY:HA3	2.13	0.47
1:E:367:VAL:CG1	1:E:375:VAL:HG21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:ARG:HA	1:A:1027:VAL:O	2.14	0.47
1:A:501:TYR:CD2	1:A:501:TYR:N	2.81	0.47
1:E:545:ILE:HD12	1:E:545:ILE:N	2.29	0.47
1:A:1010:GLU:HB3	1:A:1011:PHE:CE1	2.49	0.47
1:F:1009:PRO:HB3	3:F:1257:HOH:O	2.14	0.47
1:E:530:ASN:HD22	1:E:531:PHE:N	2.06	0.47
1:B:88:PRO:HG2	1:B:89:ASP:H	1.79	0.47
1:F:138:ALA:HB3	3:F:1293:HOH:O	2.13	0.47
1:F:591:LEU:HD11	1:F:662:LEU:HD21	1.95	0.47
1:E:322:PRO:HG2	1:E:674:ASP:OD1	2.14	0.47
1:F:765:ILE:HD11	1:F:769:PHE:HZ	1.79	0.47
1:D:131:ARG:HG2	1:D:131:ARG:HH21	1.79	0.47
1:E:53:ILE:CG2	1:E:286:LEU:HD21	2.42	0.47
1:F:48:ILE:CG2	3:F:1265:HOH:O	2.62	0.47
1:C:983:ILE:HD12	1:C:983:ILE:N	2.29	0.47
1:F:765:ILE:HD11	1:F:769:PHE:CZ	2.48	0.47
1:C:462:ALA:HA	1:C:481:HIS:O	2.13	0.47
1:D:837:LEU:HB2	1:D:845:ARG:HB2	1.96	0.47
1:E:638:ASP:HB3	1:E:651:ARG:HB3	1.97	0.47
1:D:501:TYR:CD2	1:D:501:TYR:N	2.82	0.47
1:E:1010:GLU:HB3	1:E:1011:PHE:CE1	2.50	0.47
1:A:336:LEU:O	1:A:337:ILE:HD13	2.13	0.47
1:A:578:ILE:HD11	1:A:580:VAL:CG2	2.41	0.47
1:A:322:PRO:HG3	1:A:673:THR:O	2.14	0.47
1:E:605:GLU:CG	1:F:524:PRO:HD3	2.45	0.47
1:E:993:GLY:H	2:E:1214:DKT:HE11	1.79	0.47
1:C:336:LEU:O	1:C:337:ILE:HD13	2.15	0.47
1:E:53:ILE:HG23	1:E:286:LEU:CD2	2.41	0.47
1:D:87:PHE:HB3	1:D:88:PRO:CD	2.43	0.47
1:F:983:ILE:HD12	1:F:983:ILE:N	2.29	0.47
1:F:703:ASN:OD1	1:F:706:VAL:HG23	2.14	0.47
1:C:43:LEU:HD22	1:C:55:PHE:CE1	2.50	0.47
1:A:837:LEU:HB2	1:A:845:ARG:HB2	1.96	0.47
1:C:393:ARG:NH1	1:E:558:SER:HA	2.30	0.47
1:A:53:ILE:HG23	1:A:286:LEU:CD2	2.42	0.47
1:A:591:LEU:HD11	1:A:662:LEU:HD21	1.96	0.47
1:F:887:MET:O	1:F:920:VAL:HG22	2.15	0.47
1:C:57:CYS:HB3	1:C:62:TRP:NE1	2.28	0.47
1:D:872:HIS:HE1	1:D:902:GLU:OE1	1.97	0.47
1:F:799:GLY:O	1:F:800:ILE:HG23	2.14	0.47
1:D:515:LEU:HD23	1:D:539:PRO:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:605:GLU:CG	1:D:524:PRO:HD3	2.45	0.47
1:E:515:LEU:HD23	1:E:539:PRO:HA	1.97	0.47
1:D:131:ARG:HH12	2:D:1214:DKT:CD6	2.27	0.47
1:B:284:ARG:NE	3:B:1320:HOH:O	2.46	0.47
1:A:87:PHE:CB	1:A:88:PRO:HD2	2.42	0.47
1:D:322:PRO:HG2	1:D:674:ASP:OD1	2.13	0.47
1:A:82:ASN:N	1:A:82:ASN:HD22	2.11	0.47
1:A:703:ASN:HD22	1:A:703:ASN:C	2.18	0.47
1:A:164:ARG:NH2	1:A:166:GLU:OE1	2.48	0.47
1:D:256:SER:OG	1:D:267:HIS:HE1	1.97	0.47
1:D:638:ASP:HB3	1:D:651:ARG:HB3	1.96	0.47
1:A:694:TRP:HA	1:A:738:MET:CE	2.45	0.47
1:C:489:LYS:HG3	1:C:491:PHE:CE1	2.49	0.47
1:C:789:GLU:CB	3:D:1308:HOH:O	2.63	0.47
1:F:579:ASN:HA	3:F:1264:HOH:O	2.14	0.47
1:E:867:ASN:HD22	1:E:867:ASN:N	2.13	0.47
1:F:467:LEU:N	3:F:1283:HOH:O	2.47	0.47
1:E:204:GLY:O	1:E:206:ARG:HG3	2.15	0.47
1:D:897:ARG:CZ	3:D:1267:HOH:O	2.62	0.47
1:F:438:PRO:HA	3:F:1276:HOH:O	2.15	0.47
1:A:703:ASN:OD1	1:A:706:VAL:HG23	2.14	0.47
1:C:734:VAL:HG12	3:C:1306:HOH:O	2.13	0.47
1:A:799:GLY:O	1:A:800:ILE:HG23	2.14	0.47
1:A:124:PHE:HB3	1:A:152:ALA:CB	2.45	0.47
1:F:638:ASP:HB3	1:F:651:ARG:HB3	1.96	0.47
1:D:603:HIS:HD2	1:D:604:GLY:O	1.98	0.47
1:E:162:LEU:HD21	1:E:180:ALA:HB3	1.97	0.47
1:F:319:ILE:HG23	1:F:677:PRO:HB3	1.96	0.47
1:B:545:ILE:N	1:B:545:ILE:HD12	2.29	0.47
1:D:598:TYR:HE1	3:D:1310:HOH:O	1.96	0.47
1:A:225:ILE:O	1:A:261:GLY:HA3	2.14	0.47
1:A:936:ASP:HB3	1:A:944:SER:HB3	1.97	0.47
1:A:342:ARG:O	3:A:1241:HOH:O	2.20	0.47
1:A:57:CYS:HB3	1:A:62:TRP:CD1	2.50	0.47
1:D:627:ARG:C	3:D:1264:HOH:O	2.52	0.47
1:F:550:ASN:C	1:F:550:ASN:OD1	2.53	0.47
1:E:293:ILE:HG22	1:E:306:ILE:HD12	1.96	0.47
1:C:155:PRO:HG2	1:C:156:PHE:CD1	2.50	0.47
1:B:460:PHE:CE2	1:B:568:LEU:HD11	2.50	0.47
1:C:200:PRO:O	1:C:740:GLY:HA3	2.15	0.47
1:D:57:CYS:HB3	1:D:62:TRP:NE1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:885:PRO:O	1:E:915:ASN:HA	2.15	0.47
1:C:146:LEU:HD23	1:C:165:VAL:HG21	1.96	0.47
1:F:986:ARG:HA	1:F:1027:VAL:O	2.15	0.47
1:E:936:ASP:OD2	1:F:1011:PHE:HB3	2.15	0.46
1:A:190:ARG:C	3:A:1266:HOH:O	2.53	0.46
1:C:53:ILE:HG23	1:C:286:LEU:CD2	2.44	0.46
1:A:353:THR:HG23	1:A:354:TYR:CD1	2.50	0.46
1:A:983:ILE:HD12	1:A:983:ILE:N	2.30	0.46
1:E:243:TYR:CD2	1:E:256:SER:HB3	2.50	0.46
1:E:546:PRO:CG	1:E:567:ASP:HB3	2.45	0.46
1:C:521:ASP:OD1	1:D:604:GLY:HA3	2.16	0.46
1:B:444:SER:OG	1:B:466:PRO:HG2	2.16	0.46
1:A:550:ASN:OD1	1:A:550:ASN:C	2.54	0.46
1:C:473:ASP:HA	1:D:904:SER:CB	2.45	0.46
1:F:710:ILE:HD13	1:F:713:ARG:NH2	2.29	0.46
1:C:189:ARG:C	3:C:1215:HOH:O	2.53	0.46
1:B:322:PRO:HG2	1:B:674:ASP:OD1	2.14	0.46
1:C:913:ARG:O	1:C:914:PHE:HB2	2.15	0.46
1:C:765:ILE:HD11	1:C:769:PHE:HZ	1.80	0.46
1:F:568:LEU:HB3	1:F:571:MET:CE	2.45	0.46
1:D:442:GLU:OE2	1:D:481:HIS:HD2	1.99	0.46
1:B:799:GLY:O	1:B:800:ILE:HG23	2.16	0.46
1:E:128:SER:OG	3:E:1230:HOH:O	1.97	0.46
1:F:768:ASP:HB2	1:F:780:LYS:HB3	1.97	0.46
1:A:64:HIS:HB2	1:A:71:THR:HG23	1.97	0.46
1:D:365:ARG:HG2	1:D:365:ARG:HH21	1.80	0.46
1:F:545:ILE:HD12	1:F:545:ILE:N	2.30	0.46
1:F:204:GLY:O	1:F:206:ARG:HG3	2.15	0.46
1:D:82:ASN:ND2	1:D:96:ARG:HH21	2.13	0.46
1:B:49:HIS:CD2	3:B:1225:HOH:O	2.67	0.46
1:E:57:CYS:HB3	1:E:62:TRP:CD1	2.50	0.46
1:D:1010:GLU:HB3	1:D:1011:PHE:CE1	2.50	0.46
1:C:869:ARG:NH2	3:C:1310:HOH:O	2.48	0.46
1:A:802:PRO:O	1:A:805:TYR:HB2	2.16	0.46
1:A:222:PHE:H	1:A:1038:HIS:CD2	2.34	0.46
1:B:45:ASN:HB3	1:B:277:HIS:CE1	2.51	0.46
1:B:93:ILE:HD12	1:B:111:TYR:HD2	1.80	0.46
1:C:771:LEU:CA	3:C:1234:HOH:O	2.62	0.46
1:A:143:ASP:CG	3:A:1291:HOH:O	2.54	0.46
1:E:88:PRO:CB	3:E:1234:HOH:O	2.52	0.46
1:A:87:PHE:HB3	1:A:88:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:618:VAL:CG2	1:C:631:GLU:HG3	2.45	0.46
1:B:64:HIS:HB2	1:B:71:THR:HG23	1.96	0.46
1:D:994:ILE:O	1:D:994:ILE:HD12	2.16	0.46
1:E:82:ASN:HD21	1:E:96:ARG:HG2	1.80	0.46
1:D:243:TYR:CD2	1:D:256:SER:HB3	2.51	0.46
1:A:57:CYS:HB3	1:A:62:TRP:NE1	2.31	0.46
1:E:258:ASP:C	1:E:260:ASP:H	2.18	0.46
1:C:603:HIS:HD2	1:C:604:GLY:O	1.98	0.46
1:E:131:ARG:HH12	2:E:1214:DKT:CD6	2.29	0.46
1:C:710:ILE:HD13	1:C:713:ARG:NH2	2.30	0.46
1:D:53:ILE:CG2	1:D:286:LEU:HD21	2.43	0.46
1:B:765:ILE:HD11	1:B:769:PHE:CZ	2.51	0.46
1:C:180:ALA:CA	3:C:1311:HOH:O	2.63	0.46
1:C:676:ARG:HG2	3:C:1236:HOH:O	2.15	0.46
1:F:546:PRO:HG2	1:F:567:ASP:HB3	1.97	0.46
1:F:770:LYS:O	1:F:777:VAL:HG12	2.16	0.46
1:D:460:PHE:CE2	1:D:568:LEU:HD11	2.50	0.46
1:E:442:GLU:OE2	1:E:481:HIS:HD2	1.99	0.46
1:D:200:PRO:O	1:D:740:GLY:HA3	2.16	0.46
1:C:788:ASN:ND2	3:C:1338:HOH:O	2.37	0.46
1:F:462:ALA:HA	1:F:481:HIS:O	2.16	0.46
1:B:642:SER:HB3	1:B:647:THR:HB	1.96	0.46
1:E:497:ASN:HB2	3:E:1278:HOH:O	2.16	0.46
1:F:744:THR:HG22	1:F:745:SER:H	1.80	0.46
1:C:960:ASN:N	3:C:1247:HOH:O	2.48	0.46
1:F:687:LEU:HD23	1:F:722:VAL:HG11	1.97	0.46
1:F:381:THR:CA	3:F:1251:HOH:O	2.63	0.46
1:D:285:ILE:HD12	1:D:296:PHE:HD2	1.81	0.46
1:C:768:ASP:HB2	1:C:780:LYS:HB3	1.98	0.46
1:F:64:HIS:HB2	1:F:71:THR:HG23	1.98	0.46
1:D:40:PRO:HG2	1:D:724:LEU:CD2	2.40	0.46
1:A:765:ILE:HD11	1:A:769:PHE:CZ	2.51	0.46
1:C:789:GLU:HB2	3:D:1308:HOH:O	2.16	0.46
1:D:293:ILE:HG22	1:D:306:ILE:HD12	1.98	0.46
1:A:909:ILE:HG12	1:A:956:ILE:CG2	2.46	0.46
1:E:351:SER:OG	1:E:353:THR:CG2	2.63	0.46
1:C:568:LEU:HB3	1:C:571:MET:CE	2.46	0.46
1:B:319:ILE:HG23	1:B:677:PRO:HB3	1.98	0.46
1:C:390:TYR:HD1	1:C:397:ALA:HB2	1.81	0.46
1:E:272:ASP:OD1	1:E:289:LYS:NZ	2.49	0.46
1:C:546:PRO:HG2	1:C:567:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ILE:HD11	1:B:580:VAL:CG2	2.41	0.45
1:D:558:SER:HA	1:F:393:ARG:NH1	2.31	0.45
1:C:346:PHE:CD1	3:C:1298:HOH:O	2.56	0.45
1:C:424:ASP:O	1:D:940:ARG:HD3	2.16	0.45
1:F:867:ASN:HD22	1:F:867:ASN:N	2.14	0.45
1:C:714:ILE:HG21	1:C:741:GLU:HB3	1.97	0.45
1:F:348:GLN:HB3	3:F:1299:HOH:O	2.16	0.45
1:F:367:VAL:CG1	1:F:375:VAL:HG21	2.46	0.45
1:D:367:VAL:CG1	1:D:375:VAL:HG21	2.45	0.45
1:B:823:ARG:HD2	1:E:317:ARG:HD3	1.98	0.45
1:C:118:ILE:HG22	1:F:314:PRO:HA	1.98	0.45
1:B:313:SER:O	1:E:117:GLU:HA	2.15	0.45
1:A:541:VAL:HG22	1:A:542:ILE:N	2.31	0.45
1:E:300:THR:HG22	1:E:302:LYS:HB2	1.98	0.45
1:A:545:ILE:HD12	1:A:545:ILE:N	2.32	0.45
1:A:131:ARG:HH21	1:A:131:ARG:HG2	1.81	0.45
1:F:599:SER:CA	3:F:1302:HOH:O	2.63	0.45
1:A:913:ARG:HH21	1:A:1047:GLN:NE2	2.13	0.45
1:D:82:ASN:HD21	1:D:96:ARG:HG2	1.79	0.45
1:F:890:MET:O	1:F:894:GLU:HG2	2.16	0.45
1:D:706:VAL:HG12	1:D:710:ILE:HG12	1.98	0.45
1:A:765:ILE:HD11	1:A:769:PHE:HZ	1.81	0.45
1:B:362:LEU:HD13	1:B:688:GLN:HG3	1.97	0.45
1:B:1014:TRP:CD1	1:B:1019:GLY:HA2	2.50	0.45
1:B:1014:TRP:NE1	1:B:1019:GLY:HA2	2.31	0.45
1:C:45:ASN:HA	1:C:277:HIS:CG	2.51	0.45
1:F:285:ILE:HD12	1:F:296:PHE:HD2	1.80	0.45
1:F:791:GLU:CD	1:F:861:ARG:HE	2.19	0.45
1:D:171:ASN:HB2	1:D:771:LEU:HB2	1.98	0.45
1:F:88:PRO:HG2	1:F:89:ASP:H	1.81	0.45
1:E:913:ARG:HH21	1:E:1047:GLN:NE2	2.12	0.45
