Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 04:21 PM EDT

PDB ID	:	3HT4
Title	:	Crystal Structure of the Q81A77_BACCR Protein from Bacillus cereus. Northeast Structural Genomics Consortium Target BcR213
Authors	:	Vorobiev, S.; Lew, S.; Seetharaman, J.; Wang, H.; Foote, E.; Ciccosanti, C.; Janjua, H.; Xiao, R.; Mao, L.; Acton, T.B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2009-06-11
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

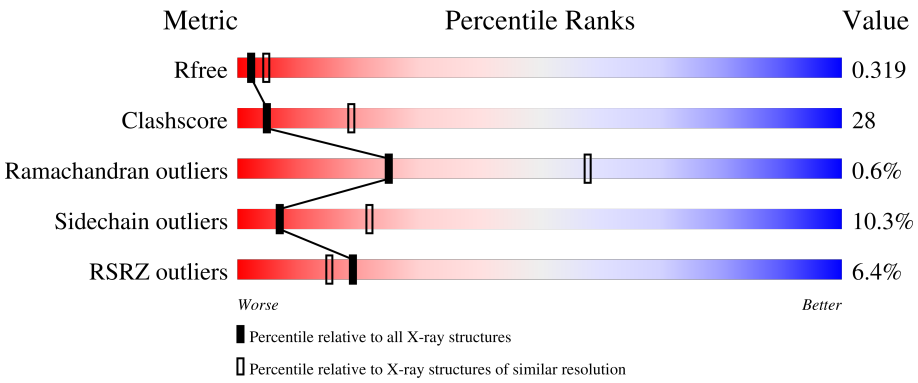
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	431	5% 45% 47% 5% •
1	B	431	4% 49% 41% 5% 6%
1	C	431	6% 50% 40% 5% 5%
1	D	431	4% 53% 38% • 5%

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Mol	Chain	Length	Quality of chain
1	E	431	5% 51% 40% • 5%
1	F	431	5% 49% 41% 5% 5%
1	G	431	7% 53% 38% • 5%
1	H	431	11% 48% 43% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 25070 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 Aluminum resistance protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	416	3151	2015	517	605	5	9	0	0	0
1	B	407	3112	1994	509	596	5	8	0	0	0
1	C	411	3123	2001	513	596	5	8	0	0	0
1	D	408	3117	1997	510	597	5	8	0	0	0
1	E	409	3117	1997	511	596	5	8	0	0	0
1	F	410	3118	1998	512	595	5	8	0	0	0
1	G	408	3102	1986	510	593	5	8	0	0	0
1	H	407	3104	1989	508	594	5	8	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	424	LEU	-	expression tag	UNP Q81A77
A	425	GLU	-	expression tag	UNP Q81A77
A	426	HIS	-	expression tag	UNP Q81A77
A	427	HIS	-	expression tag	UNP Q81A77
A	428	HIS	-	expression tag	UNP Q81A77
A	429	HIS	-	expression tag	UNP Q81A77
A	430	HIS	-	expression tag	UNP Q81A77
A	431	HIS	-	expression tag	UNP Q81A77
B	424	LEU	-	expression tag	UNP Q81A77
B	425	GLU	-	expression tag	UNP Q81A77
B	426	HIS	-	expression tag	UNP Q81A77
B	427	HIS	-	expression tag	UNP Q81A77
B	428	HIS	-	expression tag	UNP Q81A77

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Chain	Residue	Modelled	Actual	Comment	Reference
B	429	HIS	-	expression tag	UNP Q81A77
B	430	HIS	-	expression tag	UNP Q81A77
B	431	HIS	-	expression tag	UNP Q81A77
C	424	LEU	-	expression tag	UNP Q81A77
C	425	GLU	-	expression tag	UNP Q81A77
C	426	HIS	-	expression tag	UNP Q81A77
C	427	HIS	-	expression tag	UNP Q81A77
C	428	HIS	-	expression tag	UNP Q81A77
C	429	HIS	-	expression tag	UNP Q81A77
C	430	HIS	-	expression tag	UNP Q81A77
C	431	HIS	-	expression tag	UNP Q81A77
D	424	LEU	-	expression tag	UNP Q81A77
D	425	GLU	-	expression tag	UNP Q81A77
D	426	HIS	-	expression tag	UNP Q81A77
D	427	HIS	-	expression tag	UNP Q81A77
D	428	HIS	-	expression tag	UNP Q81A77
D	429	HIS	-	expression tag	UNP Q81A77
D	430	HIS	-	expression tag	UNP Q81A77
D	431	HIS	-	expression tag	UNP Q81A77
E	424	LEU	-	expression tag	UNP Q81A77
E	425	GLU	-	expression tag	UNP Q81A77
E	426	HIS	-	expression tag	UNP Q81A77
E	427	HIS	-	expression tag	UNP Q81A77
E	428	HIS	-	expression tag	UNP Q81A77
E	429	HIS	-	expression tag	UNP Q81A77
E	430	HIS	-	expression tag	UNP Q81A77
E	431	HIS	-	expression tag	UNP Q81A77
F	424	LEU	-	expression tag	UNP Q81A77
F	425	GLU	-	expression tag	UNP Q81A77
F	426	HIS	-	expression tag	UNP Q81A77
F	427	HIS	-	expression tag	UNP Q81A77
F	428	HIS	-	expression tag	UNP Q81A77
F	429	HIS	-	expression tag	UNP Q81A77
F	430	HIS	-	expression tag	UNP Q81A77
F	431	HIS	-	expression tag	UNP Q81A77
G	424	LEU	-	expression tag	UNP Q81A77
G	425	GLU	-	expression tag	UNP Q81A77
G	426	HIS	-	expression tag	UNP Q81A77
G	427	HIS	-	expression tag	UNP Q81A77
G	428	HIS	-	expression tag	UNP Q81A77
G	429	HIS	-	expression tag	UNP Q81A77
G	430	HIS	-	expression tag	UNP Q81A77

