Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 07:53 AM EDT

PDB ID	:	4EEB
Title	:	CorA coiled-coil mutant under Mg2+ absence
Authors	:	Pfoh, R.; Pai, E.F.
Deposited on	:	2012-03-28
Resolution	:	3.80 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:

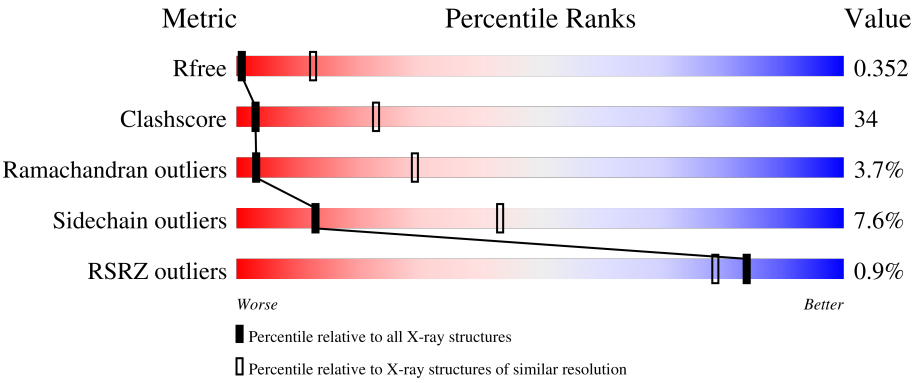
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	330	2% 43% 48% 5% 5%
1	B	330	. 44% 46% 5% .
1	C	330	. 46% 44% 5% 5%
1	D	330	44% 43% 8% 5%
1	E	330	. 39% 50% 6% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12988 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 Magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2593	1688	418	478	9			
1	B	316	Total	C	N	O	S	0	0	0
			2606	1697	419	481	9			
1	C	314	Total	C	N	O	S	0	0	0
			2593	1688	418	478	9			
1	D	314	Total	C	N	O	S	0	0	0
			2593	1688	418	478	9			
1	E	314	Total	C	N	O	S	0	0	0
			2593	1688	418	478	9			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q9WZ31
A	23	SER	-	expression tag	UNP Q9WZ31
A	24	HIS	-	expression tag	UNP Q9WZ31
A	25	MET	-	expression tag	UNP Q9WZ31
A	222	ALA	ARG	engineered mutation	UNP Q9WZ31
A	223	ALA	LYS	engineered mutation	UNP Q9WZ31
B	22	GLY	-	expression tag	UNP Q9WZ31
B	23	SER	-	expression tag	UNP Q9WZ31
B	24	HIS	-	expression tag	UNP Q9WZ31
B	25	MET	-	expression tag	UNP Q9WZ31
B	222	ALA	ARG	engineered mutation	UNP Q9WZ31
B	223	ALA	LYS	engineered mutation	UNP Q9WZ31
C	22	GLY	-	expression tag	UNP Q9WZ31
C	23	SER	-	expression tag	UNP Q9WZ31
C	24	HIS	-	expression tag	UNP Q9WZ31
C	25	MET	-	expression tag	UNP Q9WZ31
C	222	ALA	ARG	engineered mutation	UNP Q9WZ31
C	223	ALA	LYS	engineered mutation	UNP Q9WZ31
D	22	GLY	-	expression tag	UNP Q9WZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	23	SER	-	expression tag	UNP Q9WZ31
D	24	HIS	-	expression tag	UNP Q9WZ31
D	25	MET	-	expression tag	UNP Q9WZ31
D	222	ALA	ARG	engineered mutation	UNP Q9WZ31
D	223	ALA	LYS	engineered mutation	UNP Q9WZ31
E	22	GLY	-	expression tag	UNP Q9WZ31
E	23	SER	-	expression tag	UNP Q9WZ31
E	24	HIS	-	expression tag	UNP Q9WZ31
E	25	MET	-	expression tag	UNP Q9WZ31
E	222	ALA	ARG	engineered mutation	UNP Q9WZ31
E	223	ALA	LYS	engineered mutation	UNP Q9WZ31

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cs 1 1	0	0
2	B	3	Total Cs 3 3	0	0
2	C	1	Total Cs 1 1	0	0
2	D	1	Total Cs 1 1	0	0
2	E	3	Total Cs 3 3	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

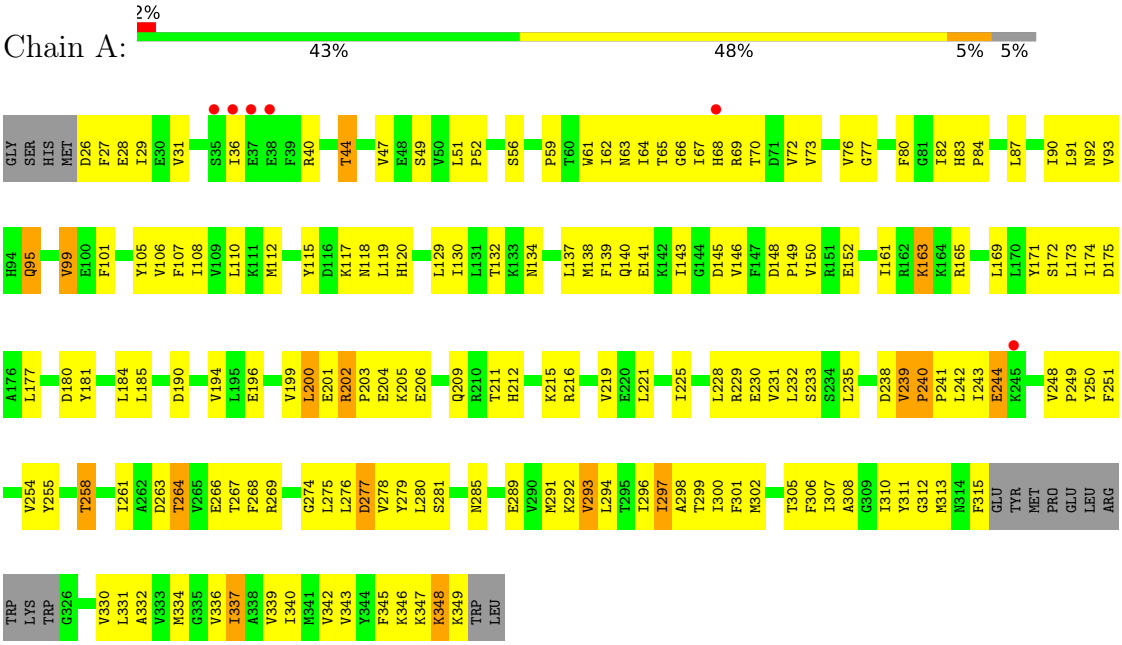
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

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.

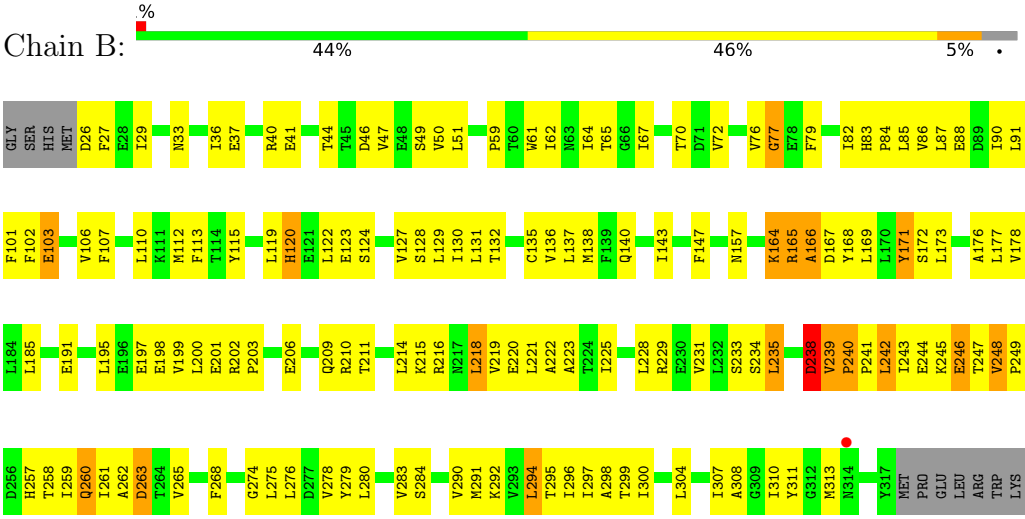
• Molecule 1: Magnesium transport protein CorA

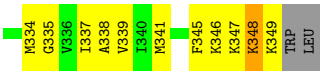
Chain A:



• Molecule 1: Magnesium transport protein CorA

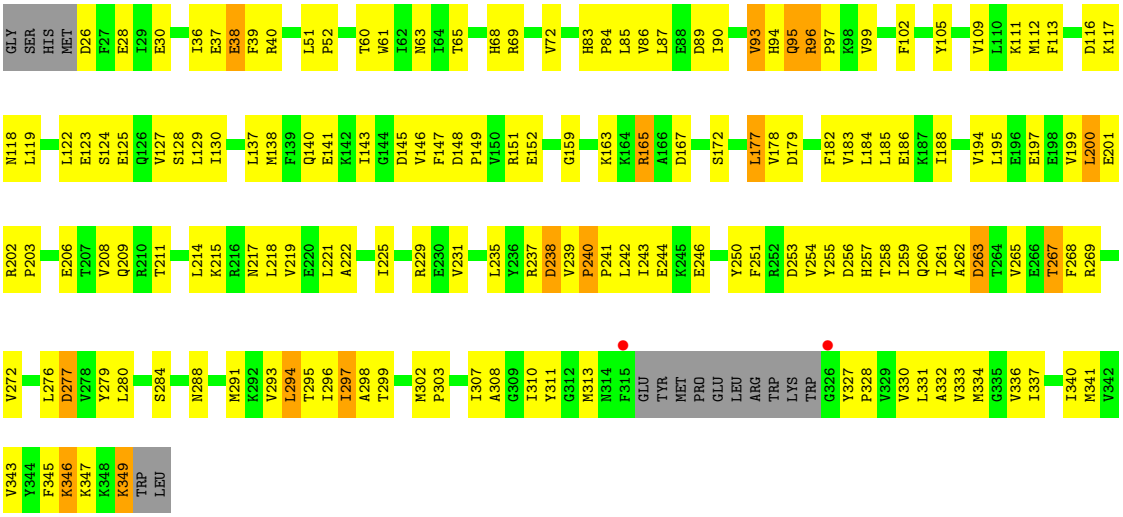
Chain B:





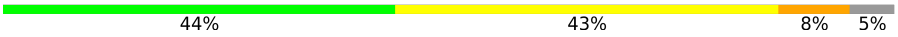
• Molecule 1: Magnesium transport protein CorA

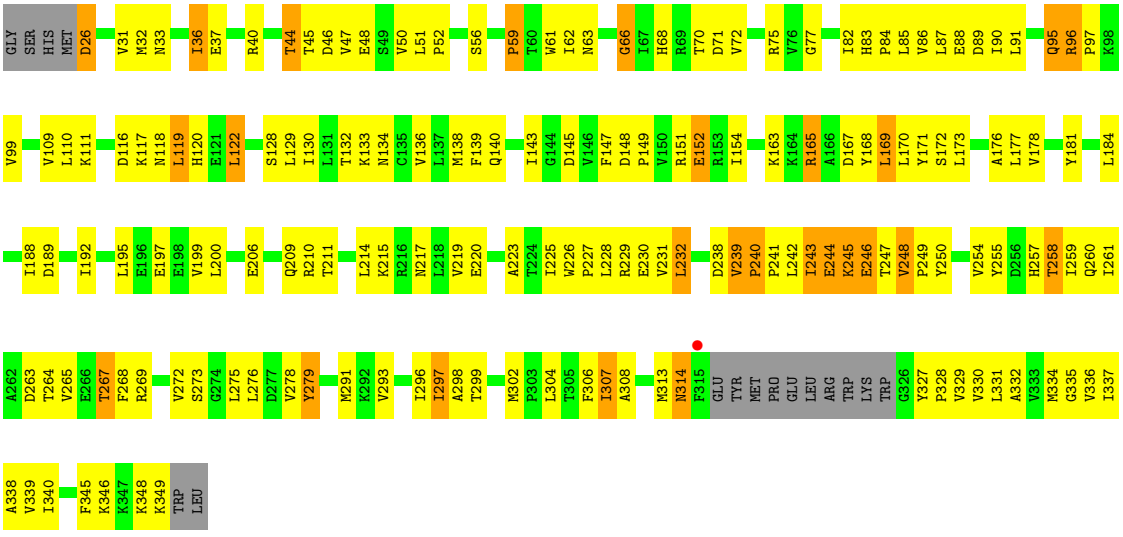
Chain C:



• Molecule 1: Magnesium transport protein CorA

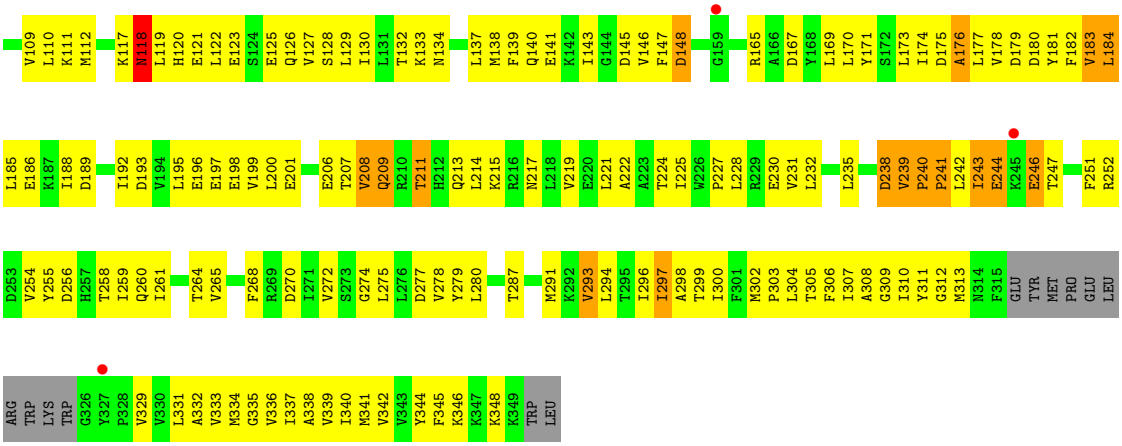
Chain D:





• Molecule 1: Magnesium transport protein CorA

Chain E:


V109 L110 K111 M112 K117 N118 L119 H120 E121 L122 E123 S124 E125 Q126 V127 S128 L129 I130 L131 T132 K133 N134 L137 M138 F139 Q140 E141 K142 I143 G144 D145 V146 F147 D148 G159 R165 A166 D167 Y168 L169 L170 Y171 S172 L173 I174 D175 A176 L177 V178 D179 D180 Y181 F182 V183 L184
L185 E186 K187 I188 D189 I192 D193 V194 L195 E196 E197 E198 V199 L200 E201 E206 T207 V208 Q209 R210 T211 H212 Q213 L214 K215 R216 N217 L218 V219 E220 L221 A222 A223 T224 I225 W226 P227 L228 R229 E230 V231 L232 L235 D238 V239 P240 P241 L242 I243 E244 K245 E246 T247 F251 R252
D253 V254 Y255 D256 H257 T258 I259 Q260 I261 T264 V265 F268 R269 D270 I271 V272 S273 G274 L275 L276 D277 V278 Y279 L280 T287 M291 K292 V293 L294 T295 I296 I297 A298 T299 I300 F301 M302 P303 L304 T305 F306 I307 A308 G309 I310 Y311 G312 M313 N314 F315 GLU TYR MET PRO GLU LEU
ARG TRP LYS TRP G326 Y327 P328 V329 V330 L331 A332 V333 M334 G335 V336 I337 A338 V339 I340 M341 V342 V343 Y344 F345 K346 K347 K348 K349 TRP LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	125.60Å 221.90Å 106.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 3.80 19.89 – 3.80	Depositor EDS
% Data completeness (in resolution range)	80.4 (19.92-3.80) 80.4 (19.89-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.82Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.299 , 0.343 0.297 , 0.352	Depositor DCC
R_{free} test set	1189 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	121.3	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 37.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12988	wwPDB-VP
Average B, all atoms (Å^2)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.60	1/2646 (0.0%)	0.67	0/3588
1	B	0.62	0/2660	0.72	0/3609
1	C	0.68	0/2646	0.72	0/3588
1	D	0.66	0/2646	0.73	0/3588
1	E	0.58	0/2646	0.69	0/3588
All	All	0.63	1/13244 (0.0%)	0.71	0/17961

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	GLU	CD-OE2	5.12	1.31	1.25

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	2593	0	2629	183	0
1	B	2606	0	2630	211	0
1	C	2593	0	2630	170	0
1	D	2593	0	2630	211	0
1	E	2593	0	2629	187	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	3	0	0	0	0
3	B	1	0	0	0	0
All	All	12988	0	13148	883	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 34.