1:B:703:ASN:C	1:B:703:ASN:HD22	2.19	0.45
1:F:684:GLU:HG3	1:F:685:GLU:N	2.32	0.45
1:F:515:LEU:HD23	1:F:539:PRO:HA	1.99	0.45
1:D:300:THR:HG22	1:D:302:LYS:HB2	1.97	0.45
1:D:909:ILE:HG12	1:D:956:ILE:CG2	2.46	0.45
1:E:746:HIS:HA	1:E:748:TYR:CE2	2.51	0.45
1:A:190:ARG:HB3	3:A:1266:HOH:O	2.15	0.45
1:D:983:ILE:HD12	1:D:983:ILE:N	2.29	0.45
1:C:618:VAL:HG21	1:C:631:GLU:HG3	1.98	0.45
1:F:57:CYS:HB3	1:F:62:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:PHE:H	1:B:1038:HIS:CD2	2.35	0.45
1:D:362:LEU:HD13	1:D:688:GLN:HG3	1.97	0.45
1:B:694:TRP:HA	1:B:738:MET:CE	2.47	0.45
1:E:889:MET:SD	1:F:522:PRO:HG2	2.56	0.45
1:B:57:CYS:HB3	1:B:62:TRP:NE1	2.30	0.45
1:C:887:MET:O	1:C:920:VAL:HG22	2.17	0.45
1:A:568:LEU:HB3	1:A:571:MET:HE1	1.99	0.45
1:C:57:CYS:HB3	1:C:62:TRP:CD1	2.51	0.45
1:B:45:ASN:HA	1:B:277:HIS:CG	2.51	0.45
1:F:442:GLU:OE2	1:F:481:HIS:HD2	1.99	0.45
1:C:347:ILE:HG12	1:C:392:TYR:CD2	2.52	0.45
1:A:546:PRO:HG2	1:A:567:ASP:HB3	1.98	0.45
1:F:1010:GLU:HB3	1:F:1011:PHE:CE1	2.52	0.45
1:C:317:ARG:CD	1:F:823:ARG:HD2	2.43	0.45
1:A:744:THR:HG22	1:A:745:SER:H	1.80	0.45
1:A:243:TYR:CD2	1:A:256:SER:HB3	2.52	0.45
1:C:243:TYR:CD2	1:C:256:SER:HB3	2.52	0.45
1:A:603:HIS:CD2	1:A:604:GLY:O	2.70	0.45
1:F:390:TYR:HD1	1:F:397:ALA:HB2	1.81	0.45
1:D:728:ARG:HG3	1:D:754:PHE:CE1	2.50	0.45
1:D:894:GLU:OE2	1:D:894:GLU:HA	2.17	0.45
1:C:46:PRO:HB2	1:C:286:LEU:CD2	2.46	0.45
1:F:714:ILE:HG21	1:F:741:GLU:HG3	1.99	0.45
1:E:707:ALA:HB2	3:F:1216:HOH:O	2.16	0.45
1:E:524:PRO:HD3	1:F:605:GLU:HG2	1.99	0.45
1:C:522:PRO:CG	1:D:889:MET:SD	3.05	0.45
1:F:894:GLU:OE2	1:F:894:GLU:HA	2.17	0.45
1:E:82:ASN:ND2	1:E:96:ARG:HH21	2.14	0.45
1:B:887:MET:O	1:B:920:VAL:HG22	2.16	0.45
1:E:460:PHE:CE2	1:E:568:LEU:HD11	2.52	0.45
1:C:936:ASP:HB3	1:C:944:SER:HB3	1.99	0.45
1:B:57:CYS:HB3	1:B:62:TRP:CD1	2.51	0.45
1:D:739:GLN:NE2	3:D:1229:HOH:O	2.49	0.45
1:D:444:SER:OG	1:D:466:PRO:HG2	2.17	0.45
1:F:45:ASN:HA	1:F:277:HIS:CG	2.52	0.45
1:B:347:ILE:HG12	1:B:392:TYR:CD2	2.52	0.45
1:A:45:ASN:HA	1:A:277:HIS:CG	2.52	0.45
1:F:694:TRP:HA	1:F:738:MET:CE	2.47	0.45
1:D:279:ASN:HD22	1:D:279:ASN:HA	1.58	0.45
1:C:638:ASP:HB3	1:C:651:ARG:HB3	1.99	0.45
1:B:1010:GLU:HB3	1:B:1011:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:NE2	1:A:270:PHE:H	2.05	0.45
1:C:351:SER:CB	1:C:353:THR:HG22	2.45	0.45
1:D:639:LEU:HD23	1:D:640:ARG:N	2.32	0.45
1:B:710:ILE:HD13	1:B:713:ARG:NH2	2.32	0.45
1:A:714:ILE:HG21	1:A:741:GLU:HB3	1.99	0.45
1:A:319:ILE:HG23	1:A:677:PRO:HB3	1.98	0.45
1:E:285:ILE:HD12	1:E:296:PHE:CD2	2.52	0.45
1:E:909:ILE:HG12	1:E:956:ILE:CG2	2.47	0.45
1:E:890:MET:O	1:E:894:GLU:HG2	2.16	0.45
1:D:347:ILE:HG12	1:D:392:TYR:CD2	2.51	0.45
1:B:925:ILE:HB	3:B:1243:HOH:O	2.17	0.45
1:D:363:ARG:HA	1:D:363:ARG:HD3	1.76	0.45
1:C:88:PRO:HG2	1:C:89:ASP:H	1.82	0.45
1:C:986:ARG:HA	1:C:1027:VAL:O	2.17	0.45
1:A:155:PRO:HG2	1:A:156:PHE:CD1	2.52	0.45
1:F:285:ILE:HD12	1:F:296:PHE:CD2	2.52	0.45
1:D:746:HIS:HA	1:D:748:TYR:CE2	2.52	0.45
1:B:728:ARG:HG3	1:B:754:PHE:CE1	2.52	0.45
1:C:533:PHE:HB3	1:C:536:VAL:HG11	1.99	0.45
1:F:125:SER:CB	1:F:762:SER:HB2	2.47	0.45
1:C:966:ASP:HA	3:C:1276:HOH:O	2.16	0.44
1:C:218:ASN:HB3	1:C:221:ALA:HB3	1.98	0.44
1:B:714:ILE:HG21	1:B:741:GLU:HB3	2.00	0.44
1:A:145:ASN:CB	3:A:1264:HOH:O	2.65	0.44
1:F:320:SER:HA	3:F:1218:HOH:O	2.17	0.44
1:E:942:THR:OG1	1:F:468:LYS:CE	2.65	0.44
1:E:983:ILE:N	1:E:983:ILE:HD12	2.32	0.44
1:E:442:GLU:CG	3:E:1242:HOH:O	2.63	0.44
1:A:200:PRO:O	1:A:740:GLY:HA3	2.17	0.44
1:A:293:ILE:HG22	1:A:306:ILE:HD12	1.98	0.44
1:B:285:ILE:HD12	1:B:296:PHE:HD2	1.83	0.44
1:D:809:ASP:HB3	1:D:814:THR:HA	1.99	0.44
1:F:501:TYR:CD2	1:F:501:TYR:N	2.85	0.44
1:C:694:TRP:HA	1:C:738:MET:CE	2.48	0.44
1:D:204:GLY:O	1:D:206:ARG:HG3	2.18	0.44
1:D:364:ILE:C	3:D:1325:HOH:O	2.54	0.44
1:B:225:ILE:O	1:B:261:GLY:HA3	2.17	0.44
1:B:684:GLU:HG3	1:B:685:GLU:N	2.32	0.44
1:E:993:GLY:N	1:E:1011:PHE:O	2.50	0.44
1:E:942:THR:OG1	1:F:468:LYS:HE2	2.17	0.44
1:F:109:TYR:HD1	3:F:1217:HOH:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:PRO:HG3	1:B:673:THR:O	2.17	0.44
1:C:196:THR:CA	3:C:1274:HOH:O	2.62	0.44
1:D:390:TYR:HD1	1:D:397:ALA:HB2	1.83	0.44
1:F:1014:TRP:CD1	1:F:1019:GLY:HA2	2.53	0.44
1:A:467:LEU:HD21	1:A:496:GLU:HB3	1.99	0.44
1:B:731:LEU:O	1:B:731:LEU:HD22	2.17	0.44
1:C:131:ARG:HH21	1:C:131:ARG:HG2	1.82	0.44
1:A:322:PRO:HG2	1:A:674:ASP:OD1	2.17	0.44
1:F:243:TYR:CD2	1:F:256:SER:HB3	2.52	0.44
1:D:976:LYS:NZ	1:D:1017:ASP:HB2	2.32	0.44
1:C:440:VAL:CG1	3:C:1267:HOH:O	2.65	0.44
1:C:604:GLY:HA3	1:D:521:ASP:OD1	2.18	0.44
1:D:885:PRO:O	1:D:915:ASN:HA	2.17	0.44
1:E:359:PRO:HA	3:E:1251:HOH:O	2.16	0.44
1:E:45:ASN:HA	1:E:277:HIS:CG	2.53	0.44
1:E:91:ARG:NH1	1:E:114:GLU:HB2	2.32	0.44
1:D:131:ARG:HH12	2:D:1214:DKT:HD61	1.83	0.44
1:B:131:ARG:HH12	2:B:1214:DKT:CD6	2.31	0.44
1:C:603:HIS:CD2	1:C:604:GLY:O	2.71	0.44
1:C:1014:TRP:CD1	1:C:1019:GLY:HA2	2.53	0.44
1:C:285:ILE:HD12	1:C:296:PHE:HD2	1.82	0.44
1:C:99:ARG:HD2	1:C:760:PHE:CZ	2.52	0.44
1:D:694:TRP:HA	1:D:738:MET:CE	2.47	0.44
1:A:1014:TRP:CD1	1:A:1019:GLY:HA2	2.53	0.44
1:C:679:VAL:N	3:C:1291:HOH:O	2.50	0.44
1:D:87:PHE:CB	1:D:88:PRO:HD2	2.42	0.44
1:C:279:ASN:HD22	1:C:279:ASN:HA	1.57	0.44
1:D:57:CYS:HB3	1:D:62:TRP:CD1	2.52	0.44
1:D:43:LEU:HD22	1:D:55:PHE:CE1	2.53	0.44
1:C:746:HIS:HA	1:C:748:TYR:CE2	2.52	0.44
1:B:131:ARG:HH21	1:B:131:ARG:HG2	1.83	0.44
1:F:162:LEU:HG	3:F:1295:HOH:O	2.18	0.44
1:B:662:LEU:O	1:B:662:LEU:HD12	2.18	0.44
1:F:322:PRO:HG3	1:F:673:THR:O	2.17	0.44
1:B:393:ARG:CZ	1:F:558:SER:HA	2.48	0.44
1:D:45:ASN:HA	1:D:277:HIS:CG	2.53	0.44
1:B:462:ALA:HA	1:B:481:HIS:O	2.18	0.44
1:B:363:ARG:HA	1:B:363:ARG:HD3	1.76	0.44
1:B:546:PRO:HG2	1:B:567:ASP:HB3	2.00	0.44
1:B:131:ARG:HA	3:B:1226:HOH:O	2.17	0.44
1:C:40:PRO:HG2	1:C:724:LEU:CD2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:PRO:HD3	1:F:288:SER:HB3	2.00	0.44
1:C:322:PRO:HG2	1:C:674:ASP:OD1	2.17	0.44
1:D:913:ARG:HH21	1:D:1047:GLN:NE2	2.12	0.44
1:A:82:ASN:HD21	1:A:96:ARG:HH21	1.65	0.44
1:D:684:GLU:HG3	1:D:685:GLU:N	2.33	0.44
1:E:976:LYS:NZ	3:E:1264:HOH:O	2.25	0.44
1:E:462:ALA:HA	1:E:481:HIS:O	2.17	0.44
1:D:618:VAL:CG2	1:D:631:GLU:HG3	2.48	0.44
1:F:146:LEU:HD23	1:F:165:VAL:HG21	1.99	0.44
1:B:200:PRO:O	1:B:740:GLY:HA3	2.16	0.44
1:C:764:ARG:HH21	1:C:764:ARG:HG2	1.83	0.44
1:E:550:ASN:C	1:E:550:ASN:OD1	2.56	0.44
1:D:131:ARG:NH1	2:D:1214:DKT:HD62	2.33	0.43
1:E:1031:VAL:HG12	1:E:1033:ILE:HD12	1.99	0.43
1:C:936:ASP:OD2	1:D:1011:PHE:HB3	2.17	0.43
1:E:894:GLU:HA	1:E:894:GLU:OE2	2.17	0.43
1:A:1014:TRP:NE1	1:A:1019:GLY:HA2	2.33	0.43
1:D:731:LEU:HD13	1:D:735:ILE:HD12	1.99	0.43
1:A:175:LEU:O	1:A:177:LEU:HG	2.18	0.43
1:A:809:ASP:HB3	1:A:814:THR:HA	2.00	0.43
1:A:728:ARG:HG3	1:A:754:PHE:CE1	2.53	0.43
1:D:162:LEU:HD21	1:D:180:ALA:HB3	1.99	0.43
1:F:467:LEU:HD12	1:F:467:LEU:C	2.38	0.43
1:C:131:ARG:HH12	2:C:1214:DKT:CD6	2.30	0.43
1:A:350:VAL:HG23	1:A:351:SER:N	2.33	0.43
1:F:322:PRO:HG2	1:F:674:ASP:OD1	2.18	0.43
1:D:897:ARG:NH1	3:D:1267:HOH:O	2.50	0.43
1:B:703:ASN:OD1	1:B:706:VAL:HG23	2.18	0.43
1:C:99:ARG:HD2	1:C:760:PHE:CE2	2.52	0.43
1:C:125:SER:CB	1:C:762:SER:HB2	2.48	0.43
1:F:444:SER:OG	1:F:466:PRO:HG2	2.18	0.43
1:B:588:ILE:C	1:B:588:ILE:HD13	2.38	0.43
1:C:501:TYR:CD2	1:C:501:TYR:N	2.86	0.43
1:C:993:GLY:N	1:C:1011:PHE:O	2.51	0.43
1:B:861:ARG:HB3	3:B:1236:HOH:O	2.17	0.43
1:D:462:ALA:HA	1:D:481:HIS:O	2.19	0.43
1:A:45:ASN:HB3	1:A:277:HIS:CE1	2.54	0.43
1:A:146:LEU:HD23	1:A:165:VAL:HG21	2.01	0.43
1:A:602:VAL:HA	3:A:1267:HOH:O	2.18	0.43
1:C:770:LYS:O	1:C:777:VAL:HG12	2.18	0.43
1:D:319:ILE:HG23	1:D:677:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:PRO:HG3	1:D:789:GLU:HG3	1.99	0.43
1:A:444:SER:OG	1:A:466:PRO:HG2	2.19	0.43
1:F:909:ILE:HG12	1:F:956:ILE:CG2	2.48	0.43
1:A:347:ILE:HG12	1:A:392:TYR:CD2	2.54	0.43
1:B:638:ASP:HB3	1:B:651:ARG:HB3	2.01	0.43
1:E:87:PHE:HB3	1:E:88:PRO:CD	2.40	0.43
1:F:82:ASN:ND2	1:F:96:ARG:HH21	2.15	0.43
1:C:684:GLU:HG3	1:C:685:GLU:N	2.32	0.43
1:B:765:ILE:HD11	1:B:769:PHE:HZ	1.84	0.43
1:E:618:VAL:CG2	1:E:631:GLU:HG3	2.48	0.43
1:B:442:GLU:OE2	1:B:481:HIS:HD2	2.01	0.43
1:B:218:ASN:HB3	1:B:221:ALA:HB3	1.99	0.43
1:E:648:VAL:O	1:E:659:THR:HA	2.19	0.43
1:E:200:PRO:O	1:E:740:GLY:HA3	2.18	0.43
1:B:279:ASN:HA	3:B:1261:HOH:O	2.17	0.43
1:C:272:ASP:OD1	1:C:289:LYS:NZ	2.52	0.43
1:A:731:LEU:O	1:A:731:LEU:HD22	2.18	0.43
1:C:648:VAL:O	1:C:659:THR:HA	2.18	0.43
1:F:131:ARG:HH12	2:F:1214:DKT:CD6	2.32	0.43
1:C:53:ILE:HD11	1:C:295:ILE:HD11	2.00	0.43
1:B:143:ASP:CG	3:B:1287:HOH:O	2.57	0.43
1:E:662:LEU:HD12	1:E:662:LEU:O	2.19	0.43
1:F:599:SER:HB2	3:F:1302:HOH:O	2.16	0.43
1:F:82:ASN:N	1:F:82:ASN:HD22	2.12	0.43
