Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2023 – 11:02 PM EDT

PDB ID	:	4OFW
Title	:	Crystal Structure of Arabidopsis thaliana DJ-1d
Authors	:	Choi, D.; Kim, J.; Ryu, K.-S.; Park, C.
Deposited on	:	2014-01-15
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

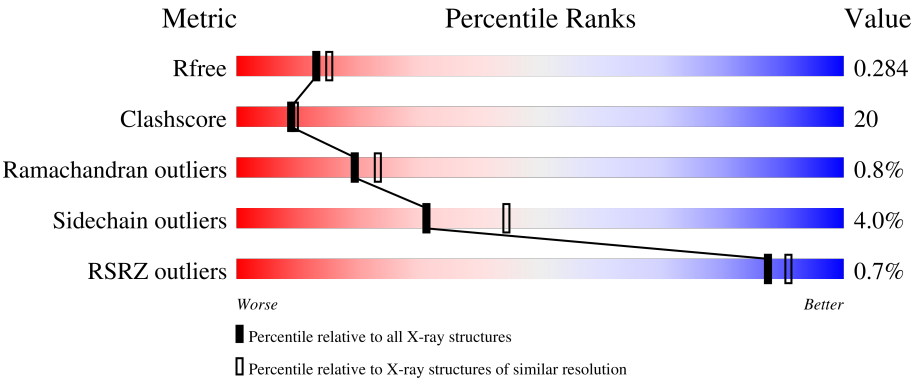
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	387	64% 32%
1	B	387	65% 33%
1	C	387	67% 29%
1	D	387	61% 37%
1	E	387	66% 32%

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Mol	Chain	Length	Quality of chain
1	F	387	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18086 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 Protein DJ-1 homolog D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	B	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	C	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	D	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	E	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	F	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	ASP	conflict	UNP Q9M8R4
A	389	HIS	-	expression tag	UNP Q9M8R4
B	238	GLU	ASP	conflict	UNP Q9M8R4
B	389	HIS	-	expression tag	UNP Q9M8R4
C	238	GLU	ASP	conflict	UNP Q9M8R4
C	389	HIS	-	expression tag	UNP Q9M8R4
D	238	GLU	ASP	conflict	UNP Q9M8R4
D	389	HIS	-	expression tag	UNP Q9M8R4
E	238	GLU	ASP	conflict	UNP Q9M8R4
E	389	HIS	-	expression tag	UNP Q9M8R4
F	238	GLU	ASP	conflict	UNP Q9M8R4
F	389	HIS	-	expression tag	UNP Q9M8R4

- Molecule 2 is water.

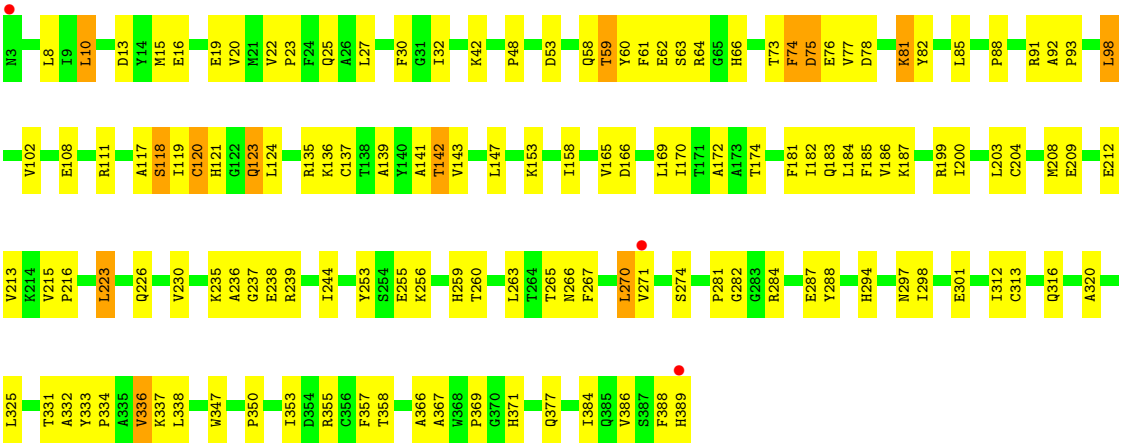
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	97	Total O 97 97	0	0
2	B	81	Total O 81 81	0	0
2	C	96	Total O 96 96	0	0
2	D	100	Total O 100 100	0	0
2	E	82	Total O 82 82	0	0
2	F	86	Total O 86 86	0	0

3 Residue-property plots (i)

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

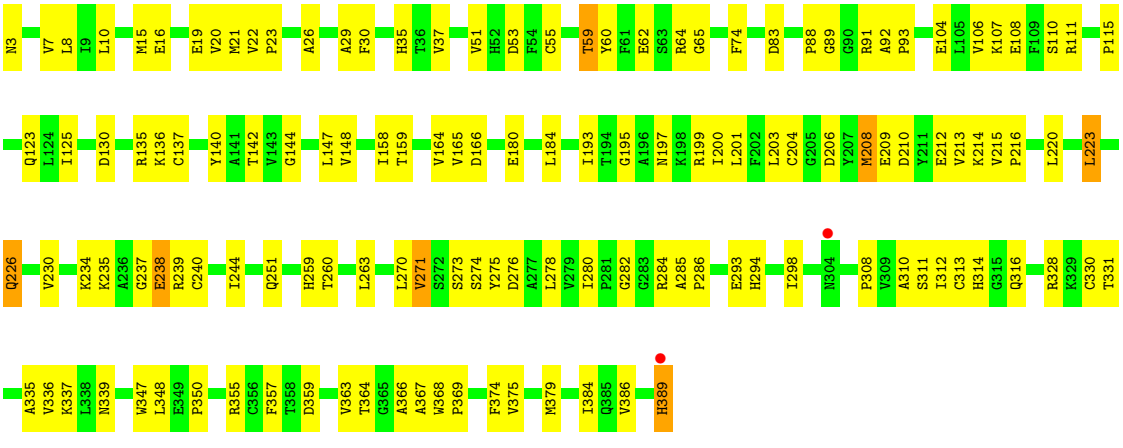
• Molecule 1: Protein DJ-1 homolog D

Chain A:



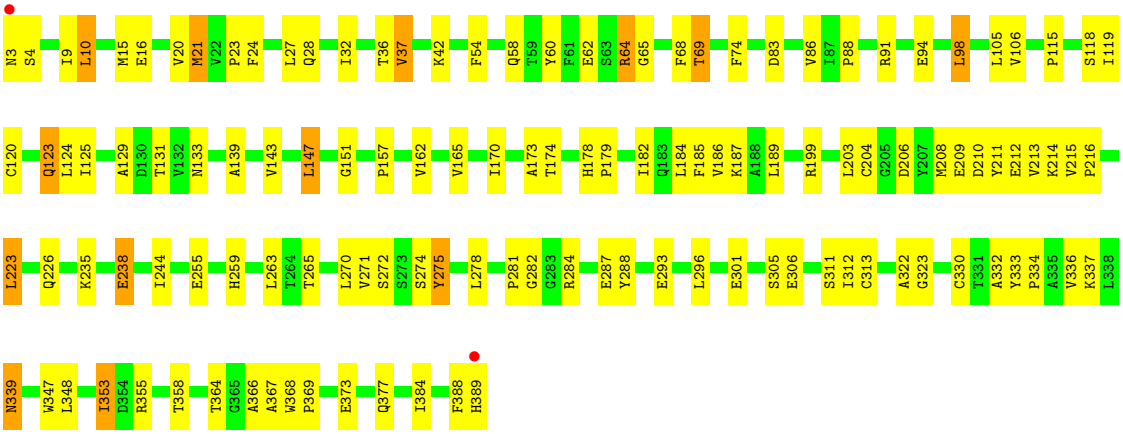
• Molecule 1: Protein DJ-1 homolog D

Chain B:



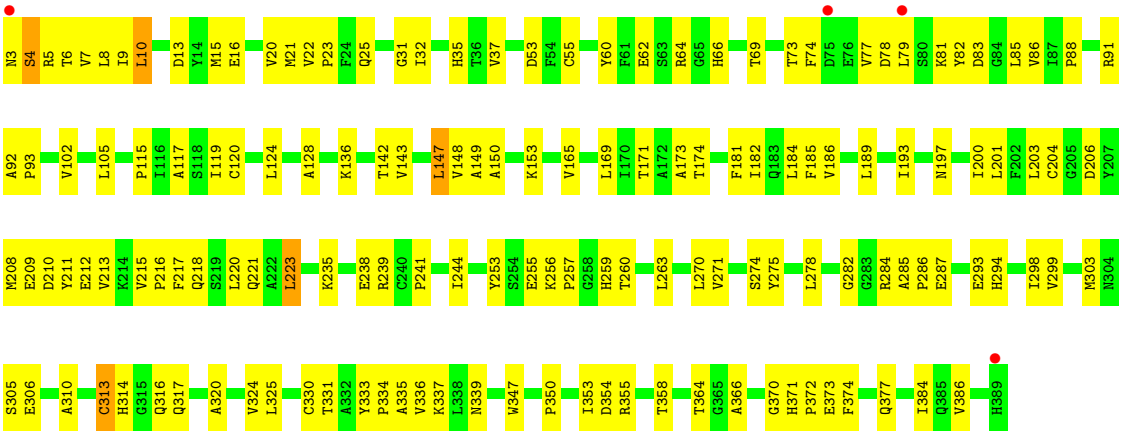
• Molecule 1: Protein DJ-1 homolog D

Chain C:



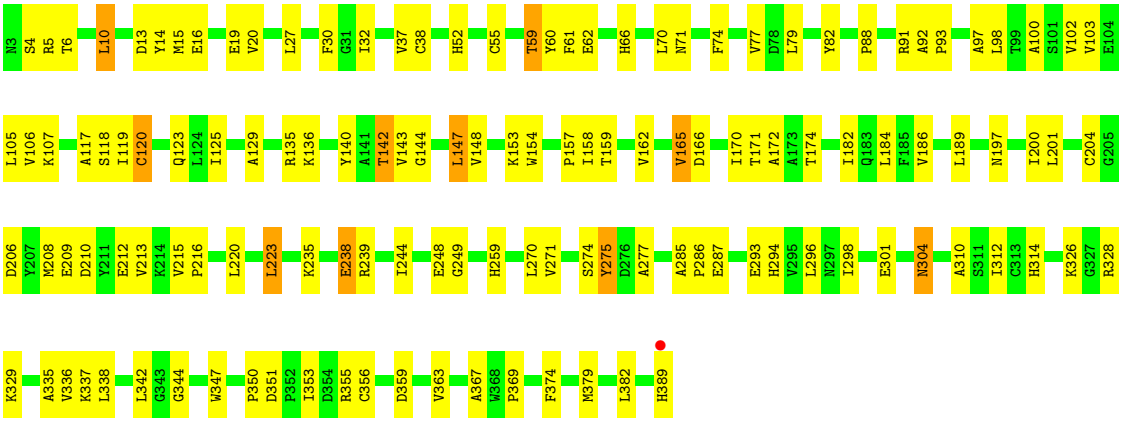
• Molecule 1: Protein DJ-1 homolog D

Chain D:



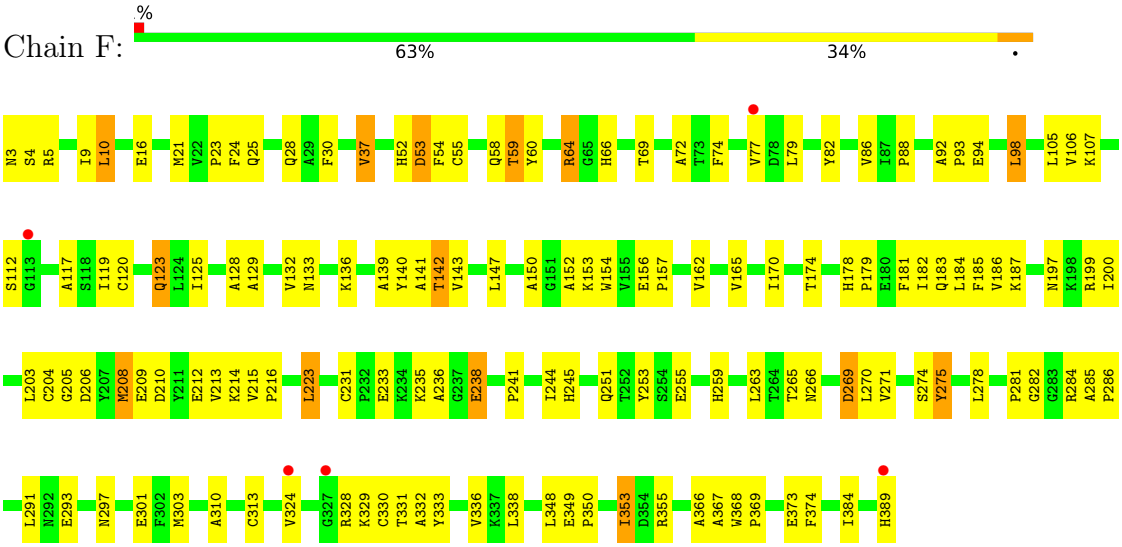
• Molecule 1: Protein DJ-1 homolog D

Chain E:



• Molecule 1: Protein DJ-1 homolog D

Chain F:


%
63%
34%
N3 S4 R5 I9 L10 E16 M21 V22 P23 F24 Q25 Q28 A29 F30 V37 H52 D53 F54 C55 Q58 T59 Y60 R64 G65 H66 T69 A72 T73 F74 V77 D78 L79 Y82 V86 I87 P88 A92 P93 E94 L98 L105 V106 K107
S112 G113 A117 S118 I119 C120 Q123 L124 I125 A128 A129 V132 N133 K136 A139 Y140 A141 T142 V143 L147 A150 G151 A152 K153 W154 V155 E156 P157 V162 V165 I170 T174 H178 P179 E180 F181 I182 Q183 L184 F185 V186 K187 N197 K198 R199 I200
L203 C204 G205 D206 Y207 M208 E209 D210 Y211 E212 V213 K214 V215 P216 L223 C231 P232 E233 K234 K235 A236 G237 E238 P241 I244 H245 Q251 T252 Y253 S254 E255 H259 L263 T264 T265 N266 D269 L270 V271 S274 Y275 L278 P281 G282 G283 R284 A285 P286
L291 N292 E293 N297 E301 F302 M303 A310 C313 V324 G327 R328 K329 C330 T331 A332 Y333 V336 K337 L338 L348 E349 P350 I353 D354 R355 A366 A367 W368 P369 E373 F374 I384 H389

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.56Å 115.05Å 115.53Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 47.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.30) 95.9 (47.96-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.29Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.243 , 0.284 0.243 , 0.284	Depositor DCC
R_{free} test set	11742 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18086	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1795e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/2994	0.62	0/4075
1	B	0.37	0/2994	0.62	0/4075
1	C	0.39	0/2994	0.64	0/4075
1	D	0.39	0/2994	0.62	0/4075
1	E	0.38	0/2994	0.63	0/4075
1	F	0.39	0/2994	0.64	0/4075
All	All	0.38	0/17964	0.63	0/24450

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	2924	0	2872	131	0
1	B	2924	0	2872	119	0
1	C	2924	0	2872	110	0
1	D	2924	0	2872	122	0
1	E	2924	0	2872	116	0
1	F	2924	0	2872	134	0
2	A	97	0	0	22	0
2	B	81	0	0	11	0
2	C	96	0	0	14	0
2	D	100	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	82	0	0	13	0
2	F	86	0	0	15	0
All	All	18086	0	17232	701	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 20.