All (883) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:VAL:CG2	1:D:231:VAL:HG13	1.63	1.27
1:B:99:VAL:CG2	1:B:231:VAL:HG13	1.72	1.18
1:E:99:VAL:CG2	1:E:231:VAL:HG13	1.74	1.16
1:B:99:VAL:HG23	1:B:231:VAL:HG13	1.30	1.11
1:A:239:VAL:HG11	1:A:248:VAL:CG2	1.80	1.10
1:D:261:ILE:O	1:D:265:VAL:HG23	1.50	1.08
1:A:296:ILE:O	1:A:299:THR:HG22	1.55	1.07
1:E:255:TYR:O	1:E:258:THR:HG22	1.56	1.05
1:C:222:ALA:HB2	1:C:265:VAL:HG11	1.31	1.05
1:E:304:LEU:HD23	1:E:307:ILE:HD11	1.38	1.05
1:E:99:VAL:HG23	1:E:231:VAL:HG13	1.07	1.04
1:D:99:VAL:HG21	1:D:231:VAL:HG13	1.33	1.04
1:A:211:THR:HG21	1:A:276:LEU:HD13	1.41	1.01
1:B:255:TYR:O	1:B:258:THR:HG22	1.61	1.00
1:A:255:TYR:O	1:A:258:THR:HG22	1.59	0.99
1:A:215:LYS:O	1:A:219:VAL:HG23	1.64	0.95
1:C:211:THR:HG21	1:C:276:LEU:HD13	1.48	0.94
1:D:331:LEU:HD23	1:D:334:MET:CE	1.98	0.93
1:E:99:VAL:CG2	1:E:231:VAL:CG1	2.46	0.93
1:B:215:LYS:O	1:B:219:VAL:HG23	1.70	0.92
1:D:99:VAL:HG23	1:D:231:VAL:HG13	1.51	0.91
1:A:313:MET:HE1	1:B:308:ALA:O	1.69	0.91
1:B:99:VAL:CG2	1:B:231:VAL:CG1	2.49	0.91
1:B:307:ILE:HD11	1:B:334:MET:HG2	1.54	0.90
1:D:296:ILE:HA	1:D:299:THR:HG22	1.54	0.90
1:E:82:ILE:HD13	1:E:130:ILE:HD13	1.54	0.90
1:D:199:VAL:HG13	1:D:279:TYR:HB2	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG11	1:A:248:VAL:HG21	1.53	0.89
1:B:182:PHE:HA	1:B:185:LEU:HD12	1.54	0.89
1:B:313:MET:HA	1:B:313:MET:HE2	1.55	0.88
1:A:47:VAL:HG21	1:A:72:VAL:HG13	1.55	0.88
1:A:232:LEU:HD23	1:A:235:LEU:HD22	1.54	0.87
1:E:64:ILE:HD13	1:E:139:PHE:CE1	2.09	0.87
1:B:280:LEU:HD23	1:C:280:LEU:HD21	1.57	0.87
1:D:313:MET:HE1	1:E:308:ALA:O	1.76	0.85
1:E:99:VAL:HG23	1:E:231:VAL:CG1	1.99	0.85
1:A:239:VAL:HG11	1:A:248:VAL:HG22	1.56	0.85
1:E:65:THR:HG21	1:E:143:ILE:HD13	1.57	0.85
1:C:167:ASP:HB2	1:C:242:LEU:HD23	1.56	0.85
1:D:122:LEU:HD22	1:D:217:ASN:ND2	1.92	0.84
1:A:336:VAL:O	1:A:340:ILE:HG23	1.77	0.84
1:C:243:ILE:HD12	1:C:246:GLU:HB2	1.59	0.84
1:A:347:LYS:O	1:A:348:LYS:HB2	1.78	0.82
1:B:240:PRO:HB2	1:B:241:PRO:CD	2.09	0.82
1:B:242:LEU:HD21	1:B:251:PHE:CE1	2.14	0.82
1:C:331:LEU:HD23	1:C:334:MET:HE2	1.60	0.82
1:D:177:LEU:HD21	1:D:181:TYR:HE1	1.44	0.82
1:E:331:LEU:HD23	1:E:334:MET:CE	2.09	0.82
1:B:225:ILE:HD13	1:B:265:VAL:HG21	1.62	0.82
1:B:88:GLU:HA	1:B:91:LEU:HD12	1.62	0.81
1:C:296:ILE:HA	1:C:299:THR:HG22	1.61	0.81
1:A:200:LEU:HD22	1:B:209:GLN:HG2	1.63	0.81
1:A:63:ASN:HB2	1:A:138:MET:HE2	1.63	0.80
1:D:165:ARG:HH12	1:D:243:ILE:HD13	1.46	0.80
1:D:184:LEU:O	1:D:188:ILE:HD12	1.81	0.80
1:A:47:VAL:CG2	1:A:72:VAL:HG13	2.11	0.80
1:A:221:LEU:O	1:A:225:ILE:HD12	1.82	0.80
1:E:29:ILE:HG21	1:E:50:VAL:HG11	1.63	0.80
1:E:184:LEU:HD12	1:E:184:LEU:O	1.82	0.80
1:D:122:LEU:HD22	1:D:217:ASN:HD22	1.47	0.79
1:C:130:ILE:HB	1:C:137:LEU:HD12	1.64	0.79
1:C:255:TYR:O	1:C:258:THR:HG22	1.82	0.79
1:E:335:GLY:O	1:E:339:VAL:HG23	1.81	0.78
1:D:239:VAL:HG11	1:D:248:VAL:CG2	2.13	0.78
1:B:51:LEU:HD22	1:B:79:PHE:CD2	2.18	0.78
1:C:65:THR:HG21	1:C:143:ILE:HG12	1.65	0.78
1:C:313:MET:HE3	1:D:308:ALA:HB1	1.66	0.78
1:B:177:LEU:HD21	1:B:181:TYR:HE1	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:VAL:O	1:D:239:VAL:HG23	1.82	0.77
1:D:47:VAL:HG22	1:D:51:LEU:HD21	1.66	0.77
1:D:109:VAL:O	1:D:110:LEU:HD23	1.84	0.77
1:C:256:ASP:HA	1:C:259:ILE:HD12	1.67	0.77
1:C:331:LEU:HD23	1:C:334:MET:CE	2.15	0.76
1:C:194:VAL:HG12	1:C:194:VAL:O	1.84	0.76
1:E:76:VAL:HG13	1:E:80:PHE:CD2	2.20	0.76
1:D:313:MET:HE2	1:D:313:MET:HA	1.67	0.76
1:C:299:THR:HG21	1:C:345:PHE:CZ	2.20	0.76
1:B:131:LEU:HD12	1:B:135:CYS:O	1.85	0.75
1:E:177:LEU:C	1:E:177:LEU:HD23	2.06	0.75
1:C:302:MET:HE2	1:D:297:ILE:HG23	1.67	0.75
1:E:165:ARG:HH12	1:E:243:ILE:HD13	1.51	0.75
1:C:310:ILE:O	1:C:313:MET:HG2	1.87	0.75
1:B:222:ALA:HB2	1:B:265:VAL:HG11	1.69	0.74
1:E:215:LYS:O	1:E:219:VAL:HG23	1.88	0.74
1:D:128:SER:O	1:D:129:LEU:HD23	1.87	0.74
1:C:99:VAL:CG2	1:C:231:VAL:HG13	2.17	0.74
1:A:70:THR:HG22	1:A:91:LEU:HD22	1.68	0.74
1:C:302:MET:CE	1:D:297:ILE:HG23	2.17	0.74
1:E:296:ILE:HG22	1:E:345:PHE:CE1	2.23	0.74
1:D:61:TRP:HB2	1:D:169:LEU:HD21	1.69	0.73
1:D:31:VAL:HG22	1:D:62:ILE:HG12	1.70	0.73
1:D:169:LEU:HD12	1:D:169:LEU:O	1.89	0.73
1:C:83:HIS:NE2	1:C:85:LEU:HD12	2.04	0.72
1:C:243:ILE:HD12	1:C:246:GLU:CB	2.18	0.72
1:C:313:MET:HE3	1:D:308:ALA:O	1.88	0.72
1:D:255:TYR:O	1:D:258:THR:HB	1.90	0.72
1:D:177:LEU:HD21	1:D:181:TYR:CE1	2.24	0.72
1:B:29:ILE:HB	1:B:44:THR:HG23	1.71	0.72
1:A:174:ILE:HG21	1:A:232:LEU:HD21	1.71	0.72
1:B:242:LEU:CD2	1:B:251:PHE:HE1	2.03	0.72
1:D:243:ILE:HD12	1:D:246:GLU:HB3	1.72	0.72
1:D:165:ARG:NH1	1:D:243:ILE:HD13	2.04	0.71
1:A:67:ILE:HD11	1:A:93:VAL:CG1	2.20	0.71
1:B:245:LYS:O	1:B:246:GLU:HB2	1.89	0.71
1:A:65:THR:HG21	1:A:143:ILE:HD13	1.71	0.71
1:E:122:LEU:HD22	1:E:217:ASN:HD22	1.56	0.71
1:E:239:VAL:HG23	1:E:239:VAL:O	1.91	0.71
1:A:269:ARG:NH1	1:E:270:ASP:OD1	2.23	0.70
1:D:99:VAL:CG2	1:D:231:VAL:CG1	2.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ILE:HD13	1:A:163:LYS:HG3	1.73	0.70
1:B:83:HIS:ND1	1:B:84:PRO:HD2	2.07	0.70
1:B:110:LEU:CD1	1:B:177:LEU:HD13	2.22	0.70
1:D:331:LEU:HD23	1:D:334:MET:HE2	1.74	0.70
1:D:297:ILE:HG22	1:D:298:ALA:N	2.07	0.70
1:B:70:THR:HG22	1:B:91:LEU:HD22	1.74	0.69
1:D:331:LEU:HD23	1:D:334:MET:HE3	1.73	0.69
1:E:331:LEU:HD23	1:E:334:MET:HE3	1.73	0.69
1:B:65:THR:HG21	1:B:143:ILE:HD13	1.74	0.69
1:B:177:LEU:HD21	1:B:181:TYR:CE1	2.28	0.69
1:C:296:ILE:HD12	1:C:297:ILE:N	2.07	0.69
1:B:99:VAL:HG22	1:B:231:VAL:HG13	1.71	0.69
1:B:347:LYS:O	1:B:348:LYS:HB2	1.92	0.69
1:B:82:ILE:HD13	1:B:130:ILE:HD13	1.73	0.69
1:B:295:THR:HG23	1:C:294:LEU:HG	1.74	0.69
1:E:84:PRO:HA	1:E:87:LEU:HD12	1.75	0.68
1:E:130:ILE:HB	1:E:137:LEU:HD12	1.74	0.68
1:B:106:VAL:O	1:B:130:ILE:HG23	1.92	0.68
1:B:313:MET:CE	1:C:311:TYR:HB2	2.24	0.68
1:A:313:MET:CE	1:B:308:ALA:O	2.42	0.68
1:D:335:GLY:O	1:D:339:VAL:HG23	1.94	0.68
1:C:225:ILE:HD12	1:C:265:VAL:HG21	1.74	0.67
1:B:242:LEU:CD2	1:B:251:PHE:CE1	2.76	0.67
1:B:65:THR:HG21	1:B:143:ILE:CD1	2.25	0.67
1:C:215:LYS:O	1:C:219:VAL:HG23	1.95	0.67
1:D:313:MET:CE	1:E:308:ALA:O	2.42	0.67
1:B:299:THR:HA	1:C:297:ILE:HG21	1.76	0.67
1:B:47:VAL:O	1:B:50:VAL:HG22	1.94	0.67
1:D:296:ILE:HA	1:D:299:THR:CG2	2.24	0.67
1:D:177:LEU:CD2	1:D:181:TYR:HE1	2.06	0.67
1:D:334:MET:O	1:D:338:ALA:HB2	1.94	0.66
1:E:256:ASP:HA	1:E:259:ILE:HD12	1.77	0.66
1:E:333:VAL:O	1:E:337:ILE:HG23	1.95	0.66
1:B:110:LEU:HD13	1:B:177:LEU:HD13	1.77	0.66
1:E:296:ILE:HA	1:E:299:THR:HG22	1.77	0.66
1:B:36:ILE:HG23	1:B:37:GLU:HG3	1.77	0.66
1:C:165:ARG:HH12	1:C:243:ILE:HD13	1.60	0.66
1:B:313:MET:CE	1:C:308:ALA:O	2.44	0.66
1:D:84:PRO:HA	1:D:87:LEU:HD12	1.78	0.66
1:D:33:ASN:ND2	1:D:59:PRO:O	2.29	0.66
1:B:130:ILE:HB	1:B:137:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:O	1:B:244:GLU:N	2.29	0.66
1:B:240:PRO:HB2	1:B:241:PRO:HD3	1.77	0.65
1:D:239:VAL:HG11	1:D:248:VAL:HG23	1.79	0.65
1:B:173:LEU:O	1:B:176:ALA:HB3	1.96	0.65
1:E:296:ILE:CD1	1:E:297:ILE:HD12	2.26	0.65
1:D:136:VAL:HG11	1:D:173:LEU:CD1	2.25	0.65
1:B:166:ALA:O	1:B:169:LEU:HB3	1.95	0.65
1:E:184:LEU:O	1:E:188:ILE:HD12	1.96	0.65
1:D:195:LEU:HD21	1:D:211:THR:HA	1.77	0.65
1:B:195:LEU:O	1:B:199:VAL:HG23	1.97	0.65
1:A:331:LEU:HA	1:A:334:MET:HE2	1.77	0.65
1:E:61:TRP:HB2	1:E:169:LEU:HD21	1.79	0.65
1:B:61:TRP:CD1	1:B:61:TRP:C	2.70	0.64
1:A:87:LEU:HD23	1:A:90:ILE:HD12	1.80	0.64
1:B:27:PHE:CZ	1:B:72:VAL:HG21	2.33	0.64
1:B:86:VAL:HG13	1:B:107:PHE:CE2	2.30	0.64
1:B:131:LEU:HD11	1:B:166:ALA:HB1	1.79	0.64
1:C:328:PRO:HA	1:C:331:LEU:HD12	1.78	0.64
1:D:178:VAL:HG21	1:D:254:VAL:CG1	2.26	0.64
1:D:296:ILE:HG22	1:D:345:PHE:CZ	2.32	0.64
1:B:247:THR:HA	1:B:250:TYR:HD2	1.60	0.64
1:C:221:LEU:HD23	1:C:265:VAL:HG22	1.78	0.64
1:D:170:LEU:O	1:D:171:TYR:C	2.35	0.64
1:A:27:PHE:CD1	1:A:69:ARG:HG3	2.33	0.64
1:E:195:LEU:O	1:E:199:VAL:HG23	1.97	0.64
1:A:56:SER:O	1:A:134:ASN:ND2	2.30	0.64
1:D:177:LEU:C	1:D:177:LEU:HD23	2.18	0.64
1:D:331:LEU:CD2	1:D:334:MET:CE	2.74	0.64
1:A:36:ILE:CD1	1:A:163:LYS:HG3	2.28	0.63
1:B:83:HIS:HE2	1:B:85:LEU:HD12	1.62	0.63
1:D:299:THR:HA	1:E:297:ILE:HG21	1.80	0.63
1:E:29:ILE:CG2	1:E:50:VAL:HG11	2.29	0.63
1:A:209:GLN:HG2	1:E:200:LEU:HD22	1.81	0.63
1:E:65:THR:HG21	1:E:143:ILE:CD1	2.29	0.63
1:A:61:TRP:HB2	1:A:169:LEU:HD21	1.80	0.63
1:B:278:VAL:HA	1:C:276:LEU:HD21	1.81	0.63
1:C:333:VAL:HA	1:C:336:VAL:HB	1.80	0.63
1:A:65:THR:HG21	1:A:143:ILE:CD1	2.28	0.62
1:A:177:LEU:O	1:A:180:ASP:HB3	1.98	0.62
1:D:32:MET:HE1	1:D:154:ILE:HB	1.81	0.62
1:B:87:LEU:HA	1:B:90:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:THR:HG22	1:D:268:PHE:N	2.13	0.62
1:E:122:LEU:HD22	1:E:217:ASN:ND2	2.15	0.62
1:A:185:LEU:HD11	1:A:261:ILE:HG23	1.79	0.62
1:A:150:VAL:HG11	1:A:173:LEU:HD23	1.81	0.62
1:B:211:THR:HG23	1:B:275:LEU:HD23	1.82	0.61
1:D:296:ILE:CA	1:D:299:THR:HG22	2.28	0.61
1:B:222:ALA:HA	1:B:225:ILE:HD12	1.83	0.61
1:E:97:PRO:HB3	1:E:228:LEU:HD12	1.83	0.61
1:B:113:PHE:CE1	1:B:124:SER:HB3	2.35	0.61
1:E:26:ASP:N	1:E:68:HIS:HE2	1.99	0.61
1:C:332:ALA:O	1:C:336:VAL:HG23	2.00	0.61
1:E:199:VAL:HG13	1:E:279:TYR:HB2	1.82	0.61
1:E:232:LEU:HD11	1:E:254:VAL:HG12	1.82	0.61
1:B:185:LEU:HD11	1:B:261:ILE:HG23	1.83	0.60
1:B:298:ALA:CB	1:C:294:LEU:HD21	2.30	0.60
1:C:313:MET:CE	1:D:308:ALA:O	2.48	0.60
1:D:199:VAL:HG13	1:D:279:TYR:CB	2.30	0.60
1:A:80:PHE:CZ	1:A:137:LEU:HD21	2.36	0.60
1:C:218:LEU:HD23	1:C:269:ARG:HA	1.83	0.60
1:A:235:LEU:HD23	1:A:251:PHE:CE2	2.37	0.60
1:A:289:GLU:O	1:A:293:VAL:HG23	2.00	0.60
1:B:242:LEU:HD21	1:B:251:PHE:CZ	2.37	0.60
1:A:165:ARG:HH12	1:A:243:ILE:HD13	1.67	0.60
1:A:299:THR:HG23	1:A:300:ILE:HG23	1.82	0.60
1:C:83:HIS:ND1	1:C:84:PRO:HD2	2.17	0.60
1:E:240:PRO:HB2	1:E:241:PRO:HD3	1.84	0.60
1:C:99:VAL:HG22	1:C:231:VAL:HG13	1.82	0.60
1:D:242:LEU:O	1:D:243:ILE:C	2.40	0.60
1:A:313:MET:HE2	1:A:313:MET:HA	1.84	0.60
1:C:240:PRO:HB2	1:C:241:PRO:CD	2.32	0.60
1:E:232:LEU:CD1	1:E:254:VAL:HG12	2.31	0.60
1:A:63:ASN:CB	1:A:138:MET:HE2	2.31	0.59
1:A:301:PHE:O	1:A:305:THR:OG1	2.10	0.59
1:E:240:PRO:HB2	1:E:241:PRO:CD	2.32	0.59
1:C:302:MET:HE2	1:D:297:ILE:CG2	2.31	0.59
1:B:310:ILE:O	1:B:313:MET:HG2	2.03	0.59
1:D:291:MET:HE1	1:E:291:MET:HG2	1.84	0.59
1:A:64:ILE:HD12	1:A:139:PHE:CE1	2.37	0.59
1:A:110:LEU:HD22	1:A:228:LEU:HD13	1.83	0.59
1:E:171:TYR:HE1	1:E:254:VAL:HG23	1.67	0.59
1:B:261:ILE:O	1:B:265:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:HG22	1:B:298:ALA:N	2.16	0.59
1:C:311:TYR:HE2	1:C:330:VAL:HG21	1.68	0.59
1:D:184:LEU:O	1:D:188:ILE:CD1	2.51	0.59
1:C:148:ASP:N	1:C:149:PRO:HD2	2.17	0.59
1:C:267:THR:HG22	1:C:268:PHE:N	2.17	0.59
1:A:339:VAL:HA	1:A:342:VAL:HG23	1.85	0.59
1:C:296:ILE:HA	1:C:299:THR:CG2	2.30	0.59
1:B:238:ASP:O	1:B:239:VAL:HG22	2.03	0.58
1:E:231:VAL:O	1:E:235:LEU:HD13	2.03	0.58
1:A:200:LEU:HD22	1:B:209:GLN:CG	2.32	0.58
1:E:268:PHE:O	1:E:272:VAL:HG23	2.03	0.58
1:C:222:ALA:HB2	1:C:265:VAL:CG1	2.20	0.58
1:D:245:LYS:O	1:D:246:GLU:HG2	2.03	0.58
1:D:299:THR:HG21	1:D:345:PHE:CZ	2.38	0.58
1:E:66:GLY:HA2	1:E:141:GLU:O	2.03	0.58
1:A:291:MET:HB3	1:B:290:VAL:HG11	1.85	0.58
1:C:97:PRO:HA	1:C:109:VAL:O	2.03	0.58
1:A:115:TYR:OH	1:A:120:HIS:HA	2.04	0.58
1:B:65:THR:HG21	1:B:143:ILE:CG1	2.33	0.58
1:E:296:ILE:HD12	1:E:297:ILE:HD12	1.85	0.58
1:A:110:LEU:HD22	1:A:228:LEU:CD1	2.34	0.58
1:B:99:VAL:HG22	1:B:231:VAL:CG1	2.29	0.58
1:B:138:MET:SD	1:B:147:PHE:CE2	2.97	0.57
1:C:60:THR:CG2	1:C:61:TRP:N	2.66	0.57
1:C:165:ARG:NH1	1:C:243:ILE:HD13	2.18	0.57
1:C:260:GLN:HA	1:D:96:ARG:HH21	1.69	0.57
1:D:330:VAL:O	1:D:334:MET:HG3	2.04	0.57
1:E:313:MET:HA	1:E:313:MET:HE2	1.87	0.57
1:B:178:VAL:HG21	1:B:254:VAL:HG12	1.86	0.57
1:C:63:ASN:OD1	1:C:138:MET:HE2	2.03	0.57
1:D:82:ILE:HG22	1:D:87:LEU:HG	1.86	0.57
1:D:122:LEU:CD2	1:D:217:ASN:HD22	2.15	0.57
1:B:240:PRO:CB	1:B:241:PRO:CD	2.82	0.57
1:E:185:LEU:O	1:E:186:GLU:C	2.42	0.57
1:E:252:ARG:O	1:E:255:TYR:HB3	2.04	0.57
1:A:171:TYR:CE1	1:A:250:TYR:HB3	2.40	0.57
1:D:171:TYR:O	1:D:172:SER:C	2.41	0.57
1:D:225:ILE:HD13	1:D:261:ILE:CG2	2.34	0.57
1:D:306:PHE:CD1	1:D:307:ILE:HG23	2.40	0.57
1:E:77:GLY:CA	1:E:87:LEU:HD21	2.34	0.57
1:A:31:VAL:HG22	1:A:62:ILE:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:LEU:CD2	1:B:181:TYR:HE1	2.17	0.57
1:B:248:VAL:HG12	1:B:249:PRO:CD	2.35	0.57
1:E:185:LEU:HA	1:E:188:ILE:HD12	1.86	0.57
1:E:329:VAL:O	1:E:333:VAL:HG23	2.05	0.57
1:E:118:ASN:OD1	1:E:119:LEU:N	2.37	0.57
1:E:242:LEU:O	1:E:243:ILE:C	2.42	0.56
1:B:169:LEU:O	1:B:172:SER:N	2.38	0.56
1:B:313:MET:HA	1:B:313:MET:CE	2.33	0.56
1:E:225:ILE:HD12	1:E:265:VAL:HG21	1.87	0.56
1:E:165:ARG:NH1	1:E:243:ILE:HD13	2.19	0.56
1:C:240:PRO:HB2	1:C:241:PRO:HD3	1.87	0.56
1:A:112:MET:SD	1:A:146:VAL:HG13	2.46	0.56
1:B:112:MET:CE	1:B:127:VAL:HG21	2.35	0.56
1:A:298:ALA:HA	1:E:302:MET:HE2	1.87	0.56
1:B:234:SER:O	1:B:238:ASP:HB2	2.05	0.56
1:D:71:ASP:OD1	1:D:71:ASP:N	2.39	0.56
1:D:297:ILE:CG2	1:D:298:ALA:N	2.68	0.56
1:D:47:VAL:HB	1:D:72:VAL:HG13	1.88	0.56
1:D:118:ASN:O	1:D:120:HIS:CE1	2.59	0.56
1:E:235:LEU:HD23	1:E:251:PHE:CD2	2.41	0.56