1:C:236:VAL:HG23	1:C:243:TYR:HB2	2.00	0.43
1:F:347:ILE:HG12	1:F:392:TYR:CD2	2.54	0.43
1:B:515:LEU:HD23	1:B:539:PRO:HA	2.00	0.43
1:E:390:TYR:HD1	1:E:397:ALA:HB2	1.83	0.43
1:E:319:ILE:HG23	1:E:677:PRO:HB3	2.01	0.43
1:F:93:ILE:HD12	1:F:111:TYR:HD2	1.82	0.43
1:E:588:ILE:C	1:E:588:ILE:HD13	2.39	0.43
1:A:204:GLY:O	1:A:206:ARG:HG3	2.17	0.43
1:A:164:ARG:HD3	3:A:1264:HOH:O	2.18	0.43
1:C:687:LEU:HD23	1:C:722:VAL:HG11	2.00	0.43
1:F:989:GLY:C	3:F:1256:HOH:O	2.56	0.43
1:D:546:PRO:CG	1:D:567:ASP:HB3	2.49	0.43
1:F:424:ASP:CB	3:F:1238:HOH:O	2.67	0.43
1:A:406:ASN:HD22	1:A:424:ASP:CG	2.22	0.43
1:C:791:GLU:CD	1:C:861:ARG:HE	2.22	0.43
1:C:894:GLU:HA	1:C:894:GLU:OE2	2.18	0.43
1:E:363:ARG:HA	1:E:363:ARG:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:588:ILE:HD13	1:C:588:ILE:C	2.38	0.43
1:C:217:VAL:HG23	1:C:218:ASN:N	2.34	0.43
1:A:765:ILE:N	1:A:765:ILE:HD13	2.33	0.43
1:F:406:ASN:HD22	1:F:424:ASP:CG	2.21	0.43
1:C:297:ASN:O	1:C:301:GLU:N	2.48	0.43
1:E:750:MET:HG2	3:E:1284:HOH:O	2.18	0.43
1:F:293:ILE:HG22	1:F:306:ILE:HD12	1.99	0.43
1:A:131:ARG:HH12	2:A:1214:DKT:CD6	2.32	0.43
1:D:351:SER:OG	1:D:353:THR:CG2	2.63	0.43
1:F:53:ILE:HG23	1:F:286:LEU:CD2	2.43	0.43
1:F:605:GLU:HG2	3:F:1235:HOH:O	2.18	0.43
1:A:618:VAL:CG2	1:A:631:GLU:HG3	2.49	0.43
1:B:540:PHE:HE1	3:B:1307:HOH:O	2.01	0.43
1:E:1010:GLU:HB3	1:E:1011:PHE:CD1	2.54	0.43
1:E:131:ARG:NH1	2:E:1214:DKT:HD62	2.34	0.43
1:C:1010:GLU:HB3	1:C:1011:PHE:CE1	2.53	0.43
1:B:46:PRO:HD3	1:B:288:SER:HB3	1.99	0.43
1:F:714:ILE:HG21	1:F:741:GLU:HB3	1.99	0.43
1:F:353:THR:HG23	1:F:354:TYR:CD1	2.54	0.43
1:A:460:PHE:CE2	1:A:568:LEU:HD11	2.53	0.43
1:B:201:HIS:O	1:B:740:GLY:HA2	2.19	0.43
1:C:809:ASP:HB3	1:C:814:THR:HA	2.01	0.43
1:B:1008:GLN:HE21	1:B:1008:GLN:HB2	1.65	0.43
1:E:322:PRO:HG3	1:E:673:THR:O	2.18	0.43
1:F:603:HIS:HD2	1:F:604:GLY:O	2.02	0.43
1:E:706:VAL:HG12	1:E:710:ILE:HG12	1.99	0.43
1:C:442:GLU:OE2	1:C:481:HIS:HD2	2.02	0.43
1:C:201:HIS:O	1:C:740:GLY:HA2	2.19	0.43
1:E:799:GLY:O	1:E:800:ILE:HG23	2.17	0.43
1:A:981:LYS:HB2	3:A:1254:HOH:O	2.18	0.43
1:D:716:GLU:HB3	3:D:1279:HOH:O	2.18	0.43
1:B:43:LEU:HD22	1:B:55:PHE:CE1	2.53	0.43
1:D:550:ASN:OD1	1:D:550:ASN:C	2.56	0.43
1:C:131:ARG:NH1	2:C:1214:DKT:HD62	2.34	0.42
1:D:562:GLU:HA	3:D:1291:HOH:O	2.19	0.42
1:C:245:ILE:HD12	3:C:1223:HOH:O	2.18	0.42
1:B:791:GLU:CD	1:B:861:ARG:HE	2.22	0.42
1:B:284:ARG:CD	3:B:1222:HOH:O	2.56	0.42
1:E:88:PRO:HG2	1:E:89:ASP:H	1.83	0.42
1:C:367:VAL:CG1	1:C:375:VAL:HG21	2.48	0.42
1:B:470:GLY:O	1:B:473:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:706:VAL:HG12	1:A:710:ILE:HG12	2.01	0.42
1:C:498:SER:CB	3:C:1320:HOH:O	2.67	0.42
1:D:776:TYR:CE1	1:D:821:ILE:HB	2.53	0.42
1:B:976:LYS:NZ	1:B:1017:ASP:HB2	2.34	0.42
1:E:1014:TRP:CD1	1:E:1019:GLY:HA2	2.53	0.42
1:D:369:ARG:HH21	1:D:369:ARG:HG3	1.83	0.42
1:C:545:ILE:N	1:C:545:ILE:HD12	2.34	0.42
1:D:138:ALA:HB1	1:D:183:ILE:HG22	2.00	0.42
1:C:234:SER:O	1:C:278:LEU:HB2	2.19	0.42
1:E:578:ILE:O	1:E:580:VAL:N	2.50	0.42
1:C:823:ARG:HD2	1:F:317:ARG:CD	2.42	0.42
1:D:96:ARG:HH21	1:D:96:ARG:HG2	1.84	0.42
1:A:684:GLU:HG3	1:A:685:GLU:N	2.33	0.42
1:D:687:LEU:HD23	1:D:722:VAL:HG11	2.00	0.42
1:E:639:LEU:HD23	1:E:640:ARG:N	2.34	0.42
1:C:909:ILE:HG12	1:C:956:ILE:CG2	2.49	0.42
1:C:362:LEU:HD13	1:C:688:GLN:HG3	2.01	0.42
1:F:882:ILE:HG22	1:F:883:HIS:N	2.34	0.42
1:F:43:LEU:HD22	1:F:55:PHE:CE1	2.54	0.42
1:E:369:ARG:HG3	1:E:369:ARG:HH21	1.82	0.42
1:C:46:PRO:HD3	1:C:288:SER:HB3	2.01	0.42
1:A:53:ILE:HD11	1:A:295:ILE:HD11	2.01	0.42
1:F:351:SER:CB	1:F:353:THR:HG22	2.49	0.42
1:B:82:ASN:ND2	1:B:96:ARG:HH21	2.16	0.42
1:B:618:VAL:CG2	1:B:631:GLU:HG3	2.49	0.42
1:E:633:LYS:HE2	1:E:633:LYS:HB2	1.88	0.42
1:B:568:LEU:HB3	1:B:571:MET:HE2	2.01	0.42
1:D:285:ILE:HD12	1:D:296:PHE:CD2	2.54	0.42
1:C:890:MET:O	1:C:894:GLU:HG2	2.19	0.42
1:E:64:HIS:HB2	1:E:71:THR:HG23	2.02	0.42
1:E:59:ASP:N	1:E:59:ASP:OD2	2.52	0.42
1:D:936:ASP:HB3	1:D:944:SER:HB3	2.01	0.42
1:E:351:SER:CB	1:E:353:THR:HG22	2.49	0.42
1:F:350:VAL:HG23	1:F:351:SER:N	2.34	0.42
1:B:744:THR:HG22	1:B:745:SER:H	1.82	0.42
1:A:604:GLY:HA3	1:B:521:ASP:CG	2.40	0.42
1:B:546:PRO:CG	1:B:567:ASP:HB3	2.50	0.42
1:B:390:TYR:HD1	1:B:397:ALA:HB2	1.85	0.42
1:E:43:LEU:HD22	1:E:55:PHE:CE1	2.54	0.42
1:B:162:LEU:HD21	1:B:180:ALA:HB3	2.01	0.42
1:E:789:GLU:HG3	1:F:577:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ARG:HH12	2:E:1214:DKT:HD61	1.83	0.42
1:B:46:PRO:HB2	1:B:286:LEU:CD2	2.50	0.42
1:B:53:ILE:HD11	1:B:295:ILE:HD11	2.02	0.42
1:F:533:PHE:HB3	1:F:536:VAL:HG11	2.01	0.42
1:B:1031:VAL:HG12	1:B:1033:ILE:HD12	2.01	0.42
1:B:1032:GLU:C	1:B:1033:ILE:HD12	2.39	0.42
1:C:546:PRO:CG	1:C:567:ASP:HB3	2.50	0.42
1:F:45:ASN:HB3	1:F:277:HIS:CE1	2.54	0.42
1:E:715:TYR:CZ	1:E:719:ARG:HD2	2.55	0.42
1:A:515:LEU:HD23	1:A:539:PRO:HA	2.01	0.42
1:B:91:ARG:CZ	3:B:1273:HOH:O	2.67	0.42
1:A:218:ASN:HB3	1:A:221:ALA:HB3	2.00	0.42
1:D:506:ASP:HB2	3:D:1246:HOH:O	2.19	0.42
1:A:285:ILE:HD12	1:A:296:PHE:HD2	1.84	0.42
1:F:91:ARG:NH1	1:F:114:GLU:HB2	2.35	0.42
1:F:746:HIS:HB2	3:F:1257:HOH:O	2.18	0.42
1:D:568:LEU:HB3	1:D:571:MET:HE1	2.01	0.42
1:C:904:SER:CB	1:D:473:ASP:HA	2.49	0.42
1:B:82:ASN:N	1:B:82:ASN:HD22	2.14	0.42
1:D:201:HIS:O	1:D:740:GLY:HA2	2.18	0.42
1:E:644:ASP:OD2	1:E:646:LYS:HB2	2.20	0.42
1:D:91:ARG:NH1	1:D:114:GLU:HB2	2.34	0.42
1:A:735:ILE:HG22	1:A:739:GLN:HE21	1.84	0.42
1:F:588:ILE:HD13	1:F:588:ILE:C	2.39	0.42
1:F:131:ARG:NH1	2:F:1214:DKT:HD62	2.35	0.42
1:E:904:SER:CB	1:F:473:ASP:HA	2.50	0.42
1:E:871:VAL:HG22	1:E:1052:ILE:CD1	2.44	0.42
1:D:578:ILE:O	1:D:580:VAL:N	2.51	0.42
1:B:353:THR:HG23	1:B:354:TYR:CD1	2.54	0.42
1:C:868:ARG:HH12	1:D:497:ASN:HD22	1.67	0.42
1:C:1032:GLU:C	1:C:1033:ILE:HD12	2.40	0.42
1:F:579:ASN:HB2	3:F:1285:HOH:O	2.20	0.42
1:D:890:MET:O	1:D:894:GLU:HG2	2.19	0.42
1:C:387:LEU:HD22	1:C:388:GLY:H	1.85	0.42
1:E:809:ASP:HB3	1:E:814:THR:HA	2.02	0.42
1:A:882:ILE:HG22	1:A:883:HIS:N	2.34	0.42
1:C:535:VAL:HG12	1:C:583:GLY:HA2	2.01	0.42
1:C:314:PRO:HA	1:F:118:ILE:HG22	2.00	0.42
1:E:840:LYS:N	3:E:1295:HOH:O	2.52	0.42
1:A:184:LEU:HD13	1:A:237:ILE:HG13	2.02	0.42
1:D:130:GLY:N	3:D:1286:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:LEU:HD23	1:C:539:PRO:HA	2.01	0.42
1:B:746:HIS:HA	1:B:748:TYR:CE2	2.53	0.42
1:C:141:ASP:OD2	1:C:141:ASP:C	2.58	0.42
1:F:993:GLY:N	1:F:1011:PHE:O	2.52	0.42
1:C:662:LEU:HD12	1:C:662:LEU:O	2.19	0.42
1:A:766:ALA:HB3	1:A:793:SER:CA	2.48	0.42
1:B:367:VAL:CG1	1:B:375:VAL:HG21	2.50	0.42
1:A:335:ASP:HA	3:A:1262:HOH:O	2.19	0.42
1:E:406:ASN:HD22	1:E:424:ASP:CG	2.22	0.42
1:B:59:ASP:N	1:B:59:ASP:OD2	2.50	0.42
1:A:530:ASN:HD22	1:A:531:PHE:N	2.10	0.42
1:E:53:ILE:HD11	1:E:295:ILE:HD11	2.02	0.42
1:B:351:SER:CB	1:B:353:THR:HG22	2.50	0.42
1:F:201:HIS:O	1:F:740:GLY:HA2	2.20	0.42
1:B:538:LYS:HB3	3:B:1307:HOH:O	2.19	0.42
1:C:293:ILE:HG22	1:C:306:ILE:HD12	2.01	0.42
1:A:162:LEU:HD21	1:A:180:ALA:HB3	2.01	0.42
1:A:638:ASP:HB3	1:A:651:ARG:HB3	2.01	0.42
1:F:648:VAL:O	1:F:659:THR:HA	2.19	0.42
1:D:526:ARG:NH1	3:D:1288:HOH:O	2.52	0.42
1:F:217:VAL:HG23	1:F:218:ASN:N	2.35	0.42
1:D:588:ILE:C	1:D:588:ILE:HD13	2.39	0.42
1:B:624:VAL:HG23	1:B:625:LYS:N	2.35	0.42
1:C:351:SER:OG	1:C:353:THR:CG2	2.63	0.42
1:F:618:VAL:CG2	1:F:631:GLU:HG3	2.50	0.42
1:D:703:ASN:C	1:D:703:ASN:ND2	2.72	0.42
1:D:882:ILE:HD11	1:D:899:PHE:HA	2.02	0.42
1:C:605:GLU:HG2	1:D:524:PRO:HD3	2.01	0.42
1:D:46:PRO:HD3	1:D:288:SER:HB3	2.02	0.42
1:D:929:MET:HB3	3:D:1219:HOH:O	2.19	0.42
1:F:414:ARG:NH1	1:F:644:ASP:HA	2.35	0.42
1:C:799:GLY:O	1:C:800:ILE:HG23	2.20	0.42
1:F:300:THR:HG22	1:F:302:LYS:HB2	2.01	0.42
1:D:715:TYR:CZ	1:D:719:ARG:HD2	2.55	0.42
1:C:562:GLU:C	1:C:564:GLY:H	2.23	0.41
1:C:744:THR:HG22	1:C:745:SER:H	1.82	0.41
1:D:710:ILE:HD13	1:D:713:ARG:NH2	2.35	0.41
1:F:452:PHE:CB	1:F:463:TYR:HB3	2.51	0.41
1:C:524:PRO:HD3	1:D:605:GLU:HG2	2.01	0.41
1:F:546:PRO:CG	1:F:567:ASP:HB3	2.49	0.41
1:F:809:ASP:HB3	1:F:814:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:LYS:O	1:A:777:VAL:HG12	2.20	0.41
1:B:184:LEU:HB2	1:B:191:VAL:HB	2.02	0.41
1:C:532:SER:OG	1:C:534:GLU:OE1	2.38	0.41
1:D:532:SER:OG	1:D:534:GLU:OE1	2.38	0.41
1:E:936:ASP:HB3	1:E:944:SER:HB3	2.02	0.41
1:C:771:LEU:HD13	3:C:1234:HOH:O	2.19	0.41
1:F:272:ASP:OD1	1:F:289:LYS:NZ	2.51	0.41
1:F:746:HIS:HA	1:F:748:TYR:CE2	2.55	0.41
1:C:633:LYS:HE2	1:C:633:LYS:HB2	1.88	0.41
1:F:155:PRO:HG2	1:F:156:PHE:CD1	2.55	0.41
1:E:155:PRO:HG2	1:E:156:PHE:CD1	2.54	0.41
1:D:573:LYS:HA	3:D:1252:HOH:O	2.21	0.41
1:F:764:ARG:HH21	1:F:764:ARG:HG2	1.85	0.41
1:E:605:GLU:HG3	1:F:524:PRO:HD3	2.02	0.41
1:C:406:ASN:HD22	1:C:424:ASP:CG	2.23	0.41