All (701) 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:B:197:ASN:HA	2:B:468:HOH:O	1.59	1.00
1:F:133:ASN:HA	2:F:460:HOH:O	1.66	0.95
1:B:20:VAL:HB	2:B:455:HOH:O	1.66	0.94
1:F:353:ILE:HD12	1:F:353:ILE:H	1.28	0.94
1:D:7:VAL:HG23	2:D:486:HOH:O	1.70	0.91
1:B:59:THR:HG22	2:B:450:HOH:O	1.73	0.89
1:E:79:LEU:HD21	1:E:105:LEU:HG	1.56	0.87
1:E:287:GLU:OE1	1:F:142:THR:HG21	1.74	0.87
1:F:72:ALA:HB3	2:F:463:HOH:O	1.73	0.87
1:C:389:HIS:HB3	2:C:457:HOH:O	1.75	0.87
1:F:21:MET:HE2	1:F:25:GLN:HG3	1.56	0.86
1:E:335:ALA:HA	1:F:98:LEU:HD13	1.58	0.85
1:A:30:PHE:HB2	2:A:434:HOH:O	1.76	0.84
1:D:239:ARG:HH21	1:D:260:THR:HG23	1.39	0.84
1:C:353:ILE:H	1:C:353:ILE:HD12	1.41	0.84
2:E:418:HOH:O	1:F:59:THR:HG21	1.77	0.83
1:B:15:MET:SD	1:B:20:VAL:HG21	2.20	0.82
1:B:37:VAL:HG21	1:B:74:PHE:HA	1.61	0.81
1:D:78:ASP:OD2	1:D:81:LYS:HD3	1.81	0.80
1:A:108:GLU:HA	1:A:111:ARG:NH1	1.97	0.80
1:A:16:GLU:OE2	1:A:259:HIS:HE1	1.64	0.80
1:B:210:ASP:OD2	1:B:259:HIS:HD2	1.66	0.79
1:B:55:CYS:HB3	2:B:445:HOH:O	1.82	0.79
1:E:215:VAL:HB	1:E:216:PRO:HD3	1.64	0.79
1:B:335:ALA:HA	1:C:98:LEU:HD13	1.65	0.78
1:D:21:MET:HG3	1:D:211:TYR:CZ	2.18	0.78
1:D:330:CYS:HB2	1:D:364:THR:HG21	1.64	0.77
1:E:37:VAL:HG21	1:E:74:PHE:HA	1.67	0.76
1:D:53:ASP:OD1	1:D:260:THR:HG22	1.86	0.76
1:B:215:VAL:HB	1:B:216:PRO:HD3	1.68	0.76
1:F:69:THR:HB	2:F:407:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:THR:HG21	2:C:413:HOH:O	1.84	0.75
1:F:150:ALA:O	2:F:460:HOH:O	2.03	0.75
1:A:142:THR:HG21	1:C:287:GLU:OE2	1.87	0.74
1:A:239:ARG:HH21	1:A:260:THR:HG23	1.51	0.74
1:A:61:PHE:HB3	2:A:454:HOH:O	1.88	0.74
1:D:235:LYS:H	1:D:238:GLU:HG3	1.52	0.74
1:E:210:ASP:OD2	1:E:259:HIS:HD2	1.71	0.73
1:C:179:PRO:HG2	2:C:414:HOH:O	1.86	0.73
1:F:16:GLU:OE2	1:F:259:HIS:HE1	1.71	0.73
1:D:79:LEU:HD12	1:D:79:LEU:H	1.53	0.73
1:A:32:ILE:HG13	2:A:434:HOH:O	1.88	0.73
1:A:22:VAL:HB	1:A:23:PRO:HD3	1.68	0.73
1:C:133:ASN:HA	1:C:151:GLY:O	1.88	0.72
1:D:203:LEU:HG	1:D:278:LEU:HD11	1.70	0.72
1:F:23:PRO:HD3	2:F:419:HOH:O	1.88	0.72
1:C:133:ASN:HB2	2:C:472:HOH:O	1.89	0.72
1:F:182:ILE:O	1:F:186:VAL:HG23	1.89	0.72
1:B:209:GLU:HB3	1:B:212:GLU:HB2	1.72	0.72
1:B:237:GLY:HA3	1:D:235:LYS:NZ	2.03	0.72
1:B:239:ARG:HH21	1:B:260:THR:HG23	1.52	0.72
1:B:235:LYS:O	1:B:238:GLU:HG2	1.89	0.72
1:E:248:GLU:HB3	2:E:464:HOH:O	1.90	0.71
1:E:208:MET:HG3	1:E:213:VAL:HG21	1.71	0.71
1:A:136:LYS:HA	1:A:153:LYS:HB2	1.72	0.71
1:D:208:MET:HG3	1:D:213:VAL:HG21	1.72	0.71
1:F:204:CYS:HA	1:F:208:MET:HE1	1.71	0.71
1:A:19:GLU:HB2	2:A:483:HOH:O	1.90	0.71
1:D:235:LYS:H	1:D:238:GLU:CG	2.03	0.71
1:C:203:LEU:HG	1:C:278:LEU:HD11	1.73	0.70
1:A:88:PRO:HB3	2:A:483:HOH:O	1.92	0.70
1:E:37:VAL:CG2	1:E:74:PHE:HA	2.21	0.70
1:F:37:VAL:HG21	1:F:74:PHE:HA	1.72	0.70
1:E:165:VAL:HG22	1:E:184:LEU:HD13	1.74	0.70
1:F:265:THR:HG22	2:F:434:HOH:O	1.91	0.69
1:D:16:GLU:OE2	1:D:259:HIS:HE1	1.74	0.69
1:A:15:MET:SD	1:A:20:VAL:HG21	2.32	0.69
1:F:154:TRP:HE1	1:F:156:GLU:HG2	1.57	0.69
1:C:339:ASN:HD22	1:C:339:ASN:H	1.40	0.69
1:E:120:CYS:SG	2:E:478:HOH:O	2.49	0.69
1:A:183:GLN:HE21	1:A:187:LYS:HE3	1.58	0.69
1:D:119:ILE:HD11	1:D:174:THR:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:389:HIS:HB3	2:F:466:HOH:O	1.91	0.68
1:A:182:ILE:O	1:A:186:VAL:HG23	1.94	0.68
1:B:235:LYS:H	1:B:238:GLU:HG3	1.58	0.68
1:A:200:ILE:HD12	1:A:200:ILE:N	2.09	0.68
1:D:182:ILE:O	1:D:186:VAL:HG23	1.93	0.68
1:A:282:GLY:HA3	1:A:313:CYS:HB3	1.76	0.67
1:B:158:ILE:HD12	1:B:159:THR:N	2.09	0.67
1:F:165:VAL:HG23	1:F:184:LEU:HD13	1.77	0.67
1:F:203:LEU:HG	1:F:278:LEU:HD11	1.77	0.67
1:D:313:CYS:SG	2:D:498:HOH:O	2.50	0.67
1:E:103:VAL:O	1:E:107:LYS:HG3	1.94	0.67
1:B:235:LYS:H	1:B:238:GLU:CG	2.07	0.67
1:A:256:LYS:HG2	2:A:402:HOH:O	1.95	0.67
1:E:30:PHE:CZ	1:E:223:LEU:HD13	2.30	0.66
1:D:253:TYR:O	1:E:91:ARG:NH2	2.28	0.66
1:F:21:MET:CE	1:F:25:GLN:HG3	2.25	0.66
1:F:235:LYS:H	1:F:238:GLU:HG3	1.61	0.66
1:B:165:VAL:CG2	1:B:184:LEU:HD13	2.25	0.66
1:B:282:GLY:HA3	1:B:313:CYS:HB3	1.78	0.66
1:C:182:ILE:O	1:C:186:VAL:HG23	1.96	0.66
1:A:53:ASP:OD1	1:A:260:THR:HG22	1.96	0.66
1:B:22:VAL:HB	1:B:23:PRO:HD3	1.78	0.66
1:F:208:MET:HE2	1:F:281:PRO:HB2	1.77	0.65
1:D:218:GLN:HG2	2:D:463:HOH:O	1.95	0.65
1:E:182:ILE:O	1:E:186:VAL:HG23	1.97	0.65
1:A:119:ILE:HD11	1:A:174:THR:O	1.97	0.65
1:E:350:PRO:HB2	2:E:461:HOH:O	1.96	0.65
1:F:120:CYS:SG	2:F:479:HOH:O	2.53	0.65
1:F:213:VAL:HG13	1:F:214:LYS:N	2.11	0.65
1:C:23:PRO:HD3	2:C:437:HOH:O	1.96	0.64
1:C:355:ARG:HB3	2:C:453:HOH:O	1.96	0.64
1:B:235:LYS:N	1:B:238:GLU:HG3	2.13	0.64
1:B:237:GLY:HA3	1:D:235:LYS:HZ2	1.59	0.64
1:A:62:GLU:OE1	1:A:91:ARG:HD3	1.98	0.64
1:D:3:ASN:O	1:D:4:SER:HB2	1.96	0.64
1:E:5:ARG:NH2	1:E:189:LEU:O	2.31	0.64
1:B:330:CYS:HB2	1:B:364:THR:HG21	1.79	0.64
1:C:37:VAL:HG22	1:C:74:PHE:N	2.13	0.64
1:D:320:ALA:HB2	1:D:325:LEU:HD12	1.77	0.64
1:D:355:ARG:HA	1:D:373:GLU:OE1	1.98	0.64
1:F:333:TYR:O	1:F:336:VAL:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:VAL:HG13	1:C:74:PHE:HD1	1.63	0.64
1:C:209:GLU:HB3	1:C:212:GLU:HB2	1.80	0.64
1:D:169:LEU:HG	2:D:457:HOH:O	1.98	0.64
1:F:21:MET:CE	1:F:24:PHE:HD2	2.11	0.64
1:A:120:CYS:SG	2:A:488:HOH:O	2.52	0.63
1:F:154:TRP:NE1	1:F:156:GLU:HG2	2.12	0.63
1:A:20:VAL:HG22	1:A:88:PRO:HB3	1.80	0.63
1:C:21:MET:HG3	1:C:211:TYR:CZ	2.33	0.63
1:C:330:CYS:HA	1:C:348:LEU:HD12	1.80	0.63
1:E:355:ARG:HD2	2:E:429:HOH:O	1.97	0.63
1:C:16:GLU:OE2	1:C:259:HIS:HE1	1.80	0.63
1:D:117:ALA:HB1	1:D:181:PHE:CZ	2.33	0.63
1:A:19:GLU:CB	2:A:483:HOH:O	2.43	0.63
1:A:284:ARG:NH1	1:B:60:TYR:O	2.24	0.63
1:F:204:CYS:HA	1:F:208:MET:CE	2.29	0.63
1:A:78:ASP:OD2	1:A:81:LYS:HD3	1.99	0.62
1:C:15:MET:SD	1:C:20:VAL:HG21	2.39	0.62
1:C:120:CYS:SG	2:C:490:HOH:O	2.46	0.62
1:C:305:SER:O	1:C:306:GLU:HB2	1.99	0.62
1:F:313:CYS:HA	1:F:366:ALA:O	1.99	0.62
1:F:140:TYR:HD2	1:F:142:THR:HB	1.65	0.62
1:E:5:ARG:HH11	1:E:389:HIS:H	1.48	0.62
1:D:77:VAL:HG13	1:D:82:TYR:HE1	1.64	0.62
1:F:330:CYS:HA	1:F:348:LEU:HD12	1.80	0.62
1:A:333:TYR:CD1	1:A:334:PRO:HD2	2.35	0.61
1:F:353:ILE:H	1:F:353:ILE:CD1	2.04	0.61
1:A:74:PHE:O	1:A:76:GLU:N	2.34	0.61
1:B:209:GLU:O	1:B:213:VAL:HG23	2.00	0.61
1:E:15:MET:SD	1:E:20:VAL:HG21	2.41	0.61