1:A:201:GLU:C	1:A:203:PRO:HD3	2.27	0.56
1:D:48:GLU:OE2	1:D:75:ARG:NE	2.38	0.56
1:B:247:THR:HG22	1:B:250:TYR:HB2	1.87	0.56
1:C:336:VAL:O	1:C:340:ILE:HG23	2.06	0.56
1:B:119:LEU:O	1:B:120:HIS:C	2.44	0.55
1:B:248:VAL:HG12	1:B:249:PRO:HD3	1.87	0.55
1:D:227:PRO:O	1:D:228:LEU:C	2.41	0.55
1:D:229:ARG:HA	1:D:258:THR:CG2	2.36	0.55
1:E:109:VAL:O	1:E:110:LEU:HD23	2.05	0.55
1:E:225:ILE:CD1	1:E:265:VAL:HG21	2.37	0.55
1:A:331:LEU:HD23	1:A:334:MET:CE	2.36	0.55
1:B:83:HIS:NE2	1:B:85:LEU:HD12	2.21	0.55
1:B:185:LEU:HD11	1:B:261:ILE:CG2	2.35	0.55
1:C:113:PHE:CE1	1:C:124:SER:HB3	2.40	0.55
1:B:65:THR:HG21	1:B:143:ILE:HG12	1.88	0.55
1:D:165:ARG:NH1	1:D:243:ILE:HG21	2.20	0.55
1:B:229:ARG:HH11	1:B:259:ILE:HG23	1.71	0.55
1:C:147:PHE:O	1:C:151:ARG:HG3	2.07	0.55
1:C:295:THR:CG2	1:D:293:VAL:HG11	2.36	0.55
1:A:117:LYS:O	1:A:119:LEU:N	2.39	0.55
1:B:300:ILE:HG22	1:B:341:MET:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:GLY:O	1:B:339:VAL:HG23	2.06	0.55
1:A:248:VAL:N	1:A:249:PRO:HD2	2.22	0.55
1:C:36:ILE:HG23	1:C:37:GLU:HG3	1.88	0.55
1:E:306:PHE:HD1	1:E:307:ILE:HG23	1.72	0.55
1:A:66:GLY:N	1:A:140:GLN:O	2.40	0.55
1:A:291:MET:HE3	1:B:290:VAL:CG1	2.37	0.55
1:D:240:PRO:HB2	1:D:241:PRO:CD	2.36	0.55
1:A:70:THR:HG22	1:A:91:LEU:CD2	2.37	0.55
1:C:194:VAL:O	1:C:194:VAL:CG1	2.54	0.55
1:D:275:LEU:O	1:D:278:VAL:N	2.37	0.55
1:D:296:ILE:O	1:D:299:THR:HG22	2.07	0.55
1:A:47:VAL:HG21	1:A:72:VAL:CG1	2.33	0.55
1:C:63:ASN:HA	1:C:138:MET:HB3	1.89	0.55
1:E:338:ALA:O	1:E:342:VAL:HG23	2.06	0.55
1:D:225:ILE:HD13	1:D:261:ILE:HG22	1.89	0.54
1:A:63:ASN:HB2	1:A:138:MET:CE	2.35	0.54
1:C:200:LEU:HD22	1:D:209:GLN:HG3	1.88	0.54
1:C:295:THR:HG21	1:D:293:VAL:HG11	1.89	0.54
1:B:136:VAL:HG11	1:B:173:LEU:CD1	2.37	0.54
1:E:51:LEU:CD2	1:E:76:VAL:HG22	2.36	0.54
1:B:296:ILE:HA	1:B:299:THR:HG22	1.90	0.54
1:D:229:ARG:HA	1:D:258:THR:HG21	1.89	0.54
1:D:296:ILE:HD12	1:D:297:ILE:N	2.22	0.54
1:B:112:MET:HE2	1:B:127:VAL:HG21	1.90	0.54
1:C:296:ILE:O	1:C:299:THR:HG22	2.07	0.54
1:E:192:ILE:O	1:E:193:ASP:C	2.46	0.54
1:A:239:VAL:HG12	1:A:242:LEU:CD1	2.37	0.54
1:D:83:HIS:ND1	1:D:84:PRO:HD2	2.23	0.54
1:A:61:TRP:HZ2	1:A:138:MET:HE1	1.73	0.54
1:B:131:LEU:HD13	1:B:136:VAL:CG2	2.38	0.54
1:B:201:GLU:C	1:B:203:PRO:HD3	2.28	0.54
1:B:225:ILE:CG2	1:B:262:ALA:HB2	2.38	0.54
1:B:263:ASP:CB	1:C:96:ARG:NH2	2.70	0.54
1:B:313:MET:HE3	1:C:308:ALA:O	2.05	0.54
1:C:130:ILE:CB	1:C:137:LEU:HD12	2.35	0.54
1:E:47:VAL:HB	1:E:72:VAL:HG13	1.88	0.54
1:A:36:ILE:HD13	1:A:163:LYS:CG	2.38	0.54
1:A:87:LEU:HD23	1:A:90:ILE:CD1	2.38	0.54
1:B:225:ILE:HG22	1:B:262:ALA:HB2	1.89	0.54
1:C:188:ILE:HG23	1:C:214:LEU:HD11	1.89	0.54
1:D:110:LEU:HD13	1:D:177:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:VAL:O	1:D:275:LEU:N	2.37	0.54
1:C:93:VAL:HG23	1:C:94:HIS:CE1	2.42	0.54
1:B:296:ILE:HD12	1:B:296:ILE:C	2.28	0.53
1:B:313:MET:HE1	1:C:308:ALA:O	2.07	0.53
1:D:313:MET:HE2	1:D:313:MET:CA	2.36	0.53
1:A:148:ASP:O	1:A:152:GLU:HG2	2.08	0.53
1:A:190:ASP:O	1:A:194:VAL:HG23	2.09	0.53
1:D:148:ASP:N	1:D:149:PRO:HD2	2.23	0.53
1:D:215:LYS:O	1:D:219:VAL:HG23	2.09	0.53
1:A:209:GLN:CG	1:E:200:LEU:HD22	2.39	0.53
1:D:122:LEU:HD21	1:D:220:GLU:OE1	2.07	0.53
1:D:260:GLN:HE22	1:E:95:GLN:HA	1.73	0.53
1:E:227:PRO:O	1:E:230:GLU:N	2.42	0.53
1:A:77:GLY:HA3	1:A:87:LEU:HD11	1.90	0.53
1:C:260:GLN:O	1:C:263:ASP:HB2	2.08	0.53
1:A:291:MET:CE	1:B:290:VAL:HG12	2.38	0.53
1:D:51:LEU:N	1:D:52:PRO:HD2	2.24	0.53
1:D:248:VAL:HG12	1:D:249:PRO:CD	2.38	0.53
1:E:109:VAL:HG11	1:E:126:GLN:OE1	2.09	0.53
1:A:294:LEU:CD2	1:B:294:LEU:HD11	2.38	0.53
1:C:36:ILE:HD13	1:C:163:LYS:HG3	1.91	0.53
1:E:64:ILE:CD1	1:E:139:PHE:CE1	2.89	0.53
1:B:238:ASP:C	1:B:239:VAL:HG22	2.29	0.53
1:C:102:PHE:CG	1:C:105:TYR:CE1	2.97	0.53
1:C:148:ASP:O	1:C:152:GLU:HG2	2.08	0.53
1:C:211:THR:CG2	1:C:276:LEU:HD13	2.31	0.53
1:D:177:LEU:CD2	1:D:181:TYR:CE1	2.86	0.53
1:E:300:ILE:O	1:E:304:LEU:HD12	2.09	0.53
1:A:83:HIS:ND1	1:A:84:PRO:HD2	2.24	0.53
1:B:216:ARG:O	1:B:219:VAL:HB	2.08	0.53
1:C:296:ILE:CA	1:C:299:THR:HG22	2.35	0.53
1:D:239:VAL:O	1:D:239:VAL:CG2	2.53	0.53
1:A:36:ILE:HD13	1:A:163:LYS:HA	1.91	0.53
1:A:199:VAL:HG13	1:A:279:TYR:HA	1.91	0.53
1:B:222:ALA:HB2	1:B:265:VAL:CG1	2.37	0.53
1:B:110:LEU:HD12	1:B:177:LEU:HD13	1.90	0.52
1:C:93:VAL:HG23	1:C:94:HIS:NE2	2.24	0.52
1:E:60:THR:HG22	1:E:61:TRP:N	2.25	0.52
1:B:67:ILE:HG23	1:B:140:GLN:O	2.09	0.52
1:D:178:VAL:HG21	1:D:254:VAL:HG12	1.90	0.52
1:C:229:ARG:HG3	1:C:258:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:TYR:CE2	1:C:330:VAL:HG21	2.45	0.52
1:B:178:VAL:HG21	1:B:254:VAL:CG1	2.39	0.52
1:C:183:VAL:HG13	1:C:186:GLU:OE2	2.09	0.52
1:A:307:ILE:O	1:A:310:ILE:HG12	2.09	0.52
1:C:185:LEU:HD11	1:C:261:ILE:HD13	1.92	0.52
1:D:132:THR:O	1:D:132:THR:HG23	2.10	0.52
1:D:250:TYR:O	1:D:254:VAL:HG23	2.10	0.52
1:E:296:ILE:HD11	1:E:297:ILE:HD12	1.91	0.52
1:E:307:ILE:HA	1:E:310:ILE:HD13	1.91	0.52
1:A:47:VAL:HG22	1:A:47:VAL:O	2.09	0.52
1:A:61:TRP:CZ2	1:A:138:MET:HE1	2.44	0.52
1:D:248:VAL:HG12	1:D:249:PRO:HD3	1.92	0.52
1:B:200:LEU:CD2	1:C:209:GLN:HG3	2.39	0.52
1:B:229:ARG:NH1	1:B:259:ILE:HG23	2.25	0.52
1:B:182:PHE:CA	1:B:185:LEU:HD12	2.32	0.52
1:D:240:PRO:HB2	1:D:241:PRO:HD3	1.91	0.52
1:D:304:LEU:HD23	1:D:307:ILE:HD11	1.91	0.52
1:A:232:LEU:HD13	1:A:254:VAL:HG12	1.91	0.51
1:B:77:GLY:HA3	1:B:87:LEU:HD21	1.92	0.51
1:C:99:VAL:HG21	1:C:235:LEU:CD1	2.40	0.51
1:E:77:GLY:HA3	1:E:87:LEU:HD21	1.90	0.51
1:E:78:GLU:O	1:E:81:GLY:N	2.40	0.51
1:A:26:ASP:O	1:A:68:HIS:NE2	2.36	0.51
1:C:302:MET:HB2	1:C:303:PRO:CD	2.40	0.51
1:D:197:GLU:O	1:D:200:LEU:HD12	2.10	0.51
1:E:117:LYS:O	1:E:118:ASN:HB3	2.10	0.51
1:A:242:LEU:HD22	1:A:251:PHE:CE1	2.45	0.51
1:B:200:LEU:HD22	1:C:209:GLN:HG3	1.93	0.51
1:D:244:GLU:O	1:D:246:GLU:N	2.43	0.51
1:B:311:TYR:HE2	1:B:330:VAL:HG21	1.74	0.51
1:A:77:GLY:HA3	1:A:87:LEU:CD1	2.40	0.51
1:E:182:PHE:HA	1:E:185:LEU:HD12	1.91	0.51
1:A:299:THR:HG21	1:A:345:PHE:CE1	2.46	0.51
1:C:201:GLU:C	1:C:203:PRO:HD3	2.31	0.51
1:D:119:LEU:HD12	1:D:119:LEU:O	2.11	0.51
1:B:51:LEU:HD22	1:B:79:PHE:CG	2.45	0.51
1:B:222:ALA:CB	1:B:265:VAL:HG11	2.40	0.51
1:B:299:THR:HG21	1:B:345:PHE:CZ	2.46	0.51
1:C:242:LEU:HD22	1:C:251:PHE:CE1	2.46	0.51
1:D:272:VAL:O	1:D:275:LEU:HB2	2.10	0.51
1:D:331:LEU:CD2	1:D:334:MET:HE2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD21	1:B:294:LEU:HD11	1.92	0.50
1:B:238:ASP:O	1:B:239:VAL:O	2.29	0.50
1:C:28:GLU:OE2	1:C:143:ILE:HD11	2.11	0.50
1:C:299:THR:HG21	1:C:345:PHE:HZ	1.72	0.50
1:D:66:GLY:N	1:D:140:GLN:O	2.44	0.50
1:B:299:THR:HG23	1:B:300:ILE:HG23	1.92	0.50
1:A:61:TRP:HB2	1:A:169:LEU:CD2	2.41	0.50
1:A:82:ILE:HD13	1:A:130:ILE:CD1	2.41	0.50
1:A:101:PHE:CD1	1:A:106:VAL:HG13	2.47	0.50
1:A:298:ALA:HA	1:E:302:MET:CE	2.42	0.50
1:B:171:TYR:CD2	1:B:172:SER:N	2.79	0.50
1:D:291:MET:CE	1:E:291:MET:HG2	2.40	0.50
1:A:229:ARG:HG3	1:A:258:THR:HG23	1.92	0.50
1:C:313:MET:CE	1:D:308:ALA:HB1	2.40	0.50
1:A:47:VAL:CB	1:A:72:VAL:HG13	2.41	0.50
1:C:116:ASP:OD2	1:C:119:LEU:HB3	2.11	0.50
1:E:272:VAL:HG13	1:E:275:LEU:HD22	1.94	0.50
1:E:221:LEU:O	1:E:222:ALA:C	2.50	0.50
1:B:221:LEU:O	1:B:225:ILE:HD12	2.11	0.50
1:C:184:LEU:O	1:C:188:ILE:HD12	2.11	0.50
1:D:336:VAL:O	1:D:340:ILE:HG23	2.12	0.50
1:A:84:PRO:O	1:A:87:LEU:N	2.45	0.50
1:A:202:ARG:N	1:A:203:PRO:HD3	2.27	0.50
1:D:299:THR:HG21	1:D:345:PHE:HZ	1.76	0.50
1:E:147:PHE:O	1:E:148:ASP:C	2.50	0.50
1:C:87:LEU:HA	1:C:90:ILE:HD12	1.94	0.50
1:C:327:TYR:CZ	1:C:331:LEU:HD11	2.47	0.50
1:C:250:TYR:O	1:C:253:ASP:HB3	2.12	0.49
1:E:109:VAL:CG1	1:E:126:GLN:OE1	2.59	0.49
1:E:177:LEU:HD21	1:E:181:TYR:HE1	1.77	0.49
1:A:91:LEU:O	1:A:93:VAL:HG13	2.13	0.49
1:B:112:MET:HE2	1:B:127:VAL:CG2	2.42	0.49
1:B:313:MET:HE1	1:C:311:TYR:HB2	1.95	0.49
1:C:146:VAL:HG21	1:C:177:LEU:HA	1.94	0.49
1:D:36:ILE:CD1	1:D:163:LYS:CG	2.90	0.49
1:D:138:MET:C	1:D:139:PHE:CD2	2.85	0.49
1:A:240:PRO:HB2	1:A:241:PRO:CD	2.42	0.49
1:C:99:VAL:HG21	1:C:235:LEU:HD13	1.93	0.49
1:A:105:TYR:HB3	1:A:132:THR:HB	1.94	0.49
1:A:228:LEU:O	1:A:231:VAL:HB	2.12	0.49
1:D:120:HIS:CE1	1:D:210:ARG:HG2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:PRO:HB2	1:A:241:PRO:HD3	1.94	0.49
1:A:299:THR:CG2	1:A:300:ILE:HG23	2.43	0.49
1:B:164:LYS:HB3	1:B:168:TYR:CB	2.42	0.49
1:A:95:GLN:HA	1:E:260:GLN:HE22	1.78	0.49
1:B:298:ALA:HB1	1:C:294:LEU:HD21	1.95	0.49
1:A:171:TYR:CZ	1:A:250:TYR:HB3	2.48	0.49
1:A:165:ARG:NH1	1:A:243:ILE:HD13	2.27	0.49
1:B:62:ILE:O	1:B:138:MET:N	2.40	0.49
1:B:222:ALA:HA	1:B:225:ILE:CD1	2.43	0.49
1:D:56:SER:O	1:D:134:ASN:ND2	2.44	0.49
1:D:214:LEU:O	1:D:215:LYS:C	2.50	0.49
1:D:314:ASN:N	1:D:314:ASN:HD22	2.11	0.49
1:E:185:LEU:O	1:E:188:ILE:N	2.46	0.49
1:E:336:VAL:O	1:E:340:ILE:HG23	2.13	0.49
1:A:235:LEU:HD23	1:A:251:PHE:CD2	2.48	0.48
1:A:308:ALA:HB1	1:E:309:GLY:O	2.13	0.48
1:B:90:ILE:HG22	1:B:90:ILE:O	2.12	0.48
1:B:257:HIS:O	1:B:260:GLN:HB3	2.13	0.48
1:D:31:VAL:HG12	1:D:32:MET:N	2.28	0.48
1:A:291:MET:HE2	1:B:291:MET:HG2	1.96	0.48
1:A:302:MET:HG2	1:E:302:MET:HE1	1.95	0.48
1:B:82:ILE:CD1	1:B:130:ILE:HD13	2.42	0.48
1:C:219:VAL:HG22	1:C:269:ARG:HH11	1.77	0.48
1:D:167:ASP:OD1	1:D:168:TYR:N	2.46	0.48
1:A:175:ASP:OD1	1:A:254:VAL:HG22	2.13	0.48
1:B:242:LEU:HD22	1:B:251:PHE:HE1	1.75	0.48
1:C:343:VAL:HG12	1:C:343:VAL:O	2.13	0.48
1:D:99:VAL:HG23	1:D:231:VAL:CG1	2.34	0.48
1:A:129:LEU:HD23	1:A:138:MET:HA	1.96	0.48
1:C:310:ILE:HG22	1:D:308:ALA:CB	2.44	0.48
1:A:209:GLN:O	1:A:212:HIS:N	2.46	0.48
1:A:306:PHE:O	1:A:310:ILE:HG23	2.13	0.48
1:C:225:ILE:CD1	1:C:265:VAL:HG21	2.40	0.48
1:E:241:PRO:O	1:E:242:LEU:HG	2.14	0.48
1:A:232:LEU:HD23	1:A:235:LEU:CD2	2.35	0.48
1:B:180:ASP:O	1:B:183:VAL:HB	2.13	0.48
1:C:182:PHE:HA	1:C:185:LEU:HD12	1.95	0.48
1:E:69:ARG:O	1:E:73:VAL:HG23	2.13	0.48
1:B:294:LEU:CD2	1:B:294:LEU:O	2.62	0.48
1:C:299:THR:HG21	1:C:345:PHE:CE1	2.48	0.48
1:D:70:THR:HG22	1:D:91:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ARG:HH11	1:D:243:ILE:HG21	1.77	0.48
1:D:178:VAL:HG11	1:D:257:HIS:HB2	1.96	0.48
1:E:197:GLU:O	1:E:198:GLU:C	2.52	0.48
1:A:51:LEU:HD21	1:A:76:VAL:HG22	1.95	0.48
1:A:232:LEU:CD2	1:A:235:LEU:HD22	2.35	0.48
1:A:297:ILE:HG21	1:E:299:THR:HA	1.96	0.48
1:B:167:ASP:O	1:B:168:TYR:C	2.51	0.48
1:D:36:ILE:CD1	1:D:163:LYS:HG3	2.43	0.48
1:D:331:LEU:HA	1:D:334:MET:HE2	1.96	0.48
1:A:347:LYS:O	1:A:348:LYS:CB	2.56	0.48
1:C:242:LEU:HD22	1:C:251:PHE:HE1	1.79	0.48
1:C:295:THR:CG2	1:D:293:VAL:CG1	2.92	0.48
1:E:99:VAL:CG2	1:E:231:VAL:HG12	2.41	0.48
1:E:306:PHE:CE2	1:E:310:ILE:HG21	2.49	0.48
1:E:306:PHE:CZ	1:E:310:ILE:HG21	2.49	0.48
1:A:239:VAL:CG1	1:A:248:VAL:HG22	2.36	0.48
1:A:291:MET:HE1	1:B:290:VAL:HG12	1.96	0.48
1:B:225:ILE:HG21	1:B:262:ALA:HA	1.95	0.48
1:D:188:ILE:O	1:D:189:ASP:C	2.52	0.48
1:E:185:LEU:HD22	1:E:264:THR:HG21	1.95	0.48
1:A:177:LEU:O	1:A:180:ASP:CB	2.60	0.47
1:A:204:GLU:HG2	1:A:205:LYS:H	1.79	0.47
1:B:33:ASN:ND2	1:B:59:PRO:O	2.47	0.47
1:D:36:ILE:HG23	1:D:37:GLU:N	2.29	0.47
1:D:44:THR:OG1	1:D:45:THR:N	2.47	0.47
1:E:184:LEU:O	1:E:188:ILE:CD1	2.62	0.47
1:A:274:GLY:O	1:A:277:ASP:N	2.46	0.47
1:B:311:TYR:CE2	1:B:330:VAL:HG21	2.48	0.47
1:C:185:LEU:HD11	1:C:261:ILE:HG23	1.95	0.47
1:D:36:ILE:HD11	1:D:163:LYS:HG2	1.95	0.47
1:D:116:ASP:OD1	1:D:117:LYS:O	2.32	0.47
1:D:177:LEU:HD23	1:D:177:LEU:O	2.13	0.47
1:E:181:TYR:O	1:E:184:LEU:HB3	2.14	0.47
1:B:102:PHE:O	1:B:103:GLU:C	2.53	0.47
1:B:247:THR:O	1:B:250:TYR:N	2.47	0.47
1:D:47:VAL:CG2	1:D:51:LEU:HD21	2.39	0.47
1:C:99:VAL:HG11	1:C:235:LEU:HD11	1.95	0.47
1:D:169:LEU:HD12	1:D:169:LEU:C	2.34	0.47
1:B:177:LEU:HD23	1:B:177:LEU:C	2.35	0.47
1:C:167:ASP:HB2	1:C:242:LEU:CD2	2.36	0.47
1:A:161:ILE:HD12	1:A:172:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ALA:O	1:A:336:VAL:HG23	2.15	0.47
1:B:274:GLY:HA3	1:C:215:LYS:HZ1	1.80	0.47
1:B:278:VAL:HG13	1:C:208:VAL:HG12	1.96	0.47
1:B:307:ILE:CD1	1:B:334:MET:HG2	2.37	0.47
1:C:288:ASN:O	1:C:291:MET:HB2	2.15	0.47
1:D:232:LEU:HD13	1:D:258:THR:OG1	2.15	0.47
1:D:242:LEU:O	1:D:244:GLU:N	2.46	0.47
1:D:332:ALA:O	1:D:336:VAL:HG23	2.14	0.47
1:E:51:LEU:HD21	1:E:76:VAL:HG22	1.97	0.47
1:E:275:LEU:O	1:E:278:VAL:HB	2.14	0.47
1:E:307:ILE:HA	1:E:310:ILE:CD1	2.44	0.47
1:B:220:GLU:O	1:B:223:ALA:HB3	2.15	0.47
1:C:69:ARG:HB3	1:C:72:VAL:HG23	1.97	0.47
1:C:125:GLU:HG3	1:C:141:GLU:HB2	1.97	0.47
1:D:89:ASP:O	1:D:90:ILE:C	2.53	0.47
1:C:346:LYS:CE	1:C:349:LYS:HZ1	2.28	0.47
1:B:36:ILE:HG23	1:B:37:GLU:N	2.30	0.47
1:B:61:TRP:CD1	1:B:61:TRP:O	2.68	0.47
1:C:254:VAL:O	1:C:257:HIS:N	2.48	0.47
1:E:111:LYS:O	1:E:177:LEU:HD11	2.14	0.47
1:E:293:VAL:HG12	1:E:294:LEU:N	2.30	0.47
1:B:240:PRO:HG2	1:B:241:PRO:HD2	1.97	0.46
1:B:295:THR:HG21	1:C:293:VAL:HG12	1.96	0.46
1:E:171:TYR:CE1	1:E:254:VAL:HG23	2.49	0.46
1:E:206:GLU:O	1:E:209:GLN:HB2	2.14	0.46
1:E:244:GLU:O	1:E:246:GLU:N	2.48	0.46
1:A:67:ILE:HD11	1:A:93:VAL:HG11	1.95	0.46
1:A:148:ASP:N	1:A:149:PRO:HD2	2.30	0.46
1:A:199:VAL:HG13	1:A:279:TYR:CA	2.45	0.46
1:A:299:THR:CG2	1:A:300:ILE:N	2.78	0.46
1:C:51:LEU:N	1:C:52:PRO:HD2	2.30	0.46