1:A:546:PRO:CG	1:A:567:ASP:HB3	2.50	0.41
1:B:217:VAL:HG23	1:B:218:ASN:N	2.35	0.41
1:D:387:LEU:HD22	1:D:388:GLY:H	1.84	0.41
1:D:109:TYR:CE2	1:D:120:ARG:HB2	2.55	0.41
1:D:64:HIS:HB2	1:D:71:THR:HG23	2.01	0.41
1:D:799:GLY:O	1:D:800:ILE:HG23	2.19	0.41
1:C:386:PHE:N	1:C:386:PHE:CD1	2.88	0.41
1:A:363:ARG:HD3	1:A:363:ARG:HA	1.77	0.41
1:F:59:ASP:OD2	1:F:59:ASP:N	2.53	0.41
1:A:1010:GLU:HB3	1:A:1011:PHE:CD1	2.55	0.41
1:C:82:ASN:HD21	1:C:96:ARG:HH21	1.67	0.41
1:F:662:LEU:HD12	1:F:662:LEU:O	2.21	0.41
1:C:1008:GLN:HB2	1:C:1008:GLN:HE21	1.68	0.41
1:B:155:PRO:HG2	1:B:156:PHE:CD1	2.56	0.41
1:B:285:ILE:HD12	1:B:296:PHE:CD2	2.54	0.41
1:D:44:LEU:HD13	1:D:733:ASN:ND2	2.35	0.41
1:F:872:HIS:HE1	1:F:902:GLU:OE1	2.03	0.41
1:B:809:ASP:HB3	1:B:814:THR:HA	2.02	0.41
1:C:363:ARG:HA	1:C:363:ARG:HD3	1.79	0.41
1:B:936:ASP:HB3	1:B:944:SER:HB3	2.00	0.41
1:F:270:PHE:CD2	1:F:289:LYS:HE2	2.55	0.41
1:E:295:ILE:HG13	1:E:306:ILE:HD11	2.03	0.41
1:A:351:SER:OG	1:A:353:THR:CG2	2.65	0.41
1:C:530:ASN:HD22	1:C:531:PHE:N	2.13	0.41
1:A:578:ILE:O	1:A:580:VAL:N	2.54	0.41
1:D:88:PRO:HG2	1:D:89:ASP:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:ASN:HD22	1:D:424:ASP:CG	2.23	0.41
1:C:285:ILE:HD12	1:C:296:PHE:CD2	2.56	0.41
1:A:285:ILE:HD12	1:A:296:PHE:CD2	2.56	0.41
1:E:54:ILE:HG23	1:E:86:PHE:CZ	2.56	0.41
1:E:146:LEU:HD23	1:E:165:VAL:HG21	2.02	0.41
1:B:194:ARG:HD2	3:B:1279:HOH:O	2.20	0.41
1:A:91:ARG:NH1	1:A:114:GLU:HB2	2.36	0.41
1:C:550:ASN:OD1	1:C:550:ASN:C	2.58	0.41
1:A:131:ARG:HH12	2:A:1214:DKT:HD61	1.85	0.41
1:C:706:VAL:HG12	1:C:710:ILE:HG12	2.02	0.41
1:C:124:PHE:HB3	1:C:152:ALA:HB1	2.01	0.41
1:E:703:ASN:C	1:E:703:ASN:ND2	2.73	0.41
1:A:522:PRO:CG	1:B:889:MET:SD	3.07	0.41
1:A:367:VAL:CG1	1:A:375:VAL:HG21	2.51	0.41
1:F:936:ASP:HB3	1:F:944:SER:HB3	2.01	0.41
1:B:753:THR:HB	3:B:1319:HOH:O	2.21	0.41
1:C:45:ASN:HB3	1:C:277:HIS:CE1	2.55	0.41
1:B:731:LEU:HD13	1:B:735:ILE:HD12	2.03	0.41
1:A:715:TYR:CZ	1:A:719:ARG:HD2	2.55	0.41
1:C:175:LEU:O	1:C:177:LEU:HG	2.20	0.41
1:A:462:ALA:HA	1:A:481:HIS:O	2.20	0.41
1:E:904:SER:OG	1:F:473:ASP:HA	2.20	0.41
1:B:131:ARG:HH12	2:B:1214:DKT:HD61	1.85	0.41
1:C:322:PRO:HG3	1:C:673:THR:O	2.20	0.41
1:E:470:GLY:O	1:E:473:ASP:HB2	2.20	0.41
1:B:706:VAL:HG12	1:B:710:ILE:HG12	2.02	0.41
1:D:1032:GLU:C	1:D:1033:ILE:HD12	2.41	0.41
1:F:537:SER:HB3	1:F:583:GLY:O	2.21	0.41
1:D:467:LEU:HD21	1:D:496:GLU:HB3	2.02	0.41
1:A:414:ARG:NH1	1:A:644:ASP:HA	2.35	0.41
1:B:565:GLU:HG2	1:B:566:TYR:N	2.35	0.41
1:E:497:ASN:ND2	1:F:868:ARG:HH12	2.19	0.41
1:F:65:ASP:CA	3:F:1222:HOH:O	2.65	0.41
1:C:681:SER:OG	1:C:684:GLU:HG2	2.21	0.41
1:E:45:ASN:N	1:E:45:ASN:ND2	2.66	0.41
1:B:467:LEU:HD21	1:B:496:GLU:HB3	2.03	0.41
1:E:694:TRP:HA	1:E:738:MET:CE	2.51	0.41
1:C:425:ARG:O	1:C:426:PHE:HB2	2.20	0.41
1:A:693:ALA:HB2	1:A:1006:LEU:HD11	2.03	0.41
1:B:1010:GLU:HB3	1:B:1011:PHE:CD1	2.56	0.41
1:C:887:MET:HB2	1:C:917:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:GLN:NE2	1:D:253:GLN:HA	2.36	0.41
1:B:253:GLN:HA	1:B:253:GLN:NE2	2.35	0.41
1:F:46:PRO:HB2	1:F:286:LEU:CD2	2.51	0.41
1:F:1014:TRP:NE1	1:F:1019:GLY:HA2	2.36	0.41
1:C:777:VAL:HG22	1:C:778:VAL:N	2.35	0.41
1:A:442:GLU:OE2	1:A:481:HIS:HD2	2.04	0.41
1:B:840:LYS:N	3:B:1294:HOH:O	2.54	0.41
1:B:54:ILE:HG23	1:B:86:PHE:CZ	2.55	0.41
1:F:729:TYR:O	1:F:732:SER:HB3	2.21	0.41
1:F:369:ARG:HH21	1:F:369:ARG:HG3	1.85	0.41
1:D:764:ARG:HH21	1:D:764:ARG:HG2	1.85	0.41
1:B:550:ASN:C	1:B:550:ASN:OD1	2.59	0.41
1:A:131:ARG:NH1	2:A:1214:DKT:HD62	2.35	0.41
1:F:1010:GLU:HB3	1:F:1011:PHE:CD1	2.55	0.41
1:B:131:ARG:NH1	2:B:1214:DKT:HD62	2.36	0.41
1:E:134:PHE:CB	3:E:1286:HOH:O	2.54	0.41
1:B:287:PHE:CZ	1:B:294:TYR:HB2	2.56	0.41
1:F:203:LYS:HE3	1:F:741:GLU:OE1	2.21	0.41
1:E:976:LYS:NZ	1:E:1017:ASP:HB2	2.35	0.41
1:F:518:ARG:C	3:F:1221:HOH:O	2.59	0.41
1:A:256:SER:OG	1:A:267:HIS:CE1	2.70	0.41
1:A:147:ILE:CD1	3:A:1264:HOH:O	2.69	0.41
1:F:236:VAL:HG23	1:F:243:TYR:HB2	2.03	0.41
1:B:236:VAL:HG23	1:B:243:TYR:HB2	2.01	0.41
1:A:1031:VAL:HG12	1:A:1033:ILE:HD12	2.02	0.41
1:F:222:PHE:H	1:F:1038:HIS:HD2	1.69	0.41
1:C:1031:VAL:HG11	1:C:1050:TYR:CZ	2.56	0.41
1:D:1010:GLU:HB3	1:D:1011:PHE:CD1	2.56	0.41
1:D:45:ASN:HB3	1:D:277:HIS:CE1	2.56	0.41
1:B:91:ARG:NH2	3:B:1273:HOH:O	2.53	0.41
1:F:644:ASP:OD2	1:F:646:LYS:HB2	2.21	0.41
1:B:603:HIS:HD2	1:B:604:GLY:O	2.04	0.41
1:C:448:MET:HB2	3:C:1277:HOH:O	2.20	0.41
1:B:369:ARG:HH21	1:B:369:ARG:HG3	1.86	0.41
1:D:644:ASP:OD2	1:D:646:LYS:HB2	2.20	0.41
1:C:93:ILE:HD12	1:C:111:TYR:HD2	1.85	0.41
1:F:297:ASN:O	1:F:301:GLU:N	2.46	0.41
1:A:43:LEU:HD22	1:A:55:PHE:CE1	2.55	0.41
1:D:425:ARG:O	1:D:426:PHE:HB2	2.21	0.41
1:C:715:TYR:CZ	1:C:719:ARG:HD2	2.56	0.41
1:B:993:GLY:N	1:B:1011:PHE:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:HH12	2:C:1214:DKT:HD61	1.86	0.41
1:D:253:GLN:HE21	1:D:253:GLN:HA	1.86	0.41
1:C:353:THR:HG23	1:C:354:TYR:CD1	2.55	0.41
1:F:578:ILE:O	1:F:580:VAL:N	2.54	0.41
1:E:317:ARG:CZ	3:E:1226:HOH:O	2.69	0.41
1:A:764:ARG:HG2	1:A:764:ARG:HH21	1.86	0.41
1:C:524:PRO:HD3	1:D:605:GLU:HG3	2.02	0.41
1:A:217:VAL:HG23	1:A:218:ASN:N	2.36	0.41
1:E:731:LEU:HD13	1:E:735:ILE:HD12	2.01	0.41
1:A:313:SER:O	1:D:117:GLU:HA	2.21	0.41
1:D:125:SER:CB	1:D:762:SER:HB2	2.50	0.41
1:E:728:ARG:HG3	1:E:754:PHE:CE1	2.56	0.41
1:C:976:LYS:NZ	1:C:1017:ASP:HB2	2.36	0.41
1:E:522:PRO:HG2	1:F:889:MET:SD	2.61	0.41
1:B:764:ARG:HG2	1:B:764:ARG:HH21	1.86	0.41
1:A:993:GLY:N	1:A:1011:PHE:O	2.54	0.40
1:C:1010:GLU:HB3	1:C:1011:PHE:CD1	2.56	0.40
1:B:532:SER:OG	1:B:534:GLU:OE1	2.39	0.40
1:E:203:LYS:HE3	1:E:741:GLU:OE1	2.20	0.40
1:A:489:LYS:HE2	1:A:491:PHE:HZ	1.85	0.40
1:F:499:HIS:CD2	3:F:1263:HOH:O	2.71	0.40
1:B:363:ARG:NH2	3:B:1281:HOH:O	2.37	0.40
1:B:770:LYS:O	1:B:777:VAL:HG12	2.21	0.40
1:F:776:TYR:CE1	1:F:821:ILE:HB	2.56	0.40
1:F:387:LEU:HD22	1:F:388:GLY:H	1.86	0.40
1:C:906:GLN:O	1:C:953:GLY:HA3	2.22	0.40
1:B:387:LEU:HD22	1:B:388:GLY:H	1.86	0.40
1:C:369:ARG:HG3	1:C:369:ARG:HH21	1.86	0.40
1:B:53:ILE:HG23	1:B:286:LEU:CD2	2.45	0.40
1:E:1000:LEU:HB2	1:E:1004:THR:HB	2.04	0.40
1:C:1014:TRP:NE1	1:C:1019:GLY:HA2	2.36	0.40
1:E:201:HIS:O	1:E:740:GLY:HA2	2.22	0.40
1:B:184:LEU:HD13	1:B:237:ILE:HG13	2.02	0.40
1:B:715:TYR:CZ	1:B:719:ARG:HD2	2.56	0.40
1:D:884:ILE:HG22	1:D:886:ASP:O	2.21	0.40
1:C:393:ARG:HH12	1:E:557:ARG:HG3	1.87	0.40
1:D:287:PHE:CZ	1:D:294:TYR:HB2	2.57	0.40
1:C:368:ARG:CZ	3:C:1251:HOH:O	2.69	0.40
1:A:904:SER:OG	1:B:473:ASP:HA	2.22	0.40
1:E:710:ILE:HD13	1:E:713:ARG:NH2	2.36	0.40
1:C:660:PHE:HB3	1:C:668:GLU:CB	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:HD11	3:A:1264:HOH:O	2.21	0.40
1:B:243:TYR:CD2	1:B:256:SER:HB3	2.55	0.40
1:D:467:LEU:HD12	1:D:467:LEU:C	2.41	0.40
1:E:776:TYR:CE1	1:E:821:ILE:HB	2.56	0.40
1:E:46:PRO:HD3	1:E:288:SER:HB3	2.03	0.40
1:F:184:LEU:HD13	1:F:237:ILE:HG13	2.03	0.40
1:F:976:LYS:NZ	1:F:1017:ASP:HB2	2.36	0.40
1:A:46:PRO:HD3	1:A:288:SER:HB3	2.02	0.40
1:A:746:HIS:HA	1:A:748:TYR:CE2	2.56	0.40
1:C:287:PHE:CZ	1:C:294:TYR:HB2	2.57	0.40
1:F:526:ARG:NH2	3:F:1225:HOH:O	2.53	0.40
1:A:317:ARG:HB3	3:A:1294:HOH:O	2.21	0.40
1:C:912:VAL:HG11	1:C:970:PHE:CE2	2.57	0.40
1:C:977:LEU:HB2	1:C:979:LEU:HD13	2.03	0.40
1:E:684:GLU:HG3	1:E:685:GLU:N	2.35	0.40
1:B:913:ARG:O	1:B:914:PHE:HB2	2.20	0.40
1:E:532:SER:OG	1:E:534:GLU:OE1	2.39	0.40
1:E:467:LEU:HD21	1:E:496:GLU:HB3	2.03	0.40
1:F:977:LEU:HB2	1:F:979:LEU:HD13	2.03	0.40
1:E:768:ASP:HB2	1:E:780:LYS:HB3	2.04	0.40
1:D:1000:LEU:HB2	1:D:1004:THR:HB	2.03	0.40
1:E:882:ILE:HD11	1:E:899:PHE:HA	2.03	0.40
1:A:164:ARG:CG	3:A:1264:HOH:O	2.65	0.40
1:B:256:SER:OG	1:B:267:HIS:CE1	2.72	0.40
1:E:236:VAL:HG23	1:E:243:TYR:HB2	2.03	0.40
1:A:312:GLU:HG2	1:A:314:PRO:HD3	2.02	0.40
1:D:365:ARG:NH2	3:D:1341:HOH:O	2.38	0.40
1:D:694:TRP:HA	1:D:738:MET:HE2	2.02	0.40
1:C:537:SER:HB3	1:C:583:GLY:O	2.22	0.40
1:F:218:ASN:HB3	1:F:221:ALA:HB3	2.03	0.40
1:A:300:THR:HG22	1:A:302:LYS:HB2	2.04	0.40
1:D:648:VAL:O	1:D:659:THR:HA	2.21	0.40
1:C:91:ARG:NH1	1:C:114:GLU:HB2	2.36	0.40
1:B:414:ARG:NH1	1:B:644:ASP:HA	2.37	0.40
1:A:701:TYR:O	1:B:939:ARG:HD3	2.22	0.40
1:A:532:SER:OG	1:A:534:GLU:OE1	2.39	0.40
1:E:125:SER:CB	1:E:762:SER:HB2	2.51	0.40
1:E:407:VAL:O	1:E:998:ARG:NH1	2.55	0.40
1:C:59:ASP:OD2	1:C:59:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1071 (95%)	950 (93%)	66 (6%)	5 (0%)	34	63
1	B	1021/1071 (95%)	948 (93%)	68 (7%)	5 (0%)	34	63
1	C	1021/1071 (95%)	947 (93%)	69 (7%)	5 (0%)	34	63
1	D	1021/1071 (95%)	955 (94%)	61 (6%)	5 (0%)	34	63
1	E	1021/1071 (95%)	951 (93%)	65 (6%)	5 (0%)	34	63
1	F	1021/1071 (95%)	946 (93%)	69 (7%)	6 (1%)	30	59
All	All	6126/6426 (95%)	5697 (93%)	398 (6%)	31 (0%)	34	63