1:F:37:VAL:HB	2:F:463:HOH:O	1.99	0.61
1:B:312:ILE:HD11	1:B:367:ALA:O	1.99	0.61
1:C:282:GLY:HA3	1:C:313:CYS:HB3	1.82	0.61
1:D:3:ASN:HB2	1:D:31:GLY:O	2.01	0.61
1:A:77:VAL:HB	2:A:440:HOH:O	2.01	0.61
1:A:208:MET:SD	1:A:213:VAL:HG21	2.41	0.61
1:A:60:TYR:O	1:C:284:ARG:NH1	2.34	0.61
1:C:170:ILE:HD13	1:C:185:PHE:HA	1.82	0.61
1:E:5:ARG:NH1	1:E:389:HIS:H	1.99	0.60
1:E:338:LEU:CD2	1:E:342:LEU:HD12	2.31	0.60
1:F:200:ILE:HD12	1:F:200:ILE:N	2.16	0.60
1:C:165:VAL:CG2	1:C:184:LEU:HD13	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:GLU:OE2	1:D:284:ARG:HD3	2.01	0.60
1:E:301:GLU:HA	1:E:304:ASN:ND2	2.16	0.60
1:A:124:LEU:CD2	1:A:143:VAL:HG13	2.32	0.60
1:B:331:THR:OG1	1:B:350:PRO:HG3	2.02	0.60
1:B:53:ASP:OD1	1:B:260:THR:HG22	2.02	0.60
1:A:77:VAL:HG13	1:A:82:TYR:HE1	1.66	0.59
1:C:9:ILE:HG12	1:C:86:VAL:HB	1.83	0.59
1:B:337:LYS:HE2	1:B:347:TRP:CD1	2.38	0.59
1:D:124:LEU:HD23	1:D:143:VAL:HG13	1.83	0.59
1:B:200:ILE:CD1	1:B:220:LEU:HD13	2.33	0.59
1:C:213:VAL:HG13	1:C:214:LYS:N	2.18	0.59
1:D:73:THR:HG22	1:D:74:PHE:O	2.02	0.59
1:D:358:THR:OG1	1:D:377:GLN:NE2	2.36	0.59
1:B:64:ARG:HD2	2:B:425:HOH:O	2.03	0.59
1:B:313:CYS:HA	1:B:366:ALA:O	2.02	0.59
1:B:350:PRO:HB3	1:B:366:ALA:HB2	1.83	0.59
1:C:187:LYS:HG3	2:C:443:HOH:O	2.03	0.59
1:F:274:SER:O	1:F:275:TYR:HB2	2.03	0.59
1:B:30:PHE:CZ	1:B:223:LEU:HD13	2.37	0.59
1:B:226:GLN:HE21	1:B:226:GLN:HA	1.68	0.59
1:F:106:VAL:HG21	1:F:125:ILE:CG2	2.33	0.59
1:C:62:GLU:OE1	1:C:91:ARG:HD3	2.03	0.58
1:C:157:PRO:HA	1:C:162:VAL:HG21	1.85	0.58
1:F:3:ASN:O	1:F:4:SER:HB2	2.03	0.58
1:C:235:LYS:H	1:C:238:GLU:HG3	1.69	0.58
1:A:265:THR:HG23	2:A:460:HOH:O	2.04	0.58
1:A:77:VAL:HG13	1:A:82:TYR:CE1	2.38	0.58
1:D:22:VAL:HB	1:D:23:PRO:HD3	1.85	0.58
1:B:165:VAL:HG21	1:B:184:LEU:HD13	1.86	0.57
1:F:165:VAL:CG2	1:F:184:LEU:HD13	2.35	0.57
1:B:209:GLU:HG3	1:B:212:GLU:H	1.70	0.57
1:C:106:VAL:HG21	1:C:125:ILE:CG2	2.34	0.57
1:D:91:ARG:NH2	1:F:253:TYR:O	2.37	0.57
1:B:285:ALA:HB3	1:B:286:PRO:HD3	1.85	0.57
1:A:209:GLU:HG3	1:A:212:GLU:H	1.69	0.57
1:D:209:GLU:O	1:D:213:VAL:HG23	2.05	0.57
1:B:204:CYS:HA	1:B:208:MET:CE	2.34	0.57
1:C:255:GLU:OE2	1:C:284:ARG:NH2	2.38	0.57
1:A:353:ILE:HG12	2:A:425:HOH:O	2.03	0.57
1:B:16:GLU:OE2	1:B:259:HIS:HE1	1.88	0.57
1:F:209:GLU:HG3	1:F:212:GLU:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:HIS:CD2	1:A:244:ILE:HG23	2.40	0.56
1:A:235:LYS:O	1:A:238:GLU:HG2	2.05	0.56
1:C:3:ASN:O	1:C:4:SER:HB2	2.05	0.56
1:B:208:MET:SD	1:B:213:VAL:HG21	2.45	0.56
1:F:123:GLN:OE1	1:F:123:GLN:N	2.39	0.56
1:B:193:ILE:HG12	1:B:386:VAL:HG22	1.87	0.56
1:A:117:ALA:HB1	1:A:181:PHE:CZ	2.41	0.56
1:E:10:LEU:HD11	1:E:102:VAL:HG13	1.87	0.56
1:E:4:SER:O	1:E:5:ARG:HD3	2.06	0.56
1:D:335:ALA:HA	1:E:98:LEU:HD22	1.87	0.56
1:D:210:ASP:OD2	1:D:259:HIS:HD2	1.88	0.56
1:E:326:LYS:HD3	1:E:344:GLY:HA3	1.88	0.56
1:B:235:LYS:N	1:B:238:GLU:CG	2.69	0.56
1:C:333:TYR:O	1:C:336:VAL:HG22	2.06	0.55
1:D:193:ILE:HG12	1:D:386:VAL:HG22	1.88	0.55
1:D:200:ILE:HD12	1:D:220:LEU:HD13	1.88	0.55
1:A:123:GLN:HG2	1:A:139:ALA:HB2	1.88	0.55
1:B:230:VAL:HG21	1:B:270:LEU:HD11	1.88	0.55
1:C:223:LEU:HG	1:C:384:ILE:HG21	1.89	0.55
1:D:239:ARG:NH2	1:D:260:THR:HG23	2.17	0.55
1:E:338:LEU:HD21	1:E:342:LEU:HD12	1.87	0.55
1:B:140:TYR:HD2	1:B:142:THR:HG22	1.71	0.55
1:B:367:ALA:HB3	1:B:369:PRO:HD2	1.89	0.55
1:D:165:VAL:HG22	1:D:184:LEU:HD13	1.88	0.55
1:D:208:MET:CG	1:D:213:VAL:HG21	2.37	0.55
1:D:217:PHE:O	1:D:221:GLN:HG3	2.06	0.55
1:F:37:VAL:CG2	1:F:74:PHE:HA	2.36	0.55
1:F:37:VAL:HG13	1:F:74:PHE:HD1	1.72	0.55
1:A:59:THR:HG22	1:A:60:TYR:H	1.72	0.55
1:E:147:LEU:HD23	1:E:154:TRP:CZ3	2.42	0.55
1:A:204:CYS:HA	1:A:208:MET:HE3	1.89	0.54
1:E:209:GLU:O	1:E:213:VAL:HG23	2.07	0.54
1:B:37:VAL:CG2	1:B:74:PHE:HA	2.35	0.54
1:B:184:LEU:HD23	2:B:442:HOH:O	2.07	0.54
1:B:294:HIS:O	1:B:298:ILE:HG13	2.07	0.54
1:B:280:ILE:HB	1:B:311:SER:HB2	1.89	0.54
1:E:206:ASP:OD2	1:F:58:GLN:HG3	2.07	0.54
1:E:235:LYS:H	1:E:238:GLU:CG	2.20	0.54
1:F:55:CYS:HB3	2:F:415:HOH:O	2.07	0.54
1:F:349:GLU:CD	1:F:350:PRO:HD2	2.28	0.54
1:B:212:GLU:HG3	1:B:368:TRP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:355:ARG:HG2	1:F:355:ARG:HH21	1.71	0.54
1:C:119:ILE:HD11	1:C:174:THR:O	2.07	0.54
1:E:338:LEU:HD12	1:F:128:ALA:HB2	1.88	0.54
1:A:10:LEU:O	1:A:88:PRO:HD2	2.08	0.54
1:F:64:ARG:HD3	2:F:437:HOH:O	2.08	0.54
1:A:119:ILE:HG13	1:A:172:ALA:HB3	1.89	0.54
1:F:21:MET:HE3	1:F:24:PHE:HD2	1.72	0.54
1:F:213:VAL:HG13	1:F:214:LYS:H	1.73	0.54
1:D:16:GLU:O	1:D:20:VAL:HG23	2.08	0.54
1:F:233:GLU:HG3	1:F:233:GLU:O	2.07	0.54
1:C:210:ASP:OD2	1:C:259:HIS:HD2	1.90	0.53
1:D:212:GLU:HA	1:D:371:HIS:HE2	1.73	0.53
1:D:353:ILE:HD12	1:D:354:ASP:H	1.72	0.53
1:A:15:MET:CG	1:A:20:VAL:HG21	2.39	0.53
1:A:165:VAL:CG2	1:A:184:LEU:HD13	2.38	0.53
1:F:263:LEU:HD22	1:F:263:LEU:H	1.72	0.53
1:B:200:ILE:HD12	1:B:220:LEU:HD13	1.89	0.53
1:B:204:CYS:HA	1:B:208:MET:HE1	1.90	0.53
1:D:15:MET:HG3	1:D:20:VAL:HG21	1.89	0.53
1:F:235:LYS:N	1:F:238:GLU:HG3	2.22	0.53
1:E:19:GLU:O	1:E:88:PRO:HB3	2.09	0.53
1:D:201:LEU:HD22	1:D:270:LEU:HD21	1.90	0.53
1:E:52:HIS:HE1	1:E:62:GLU:OE1	1.91	0.53
1:B:62:GLU:OE2	1:B:91:ARG:NH1	2.42	0.53
1:D:62:GLU:OE2	1:D:91:ARG:NH1	2.42	0.53
1:D:200:ILE:CD1	1:D:220:LEU:HD13	2.39	0.53
1:D:287:GLU:OE1	1:E:142:THR:HG21	2.08	0.53
1:A:10:LEU:HD11	1:A:102:VAL:HG13	1.90	0.53
1:C:235:LYS:N	1:C:238:GLU:HG3	2.24	0.53
1:C:271:VAL:HG13	1:C:274:SER:OG	2.09	0.53
1:A:25:GLN:NE2	1:A:371:HIS:ND1	2.55	0.53
1:E:293:GLU:OE1	1:E:293:GLU:HA	2.09	0.52
1:A:118:SER:HB3	1:A:123:GLN:OE1	2.09	0.52
1:D:8:LEU:O	1:D:85:LEU:HD12	2.09	0.52
1:C:69:THR:HG23	2:C:486:HOH:O	2.09	0.52
1:C:24:PHE:O	1:C:28:GLN:HG3	2.09	0.52
1:D:215:VAL:HB	1:D:216:PRO:HD3	1.91	0.52
1:F:255:GLU:OE2	1:F:284:ARG:HD3	2.09	0.52
1:B:240:CYS:SG	1:B:263:LEU:HD21	2.50	0.52
1:C:143:VAL:HG12	1:C:147:LEU:CD2	2.40	0.52
1:E:97:ALA:C	1:E:98:LEU:HD12	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:GLY:HA3	1:F:313:CYS:HB3	1.92	0.52
1:C:209:GLU:HG3	1:C:212:GLU:H	1.74	0.52
1:D:32:ILE:HG23	2:D:486:HOH:O	2.09	0.52
1:E:27:LEU:HD22	1:E:32:ILE:HD12	1.92	0.52
1:E:312:ILE:HD11	1:E:367:ALA:O	2.10	0.52
1:F:157:PRO:HA	1:F:162:VAL:HG21	1.91	0.52