1:E:99:VAL:HG22	1:E:231:VAL:CG1	2.43	0.46
1:E:169:LEU:O	1:E:173:LEU:HD12	2.15	0.46
1:A:298:ALA:O	1:A:299:THR:C	2.53	0.46
1:C:221:LEU:CD2	1:C:265:VAL:HG22	2.45	0.46
1:C:296:ILE:CD1	1:C:297:ILE:HD12	2.45	0.46
1:E:112:MET:SD	1:E:146:VAL:HG22	2.55	0.46
1:E:184:LEU:HD12	1:E:184:LEU:C	2.32	0.46
1:A:263:ASP:O	1:A:264:THR:C	2.54	0.46
1:B:296:ILE:HD12	1:B:297:ILE:HD12	1.98	0.46
1:C:200:LEU:HD22	1:D:209:GLN:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:GLY:O	1:D:82:ILE:HB	2.15	0.46
1:E:76:VAL:HG13	1:E:80:PHE:CE2	2.50	0.46
1:E:239:VAL:O	1:E:239:VAL:CG2	2.60	0.46
1:A:312:GLY:HA2	1:E:312:GLY:O	2.16	0.46
1:D:86:VAL:O	1:D:89:ASP:HB2	2.15	0.46
1:E:304:LEU:HD23	1:E:307:ILE:CD1	2.26	0.46
1:A:47:VAL:CG2	1:A:76:VAL:HG23	2.46	0.46
1:A:59:PRO:HA	1:A:134:ASN:HB3	1.96	0.46
1:A:93:VAL:HB	1:A:141:GLU:OE2	2.15	0.46
1:D:44:THR:OG1	1:D:46:ASP:N	2.44	0.46
1:D:140:GLN:HE22	1:D:145:ASP:CB	2.28	0.46
1:D:247:THR:O	1:D:250:TYR:N	2.49	0.46
1:B:177:LEU:CD2	1:B:181:TYR:CE1	2.95	0.46
1:E:335:GLY:O	1:E:339:VAL:CG2	2.59	0.46
1:B:131:LEU:HD13	1:B:136:VAL:HG23	1.98	0.46
1:C:95:GLN:H	1:C:111:LYS:NZ	2.14	0.46
1:D:88:GLU:O	1:D:89:ASP:C	2.54	0.46
1:D:99:VAL:HG21	1:D:231:VAL:CG1	2.24	0.46
1:D:263:ASP:O	1:D:264:THR:C	2.54	0.46
1:E:177:LEU:HD23	1:E:178:VAL:N	2.30	0.46
1:E:186:GLU:O	1:E:189:ASP:N	2.49	0.46
1:E:211:THR:HG23	1:E:275:LEU:HD23	1.96	0.46
1:B:296:ILE:HD12	1:B:297:ILE:N	2.30	0.46
1:D:31:VAL:HG21	1:D:50:VAL:HG12	1.97	0.46
1:E:56:SER:O	1:E:134:ASN:ND2	2.42	0.46
1:E:247:THR:HG22	1:E:251:PHE:CD1	2.50	0.46
1:B:274:GLY:CA	1:C:215:LYS:HZ1	2.28	0.46
1:B:279:TYR:O	1:B:283:VAL:HG23	2.15	0.46
1:D:63:ASN:C	1:D:63:ASN:OD1	2.55	0.46
1:A:231:VAL:HG12	1:A:232:LEU:N	2.30	0.45
1:A:306:PHE:CZ	1:A:310:ILE:HG21	2.51	0.45
1:B:46:ASP:OD1	1:B:46:ASP:C	2.54	0.45
1:B:106:VAL:HG12	1:B:107:PHE:N	2.31	0.45
1:B:292:LYS:NZ	1:B:349:LYS:C	2.69	0.45
1:C:30:GLU:HB3	1:C:63:ASN:HB3	1.99	0.45
1:C:179:ASP:O	1:C:182:PHE:HB2	2.16	0.45
1:C:199:VAL:HG13	1:C:279:TYR:CA	2.46	0.45
1:D:88:GLU:O	1:D:91:LEU:N	2.49	0.45
1:D:297:ILE:HG22	1:D:298:ALA:H	1.79	0.45
1:E:61:TRP:CZ2	1:E:173:LEU:HD21	2.51	0.45
1:B:238:ASP:O	1:B:239:VAL:CG2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:LEU:HD21	1:C:272:VAL:HG21	1.98	0.45
1:C:313:MET:N	1:C:313:MET:HE2	2.32	0.45
1:A:196:GLU:OE1	1:B:216:ARG:HD2	2.17	0.45
1:C:345:PHE:O	1:C:349:LYS:HB3	2.16	0.45
1:C:140:GLN:OE1	1:C:145:ASP:HB3	2.17	0.45
1:D:77:GLY:HA3	1:D:87:LEU:CD2	2.47	0.45
1:A:63:ASN:HA	1:A:138:MET:HB3	1.99	0.45
1:A:230:GLU:HA	1:A:230:GLU:OE1	2.16	0.45
1:C:302:MET:HE2	1:D:298:ALA:HA	1.99	0.45
1:D:227:PRO:O	1:D:230:GLU:N	2.50	0.45
1:A:277:ASP:N	1:A:277:ASP:OD1	2.49	0.45
1:A:291:MET:HE3	1:B:290:VAL:HB	1.99	0.45
1:A:311:TYR:HB2	1:E:313:MET:HE1	1.97	0.45
1:B:195:LEU:HD13	1:B:210:ARG:CZ	2.46	0.45
1:D:167:ASP:OD2	1:D:243:ILE:HG12	2.17	0.45
1:E:189:ASP:O	1:E:192:ILE:HB	2.15	0.45
1:A:339:VAL:HA	1:A:342:VAL:CG2	2.46	0.45
1:B:191:GLU:HB3	1:B:214:LEU:HD11	1.99	0.45
1:B:292:LYS:HZ2	1:B:349:LYS:HA	1.81	0.45
1:C:60:THR:HG22	1:C:61:TRP:N	2.31	0.45
1:D:82:ILE:CG2	1:D:87:LEU:HG	2.46	0.45
1:E:93:VAL:HG11	1:E:141:GLU:OE1	2.17	0.45
1:E:96:ARG:HD2	1:E:227:PRO:HB3	1.99	0.45
1:E:243:ILE:HD12	1:E:246:GLU:HB3	1.99	0.45
1:A:216:ARG:O	1:A:219:VAL:N	2.50	0.45
1:B:91:LEU:O	1:B:93:VAL:HG13	2.17	0.45
1:B:199:VAL:HG13	1:B:279:TYR:HB2	1.97	0.45
1:C:26:ASP:O	1:C:68:HIS:NE2	2.41	0.45
1:D:296:ILE:HG22	1:D:345:PHE:CE1	2.51	0.45
1:E:77:GLY:HA2	1:E:87:LEU:HD21	1.98	0.45
1:E:118:ASN:O	1:E:120:HIS:N	2.50	0.45
1:E:225:ILE:HD13	1:E:261:ILE:HG22	1.98	0.45
1:A:264:THR:O	1:A:267:THR:CB	2.65	0.45
1:B:101:PHE:CZ	1:B:235:LEU:HD12	2.52	0.45
1:D:132:THR:O	1:D:134:ASN:N	2.50	0.45
1:D:189:ASP:O	1:D:192:ILE:HB	2.17	0.45
1:A:239:VAL:HG12	1:A:242:LEU:HD12	1.99	0.44
1:B:242:LEU:HD21	1:B:251:PHE:HE1	1.60	0.44
1:C:261:ILE:O	1:C:262:ALA:C	2.55	0.44
1:D:306:PHE:HB2	1:E:305:THR:OG1	2.17	0.44
1:B:115:TYR:OH	1:B:120:HIS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:LEU:HA	1:D:334:MET:HB2	1.98	0.44
1:A:200:LEU:HD13	1:B:209:GLN:HE21	1.82	0.44
1:D:302:MET:HE1	1:E:298:ALA:HA	1.99	0.44
1:E:51:LEU:N	1:E:52:PRO:HD2	2.33	0.44
1:A:47:VAL:CG2	1:A:72:VAL:CG1	2.89	0.44
1:A:99:VAL:HG13	1:A:108:ILE:HG12	1.98	0.44
1:A:331:LEU:HD23	1:A:334:MET:HE2	1.98	0.44
1:B:200:LEU:HD21	1:C:209:GLN:HG2	2.00	0.44
1:E:146:VAL:HG21	1:E:177:LEU:HA	2.00	0.44
1:D:178:VAL:HG21	1:D:254:VAL:HG13	1.98	0.44
1:E:182:PHE:O	1:E:183:VAL:C	2.54	0.44
1:E:247:THR:HG22	1:E:251:PHE:CE1	2.53	0.44
1:E:332:ALA:O	1:E:336:VAL:N	2.48	0.44
1:A:51:LEU:N	1:A:52:PRO:HD2	2.32	0.44
1:D:291:MET:HE3	1:D:291:MET:HB3	1.86	0.44
1:A:90:ILE:HD13	1:A:139:PHE:CE1	2.52	0.44
1:A:339:VAL:O	1:A:343:VAL:HG23	2.17	0.44
1:C:302:MET:HE3	1:C:302:MET:HB3	1.78	0.44
1:D:247:THR:O	1:D:248:VAL:C	2.56	0.44
1:D:147:PHE:O	1:D:151:ARG:HG3	2.18	0.44
1:D:296:ILE:HD12	1:D:296:ILE:C	2.38	0.44
1:A:268:PHE:O	1:A:269:ARG:C	2.56	0.44
1:B:177:LEU:O	1:B:180:ASP:N	2.50	0.44
1:B:240:PRO:HB2	1:B:241:PRO:HD2	1.95	0.44
1:D:168:TYR:O	1:D:169:LEU:C	2.52	0.44
1:D:313:MET:SD	1:E:311:TYR:HB2	2.58	0.44
1:E:213:GLN:O	1:E:214:LEU:C	2.54	0.44
1:B:165:ARG:O	1:B:166:ALA:C	2.56	0.43
1:B:244:GLU:O	1:B:245:LYS:C	2.56	0.43
1:C:148:ASP:N	1:C:149:PRO:CD	2.81	0.43
1:C:219:VAL:HG22	1:C:269:ARG:NH1	2.32	0.43
1:C:127:VAL:HG22	1:C:140:GLN:HG2	2.01	0.43
1:C:140:GLN:HE22	1:C:145:ASP:CB	2.30	0.43
1:A:73:VAL:O	1:A:87:LEU:HD22	2.18	0.43
1:B:197:GLU:OE1	1:B:197:GLU:HA	2.19	0.43
1:E:208:VAL:O	1:E:209:GLN:C	2.55	0.43
1:A:200:LEU:HD13	1:A:201:GLU:HG3	2.00	0.43
1:D:225:ILE:CD1	1:D:265:VAL:HG21	2.47	0.43
1:E:63:ASN:HB2	1:E:138:MET:HE2	2.00	0.43
1:E:92:ASN:O	1:E:95:GLN:NE2	2.52	0.43
1:E:167:ASP:O	1:E:170:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:N	1:A:138:MET:O	2.43	0.43
1:A:221:LEU:C	1:A:225:ILE:HD12	2.37	0.43
1:A:313:MET:CE	1:A:313:MET:HA	2.49	0.43
1:D:89:ASP:OD1	1:D:95:GLN:OE1	2.37	0.43
1:D:171:TYR:CD2	1:D:172:SER:N	2.86	0.43
1:D:173:LEU:O	1:D:176:ALA:HB3	2.18	0.43
1:E:64:ILE:HD12	1:E:138:MET:O	2.18	0.43
1:A:171:TYR:HE1	1:A:254:VAL:HG23	1.83	0.43
1:A:177:LEU:C	1:A:177:LEU:HD23	2.38	0.43
1:B:129:LEU:HD23	1:B:138:MET:HA	2.00	0.43
1:C:130:ILE:CG2	1:C:137:LEU:HD12	2.48	0.43
1:B:86:VAL:HG13	1:B:107:PHE:CZ	2.54	0.43
1:D:243:ILE:O	1:D:244:GLU:O	2.37	0.43
1:E:227:PRO:O	1:E:228:LEU:C	2.57	0.43
1:C:302:MET:HE2	1:D:297:ILE:C	2.39	0.43
1:E:177:LEU:HD23	1:E:177:LEU:O	2.18	0.43
1:A:99:VAL:HG22	1:A:231:VAL:HG22	2.01	0.43
1:C:86:VAL:O	1:C:89:ASP:HB2	2.19	0.43
1:D:148:ASP:O	1:D:152:GLU:HG2	2.19	0.43
1:D:264:THR:O	1:D:267:THR:HB	2.18	0.43
1:D:272:VAL:O	1:D:273:SER:C	2.57	0.43
1:B:115:TYR:CZ	1:B:120:HIS:HA	2.54	0.43
1:C:83:HIS:HD1	1:C:84:PRO:HD2	1.84	0.43
1:B:218:LEU:HD21	1:B:268:PHE:HB3	1.99	0.42
1:B:310:ILE:HG22	1:C:308:ALA:HB2	2.01	0.42
1:C:296:ILE:HD11	1:C:297:ILE:HD12	2.01	0.42
1:B:221:LEU:C	1:B:225:ILE:HD12	2.40	0.42
1:C:128:SER:O	1:C:129:LEU:HD23	2.19	0.42
1:C:243:ILE:HD12	1:C:246:GLU:HB3	1.99	0.42
1:C:296:ILE:HD12	1:C:296:ILE:C	2.39	0.42
1:D:128:SER:HB2	1:D:139:PHE:HB2	2.00	0.42
1:D:172:SER:O	1:D:173:LEU:C	2.57	0.42
1:E:302:MET:N	1:E:303:PRO:HD2	2.35	0.42
1:A:216:ARG:NH1	1:E:196:GLU:OE1	2.52	0.42
1:B:64:ILE:CD1	1:B:76:VAL:HG21	2.50	0.42
1:B:84:PRO:O	1:B:85:LEU:C	2.58	0.42
1:D:229:ARG:HG3	1:D:258:THR:HG22	2.00	0.42
1:E:179:ASP:O	1:E:181:TYR:N	2.53	0.42
1:A:299:THR:HG23	1:A:300:ILE:N	2.34	0.42
1:C:199:VAL:HG13	1:C:279:TYR:HA	2.01	0.42
1:C:202:ARG:N	1:C:203:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:VAL:HG13	1:E:279:TYR:CB	2.47	0.42
1:E:296:ILE:O	1:E:300:ILE:HG23	2.19	0.42
1:B:46:ASP:OD2	1:B:49:SER:HB3	2.19	0.42
1:B:64:ILE:HD11	1:B:76:VAL:HG21	2.01	0.42
1:C:265:VAL:HG12	1:C:269:ARG:HG3	2.02	0.42
1:E:140:GLN:HE22	1:E:145:ASP:HB3	1.84	0.42
1:B:177:LEU:O	1:B:178:VAL:C	2.56	0.42
1:C:122:LEU:HD22	1:C:217:ASN:ND2	2.34	0.42
1:D:36:ILE:HD13	1:D:163:LYS:HA	2.02	0.42
1:D:297:ILE:O	1:D:298:ALA:C	2.58	0.42
1:E:200:LEU:HD12	1:E:201:GLU:HG2	2.02	0.42
1:E:206:GLU:O	1:E:207:THR:C	2.56	0.42
1:A:297:ILE:HG22	1:A:298:ALA:N	2.35	0.42
1:B:171:TYR:CD2	1:B:171:TYR:C	2.92	0.42
1:B:200:LEU:HD21	1:C:209:GLN:CG	2.50	0.42
1:C:99:VAL:HG11	1:C:235:LEU:CD1	2.50	0.42
1:D:77:GLY:CA	1:D:87:LEU:HD21	2.50	0.42
1:E:306:PHE:CD1	1:E:307:ILE:HG23	2.53	0.42
1:A:62:ILE:HD12	1:A:137:LEU:CD2	2.50	0.42
1:A:106:VAL:HG12	1:A:107:PHE:N	2.35	0.42
1:A:181:TYR:O	1:A:184:LEU:HB3	2.20	0.42
1:B:225:ILE:O	1:B:228:LEU:HB3	2.20	0.42
1:C:295:THR:O	1:C:299:THR:HB	2.19	0.42
1:D:302:MET:HE1	1:E:302:MET:HG2	2.02	0.42
1:E:185:LEU:HD22	1:E:264:THR:CG2	2.49	0.42
1:A:44:THR:HG21	1:A:49:SER:OG	2.20	0.42
1:A:331:LEU:HD23	1:A:334:MET:HE1	2.02	0.42
1:E:129:LEU:HD23	1:E:138:MET:HA	2.02	0.42
1:B:218:LEU:HD21	1:B:268:PHE:CB	2.50	0.42
1:B:295:THR:HA	1:C:294:LEU:HG	2.02	0.42
1:D:122:LEU:CD2	1:D:217:ASN:ND2	2.70	0.42
1:D:171:TYR:CG	1:D:172:SER:N	2.87	0.42
1:E:129:LEU:HA	1:E:137:LEU:O	2.20	0.42
1:A:266:GLU:O	1:A:267:THR:C	2.58	0.41
1:A:292:LYS:O	1:A:293:VAL:C	2.57	0.41
1:B:110:LEU:HD22	1:B:228:LEU:CD1	2.49	0.41
1:B:202:ARG:N	1:B:203:PRO:HD3	2.35	0.41
1:C:112:MET:SD	1:C:146:VAL:HG13	2.60	0.41
1:E:240:PRO:CB	1:E:241:PRO:CD	2.97	0.41
1:B:61:TRP:O	1:B:61:TRP:CG	2.73	0.41
1:C:268:PHE:O	1:C:269:ARG:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ILE:HD11	1:D:163:LYS:CG	2.49	0.41
1:D:177:LEU:CD2	1:D:177:LEU:C	2.87	0.41
1:D:177:LEU:O	1:D:178:VAL:C	2.57	0.41
1:A:308:ALA:HB2	1:E:310:ILE:HG22	2.03	0.41
1:B:112:MET:HE1	1:B:127:VAL:HG21	2.03	0.41
1:C:310:ILE:O	1:C:313:MET:HE2	2.20	0.41
1:D:239:VAL:HA	1:D:242:LEU:HD12	2.02	0.41
1:E:296:ILE:HG22	1:E:345:PHE:CZ	2.53	0.41
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.92	0.41
1:B:70:THR:HG22	1:B:91:LEU:CD2	2.45	0.41
1:B:164:LYS:HB3	1:B:168:TYR:HB3	2.02	0.41
1:B:221:LEU:HG	1:B:225:ILE:HD11	2.02	0.41
1:B:295:THR:CG2	1:C:293:VAL:HG12	2.49	0.41
1:B:330:VAL:O	1:B:334:MET:HG3	2.21	0.41
1:C:298:ALA:O	1:C:302:MET:CG	2.68	0.41
1:D:97:PRO:HG3	1:D:111:LYS:HG2	2.02	0.41
1:E:34:TYR:OH	1:E:169:LEU:HD22	2.20	0.41
1:E:171:TYR:O	1:E:174:ILE:HB	2.20	0.41
1:A:47:VAL:HG22	1:A:76:VAL:HG23	2.02	0.41
1:B:84:PRO:HA	1:B:87:LEU:HD12	2.03	0.41
1:B:86:VAL:O	1:B:87:LEU:C	2.59	0.41
1:D:129:LEU:O	1:D:130:ILE:HG13	2.21	0.41
1:A:77:GLY:CA	1:A:87:LEU:HD11	2.50	0.41
1:A:280:LEU:HD21	1:E:280:LEU:HD23	2.01	0.41
1:D:240:PRO:CB	1:D:241:PRO:CD	2.99	0.41
1:E:235:LEU:HD23	1:E:251:PHE:CE2	2.56	0.41
1:A:221:LEU:CD1	1:A:225:ILE:HD11	2.50	0.41
1:C:277:ASP:N	1:C:277:ASP:OD1	2.54	0.41
1:E:232:LEU:HD13	1:E:258:THR:HB	2.03	0.41
1:A:51:LEU:CD2	1:A:76:VAL:HG22	2.51	0.41
1:B:292:LYS:HZ1	1:B:349:LYS:C	2.23	0.41
1:E:175:ASP:O	1:E:176:ALA:C	2.59	0.41
1:B:304:LEU:HD11	1:B:338:ALA:HB2	2.03	0.41
1:C:117:LYS:O	1:C:119:LEU:N	2.53	0.41
1:C:221:LEU:HD23	1:C:265:VAL:CG2	2.47	0.41
1:C:302:MET:HE2	1:D:298:ALA:N	2.35	0.41
1:E:256:ASP:CA	1:E:259:ILE:HD12	2.49	0.41
1:A:65:THR:HG21	1:A:143:ILE:CG1	2.50	0.41
1:C:38:GLU:HG2	1:C:39:PHE:N	2.36	0.41
1:C:302:MET:HB2	1:C:303:PRO:HD3	2.02	0.41
1:D:329:VAL:HA	1:D:332:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:GLU:HG3	1:E:141:GLU:HB2	2.03	0.41
1:E:206:GLU:O	1:E:209:GLN:N	2.54	0.41
1:C:337:ILE:O	1:C:341:MET:HG2	2.21	0.40
1:D:243:ILE:HD12	1:D:246:GLU:CB	2.47	0.40
1:D:275:LEU:O	1:D:276:LEU:C	2.59	0.40
1:D:296:ILE:C	1:D:299:THR:HG22	2.42	0.40
1:E:53:PHE:O	1:E:54:ARG:C	2.60	0.40
1:B:177:LEU:HD23	1:B:178:VAL:N	2.37	0.40
1:B:297:ILE:O	1:B:298:ALA:C	2.59	0.40
1:C:195:LEU:C	1:C:197:GLU:H	2.23	0.40
1:D:171:TYR:HE1	1:D:254:VAL:CG2	2.35	0.40
1:D:327:TYR:N	1:D:328:PRO:HD2	2.36	0.40
1:E:127:VAL:HA	1:E:139:PHE:O	2.21	0.40
1:B:65:THR:CG2	1:B:143:ILE:HD13	2.49	0.40
1:D:26:ASP:O	1:D:68:HIS:NE2	2.44	0.40
1:D:195:LEU:HD21	1:D:211:THR:CA	2.50	0.40
1:E:224:THR:O	1:E:228:LEU:HB2	2.21	0.40
1:E:225:ILE:HD13	1:E:261:ILE:CG2	2.52	0.40
1:E:341:MET:O	1:E:344:TYR:HB3	2.22	0.40
1:A:242:LEU:O	1:A:243:ILE:C	2.59	0.40
1:A:278:VAL:HA	1:B:276:LEU:HD21	2.02	0.40
1:A:330:VAL:HG12	1:A:334:MET:HG3	2.02	0.40
1:A:337:ILE:HA	1:A:340:ILE:HG12	2.04	0.40
1:D:259:ILE:O	1:D:260:GLN:C	2.60	0.40
1:D:299:THR:HG21	1:D:345:PHE:CE1	2.56	0.40
1:D:337:ILE:HA	1:D:340:ILE:HG12	2.03	0.40
1:E:177:LEU:HD21	1:E:181:TYR:CE1	2.57	0.40
1:E:274:GLY:O	1:E:277:ASP:HB2	2.21	0.40
1:A:29:ILE:HB	1:A:44:THR:O	2.21	0.40
1:A:330:VAL:O	1:A:334:MET:HG3	2.21	0.40
1:B:101:PHE:CD1	1:B:240:PRO:HG3	2.57	0.40
1:D:223:ALA:O	1:D:227:PRO:CD	2.69	0.40
1:D:225:ILE:HD12	1:D:265:VAL:HG21	2.04	0.40
1:E:127:VAL:HG22	1:E:140:GLN:HG2	2.03	0.40
1:E:132:THR:O	1:E:134:ASN:N	2.54	0.40
1:E:178:VAL:O	1:E:181:TYR:HB2	2.22	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	310/330 (94%)	255 (82%)	47 (15%)	8 (3%)	5	36
1	B	312/330 (94%)	251 (80%)	50 (16%)	11 (4%)	3	31
1	C	310/330 (94%)	255 (82%)	48 (16%)	7 (2%)	6	38
1	D	310/330 (94%)	246 (79%)	52 (17%)	12 (4%)	3	28
1	E	310/330 (94%)	250 (81%)	41 (13%)	19 (6%)	1	20
All	All	1552/1650 (94%)	1257 (81%)	238 (15%)	57 (4%)	3	29