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	ASN
1	B	579	ASN
1	C	579	ASN
1	D	579	ASN
1	E	579	ASN
1	F	579	ASN
1	A	562	GLU
1	B	562	GLU
1	C	562	GLU
1	D	562	GLU
1	E	562	GLU
1	F	562	GLU
1	A	220	GLY
1	A	259	LEU
1	B	220	GLY
1	B	259	LEU
1	C	220	GLY
1	D	220	GLY
1	E	220	GLY
1	F	220	GLY

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Mol	Chain	Res	Type
1	C	259	LEU
1	C	919	PHE
1	D	259	LEU
1	D	919	PHE
1	E	259	LEU
1	E	919	PHE
1	F	259	LEU
1	F	919	PHE
1	B	919	PHE
1	A	919	PHE
1	F	1009	PRO

5.3.2 Protein sidechains (i)

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	883/928 (95%)	842 (95%)	41 (5%)	33	64
1	B	882/928 (95%)	841 (95%)	41 (5%)	33	64
1	C	882/928 (95%)	840 (95%)	42 (5%)	31	62
1	D	882/928 (95%)	841 (95%)	41 (5%)	33	64
1	E	883/928 (95%)	839 (95%)	44 (5%)	30	60
1	F	882/928 (95%)	841 (95%)	41 (5%)	33	64
All	All	5294/5568 (95%)	5044 (95%)	250 (5%)	32	63

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	46	PRO
1	A	61	LEU
1	A	75	VAL
1	A	82	ASN
1	A	104	ASN
1	A	128	SER

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Mol	Chain	Res	Type
1	A	209	THR
1	A	260	ASP
1	A	279	ASN
1	A	297	ASN
1	A	351	SER
1	A	353	THR
1	A	368	ARG
1	A	403	ASN
1	A	423	ASN
1	A	429	MET
1	A	473	ASP
1	A	481	HIS
1	A	496	GLU
1	A	530	ASN
1	A	562	GLU
1	A	578	ILE
1	A	580	VAL
1	A	588	ILE
1	A	681	SER
1	A	703	ASN
1	A	731	LEU
1	A	738	MET
1	A	764	ARG
1	A	765	ILE
1	A	772	ASP
1	A	809	ASP
1	A	847	LEU
1	A	853	ASP
1	A	892	LEU
1	A	929	MET
1	A	1008	GLN
1	A	1015	PHE
1	A	1024	ASN
1	A	1035	TYR
1	B	44	LEU
1	B	46	PRO
1	B	61	LEU
1	B	75	VAL
1	B	82	ASN
1	B	104	ASN
1	B	128	SER
1	B	209	THR

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Mol	Chain	Res	Type
1	B	260	ASP
1	B	279	ASN
1	B	297	ASN
1	B	353	THR
1	B	368	ARG
1	B	403	ASN
1	B	415	ASN
1	B	423	ASN
1	B	429	MET
1	B	473	ASP
1	B	481	HIS
1	B	496	GLU
1	B	530	ASN
1	B	562	GLU
1	B	578	ILE
1	B	580	VAL
1	B	588	ILE
1	B	681	SER
1	B	703	ASN
1	B	731	LEU
1	B	738	MET
1	B	764	ARG
1	B	765	ILE
1	B	772	ASP
1	B	809	ASP
1	B	847	LEU
1	B	853	ASP
1	B	892	LEU
1	B	929	MET
1	B	1008	GLN
1	B	1015	PHE
1	B	1024	ASN
1	B	1035	TYR
1	C	44	LEU
1	C	61	LEU
1	C	71	THR
1	C	75	VAL
1	C	82	ASN
1	C	104	ASN
1	C	128	SER
1	C	209	THR
1	C	260	ASP

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Mol	Chain	Res	Type
1	C	279	ASN
1	C	297	ASN
1	C	353	THR
1	C	368	ARG
1	C	403	ASN
1	C	415	ASN
1	C	423	ASN
1	C	429	MET
1	C	473	ASP
1	C	481	HIS
1	C	496	GLU
1	C	530	ASN
1	C	562	GLU
1	C	578	ILE
1	C	580	VAL
1	C	588	ILE
1	C	593	SER
1	C	681	SER
1	C	703	ASN
1	C	731	LEU
1	C	738	MET
1	C	764	ARG
1	C	765	ILE
1	C	772	ASP
1	C	809	ASP
1	C	847	LEU
1	C	853	ASP
1	C	892	LEU
1	C	929	MET
1	C	1008	GLN
1	C	1015	PHE
1	C	1024	ASN
1	C	1035	TYR
1	D	44	LEU
1	D	61	LEU
1	D	75	VAL
1	D	82	ASN
1	D	104	ASN
1	D	128	SER
1	D	209	THR
1	D	260	ASP
1	D	279	ASN

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Mol	Chain	Res	Type
1	D	297	ASN
1	D	311	LEU
1	D	351	SER
1	D	353	THR
1	D	368	ARG
1	D	403	ASN
1	D	415	ASN
1	D	423	ASN
1	D	429	MET
1	D	473	ASP
1	D	481	HIS
1	D	496	GLU
1	D	530	ASN
1	D	562	GLU
1	D	578	ILE
1	D	588	ILE
1	D	681	SER
1	D	703	ASN
1	D	731	LEU
1	D	738	MET
1	D	764	ARG
1	D	765	ILE
1	D	772	ASP
1	D	809	ASP
1	D	847	LEU
1	D	853	ASP
1	D	892	LEU
1	D	929	MET
1	D	1008	GLN
1	D	1015	PHE
1	D	1024	ASN
1	D	1035	TYR
1	E	44	LEU
1	E	46	PRO
1	E	59	ASP
1	E	61	LEU
1	E	75	VAL
1	E	82	ASN
1	E	104	ASN
1	E	128	SER
1	E	209	THR
1	E	260	ASP

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Mol	Chain	Res	Type
1	E	279	ASN
1	E	297	ASN
1	E	311	LEU
1	E	351	SER
1	E	353	THR
1	E	368	ARG
1	E	403	ASN
1	E	415	ASN
1	E	423	ASN
1	E	429	MET
1	E	473	ASP
1	E	481	HIS
1	E	496	GLU
1	E	530	ASN
1	E	562	GLU
1	E	578	ILE
1	E	588	ILE
1	E	681	SER
1	E	703	ASN
1	E	731	LEU
1	E	738	MET
1	E	764	ARG
1	E	765	ILE
1	E	772	ASP
1	E	809	ASP
1	E	847	LEU
1	E	853	ASP
1	E	892	LEU
1	E	929	MET
1	E	965	SER
1	E	1008	GLN
1	E	1015	PHE
1	E	1024	ASN
1	E	1035	TYR
1	F	44	LEU
1	F	46	PRO
1	F	59	ASP
1	F	61	LEU
1	F	71	THR
1	F	75	VAL
1	F	82	ASN
1	F	104	ASN