1:F:143:VAL:HG12	1:F:143:VAL:O	2.10	0.52
1:E:140:TYR:HD2	1:E:142:THR:HB	1.75	0.52
1:E:301:GLU:HA	1:E:304:ASN:HD22	1.75	0.52
1:E:329:LYS:HG3	2:E:445:HOH:O	2.09	0.52
1:C:312:ILE:HD11	1:C:367:ALA:O	2.10	0.52
1:E:285:ALA:HB3	1:E:286:PRO:HD3	1.92	0.51
1:F:329:LYS:O	1:F:330:CYS:HB3	2.09	0.51
1:A:235:LYS:H	1:A:238:GLU:CG	2.23	0.51
1:B:348:LEU:HD13	1:B:357:PHE:CD2	2.45	0.51
1:F:293:GLU:HA	1:F:293:GLU:OE1	2.08	0.51
1:A:25:GLN:HE21	1:A:215:VAL:HG21	1.75	0.51
1:A:73:THR:HG22	1:A:74:PHE:O	2.10	0.51
1:B:20:VAL:HG22	1:B:88:PRO:HG3	1.93	0.51
1:B:51:VAL:HG13	1:B:259:HIS:CD2	2.44	0.51
1:E:204:CYS:HA	1:E:208:MET:CE	2.41	0.51
1:E:249:GLY:N	2:E:464:HOH:O	2.43	0.51
1:E:336:VAL:O	1:E:336:VAL:HG12	2.09	0.51
1:C:265:THR:HG23	2:C:419:HOH:O	2.11	0.51
1:E:37:VAL:CG2	1:E:74:PHE:CA	2.88	0.51
1:D:77:VAL:HB	2:D:470:HOH:O	2.11	0.51
1:D:208:MET:SD	1:D:213:VAL:HG21	2.51	0.51
1:A:98:LEU:HD21	1:C:337:LYS:HB3	1.93	0.51
1:D:353:ILE:HD12	1:D:354:ASP:N	2.25	0.51
1:E:123:GLN:N	1:E:123:GLN:OE1	2.43	0.51
1:B:37:VAL:CG2	1:B:74:PHE:CA	2.89	0.51
1:C:54:PHE:HB3	2:C:458:HOH:O	2.09	0.51
1:F:77:VAL:HG13	1:F:82:TYR:HE1	1.75	0.51
1:E:38:CYS:HB3	1:E:70:LEU:HD11	1.93	0.50
1:E:294:HIS:O	1:E:298:ILE:HG13	2.10	0.50
1:B:336:VAL:HG12	1:B:336:VAL:O	2.11	0.50
1:E:200:ILE:CD1	1:E:220:LEU:HD13	2.41	0.50
1:A:8:LEU:HB2	1:A:82:TYR:CD2	2.46	0.50
1:B:271:VAL:HG13	1:B:271:VAL:O	2.11	0.50
1:B:271:VAL:HG22	1:B:273:SER:HB2	1.93	0.50
1:C:368:TRP:N	1:C:369:PRO:CD	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ALA:N	1:D:286:PRO:CD	2.74	0.50
1:A:235:LYS:H	1:A:238:GLU:HG3	1.77	0.50
1:A:332:ALA:CB	1:A:336:VAL:HG23	2.41	0.50
1:D:372:PRO:HD2	2:D:425:HOH:O	2.12	0.50
1:F:235:LYS:H	1:F:238:GLU:CG	2.22	0.50
1:B:91:ARG:NH2	2:B:453:HOH:O	2.44	0.50
1:C:215:VAL:HB	1:C:216:PRO:HD3	1.93	0.50
1:E:135:ARG:HD2	1:E:166:ASP:OD2	2.12	0.50
1:C:235:LYS:H	1:C:238:GLU:CG	2.23	0.50
1:F:197:ASN:HB2	2:F:404:HOH:O	2.12	0.50
1:A:313:CYS:HA	1:A:366:ALA:O	2.11	0.50
1:B:123:GLN:N	1:B:123:GLN:OE1	2.45	0.50
1:C:353:ILE:H	1:C:353:ILE:CD1	2.08	0.50
1:F:5:ARG:HH22	1:F:389:HIS:CD2	2.30	0.50
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.77	0.50
1:D:120:CYS:SG	2:D:493:HOH:O	2.55	0.50
1:A:135:ARG:HD2	1:A:166:ASP:OD2	2.12	0.49
1:B:389:HIS:HB2	2:B:461:HOH:O	2.10	0.49
1:C:332:ALA:HB1	1:C:336:VAL:CG2	2.42	0.49
1:E:16:GLU:HB3	1:E:19:GLU:HB2	1.94	0.49
1:F:106:VAL:HG21	1:F:125:ILE:HG22	1.92	0.49
1:A:88:PRO:CA	2:A:483:HOH:O	2.60	0.49
1:C:293:GLU:OE1	1:C:293:GLU:HA	2.12	0.49
1:A:16:GLU:OE2	1:A:259:HIS:CE1	2.56	0.49
1:E:77:VAL:HG13	1:E:82:TYR:HE1	1.76	0.49
1:C:270:LEU:HD13	1:C:271:VAL:N	2.27	0.49
1:E:61:PHE:HB3	2:E:459:HOH:O	2.11	0.49
1:A:367:ALA:HB3	1:A:369:PRO:HD2	1.95	0.49
1:D:256:LYS:HG2	2:D:407:HOH:O	2.13	0.49
1:F:105:LEU:HD23	1:F:105:LEU:C	2.33	0.49
1:C:199:ARG:HB2	1:C:275:TYR:HA	1.94	0.49
1:D:148:VAL:C	1:D:150:ALA:H	2.15	0.49
1:F:205:GLY:HA2	1:F:231:CYS:SG	2.53	0.49
1:C:83:ASP:O	1:C:115:PRO:HD2	2.12	0.49
1:E:355:ARG:HG3	1:E:356:CYS:N	2.28	0.49
1:F:269:ASP:N	1:F:269:ASP:OD2	2.45	0.49
1:C:274:SER:O	1:C:275:TYR:HB2	2.12	0.49
1:A:92:ALA:N	1:A:93:PRO:CD	2.76	0.49
1:B:314:HIS:HA	1:B:336:VAL:HG21	1.93	0.49
1:A:98:LEU:HD22	1:C:334:PRO:O	2.13	0.48
1:D:171:THR:HG23	2:D:457:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:LYS:HG3	1:D:257:PRO:HD2	1.94	0.48
1:E:351:ASP:N	2:E:461:HOH:O	2.46	0.48
1:F:154:TRP:HE1	1:F:156:GLU:CG	2.22	0.48
1:B:336:VAL:HA	1:B:339:ASN:HD22	1.78	0.48
1:C:178:HIS:N	1:C:179:PRO:HD2	2.28	0.48
1:D:32:ILE:CG2	2:D:486:HOH:O	2.60	0.48
1:E:337:LYS:HE2	1:E:347:TRP:CD1	2.48	0.48
1:A:8:LEU:O	1:A:85:LEU:HD12	2.13	0.48
1:A:15:MET:HG3	1:A:20:VAL:HG21	1.95	0.48
1:D:331:THR:OG1	1:D:350:PRO:HB3	2.13	0.48
1:F:212:GLU:OE1	1:F:313:CYS:HB2	2.13	0.48
1:A:58:GLN:HG3	1:C:206:ASP:OD2	2.13	0.48
1:B:16:GLU:HB3	1:B:19:GLU:HB2	1.94	0.48
1:D:66:HIS:CD2	1:D:244:ILE:HG23	2.48	0.48
1:C:353:ILE:HD12	1:C:353:ILE:N	2.20	0.48
1:D:55:CYS:HB3	2:D:442:HOH:O	2.13	0.48
1:D:64:ARG:NH1	2:D:429:HOH:O	2.45	0.48
1:E:157:PRO:HA	1:E:162:VAL:HG21	1.95	0.48
1:E:298:ILE:HG12	2:E:474:HOH:O	2.13	0.48
1:A:332:ALA:HB1	1:A:336:VAL:CG2	2.44	0.48
1:B:180:GLU:O	1:B:184:LEU:HG	2.14	0.48
1:D:271:VAL:HG13	1:D:274:SER:OG	2.14	0.48
1:F:206:ASP:OD1	1:F:241:PRO:HD2	2.13	0.48
1:E:274:SER:O	1:E:275:TYR:HB2	2.13	0.48
1:A:255:GLU:OE1	1:A:284:ARG:NH2	2.46	0.48
1:A:320:ALA:HB2	1:A:325:LEU:HD12	1.95	0.48
1:A:316:GLN:OE1	1:A:316:GLN:N	2.44	0.47
1:F:353:ILE:HD12	1:F:353:ILE:N	2.12	0.47
1:A:358:THR:OG1	1:A:377:GLN:NE2	2.48	0.47
1:D:92:ALA:N	1:D:93:PRO:CD	2.77	0.47
1:D:316:GLN:N	1:D:316:GLN:OE1	2.47	0.47
1:E:117:ALA:HA	1:E:170:ILE:O	2.14	0.47
1:A:136:LYS:O	1:A:137:CYS:HB3	2.14	0.47
1:C:37:VAL:CG2	1:C:74:PHE:N	2.78	0.47
1:F:77:VAL:HG13	1:F:82:TYR:CE1	2.49	0.47
1:B:368:TRP:N	1:B:369:PRO:CD	2.78	0.47
1:C:339:ASN:HD22	1:C:339:ASN:N	2.09	0.47
1:D:201:LEU:HD21	1:D:270:LEU:HD11	1.96	0.47
1:A:117:ALA:HB1	1:A:181:PHE:CE1	2.50	0.47
1:B:280:ILE:HB	1:B:311:SER:CB	2.45	0.47
1:C:313:CYS:HA	1:C:366:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ARG:NH2	2:D:446:HOH:O	2.48	0.47
1:D:223:LEU:HG	1:D:384:ILE:HG21	1.95	0.47
1:D:310:ALA:HB1	1:D:374:PHE:CZ	2.50	0.47
1:E:100:ALA:HB3	2:E:437:HOH:O	2.14	0.47
1:E:144:GLY:O	1:E:148:VAL:HG23	2.14	0.47
1:E:158:ILE:HG13	1:E:159:THR:HG23	1.96	0.47
1:A:25:GLN:NE2	1:A:215:VAL:HG21	2.30	0.47
1:B:37:VAL:HG21	1:B:74:PHE:CA	2.38	0.47
1:E:59:THR:HG22	1:E:60:TYR:H	1.80	0.47
1:E:140:TYR:CD2	1:E:142:THR:HB	2.50	0.47
1:F:123:GLN:HG2	1:F:139:ALA:HB2	1.95	0.47
1:A:208:MET:HG3	1:A:213:VAL:HG21	1.97	0.47
1:F:263:LEU:HD22	1:F:263:LEU:N	2.30	0.47
1:F:199:ARG:HB2	1:F:275:TYR:HA	1.97	0.46
1:B:83:ASP:O	1:B:115:PRO:HD2	2.15	0.46
1:C:143:VAL:HG12	1:C:147:LEU:HD22	1.97	0.46
1:D:7:VAL:HG12	1:D:8:LEU:N	2.31	0.46
1:D:299:VAL:O	1:D:303:MET:HG2	2.15	0.46
1:E:337:LYS:HB3	1:F:98:LEU:HD21	1.98	0.46
1:D:204:CYS:HA	1:D:208:MET:HE3	1.97	0.46
1:D:6:THR:HG22	1:D:82:TYR:CD2	2.50	0.46
1:E:204:CYS:HA	1:E:208:MET:HE3	1.98	0.46
1:A:74:PHE:O	1:A:75:ASP:C	2.54	0.46
1:A:208:MET:HE2	1:A:213:VAL:HG22	1.97	0.46
1:B:62:GLU:OE1	1:B:91:ARG:NH1	2.48	0.46