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	240	PRO
1	A	348	LYS
1	B	240	PRO
1	B	246	GLU
1	B	348	LYS
1	C	240	PRO
1	D	240	PRO
1	D	244	GLU
1	E	240	PRO
1	E	243	ILE
1	A	244	GLU
1	A	275	LEU
1	A	293	VAL
1	B	103	GLU
1	B	157	ASN
1	B	239	VAL
1	C	238	ASP
1	C	239	VAL
1	C	244	GLU
1	D	243	ILE

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Mol	Chain	Res	Type
1	D	246	GLU
1	E	71	ASP
1	E	180	ASP
1	E	208	VAL
1	E	244	GLU
1	E	246	GLU
1	E	348	LYS
1	A	118	ASN
1	B	120	HIS
1	D	66	GLY
1	D	133	LYS
1	E	209	GLN
1	E	238	ASP
1	E	293	VAL
1	B	238	ASP
1	C	118	ASN
1	C	267	THR
1	D	59	PRO
1	E	118	ASN
1	A	239	VAL
1	B	243	ILE
1	D	239	VAL
1	D	245	LYS
1	D	258	THR
1	E	133	LYS
1	E	176	ALA
1	B	166	ALA
1	D	348	LYS
1	B	77	GLY
1	C	159	GLY
1	E	148	ASP
1	D	36	ILE
1	E	67	ILE
1	E	183	VAL
1	E	239	VAL
1	E	241	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	295/310 (95%)	273 (92%)	22 (8%)	13	44
1	B	295/310 (95%)	270 (92%)	25 (8%)	10	40
1	C	295/310 (95%)	272 (92%)	23 (8%)	12	42
1	D	295/310 (95%)	270 (92%)	25 (8%)	10	40
1	E	295/310 (95%)	278 (94%)	17 (6%)	20	51
All	All	1475/1550 (95%)	1363 (92%)	112 (8%)	13	43