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Mol	Chain	Res	Type
1	F	128	SER
1	F	260	ASP
1	F	279	ASN
1	F	297	ASN
1	F	353	THR
1	F	368	ARG
1	F	403	ASN
1	F	415	ASN
1	F	423	ASN
1	F	429	MET
1	F	473	ASP
1	F	481	HIS
1	F	496	GLU
1	F	562	GLU
1	F	578	ILE
1	F	580	VAL
1	F	588	ILE
1	F	681	SER
1	F	703	ASN
1	F	731	LEU
1	F	738	MET
1	F	764	ARG
1	F	765	ILE
1	F	772	ASP
1	F	809	ASP
1	F	847	LEU
1	F	853	ASP
1	F	892	LEU
1	F	929	MET
1	F	1008	GLN
1	F	1015	PHE
1	F	1024	ASN
1	F	1035	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	82	ASN
1	A	104	ASN
1	A	253	GLN
1	A	267	HIS

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Mol	Chain	Res	Type
1	A	279	ASN
1	A	297	ASN
1	A	403	ASN
1	A	415	ASN
1	A	423	ASN
1	A	469	HIS
1	A	481	HIS
1	A	497	ASN
1	A	511	ASN
1	A	530	ASN
1	A	603	HIS
1	A	611	GLN
1	A	703	ASN
1	A	733	ASN
1	A	739	GLN
1	A	867	ASN
1	A	872	HIS
1	A	922	GLN
1	A	930	ASN
1	A	949	ASN
1	A	1008	GLN
1	A	1024	ASN
1	A	1038	HIS
1	A	1047	GLN
1	B	45	ASN
1	B	64	HIS
1	B	82	ASN
1	B	104	ASN
1	B	253	GLN
1	B	267	HIS
1	B	279	ASN
1	B	297	ASN
1	B	403	ASN
1	B	415	ASN
1	B	423	ASN
1	B	469	HIS
1	B	481	HIS
1	B	497	ASN
1	B	511	ASN
1	B	530	ASN
1	B	603	HIS
1	B	611	GLN

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Mol	Chain	Res	Type
1	B	703	ASN
1	B	733	ASN
1	B	739	GLN
1	B	867	ASN
1	B	872	HIS
1	B	922	GLN
1	B	930	ASN
1	B	949	ASN
1	B	1008	GLN
1	B	1024	ASN
1	B	1038	HIS
1	B	1047	GLN
1	C	45	ASN
1	C	64	HIS
1	C	82	ASN
1	C	104	ASN
1	C	201	HIS
1	C	253	GLN
1	C	267	HIS
1	C	297	ASN
1	C	403	ASN
1	C	406	ASN
1	C	415	ASN
1	C	423	ASN
1	C	469	HIS
1	C	481	HIS
1	C	497	ASN
1	C	499	HIS
1	C	530	ASN
1	C	603	HIS
1	C	611	GLN
1	C	703	ASN
1	C	733	ASN
1	C	739	GLN
1	C	867	ASN
1	C	872	HIS
1	C	922	GLN
1	C	930	ASN
1	C	949	ASN
1	C	1008	GLN
1	C	1024	ASN
1	C	1038	HIS

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Mol	Chain	Res	Type
1	C	1047	GLN
1	D	45	ASN
1	D	64	HIS
1	D	82	ASN
1	D	104	ASN
1	D	195	ASN
1	D	218	ASN
1	D	253	GLN
1	D	267	HIS
1	D	279	ASN
1	D	297	ASN
1	D	403	ASN
1	D	415	ASN
1	D	423	ASN
1	D	469	HIS
1	D	481	HIS
1	D	497	ASN
1	D	499	HIS
1	D	511	ASN
1	D	530	ASN
1	D	603	HIS
1	D	611	GLN
1	D	635	ASN
1	D	703	ASN
1	D	733	ASN
1	D	739	GLN
1	D	867	ASN
1	D	872	HIS
1	D	922	GLN
1	D	930	ASN
1	D	949	ASN
1	D	1008	GLN
1	D	1024	ASN
1	D	1038	HIS
1	D	1047	GLN
1	E	45	ASN
1	E	64	HIS
1	E	82	ASN
1	E	104	ASN
1	E	195	ASN
1	E	253	GLN
1	E	267	HIS

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Mol	Chain	Res	Type
1	E	277	HIS
1	E	279	ASN
1	E	297	ASN
1	E	403	ASN
1	E	406	ASN
1	E	415	ASN
1	E	423	ASN
1	E	481	HIS
1	E	497	ASN
1	E	499	HIS
1	E	511	ASN
1	E	530	ASN
1	E	603	HIS
1	E	611	GLN
1	E	703	ASN
1	E	733	ASN
1	E	739	GLN
1	E	867	ASN
1	E	872	HIS
1	E	922	GLN
1	E	930	ASN
1	E	949	ASN
1	E	1008	GLN
1	E	1024	ASN
1	E	1038	HIS
1	E	1047	GLN
1	F	64	HIS
1	F	82	ASN
1	F	104	ASN
1	F	201	HIS
1	F	253	GLN
1	F	267	HIS
1	F	279	ASN
1	F	297	ASN
1	F	403	ASN
1	F	406	ASN
1	F	415	ASN
1	F	423	ASN
1	F	481	HIS
1	F	497	ASN
1	F	499	HIS
1	F	530	ASN

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Mol	Chain	Res	Type
1	F	603	HIS
1	F	611	GLN
1	F	703	ASN
1	F	733	ASN
1	F	739	GLN
1	F	867	ASN
1	F	872	HIS
1	F	922	GLN
1	F	930	ASN
1	F	949	ASN
1	F	1008	GLN
1	F	1024	ASN
1	F	1038	HIS
1	F	1047	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

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DKT	A	1214	1	47,57,57	3.78	26 (55%)	56,74,74	5.62	37 (66%)
2	DKT	B	1214	1	47,57,57	3.78	26 (55%)	56,74,74	5.62	37 (66%)
2	DKT	C	1214	1	47,57,57	3.78	26 (55%)	56,74,74	5.62	37 (66%)
2	DKT	D	1214	1	47,57,57	3.78	26 (55%)	56,74,74	5.63	37 (66%)
2	DKT	E	1214	1	47,57,57	3.78	26 (55%)	56,74,74	5.62	37 (66%)
2	DKT	F	1214	1	47,57,57	3.78	26 (55%)	56,74,74	5.62	37 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DKT	A	1214	1	1/1/14/19	3/53/77/77	0/3/3/3
2	DKT	B	1214	1	1/1/14/19	3/53/77/77	0/3/3/3
2	DKT	C	1214	1	1/1/14/19	3/53/77/77	0/3/3/3
2	DKT	D	1214	1	1/1/14/19	3/53/77/77	0/3/3/3
2	DKT	E	1214	1	1/1/14/19	3/53/77/77	0/3/3/3
2	DKT	F	1214	1	1/1/14/19	3/53/77/77	0/3/3/3

All (156) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1214	DKT	OC2-CC2	-5.99	1.32	1.45
2	B	1214	DKT	OC2-CC2	-5.99	1.32	1.45
2	E	1214	DKT	OC2-CC2	-5.97	1.32	1.45
2	F	1214	DKT	OC2-CC2	-5.96	1.32	1.45
2	A	1214	DKT	OC2-CC2	-5.96	1.32	1.45
2	A	1214	DKT	CA1-N	-5.93	1.32	1.45
2	C	1214	DKT	OC2-CC2	-5.93	1.32	1.45
2	B	1214	DKT	CA1-N	-5.93	1.32	1.45
2	E	1214	DKT	CA1-N	-5.92	1.32	1.45
2	D	1214	DKT	CA1-N	-5.92	1.32	1.45
2	C	1214	DKT	CA1-N	-5.89	1.32	1.45
2	F	1214	DKT	CA1-N	-5.88	1.32	1.45
2	B	1214	DKT	CA2-N1	-5.61	1.33	1.45
2	A	1214	DKT	CA2-N1	-5.60	1.33	1.45
2	E	1214	DKT	CA2-N1	-5.60	1.33	1.45
2	C	1214	DKT	CA2-N1	-5.59	1.33	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1214	DKT	CA2-N1	-5.59	1.33	1.45
2	D	1214	DKT	CA2-N1	-5.58	1.33	1.45
2	A	1214	DKT	O2-C8	-5.53	1.12	1.23
2	E	1214	DKT	O2-C8	-5.50	1.12	1.23
2	B	1214	DKT	O2-C8	-5.50	1.12	1.23
2	F	1214	DKT	O2-C8	-5.49	1.12	1.23
2	D	1214	DKT	O2-C8	-5.49	1.12	1.23
2	C	1214	DKT	O2-C8	-5.48	1.12	1.23
2	D	1214	DKT	CE1-CD1	-4.13	1.42	1.53
2	C	1214	DKT	CE1-CD1	-4.12	1.42	1.53
2	E	1214	DKT	CE1-CD1	-4.12	1.42	1.53
2	A	1214	DKT	CE1-CD1	-4.12	1.42	1.53
2	B	1214	DKT	CE1-CD1	-4.10	1.42	1.53
2	F	1214	DKT	CE1-CD1	-4.10	1.42	1.53
2	A	1214	DKT	CE6-CD5	-3.95	1.42	1.53
2	B	1214	DKT	CE6-CD5	-3.93	1.42	1.53
2	E	1214	DKT	CD5-CG4	-3.93	1.41	1.52
2	B	1214	DKT	CD5-CG4	-3.93	1.41	1.52
2	C	1214	DKT	CD5-CG4	-3.93	1.41	1.52
2	D	1214	DKT	CE6-CD5	-3.93	1.42	1.53
2	F	1214	DKT	CE6-CD5	-3.92	1.42	1.53
2	D	1214	DKT	CD5-CG4	-3.91	1.42	1.52
2	C	1214	DKT	CE6-CD5	-3.91	1.42	1.53
2	E	1214	DKT	CE6-CD5	-3.91	1.42	1.53
2	F	1214	DKT	CD5-CG4	-3.91	1.42	1.52
2	A	1214	DKT	CD5-CG4	-3.90	1.42	1.52
2	F	1214	DKT	CB1-CG1	-3.90	1.46	1.53
2	B	1214	DKT	CB1-CG1	-3.88	1.46	1.53
2	A	1214	DKT	CB1-CG1	-3.86	1.46	1.53
2	E	1214	DKT	CB1-CG1	-3.86	1.46	1.53
2	A	1214	DKT	CE2-CD2	-3.85	1.42	1.53
2	D	1214	DKT	CB1-CG1	-3.84	1.46	1.53
2	C	1214	DKT	CB1-CG1	-3.83	1.46	1.53
2	D	1214	DKT	CE2-CD2	-3.83	1.42	1.53
2	F	1214	DKT	CE2-CD2	-3.83	1.42	1.53
2	E	1214	DKT	CE2-CD2	-3.82	1.42	1.53
2	C	1214	DKT	CE2-CD2	-3.80	1.43	1.53
2	B	1214	DKT	CE2-CD2	-3.78	1.43	1.53
2	B	1214	DKT	CA3-C9	-3.70	1.42	1.52
2	A	1214	DKT	CA3-C9	-3.69	1.42	1.52
2	C	1214	DKT	CA3-C9	-3.68	1.42	1.52
2	E	1214	DKT	CA3-C9	-3.67	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1214	DKT	CA3-C9	-3.67	1.42	1.52
2	D	1214	DKT	CA3-C9	-3.65	1.42	1.52
2	D	1214	DKT	CD2-CG1	-3.63	1.42	1.52
2	A	1214	DKT	CD2-CG1	-3.63	1.42	1.52
2	C	1214	DKT	CD1-CG1	-3.62	1.42	1.52
2	B	1214	DKT	CD2-CG1	-3.62	1.42	1.52
2	E	1214	DKT	CD2-CG1	-3.61	1.42	1.52
2	C	1214	DKT	CD2-CG1	-3.61	1.42	1.52
2	F	1214	DKT	CD1-CG1	-3.60	1.42	1.52
2	D	1214	DKT	CD1-CG1	-3.60	1.42	1.52
2	A	1214	DKT	CD1-CG1	-3.59	1.42	1.52
2	E	1214	DKT	CD1-CG1	-3.59	1.42	1.52
2	F	1214	DKT	CD2-CG1	-3.59	1.42	1.52
2	B	1214	DKT	CD1-CG1	-3.59	1.42	1.52
2	A	1214	DKT	CE7-CD6	-3.46	1.43	1.53
2	E	1214	DKT	CE7-CD6	-3.45	1.43	1.53
2	F	1214	DKT	CE7-CD6	-3.45	1.43	1.53
2	D	1214	DKT	CE7-CD6	-3.45	1.43	1.53
2	C	1214	DKT	CE7-CD6	-3.44	1.43	1.53
2	B	1214	DKT	CE7-CD6	-3.43	1.43	1.53
2	B	1214	DKT	CD6-CG4	-3.33	1.43	1.52
2	D	1214	DKT	CD6-CG4	-3.32	1.43	1.52
2	A	1214	DKT	CD6-CG4	-3.29	1.43	1.52
2	E	1214	DKT	CD6-CG4	-3.29	1.43	1.52
2	F	1214	DKT	CD6-CG4	-3.29	1.43	1.52
2	C	1214	DKT	CD6-CG4	-3.29	1.43	1.52
2	D	1214	DKT	C9-N3	-3.11	1.26	1.34
2	E	1214	DKT	C9-N3	-3.11	1.26	1.34
2	C	1214	DKT	C9-N3	-3.11	1.26	1.34
2	A	1214	DKT	C9-N3	-3.11	1.26	1.34
2	F	1214	DKT	C9-N3	-3.10	1.26	1.34
2	B	1214	DKT	C9-N3	-3.08	1.26	1.34
2	C	1214	DKT	CZ1-CE2	-2.22	1.42	1.51
2	B	1214	DKT	CZ1-CE2	-2.22	1.42	1.51
2	E	1214	DKT	CZ1-CE2	-2.22	1.42	1.51
2	A	1214	DKT	CZ1-CE2	-2.21	1.42	1.51
2	D	1214	DKT	CZ1-CE2	-2.21	1.42	1.51
2	F	1214	DKT	CZ1-CE2	-2.20	1.42	1.51
2	B	1214	DKT	CZ1-CE1	-2.14	1.42	1.51
2	F	1214	DKT	CZ1-CE1	-2.14	1.42	1.51
2	D	1214	DKT	CZ1-CE1	-2.14	1.42	1.51
2	E	1214	DKT	CZ1-CE1	-2.14	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1214	DKT	CZ1-CE1	-2.13	1.42	1.51
2	C	1214	DKT	CZ1-CE1	-2.12	1.42	1.51
2	B	1214	DKT	CA4-N3	2.11	1.49	1.46
2	A	1214	DKT	CA4-N3	2.12	1.49	1.46
2	D	1214	DKT	CA4-N3	2.13	1.49	1.46
2	E	1214	DKT	CA4-N3	2.14	1.49	1.46
2	F	1214	DKT	CA4-N3	2.14	1.49	1.46
2	C	1214	DKT	CA4-N3	2.19	1.49	1.46
2	D	1214	DKT	CA2-C8	2.36	1.59	1.52
2	F	1214	DKT	CA2-C8	2.37	1.59	1.52
2	B	1214	DKT	CA2-C8	2.38	1.59	1.52
2	C	1214	DKT	CA2-C8	2.38	1.59	1.52
2	E	1214	DKT	CA2-C8	2.39	1.59	1.52
2	A	1214	DKT	CA2-C8	2.41	1.59	1.52
2	D	1214	DKT	CB4-CA4	2.50	1.56	1.54
2	E	1214	DKT	CB4-CA4	2.52	1.56	1.54
2	C	1214	DKT	CB4-CA4	2.53	1.56	1.54
2	B	1214	DKT	CB4-CA4	2.54	1.56	1.54
2	A	1214	DKT	CB4-CA4	2.54	1.56	1.54
2	F	1214	DKT	CB4-CA4	2.58	1.57	1.54
2	F	1214	DKT	C4-C1	6.65	1.55	1.38
2	A	1214	DKT	C4-C1	6.65	1.55	1.38
2	D	1214	DKT	C4-C1	6.65	1.55	1.38
2	E	1214	DKT	C4-C1	6.65	1.55	1.38
2	B	1214	DKT	C4-C1	6.67	1.55	1.38
2	C	1214	DKT	C4-C1	6.67	1.55	1.38
2	A	1214	DKT	C1-C3	6.72	1.55	1.38
2	B	1214	DKT	C1-C3	6.73	1.55	1.38
2	F	1214	DKT	C1-C3	6.74	1.55	1.38
2	C	1214	DKT	C1-C3	6.74	1.55	1.38
2	E	1214	DKT	C1-C3	6.75	1.55	1.38
2	D	1214	DKT	C1-C3	6.76	1.55	1.38
2	D	1214	DKT	C5-CC3	7.58	1.54	1.38
2	A	1214	DKT	C5-CC3	7.59	1.55	1.38
2	B	1214	DKT	C5-CC3	7.60	1.55	1.38
2	E	1214	DKT	C5-CC3	7.61	1.55	1.38
2	F	1214	DKT	C5-CC3	7.62	1.55	1.38
2	C	1214	DKT	C5-CC3	7.63	1.55	1.38
2	D	1214	DKT	C2-CC3	7.74	1.55	1.38
2	A	1214	DKT	C2-CC3	7.74	1.55	1.38
2	E	1214	DKT	C2-CC3	7.75	1.55	1.38
2	B	1214	DKT	C2-CC3	7.76	1.55	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1214	DKT	C2-CC3	7.78	1.55	1.38
2	F	1214	DKT	C2-CC3	7.79	1.55	1.38
2	C	1214	DKT	C3-C2	7.96	1.55	1.38
2	E	1214	DKT	C3-C2	7.97	1.55	1.38
2	A	1214	DKT	C3-C2	7.98	1.55	1.38
2	B	1214	DKT	C3-C2	7.98	1.55	1.38
2	D	1214	DKT	C3-C2	7.99	1.55	1.38
2	F	1214	DKT	C3-C2	8.00	1.55	1.38
2	C	1214	DKT	C4-C5	8.03	1.55	1.38
2	F	1214	DKT	C4-C5	8.06	1.55	1.38
2	E	1214	DKT	C4-C5	8.08	1.55	1.38
2	A	1214	DKT	C4-C5	8.08	1.55	1.38
2	D	1214	DKT	C4-C5	8.12	1.55	1.38
2	B	1214	DKT	C4-C5	8.13	1.55	1.38