1:B:106:VAL:HG21	1:B:125:ILE:CG2	2.45	0.46
1:D:313:CYS:HB3	2:D:498:HOH:O	2.15	0.46
1:A:200:ILE:N	1:A:200:ILE:CD1	2.78	0.46
1:B:226:GLN:HG2	2:B:441:HOH:O	2.15	0.46
1:C:185:PHE:CE2	1:C:189:LEU:HD11	2.49	0.46
1:D:153:LYS:HE2	2:D:482:HOH:O	2.15	0.46
1:E:235:LYS:H	1:E:238:GLU:HG2	1.81	0.46
1:A:183:GLN:HE21	1:A:187:LYS:CE	2.27	0.46
1:B:201:LEU:HB2	1:B:275:TYR:CD2	2.50	0.46
1:C:355:ARG:HG3	1:C:373:GLU:OE1	2.15	0.46
1:D:124:LEU:CD2	1:D:143:VAL:HG13	2.45	0.46
1:A:238:GLU:HB2	1:A:263:LEU:HD23	1.97	0.46
1:E:62:GLU:OE2	1:E:91:ARG:NH1	2.48	0.46
1:B:107:LYS:O	1:B:110:SER:HB3	2.16	0.46
1:B:239:ARG:HE	1:B:260:THR:CG2	2.29	0.46
1:D:7:VAL:CG1	1:D:8:LEU:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ILE:HG12	1:D:86:VAL:HB	1.98	0.46
1:F:245:HIS:CD2	1:F:255:GLU:HG3	2.51	0.46
1:A:271:VAL:HG13	1:A:271:VAL:O	2.15	0.46
1:C:263:LEU:N	1:C:263:LEU:HD22	2.30	0.46
1:E:270:LEU:HD13	1:E:271:VAL:N	2.31	0.46
1:F:37:VAL:CG2	1:F:74:PHE:CA	2.94	0.46
1:F:92:ALA:N	1:F:93:PRO:CD	2.79	0.46
1:C:271:VAL:HG13	1:C:271:VAL:O	2.16	0.45
1:E:200:ILE:HD13	1:E:220:LEU:HD13	1.98	0.45
1:A:123:GLN:OE1	1:A:123:GLN:N	2.49	0.45
1:B:137:CYS:HA	1:B:164:VAL:HG11	1.98	0.45
1:D:206:ASP:OD1	1:D:241:PRO:HD2	2.17	0.45
1:E:16:GLU:OE2	1:E:259:HIS:HE1	1.99	0.45
1:E:209:GLU:HG2	1:E:212:GLU:OE2	2.16	0.45
1:A:88:PRO:CB	2:A:483:HOH:O	2.56	0.45
1:B:259:HIS:CD2	1:B:259:HIS:H	2.35	0.45
1:E:6:THR:HG22	1:E:82:TYR:CD2	2.52	0.45
1:C:65:GLY:HA2	1:C:244:ILE:HD13	1.98	0.45
1:C:332:ALA:HB1	1:C:336:VAL:HG21	1.99	0.45
1:D:142:THR:HA	1:F:291:LEU:HD11	1.99	0.45
1:E:98:LEU:HD12	1:E:98:LEU:N	2.31	0.45
1:F:235:LYS:N	1:F:238:GLU:CG	2.80	0.45
1:B:328:ARG:HD2	2:B:418:HOH:O	2.15	0.45
1:D:136:LYS:HA	1:D:153:LYS:HB2	1.97	0.45
1:D:337:LYS:HG3	1:D:347:TRP:CD2	2.52	0.45
1:D:370:GLY:HA2	2:D:425:HOH:O	2.17	0.45
1:F:10:LEU:O	1:F:88:PRO:HD2	2.16	0.45
1:F:213:VAL:CG1	1:F:214:LYS:N	2.77	0.45
1:F:236:ALA:N	1:F:266:ASN:OD1	2.49	0.45
1:B:284:ARG:NH1	1:C:60:TYR:O	2.43	0.45
1:B:285:ALA:N	1:B:286:PRO:CD	2.79	0.45
1:D:235:LYS:H	1:D:238:GLU:HG2	1.80	0.45
1:A:13:ASP:OD1	1:A:48:PRO:HD2	2.17	0.45
1:C:123:GLN:HG2	1:C:139:ALA:HB2	1.99	0.45
1:D:10:LEU:HD11	1:D:102:VAL:HG13	1.98	0.45
1:D:79:LEU:H	1:D:79:LEU:CD1	2.24	0.45
1:C:165:VAL:HG23	1:C:184:LEU:HD13	1.99	0.45
1:C:296:LEU:HD22	1:C:322:ALA:HB2	1.98	0.45
1:D:8:LEU:HD12	1:D:35:HIS:O	2.16	0.45
1:E:314:HIS:HA	1:E:336:VAL:HG21	1.99	0.45
1:D:303:MET:HG3	1:D:324:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ALA:HB3	1:F:369:PRO:HD2	1.99	0.45
1:A:208:MET:CG	1:A:213:VAL:HG21	2.48	0.44
1:C:10:LEU:O	1:C:88:PRO:HD2	2.16	0.44
1:C:311:SER:O	1:C:364:THR:HA	2.18	0.44
1:F:355:ARG:HG2	1:F:355:ARG:NH2	2.31	0.44
1:B:199:ARG:HD3	1:B:274:SER:O	2.17	0.44
1:C:16:GLU:O	1:C:20:VAL:HG23	2.18	0.44
1:C:367:ALA:HB3	1:C:369:PRO:HD2	1.99	0.44
1:D:13:ASP:OD2	1:F:251:GLN:HB2	2.17	0.44
1:D:143:VAL:HG12	1:D:147:LEU:HD22	1.99	0.44
1:E:367:ALA:HB3	1:E:369:PRO:HD2	1.99	0.44
1:F:223:LEU:HG	1:F:384:ILE:HG21	1.98	0.44
1:B:26:ALA:O	1:B:29:ALA:HB3	2.17	0.44
1:D:310:ALA:HB1	1:D:374:PHE:CE1	2.52	0.44
1:E:106:VAL:HG21	1:E:125:ILE:HG22	1.99	0.44
1:E:271:VAL:O	1:E:271:VAL:HG13	2.18	0.44
1:F:21:MET:HE3	1:F:24:PHE:CD2	2.51	0.44
1:F:170:ILE:HD13	1:F:185:PHE:HA	1.99	0.44
1:A:23:PRO:HG2	2:A:449:HOH:O	2.16	0.44
1:A:386:VAL:HG12	1:A:388:PHE:CE1	2.52	0.44
1:B:30:PHE:N	1:B:30:PHE:CD2	2.85	0.44
1:B:206:ASP:OD2	1:C:58:GLN:HG3	2.18	0.44
1:F:136:LYS:HA	1:F:153:LYS:HB2	1.99	0.44
1:A:332:ALA:HB1	1:A:336:VAL:HG23	1.98	0.44
1:B:276:ASP:O	1:B:308:PRO:HD2	2.18	0.44
1:B:158:ILE:CD1	1:B:159:THR:HG23	2.48	0.44
1:C:223:LEU:HD12	1:C:223:LEU:HA	1.82	0.44
1:E:30:PHE:CE2	1:E:223:LEU:HD13	2.53	0.44
1:E:55:CYS:HB3	2:E:459:HOH:O	2.18	0.44
1:A:347:TRP:CZ2	1:A:350:PRO:HD3	2.52	0.44
1:B:135:ARG:NH2	1:B:166:ASP:O	2.51	0.44
1:C:204:CYS:SG	1:C:208:MET:HE1	2.58	0.44
1:C:235:LYS:N	1:C:238:GLU:CG	2.81	0.44
1:C:337:LYS:HA	1:C:347:TRP:CZ3	2.53	0.44
1:E:15:MET:HG3	1:E:20:VAL:HG21	1.99	0.44
1:A:271:VAL:HG13	1:A:274:SER:OG	2.18	0.44
1:B:136:LYS:O	1:B:137:CYS:HB3	2.17	0.44
1:B:200:ILE:HD13	1:B:220:LEU:HD13	1.98	0.44
1:C:213:VAL:HG13	1:C:214:LYS:H	1.80	0.44
1:D:333:TYR:CD1	1:D:334:PRO:HD2	2.52	0.44
1:E:310:ALA:HA	1:E:363:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:ILE:HA	2:E:461:HOH:O	2.17	0.44
1:F:66:HIS:CE1	1:F:244:ILE:HG23	2.52	0.44
1:A:27:LEU:O	2:A:434:HOH:O	2.21	0.44
1:F:303:MET:HG3	1:F:324:VAL:HB	2.00	0.44
1:A:25:GLN:OE1	1:A:371:HIS:HB2	2.18	0.43
1:A:287:GLU:OE1	1:B:142:THR:HG21	2.18	0.43
1:B:328:ARG:NH1	1:B:359:ASP:O	2.51	0.43
1:E:201:LEU:HB2	1:E:275:TYR:CD2	2.53	0.43
1:A:297:ASN:O	1:A:301:GLU:HG3	2.18	0.43
1:C:330:CYS:CA	1:C:348:LEU:HD12	2.46	0.43
1:E:165:VAL:CG2	1:E:184:LEU:HD13	2.46	0.43
1:B:214:LYS:HD3	2:B:405:HOH:O	2.18	0.43
1:D:117:ALA:HB1	1:D:181:PHE:CE1	2.53	0.43
1:D:282:GLY:HA3	1:D:313:CYS:HB3	2.00	0.43
1:D:320:ALA:CB	1:D:325:LEU:HD12	2.46	0.43
1:E:92:ALA:HB3	1:E:93:PRO:HD3	2.00	0.43
1:E:277:ALA:HB2	1:E:382:LEU:HD21	2.00	0.43
1:F:24:PHE:O	1:F:28:GLN:HG3	2.19	0.43
1:F:59:THR:HG22	1:F:60:TYR:CD1	2.52	0.43
1:F:66:HIS:CD2	1:F:244:ILE:HG23	2.53	0.43
1:A:59:THR:HG23	2:A:430:HOH:O	2.18	0.43
1:D:143:VAL:HG12	1:D:143:VAL:O	2.18	0.43
1:D:79:LEU:HD12	1:D:79:LEU:N	2.26	0.43
1:E:223:LEU:HD21	1:E:379:MET:HG2	2.00	0.43
1:F:213:VAL:CG1	1:F:214:LYS:H	2.31	0.43
1:C:208:MET:HE2	1:C:281:PRO:HB2	1.99	0.43
1:C:339:ASN:N	1:C:339:ASN:ND2	2.66	0.43
1:D:25:GLN:NE2	1:D:371:HIS:ND1	2.65	0.43
1:E:66:HIS:CD2	1:E:244:ILE:HG23	2.54	0.43
1:E:285:ALA:N	1:E:286:PRO:CD	2.81	0.43
1:F:117:ALA:HA	1:F:170:ILE:O	2.18	0.43
1:A:253:TYR:O	1:B:91:ARG:NH2	2.50	0.43
1:C:388:PHE:O	1:C:389:HIS:HB2	2.18	0.43
1:E:143:VAL:HG12	1:E:143:VAL:O	2.18	0.43
1:F:373:GLU:HG2	2:F:451:HOH:O	2.19	0.43
1:A:81:LYS:HE3	2:A:437:HOH:O	2.18	0.43
1:A:199:ARG:HA	1:A:226:GLN:O	2.19	0.43
1:A:223:LEU:HG	1:A:384:ILE:HG21	2.00	0.43
1:F:107:LYS:HE2	1:F:129:ALA:O	2.19	0.43
1:F:332:ALA:HB1	1:F:336:VAL:CG2	2.48	0.43
1:A:355:ARG:HG2	1:A:357:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:LYS:HA	1:E:153:LYS:HB2	2.00	0.43
1:E:310:ALA:HB1	1:E:374:PHE:CZ	2.53	0.43
1:F:183:GLN:O	1:F:187:LYS:HG2	2.18	0.43