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	40	ARG
1	A	44	THR
1	A	95	GLN
1	A	99	VAL
1	A	145	ASP
1	A	163	LYS
1	A	200	LEU
1	A	202	ARG
1	A	206	GLU
1	A	233	SER
1	A	238	ASP
1	A	258	THR
1	A	264	THR
1	A	277	ASP
1	A	281	SER
1	A	285	ASN
1	A	297	ILE
1	A	315	PHE
1	A	337	ILE
1	A	346	LYS
1	A	349	LYS
1	B	26	ASP
1	B	40	ARG
1	B	41	GLU
1	B	122	LEU
1	B	123	GLU
1	B	128	SER

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Mol	Chain	Res	Type
1	B	132	THR
1	B	164	LYS
1	B	165	ARG
1	B	171	TYR
1	B	198	GLU
1	B	206	GLU
1	B	218	LEU
1	B	233	SER
1	B	235	LEU
1	B	238	ASP
1	B	242	LEU
1	B	248	VAL
1	B	260	GLN
1	B	263	ASP
1	B	284	SER
1	B	294	LEU
1	B	327	TYR
1	B	337	ILE
1	B	346	LYS
1	C	38	GLU
1	C	40	ARG
1	C	93	VAL
1	C	95	GLN
1	C	96	ARG
1	C	123	GLU
1	C	165	ARG
1	C	172	SER
1	C	177	LEU
1	C	178	VAL
1	C	200	LEU
1	C	206	GLU
1	C	237	ARG
1	C	238	ASP
1	C	263	ASP
1	C	277	ASP
1	C	284	SER
1	C	294	LEU
1	C	297	ILE
1	C	307	ILE
1	C	346	LYS
1	C	347	LYS
1	C	349	LYS