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1214	DKT	O3-C9-CA3	-6.61	105.75	120.36
2	E	1214	DKT	O3-C9-CA3	-6.60	105.77	120.36
2	B	1214	DKT	O3-C9-CA3	-6.59	105.79	120.36
2	D	1214	DKT	O3-C9-CA3	-6.59	105.79	120.36
2	F	1214	DKT	O3-C9-CA3	-6.59	105.80	120.36
2	A	1214	DKT	O3-C9-CA3	-6.58	105.80	120.36
2	F	1214	DKT	O2-C8-N2	-5.75	111.66	122.93
2	D	1214	DKT	O2-C8-N2	-5.73	111.70	122.93
2	E	1214	DKT	O2-C8-N2	-5.73	111.71	122.93
2	C	1214	DKT	O2-C8-N2	-5.73	111.71	122.93
2	B	1214	DKT	O2-C8-N2	-5.72	111.72	122.93
2	A	1214	DKT	O2-C8-N2	-5.69	111.78	122.93
2	A	1214	DKT	O2-C8-CA2	-5.02	109.26	120.36
2	B	1214	DKT	O2-C8-CA2	-5.01	109.28	120.36
2	D	1214	DKT	O2-C8-CA2	-5.01	109.29	120.36
2	E	1214	DKT	O2-C8-CA2	-5.01	109.29	120.36
2	C	1214	DKT	O2-C8-CA2	-5.00	109.30	120.36
2	F	1214	DKT	O2-C8-CA2	-4.99	109.33	120.36
2	F	1214	DKT	O12-CC1-N	-4.66	116.73	124.86
2	A	1214	DKT	O12-CC1-N	-4.65	116.73	124.86
2	E	1214	DKT	O12-CC1-N	-4.65	116.73	124.86
2	D	1214	DKT	O12-CC1-N	-4.65	116.75	124.86
2	B	1214	DKT	O12-CC1-N	-4.64	116.76	124.86
2	C	1214	DKT	O12-CC1-N	-4.64	116.76	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1214	DKT	CB3-CA3-N2	-3.56	104.08	110.87
2	C	1214	DKT	CB3-CA3-N2	-3.56	104.08	110.87
2	E	1214	DKT	CB3-CA3-N2	-3.54	104.12	110.87
2	A	1214	DKT	CB3-CA3-N2	-3.53	104.14	110.87
2	F	1214	DKT	CB3-CA3-N2	-3.52	104.16	110.87
2	D	1214	DKT	CB3-CA3-N2	-3.52	104.16	110.87
2	B	1214	DKT	C8-CA2-N1	-3.20	102.25	111.26
2	E	1214	DKT	C8-CA2-N1	-3.18	102.29	111.26
2	F	1214	DKT	C8-CA2-N1	-3.18	102.30	111.26
2	D	1214	DKT	C8-CA2-N1	-3.18	102.31	111.26
2	D	1214	DKT	CC2-CC3-C2	-3.18	113.04	120.66
2	A	1214	DKT	C8-CA2-N1	-3.18	102.31	111.26
2	F	1214	DKT	CC2-CC3-C2	-3.17	113.04	120.66
2	C	1214	DKT	C8-CA2-N1	-3.17	102.32	111.26
2	B	1214	DKT	CC2-CC3-C2	-3.17	113.05	120.66
2	C	1214	DKT	CC2-CC3-C2	-3.17	113.06	120.66
2	A	1214	DKT	CC2-CC3-C2	-3.17	113.06	120.66
2	E	1214	DKT	CC2-CC3-C2	-3.17	113.06	120.66
2	C	1214	DKT	CB1-CG1-CD2	-2.08	106.74	111.67
2	D	1214	DKT	CB1-CG1-CD2	-2.07	106.77	111.67
2	A	1214	DKT	CB1-CG1-CD2	-2.06	106.77	111.67
2	E	1214	DKT	CB1-CG1-CD2	-2.06	106.77	111.67
2	B	1214	DKT	CB1-CG1-CD2	-2.06	106.78	111.67
2	F	1214	DKT	CB1-CG1-CD2	-2.06	106.79	111.67
2	D	1214	DKT	CB1-CA1-N	2.13	115.81	110.49
2	A	1214	DKT	CB1-CA1-N	2.14	115.82	110.49
2	F	1214	DKT	CB1-CA1-N	2.15	115.84	110.49
2	E	1214	DKT	CB1-CA1-N	2.15	115.85	110.49
2	C	1214	DKT	CB1-CA1-N	2.16	115.88	110.49
2	B	1214	DKT	CB1-CA1-N	2.17	115.90	110.49
2	B	1214	DKT	CC2-CC3-C5	2.47	126.58	120.66
2	E	1214	DKT	CC2-CC3-C5	2.47	126.60	120.66
2	A	1214	DKT	CC2-CC3-C5	2.48	126.61	120.66
2	D	1214	DKT	CC2-CC3-C5	2.48	126.61	120.66
2	F	1214	DKT	CC2-CC3-C5	2.48	126.61	120.66
2	C	1214	DKT	CC2-CC3-C5	2.48	126.61	120.66
2	A	1214	DKT	CE7-CZ3-CE6	2.58	119.53	111.27
2	C	1214	DKT	CE7-CZ3-CE6	2.59	119.56	111.27
2	B	1214	DKT	CE7-CZ3-CE6	2.59	119.57	111.27
2	E	1214	DKT	CE7-CZ3-CE6	2.60	119.58	111.27
2	F	1214	DKT	CE7-CZ3-CE6	2.60	119.58	111.27
2	D	1214	DKT	CE7-CZ3-CE6	2.60	119.59	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1214	DKT	CE2-CZ1-CE1	2.73	120.00	111.27
2	A	1214	DKT	CE2-CZ1-CE1	2.74	120.03	111.27
2	F	1214	DKT	CE2-CZ1-CE1	2.74	120.05	111.27
2	E	1214	DKT	CE2-CZ1-CE1	2.75	120.06	111.27
2	C	1214	DKT	CE2-CZ1-CE1	2.75	120.07	111.27
2	B	1214	DKT	CE2-CZ1-CE1	2.75	120.07	111.27
2	F	1214	DKT	O-C6-N1	3.14	128.65	123.01
2	A	1214	DKT	O-C6-N1	3.15	128.66	123.01
2	E	1214	DKT	O-C6-N1	3.16	128.68	123.01
2	B	1214	DKT	O-C6-N1	3.16	128.68	123.01
2	D	1214	DKT	O-C6-N1	3.17	128.71	123.01
2	C	1214	DKT	O-C6-N1	3.18	128.72	123.01
2	D	1214	DKT	CB4-CG4-CD5	3.47	119.89	111.67
2	B	1214	DKT	CB4-CG4-CD5	3.49	119.94	111.67
2	F	1214	DKT	CB4-CG4-CD5	3.49	119.94	111.67
2	E	1214	DKT	CB4-CG4-CD5	3.49	119.95	111.67
2	A	1214	DKT	CB4-CG4-CD5	3.51	119.98	111.67
2	C	1214	DKT	CB4-CG4-CD5	3.51	119.98	111.67
2	B	1214	DKT	OC2-CC1-N	3.58	118.48	110.54
2	C	1214	DKT	OC2-CC1-N	3.59	118.51	110.54
2	A	1214	DKT	OC2-CC1-N	3.60	118.52	110.54
2	E	1214	DKT	OC2-CC1-N	3.60	118.52	110.54
2	D	1214	DKT	OC2-CC1-N	3.61	118.55	110.54
2	F	1214	DKT	OC2-CC1-N	3.61	118.56	110.54
2	A	1214	DKT	CD6-CG4-CD5	3.80	118.81	109.26
2	C	1214	DKT	CD6-CG4-CD5	3.80	118.81	109.26
2	D	1214	DKT	CZ3-CE7-CD6	3.80	119.42	111.44
2	B	1214	DKT	CD6-CG4-CD5	3.81	118.83	109.26
2	E	1214	DKT	CD6-CG4-CD5	3.81	118.83	109.26
2	F	1214	DKT	CD6-CG4-CD5	3.81	118.84	109.26
2	D	1214	DKT	CD6-CG4-CD5	3.81	118.84	109.26
2	F	1214	DKT	CZ3-CE7-CD6	3.82	119.44	111.44
2	B	1214	DKT	CZ3-CE7-CD6	3.82	119.45	111.44
2	E	1214	DKT	CZ3-CE7-CD6	3.83	119.46	111.44
2	C	1214	DKT	CZ3-CE7-CD6	3.84	119.48	111.44
2	A	1214	DKT	CZ3-CE7-CD6	3.84	119.49	111.44
2	F	1214	DKT	CD2-CG1-CD1	3.90	119.07	109.26
2	C	1214	DKT	CZ1-CE1-CD1	3.91	119.63	111.44
2	B	1214	DKT	CD2-CG1-CD1	3.91	119.08	109.26
2	F	1214	DKT	CZ1-CE1-CD1	3.91	119.63	111.44
2	E	1214	DKT	CD2-CG1-CD1	3.92	119.10	109.26
2	A	1214	DKT	CD2-CG1-CD1	3.92	119.10	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1214	DKT	CZ1-CE1-CD1	3.92	119.65	111.44
2	D	1214	DKT	CD2-CG1-CD1	3.92	119.11	109.26
2	E	1214	DKT	CZ1-CE1-CD1	3.92	119.66	111.44
2	C	1214	DKT	CD2-CG1-CD1	3.92	119.12	109.26
2	A	1214	DKT	CZ1-CE1-CD1	3.93	119.67	111.44
2	D	1214	DKT	CZ1-CE1-CD1	3.93	119.68	111.44
2	C	1214	DKT	CB4-CG4-CD6	4.02	121.20	111.67
2	A	1214	DKT	CB4-CG4-CD6	4.03	121.21	111.67
2	E	1214	DKT	CB4-CG4-CD6	4.03	121.22	111.67
2	F	1214	DKT	CB4-CG4-CD6	4.03	121.23	111.67
2	B	1214	DKT	CB4-CG4-CD6	4.04	121.23	111.67
2	D	1214	DKT	CB4-CG4-CD6	4.05	121.27	111.67
2	C	1214	DKT	CZ1-CE2-CD2	4.11	120.05	111.44
2	B	1214	DKT	CZ1-CE2-CD2	4.11	120.06	111.44
2	A	1214	DKT	CZ1-CE2-CD2	4.11	120.06	111.44
2	E	1214	DKT	CZ1-CE2-CD2	4.12	120.07	111.44
2	F	1214	DKT	CZ1-CE2-CD2	4.12	120.08	111.44
2	D	1214	DKT	CZ1-CE2-CD2	4.13	120.10	111.44
2	B	1214	DKT	CZ3-CE6-CD5	4.17	120.17	111.44
2	E	1214	DKT	CZ3-CE6-CD5	4.18	120.20	111.44
2	D	1214	DKT	CZ3-CE6-CD5	4.18	120.21	111.44
2	C	1214	DKT	CZ3-CE6-CD5	4.19	120.22	111.44
2	A	1214	DKT	CZ3-CE6-CD5	4.19	120.22	111.44
2	F	1214	DKT	CZ3-CE6-CD5	4.20	120.24	111.44
2	C	1214	DKT	CE2-CD2-CG1	4.95	120.20	112.22
2	D	1214	DKT	CE2-CD2-CG1	4.95	120.20	112.22
2	B	1214	DKT	CE2-CD2-CG1	4.95	120.21	112.22
2	E	1214	DKT	CE2-CD2-CG1	4.95	120.21	112.22
2	F	1214	DKT	CE2-CD2-CG1	4.96	120.21	112.22
2	A	1214	DKT	CE2-CD2-CG1	4.98	120.25	112.22
2	C	1214	DKT	CE7-CD6-CG4	5.33	120.82	112.22
2	A	1214	DKT	CE7-CD6-CG4	5.33	120.83	112.22
2	E	1214	DKT	CE7-CD6-CG4	5.34	120.83	112.22
2	F	1214	DKT	CE7-CD6-CG4	5.35	120.84	112.22
2	B	1214	DKT	CE7-CD6-CG4	5.35	120.85	112.22
2	D	1214	DKT	CE7-CD6-CG4	5.36	120.87	112.22
2	A	1214	DKT	CE1-CD1-CG1	5.37	120.88	112.22
2	E	1214	DKT	CE1-CD1-CG1	5.38	120.91	112.22
2	D	1214	DKT	CE1-CD1-CG1	5.39	120.91	112.22
2	B	1214	DKT	CE1-CD1-CG1	5.39	120.92	112.22
2	C	1214	DKT	CE1-CD1-CG1	5.40	120.93	112.22
2	F	1214	DKT	CE1-CD1-CG1	5.41	120.95	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1214	DKT	CE6-CD5-CG4	5.48	121.05	112.22
2	D	1214	DKT	CE6-CD5-CG4	5.49	121.08	112.22
2	E	1214	DKT	CE6-CD5-CG4	5.50	121.09	112.22
2	C	1214	DKT	CE6-CD5-CG4	5.50	121.10	112.22
2	A	1214	DKT	CE6-CD5-CG4	5.52	121.12	112.22
2	B	1214	DKT	CE6-CD5-CG4	5.52	121.13	112.22
2	C	1214	DKT	CA4-N3-C9	6.39	133.37	123.43
2	F	1214	DKT	CA4-N3-C9	6.40	133.39	123.43
2	E	1214	DKT	CA4-N3-C9	6.40	133.40	123.43
2	A	1214	DKT	CA4-N3-C9	6.41	133.41	123.43
2	D	1214	DKT	CA4-N3-C9	6.43	133.44	123.43
2	B	1214	DKT	CA4-N3-C9	6.44	133.45	123.43
2	F	1214	DKT	CA3-C9-N3	6.71	132.24	116.78
2	E	1214	DKT	CA3-C9-N3	6.72	132.26	116.78
2	A	1214	DKT	CA3-C9-N3	6.72	132.26	116.78
2	D	1214	DKT	CA3-C9-N3	6.72	132.27	116.78
2	C	1214	DKT	CA3-C9-N3	6.72	132.27	116.78
2	B	1214	DKT	CA3-C9-N3	6.73	132.31	116.78
2	C	1214	DKT	CA1-N-CC1	7.16	140.48	121.12
2	D	1214	DKT	CA1-N-CC1	7.16	140.49	121.12
2	E	1214	DKT	CA1-N-CC1	7.16	140.50	121.12
2	F	1214	DKT	CA1-N-CC1	7.17	140.50	121.12
2	A	1214	DKT	CA1-N-CC1	7.17	140.51	121.12
2	B	1214	DKT	CA1-N-CC1	7.17	140.51	121.12
2	B	1214	DKT	CA3-N2-C8	9.06	141.92	121.62
2	C	1214	DKT	CA3-N2-C8	9.06	141.93	121.62
2	A	1214	DKT	CA3-N2-C8	9.07	141.93	121.62
2	E	1214	DKT	CA3-N2-C8	9.08	141.96	121.62
2	D	1214	DKT	CA3-N2-C8	9.09	141.99	121.62
2	F	1214	DKT	CA3-N2-C8	9.09	141.99	121.62
2	A	1214	DKT	CB1-CG1-CD1	9.15	133.36	111.67
2	E	1214	DKT	CB1-CG1-CD1	9.16	133.38	111.67
2	D	1214	DKT	CB1-CG1-CD1	9.16	133.38	111.67
2	F	1214	DKT	CB1-CG1-CD1	9.16	133.39	111.67
2	B	1214	DKT	CB1-CG1-CD1	9.17	133.40	111.67
2	C	1214	DKT	CB1-CG1-CD1	9.17	133.40	111.67
2	A	1214	DKT	CA2-C8-N2	9.62	138.96	116.78
2	C	1214	DKT	CA2-C8-N2	9.63	138.99	116.78
2	E	1214	DKT	CA2-C8-N2	9.64	139.00	116.78
2	B	1214	DKT	CA2-C8-N2	9.64	139.00	116.78
2	F	1214	DKT	CA2-C8-N2	9.64	139.00	116.78
2	D	1214	DKT	CA2-C8-N2	9.64	139.01	116.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1214	DKT	OC2-CC2-CC3	9.93	134.33	109.36
2	B	1214	DKT	OC2-CC2-CC3	9.93	134.34	109.36
2	A	1214	DKT	OC2-CC2-CC3	9.94	134.36	109.36
2	C	1214	DKT	OC2-CC2-CC3	9.94	134.37	109.36
2	E	1214	DKT	OC2-CC2-CC3	9.94	134.37	109.36
2	D	1214	DKT	OC2-CC2-CC3	9.94	134.37	109.36
2	F	1214	DKT	CA2-N1-C6	10.71	140.34	122.12
2	C	1214	DKT	CA2-N1-C6	10.72	140.36	122.12
2	A	1214	DKT	CA2-N1-C6	10.73	140.37	122.12
2	E	1214	DKT	CA2-N1-C6	10.73	140.38	122.12
2	B	1214	DKT	CA2-N1-C6	10.74	140.38	122.12
2	D	1214	DKT	CA2-N1-C6	10.74	140.40	122.12
2	C	1214	DKT	CC2-OC2-CC1	11.07	142.29	115.91
2	F	1214	DKT	CC2-OC2-CC1	11.09	142.33	115.91
2	E	1214	DKT	CC2-OC2-CC1	11.09	142.35	115.91
2	D	1214	DKT	CC2-OC2-CC1	11.10	142.35	115.91
2	A	1214	DKT	CC2-OC2-CC1	11.11	142.38	115.91
2	B	1214	DKT	CC2-OC2-CC1	11.12	142.40	115.91
2	F	1214	DKT	CB2-CA2-N1	13.27	136.15	110.87
2	A	1214	DKT	CB2-CA2-N1	13.28	136.16	110.87
2	D	1214	DKT	CB2-CA2-N1	13.28	136.17	110.87
2	C	1214	DKT	CB2-CA2-N1	13.28	136.17	110.87
2	E	1214	DKT	CB2-CA2-N1	13.30	136.19	110.87
2	B	1214	DKT	CB2-CA2-N1	13.31	136.22	110.87
2	B	1214	DKT	C7-CA1-N	20.00	136.07	110.17
2	F	1214	DKT	C7-CA1-N	20.04	136.13	110.17
2	C	1214	DKT	C7-CA1-N	20.04	136.13	110.17
2	E	1214	DKT	C7-CA1-N	20.07	136.16	110.17
2	A	1214	DKT	C7-CA1-N	20.07	136.16	110.17
2	D	1214	DKT	C7-CA1-N	20.09	136.19	110.17