1:A:230:VAL:HG21	1:A:270:LEU:HD11	2.01	0.43
1:E:328:ARG:NH1	1:E:359:ASP:O	2.52	0.43
1:A:235:LYS:N	1:A:238:GLU:HG3	2.34	0.42
1:A:265:THR:HG22	1:A:266:ASN:N	2.33	0.42
1:B:375:VAL:O	1:B:379:MET:HG3	2.19	0.42
1:D:334:PRO:O	1:E:98:LEU:HD22	2.18	0.42
1:E:235:LYS:H	1:E:238:GLU:HG3	1.82	0.42
1:B:195:GLY:O	1:B:384:ILE:HG12	2.18	0.42
1:B:310:ALA:HA	1:B:363:VAL:O	2.19	0.42
1:B:337:LYS:HG3	1:B:347:TRP:CD2	2.54	0.42
1:C:119:ILE:HD11	1:C:174:THR:C	2.40	0.42
1:F:52:HIS:O	1:F:53:ASP:HB3	2.19	0.42
1:F:132:VAL:CG2	1:F:152:ALA:HB2	2.49	0.42
1:F:297:ASN:O	1:F:301:GLU:HG3	2.19	0.42
1:B:335:ALA:HB1	1:C:94:GLU:HG2	2.01	0.42
1:D:128:ALA:HB2	1:F:338:LEU:HD13	2.00	0.42
1:D:314:HIS:HD2	1:D:317:GLN:NE2	2.17	0.42
1:A:170:ILE:HD12	1:A:185:PHE:HA	2.01	0.42
1:A:235:LYS:O	1:A:237:GLY:N	2.53	0.42
1:A:288:TYR:CD2	1:B:59:THR:HG23	2.54	0.42
1:A:333:TYR:O	1:A:336:VAL:HG22	2.19	0.42
1:C:123:GLN:OE1	1:C:123:GLN:N	2.51	0.42
1:A:23:PRO:O	1:A:27:LEU:HG	2.19	0.42
1:C:358:THR:OG1	1:C:377:GLN:NE2	2.52	0.42
1:D:60:TYR:O	1:F:284:ARG:NH1	2.26	0.42
1:D:294:HIS:O	1:D:298:ILE:HG13	2.19	0.42
1:F:9:ILE:HG12	1:F:86:VAL:HB	2.01	0.42
1:F:210:ASP:OD2	1:F:259:HIS:HD2	2.03	0.42
1:F:212:GLU:OE1	1:F:313:CYS:CB	2.68	0.42
1:F:331:THR:OG1	1:F:350:PRO:HB3	2.20	0.42
1:A:203:LEU:O	1:A:281:PRO:HD2	2.20	0.42
1:A:312:ILE:HG12	1:A:313:CYS:N	2.33	0.42
1:B:204:CYS:HA	1:B:208:MET:HE3	2.01	0.42
1:E:119:ILE:HG13	1:E:172:ALA:HB3	2.02	0.42
1:F:54:PHE:N	1:F:54:PHE:CD1	2.86	0.42
1:B:203:LEU:HG	1:B:278:LEU:HD11	2.02	0.42
1:C:124:LEU:CD2	1:C:143:VAL:HG13	2.50	0.42
1:D:336:VAL:HB	1:D:339:ASN:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:LEU:C	1:F:270:LEU:HD13	2.40	0.42
1:A:169:LEU:HG	2:A:442:HOH:O	2.20	0.42
1:F:328:ARG:HA	1:F:328:ARG:HD2	1.94	0.42
1:A:108:GLU:HA	1:A:111:ARG:HH12	1.80	0.42
1:A:124:LEU:HD21	1:A:143:VAL:HG13	2.01	0.42
1:B:37:VAL:CG2	1:B:74:PHE:N	2.82	0.42
1:D:3:ASN:O	1:D:4:SER:CB	2.65	0.42
1:D:5:ARG:HH21	1:D:5:ARG:HG2	1.84	0.42
1:E:106:VAL:HG21	1:E:125:ILE:CG2	2.50	0.42
1:F:165:VAL:HG22	1:F:170:ILE:HG12	2.02	0.42
1:A:42:LYS:N	1:A:42:LYS:HD3	2.33	0.41
1:A:337:LYS:HG3	1:A:347:TRP:CD2	2.55	0.41
1:B:8:LEU:HD12	1:B:35:HIS:O	2.20	0.41
1:E:13:ASP:O	1:E:14:TYR:HB2	2.20	0.41
1:A:215:VAL:HB	1:A:216:PRO:HD3	2.00	0.41
1:B:310:ALA:HB1	1:B:374:PHE:CE1	2.55	0.41
1:C:27:LEU:HD22	1:C:32:ILE:HD12	2.03	0.41
1:C:64:ARG:NH2	2:C:467:HOH:O	2.52	0.41
1:D:313:CYS:HA	1:D:366:ALA:O	2.21	0.41
1:F:271:VAL:O	1:F:271:VAL:HG13	2.20	0.41
1:C:64:ARG:HB2	2:C:420:HOH:O	2.19	0.41
1:E:71:ASN:OD1	1:E:71:ASN:C	2.58	0.41
1:E:159:THR:O	1:E:162:VAL:HG13	2.20	0.41
1:F:310:ALA:HB1	1:F:374:PHE:CZ	2.56	0.41
1:A:73:THR:C	1:A:74:PHE:O	2.58	0.41
1:B:234:LYS:HB3	1:B:238:GLU:HG3	2.02	0.41
1:C:36:THR:HG21	1:C:68:PHE:CZ	2.55	0.41
1:C:106:VAL:HG21	1:C:125:ILE:HG21	2.01	0.41
1:C:124:LEU:HD23	1:C:143:VAL:HG13	2.03	0.41
1:E:335:ALA:CB	1:F:94:GLU:HG2	2.51	0.41
1:F:285:ALA:HB3	1:F:286:PRO:HD3	2.01	0.41
1:A:119:ILE:HD11	1:A:174:THR:C	2.41	0.41
1:B:65:GLY:HA2	1:B:244:ILE:HD13	2.01	0.41
1:B:239:ARG:NH2	1:B:260:THR:HG23	2.28	0.41
1:D:235:LYS:N	1:D:238:GLU:HG3	2.27	0.41
1:E:30:PHE:N	1:E:30:PHE:CD2	2.88	0.41
1:E:107:LYS:HG2	1:E:129:ALA:HB1	2.02	0.41
1:E:119:ILE:HD11	1:E:174:THR:O	2.21	0.41
1:E:338:LEU:HD23	1:E:338:LEU:C	2.40	0.41
1:F:368:TRP:N	1:F:369:PRO:CD	2.83	0.41
1:A:120:CYS:HB3	1:A:121:HIS:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:PHE:O	1:A:270:LEU:HB2	2.21	0.41
1:C:105:LEU:HD23	1:C:105:LEU:C	2.41	0.41
1:C:120:CYS:HA	1:C:173:ALA:O	2.21	0.41
1:C:213:VAL:CG1	1:C:214:LYS:N	2.82	0.41
1:F:271:VAL:HG13	1:F:274:SER:OG	2.21	0.41
1:B:7:VAL:HG12	1:B:8:LEU:N	2.36	0.41
1:B:144:GLY:O	1:B:148:VAL:HG23	2.20	0.41
1:D:10:LEU:O	1:D:88:PRO:HD2	2.21	0.41
1:A:88:PRO:HA	2:A:483:HOH:O	2.20	0.41
1:A:294:HIS:O	1:A:298:ILE:HG13	2.20	0.41
1:A:367:ALA:CB	1:A:369:PRO:HD2	2.51	0.41
1:B:108:GLU:HA	1:B:111:ARG:NH1	2.35	0.41
1:C:272:SER:HB3	1:C:301:GLU:OE1	2.21	0.41
1:C:323:GLY:HA2	2:C:403:HOH:O	2.21	0.41
1:C:332:ALA:CB	1:C:336:VAL:CG2	2.99	0.41
1:D:173:ALA:N	2:D:411:HOH:O	2.46	0.41
1:E:235:LYS:N	1:E:238:GLU:HG2	2.36	0.41
1:E:239:ARG:HG3	1:E:239:ARG:HH11	1.85	0.41
1:F:178:HIS:N	1:F:179:PRO:CD	2.84	0.41
1:C:129:ALA:O	1:C:131:THR:HG23	2.21	0.41
1:A:32:ILE:CG1	2:A:434:HOH:O	2.57	0.40
1:A:331:THR:OG1	1:A:350:PRO:HB3	2.21	0.40
1:C:37:VAL:HG22	1:C:74:PHE:CA	2.51	0.40
1:D:91:ARG:HB3	2:D:421:HOH:O	2.21	0.40
1:F:30:PHE:CZ	1:F:223:LEU:HD13	2.57	0.40
1:F:37:VAL:CG2	1:F:74:PHE:N	2.84	0.40
1:F:119:ILE:HD11	1:F:174:THR:O	2.21	0.40
1:A:255:GLU:OE2	1:A:284:ARG:HD3	2.20	0.40
1:B:92:ALA:HB3	1:B:93:PRO:HD3	2.03	0.40
1:D:79:LEU:HD21	1:D:105:LEU:HG	2.02	0.40
1:E:118:SER:O	1:E:171:THR:HA	2.22	0.40
1:E:208:MET:HG3	1:E:213:VAL:CG2	2.45	0.40
1:E:335:ALA:HB1	1:F:94:GLU:HG2	2.03	0.40
1:F:37:VAL:CB	2:F:463:HOH:O	2.66	0.40
1:F:330:CYS:CA	1:F:348:LEU:HD12	2.48	0.40
1:A:20:VAL:HG22	1:A:88:PRO:CB	2.49	0.40
1:A:325:LEU:HB2	2:A:431:HOH:O	2.21	0.40
1:C:388:PHE:HB3	1:C:389:HIS:H	1.76	0.40
1:D:185:PHE:O	1:D:189:LEU:HG	2.22	0.40
1:D:271:VAL:HG13	1:D:271:VAL:O	2.21	0.40
1:D:305:SER:O	1:D:306:GLU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:CYS:HB3	2:F:479:HOH:O	2.20	0.40
1:B:367:ALA:CB	1:B:369:PRO:HD2	2.52	0.40
1:D:83:ASP:O	1:D:115:PRO:HD2	2.22	0.40
1:D:221:GLN:OE1	2:D:463:HOH:O	2.22	0.40
1:F:66:HIS:CE1	1:F:244:ILE:HG12	2.56	0.40
1:F:236:ALA:O	1:F:263:LEU:O	2.39	0.40
1:A:62:GLU:HG2	1:A:63:SER:N	2.37	0.40
1:A:77:VAL:HG22	2:A:461:HOH:O	2.22	0.40
1:B:19:GLU:OE1	1:B:89:GLY:HA3	2.21	0.40
1:B:130:ASP:CG	1:B:130:ASP:O	2.60	0.40
1:B:316:GLN:N	1:B:316:GLN:OE1	2.55	0.40
1:E:296:LEU:HA	1:E:296:LEU:HD23	1.87	0.40
1:F:117:ALA:HB1	1:F:181:PHE:CZ	2.56	0.40
1:F:215:VAL:HB	1:F:216:PRO:CD	2.52	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	385/387 (100%)	353 (92%)	27 (7%)	5 (1%)	12	12
1	B	385/387 (100%)	356 (92%)	27 (7%)	2 (0%)	29	35
1	C	385/387 (100%)	356 (92%)	28 (7%)	1 (0%)	41	50
1	D	385/387 (100%)	358 (93%)	24 (6%)	3 (1%)	19	23
1	E	385/387 (100%)	352 (91%)	31 (8%)	2 (0%)	29	35
1	F	385/387 (100%)	356 (92%)	24 (6%)	5 (1%)	12	12
All	All	2310/2322 (100%)	2131 (92%)	161 (7%)	18 (1%)	19	23