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Mol	Chain	Res	Type
1	D	26	ASP
1	D	40	ARG
1	D	44	THR
1	D	85	LEU
1	D	95	GLN
1	D	96	ARG
1	D	119	LEU
1	D	122	LEU
1	D	143	ILE
1	D	152	GLU
1	D	165	ARG
1	D	169	LEU
1	D	206	GLU
1	D	226	TRP
1	D	232	LEU
1	D	238	ASP
1	D	248	VAL
1	D	267	THR
1	D	269	ARG
1	D	279	TYR
1	D	297	ILE
1	D	307	ILE
1	D	314	ASN
1	D	346	LYS
1	D	349	LYS
1	E	26	ASP
1	E	28	GLU
1	E	29	ILE
1	E	40	ARG
1	E	44	THR
1	E	65	THR
1	E	95	GLN
1	E	118	ASN
1	E	121	GLU
1	E	123	GLU
1	E	128	SER
1	E	184	LEU
1	E	211	THR
1	E	238	ASP
1	E	287	THR
1	E	297	ILE
1	E	346	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	213	GLN
1	A	217	ASN
1	A	285	ASN
1	B	33	ASN
1	B	120	HIS
1	B	140	GLN
1	B	209	GLN
1	B	257	HIS
1	B	314	ASN
1	C	33	ASN
1	C	95	GLN
1	C	118	ASN
1	C	140	GLN
1	C	217	ASN
1	C	314	ASN
1	D	33	ASN
1	D	140	GLN
1	D	217	ASN
1	D	260	GLN
1	D	314	ASN
1	E	33	ASN
1	E	120	HIS
1	E	140	GLN
1	E	217	ASN
1	E	288	ASN
1	E	314	ASN

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

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	314/330 (95%)	-0.27	6 (1%)	66	59	124, 172, 239, 320	0
1	B	316/330 (95%)	-0.59	2 (0%)	89	85	110, 148, 223, 326	0
1	C	314/330 (95%)	-0.59	2 (0%)	89	85	109, 142, 210, 320	0
1	D	314/330 (95%)	-0.61	1 (0%)	94	91	112, 144, 220, 327	0
1	E	314/330 (95%)	-0.45	3 (0%)	82	76	122, 157, 227, 329	0
All	All	1572/1650 (95%)	-0.50	14 (0%)	84	79	109, 152, 229, 329	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	LYS	4.8
1	C	315	PHE	3.5
1	A	38	GLU	3.3
1	B	314	ASN	3.2
1	C	326	GLY	3.1
1	B	326	GLY	3.0
1	A	68	HIS	2.7
1	A	36	ILE	2.7
1	A	35	SER	2.5
1	D	315	PHE	2.5
1	E	327	TYR	2.4
1	E	159	GLY	2.3
1	A	37	GLU	2.2
1	E	245	LYS	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
2	CS	D	1001	1/1	0.63	0.23	158,158,158,158	1
2	CS	A	401	1/1	0.69	0.17	281,281,281,281	1
2	CS	B	1001	1/1	0.73	0.22	170,170,170,170	1
2	CS	B	1004	1/1	0.86	0.31	135,135,135,135	1
3	NA	B	1002	1/1	0.86	0.14	109,109,109,109	0
2	CS	E	401	1/1	0.87	0.15	154,154,154,154	1
2	CS	E	402	1/1	0.88	0.20	155,155,155,155	1
2	CS	B	1003	1/1	0.90	0.17	144,144,144,144	1
2	CS	C	401	1/1	0.94	0.16	178,178,178,178	1
2	CS	E	403	1/1	0.95	0.22	183,183,183,183	1

6.5 Other polymers (i)

There are no such residues in this entry.