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1214	DKT	CA1
2	F	1214	DKT	CA1
2	D	1214	DKT	CA1
2	A	1214	DKT	CA1
2	C	1214	DKT	CA1
2	E	1214	DKT	CA1

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1214	DKT	CA1-C7-C6-N1
2	E	1214	DKT	CA1-C7-C6-N1
2	F	1214	DKT	CA1-C7-C6-N1
2	D	1214	DKT	CA1-C7-C6-N1
2	C	1214	DKT	CA1-C7-C6-N1
2	A	1214	DKT	CA1-C7-C6-N1
2	A	1214	DKT	O1-C7-C6-O
2	F	1214	DKT	O1-C7-C6-O
2	D	1214	DKT	O1-C7-C6-O
2	C	1214	DKT	O1-C7-C6-O
2	B	1214	DKT	O1-C7-C6-O
2	E	1214	DKT	O1-C7-C6-O
2	C	1214	DKT	O1-C7-C6-N1
2	B	1214	DKT	O1-C7-C6-N1
2	E	1214	DKT	O1-C7-C6-N1
2	A	1214	DKT	O1-C7-C6-N1
2	F	1214	DKT	O1-C7-C6-N1
2	D	1214	DKT	O1-C7-C6-N1

There are no ring outliers.

6 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1214	DKT	16	0
2	B	1214	DKT	5	0
2	C	1214	DKT	6	0
2	D	1214	DKT	6	0
2	E	1214	DKT	13	0
2	F	1214	DKT	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1023/1071 (95%)	-0.17	10 (0%)	84	85	14, 34, 58, 85	20 (1%)
1	B	1023/1071 (95%)	-0.17	12 (1%)	81	81	15, 35, 59, 85	20 (1%)
1	C	1023/1071 (95%)	0.20	46 (4%)	37	36	20, 39, 61, 85	20 (1%)
1	D	1023/1071 (95%)	-0.12	16 (1%)	74	75	16, 36, 60, 84	20 (1%)
1	E	1023/1071 (95%)	-0.15	13 (1%)	79	79	18, 35, 60, 83	20 (1%)
1	F	1023/1071 (95%)	0.13	43 (4%)	40	39	17, 39, 61, 85	20 (1%)
All	All	6138/6426 (95%)	-0.05	140 (2%)	64	64	14, 36, 60, 85	120 (1%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	219	SER	9.9
1	B	842	GLY	6.6
1	C	219	SER	6.3
1	D	563	ALA	6.0
1	F	219	SER	5.9
1	D	220	GLY	5.7
1	E	563	ALA	5.4
1	C	842	GLY	5.3
1	C	770	LYS	5.1
1	A	842	GLY	5.1
1	C	840	LYS	4.8
1	C	841	GLY	4.8
1	C	843	ASP	4.7
1	C	88	PRO	4.6
1	D	841	GLY	4.6
1	D	219	SER	4.5
1	D	842	GLY	4.5
1	F	840	LYS	4.4
1	C	239	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	F	842	GLY	4.3
1	C	238	VAL	4.2
1	E	841	GLY	4.2
1	A	218	ASN	4.1
1	F	841	GLY	4.0
1	A	329	PHE	3.9
1	A	840	LYS	3.7
1	E	842	GLY	3.7
1	C	90	GLY	3.7
1	C	774	ASP	3.6
1	D	91	ARG	3.6
1	C	838	SER	3.6
1	C	67	LYS	3.5
1	C	168	ASP	3.4
1	F	297	ASN	3.4
1	F	91	ARG	3.3
1	C	1017	ASP	3.3
1	E	91	ARG	3.3
1	D	557	ARG	3.2
1	F	114	GLU	3.2
1	E	329	PHE	3.2
1	F	142	PRO	3.2
1	D	114	GLU	3.2
1	C	1043	GLY	3.2
1	A	563	ALA	3.2
1	C	1042	SER	3.1
1	D	329	PHE	3.1
1	B	329	PHE	3.1
1	B	611	GLN	3.1
1	C	142	PRO	3.0
1	E	220	GLY	3.0
1	C	611	GLN	3.0
1	E	557	ARG	3.0
1	C	706	VAL	2.9
1	F	667	ASP	2.9
1	F	188	GLY	2.9
1	F	563	ALA	2.9
1	C	393	ARG	2.8
1	B	840	LYS	2.8
1	F	1042	SER	2.8
1	C	114	GLU	2.7
1	B	218	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	434	GLU	2.7
1	D	393	ARG	2.7
1	F	77	ASN	2.7
1	F	706	VAL	2.7
1	C	91	ARG	2.7
1	F	435	THR	2.7
1	C	839	GLY	2.6
1	F	309	GLY	2.6
1	D	382	ARG	2.6
1	B	841	GLY	2.6
1	A	841	GLY	2.6
1	F	89	ASP	2.6
1	C	237	ILE	2.6
1	B	67	LYS	2.6
1	A	299	ASP	2.6
1	B	683	HIS	2.6
1	F	263	ASP	2.5
1	F	561	SER	2.5
1	F	770	LYS	2.5
1	F	774	ASP	2.5
1	F	220	GLY	2.5
1	D	435	THR	2.4
1	F	756	ASP	2.4
1	F	144	GLY	2.4
1	E	840	LYS	2.4
1	C	220	GLY	2.4
1	C	115	ASN	2.4
1	B	592	GLU	2.3
1	F	401	GLU	2.3
1	C	173	VAL	2.3
1	C	310	ASP	2.3
1	F	281	ASP	2.3
1	F	393	ARG	2.3
1	F	174	PRO	2.3
1	E	435	THR	2.3
1	F	298	PRO	2.3
1	A	683	HIS	2.3
1	D	840	LYS	2.3
1	C	434	GLU	2.3
1	A	716	GLU	2.3
1	C	563	ALA	2.3
1	C	445	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	843	ASP	2.2
1	C	265	ARG	2.2
1	C	240	HIS	2.2
1	F	252	GLY	2.2
1	C	318	ILE	2.2
1	C	143	ASP	2.2
1	C	299	ASP	2.2
1	C	1025	TYR	2.2
1	C	40	PRO	2.2
1	C	218	ASN	2.2
1	F	565	GLU	2.2
1	D	683	HIS	2.2
1	F	262	LYS	2.2
1	C	250	GLY	2.2
1	B	557	ARG	2.2
1	F	819	SER	2.1
1	F	839	GLY	2.1
1	E	909	ILE	2.1
1	F	683	HIS	2.1
1	F	395	GLY	2.1
1	B	563	ALA	2.1
1	D	628	LYS	2.1
1	C	877	GLY	2.1
1	F	873	GLU	2.1
1	C	819	SER	2.1
1	C	703	ASN	2.1
1	A	835	ILE	2.1
1	F	307	GLU	2.1
1	C	144	GLY	2.1
1	E	1059	LEU	2.0
1	F	308	ILE	2.0
1	B	114	GLU	2.0
1	D	218	ASN	2.0
1	E	114	GLU	2.0
1	F	716	GLU	2.0
1	C	174	PRO	2.0
1	F	414	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	DKT	A	1214	55/55	0.76	0.29	5.18	41,57,73,74	0
2	DKT	C	1214	55/55	0.75	0.35	4.53	41,57,73,74	0
2	DKT	B	1214	55/55	0.75	0.28	4.16	41,57,73,74	0
2	DKT	F	1214	55/55	0.77	0.34	3.94	41,57,73,74	0
2	DKT	E	1214	55/55	0.72	0.31	3.59	41,57,73,74	0
2	DKT	D	1214	55/55	0.78	0.29	3.10	41,57,73,74	0

6.5 Other polymers (i)

There are no such residues in this entry.