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	E	238	GLU
1	A	74	PHE
1	A	236	ALA
1	D	275	TYR
1	B	238	GLU
1	C	275	TYR
1	F	112	SER
1	D	149	ALA
1	A	141	ALA
1	D	4	SER
1	E	275	TYR
1	F	53	ASP
1	F	79	LEU
1	F	141	ALA
1	F	275	TYR
1	B	271	VAL
1	A	336	VAL

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	313/313 (100%)	298 (95%)	15 (5%)	25	36
1	B	313/313 (100%)	300 (96%)	13 (4%)	30	42
1	C	313/313 (100%)	297 (95%)	16 (5%)	24	33
1	D	313/313 (100%)	304 (97%)	9 (3%)	42	58
1	E	313/313 (100%)	304 (97%)	9 (3%)	42	58
1	F	313/313 (100%)	300 (96%)	13 (4%)	30	42
All	All	1878/1878 (100%)	1803 (96%)	75 (4%)	31	44

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU

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Mol	Chain	Res	Type
1	A	59	THR
1	A	64	ARG
1	A	81	LYS
1	A	98	LEU
1	A	118	SER
1	A	120	CYS
1	A	123	GLN
1	A	142	THR
1	A	147	LEU
1	A	158	ILE
1	A	223	LEU
1	A	270	LEU
1	A	338	LEU
1	A	389	HIS
1	B	3	ASN
1	B	10	LEU
1	B	21	MET
1	B	59	THR
1	B	104	GLU
1	B	147	LEU
1	B	208	MET
1	B	223	LEU
1	B	226	GLN
1	B	251	GLN
1	B	293	GLU
1	B	355	ARG
1	B	389	HIS
1	C	10	LEU
1	C	21	MET
1	C	37	VAL
1	C	42	LYS
1	C	64	ARG
1	C	69	THR
1	C	98	LEU
1	C	118	SER
1	C	123	GLN
1	C	147	LEU
1	C	223	LEU
1	C	226	GLN
1	C	238	GLU
1	C	288	TYR
1	C	339	ASN

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Mol	Chain	Res	Type
1	C	353	ILE
1	D	10	LEU
1	D	37	VAL
1	D	69	THR
1	D	147	LEU
1	D	197	ASN
1	D	223	LEU
1	D	263	LEU
1	D	293	GLU
1	D	313	CYS
1	E	10	LEU
1	E	59	THR
1	E	120	CYS
1	E	142	THR
1	E	147	LEU
1	E	165	VAL
1	E	197	ASN
1	E	223	LEU
1	E	304	ASN
1	F	10	LEU
1	F	37	VAL
1	F	59	THR
1	F	64	ARG
1	F	98	LEU
1	F	123	GLN
1	F	142	THR
1	F	147	LEU
1	F	208	MET
1	F	223	LEU
1	F	238	GLU
1	F	269	ASP
1	F	353	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	28	GLN
1	A	52	HIS
1	A	183	GLN
1	A	259	HIS
1	A	339	ASN

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Mol	Chain	Res	Type
1	A	377	GLN
1	A	385	GLN
1	B	28	GLN
1	B	57	HIS
1	B	226	GLN
1	B	251	GLN
1	B	259	HIS
1	B	339	ASN
1	B	385	GLN
1	C	28	GLN
1	C	52	HIS
1	C	57	HIS
1	C	183	GLN
1	C	226	GLN
1	C	259	HIS
1	C	317	GLN
1	C	339	ASN
1	C	377	GLN
1	D	3	ASN
1	D	25	GLN
1	D	183	GLN
1	D	197	ASN
1	D	259	HIS
1	D	266	ASN
1	D	317	GLN
1	D	339	ASN
1	D	377	GLN
1	E	3	ASN
1	E	28	GLN
1	E	52	HIS
1	E	57	HIS
1	E	183	GLN
1	E	197	ASN
1	E	259	HIS
1	E	294	HIS
1	E	377	GLN
1	F	35	HIS
1	F	245	HIS
1	F	259	HIS
1	F	317	GLN
1	F	339	ASN
1	F	377	GLN

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Mol	Chain	Res	Type
1	F	389	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	387/387 (100%)	-0.05	3 (0%)	86	89	16, 30, 48, 69	0
1	B	387/387 (100%)	-0.09	2 (0%)	91	94	14, 33, 49, 68	0
1	C	387/387 (100%)	-0.20	2 (0%)	91	94	15, 28, 46, 68	0
1	D	387/387 (100%)	-0.08	4 (1%)	82	86	18, 31, 49, 69	0
1	E	387/387 (100%)	-0.21	1 (0%)	94	96	15, 31, 47, 68	0
1	F	387/387 (100%)	-0.10	5 (1%)	77	81	14, 31, 48, 67	0
All	All	2322/2322 (100%)	-0.12	17 (0%)	87	91	14, 31, 48, 69	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	389	HIS	4.1
1	B	389	HIS	4.1
1	A	3	ASN	3.4
1	D	389	HIS	3.0
1	C	389	HIS	3.0
1	D	75	ASP	2.9
1	D	3	ASN	2.9
1	F	324	VAL	2.8
1	D	79	LEU	2.8
1	E	389	HIS	2.6
1	C	3	ASN	2.6
1	B	304	ASN	2.5
1	F	327	GLY	2.3
1	A	271	VAL	2.2
1	F	389	HIS	2.1
1	F	77	VAL	2.1
1	F	113	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.