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Chain	Residue	Modelled	Actual	Comment	Reference
G	431	HIS	-	expression tag	UNP Q81A77
H	424	LEU	-	expression tag	UNP Q81A77
H	425	GLU	-	expression tag	UNP Q81A77
H	426	HIS	-	expression tag	UNP Q81A77
H	427	HIS	-	expression tag	UNP Q81A77
H	428	HIS	-	expression tag	UNP Q81A77
H	429	HIS	-	expression tag	UNP Q81A77
H	430	HIS	-	expression tag	UNP Q81A77
H	431	HIS	-	expression tag	UNP Q81A77

- Molecule 2 is water.

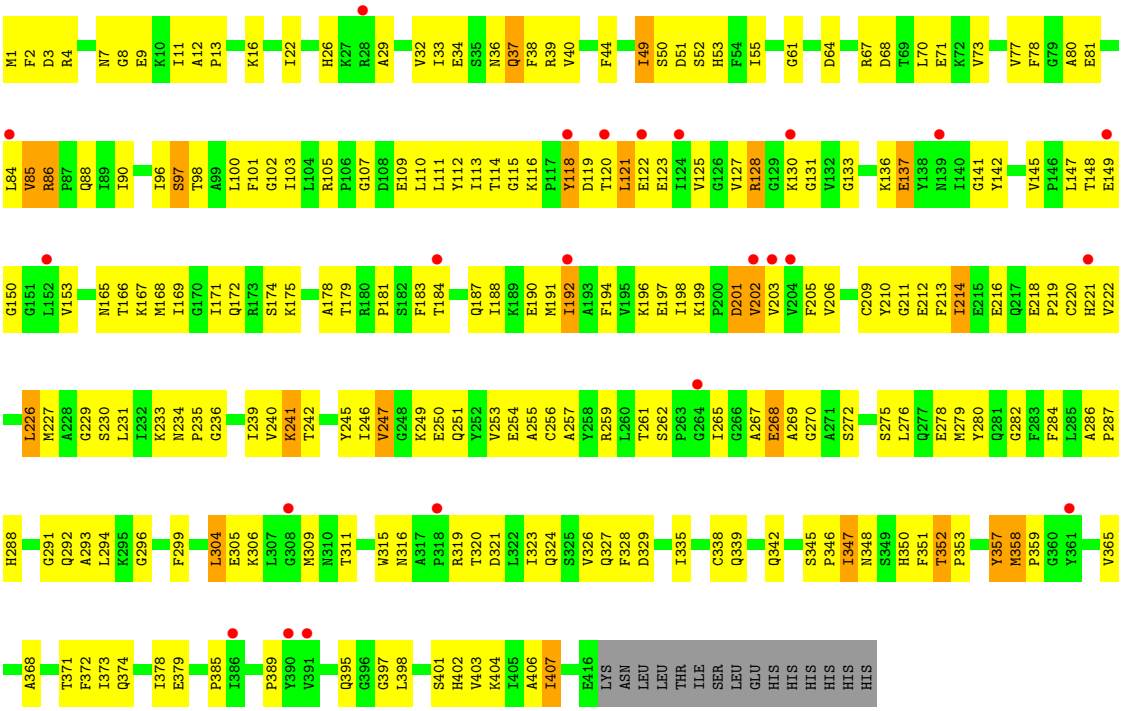
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	19	19	19	0	0
			Total	O		
2	B	16	16	16	0	0
			Total	O		
2	C	12	12	12	0	0
			Total	O		
2	D	24	24	24	0	0
			Total	O		
2	E	18	18	18	0	0
			Total	O		
2	F	18	18	18	0	0
			Total	O		
2	G	10	10	10	0	0
			Total	O		
2	H	9	9	9	0	0

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.

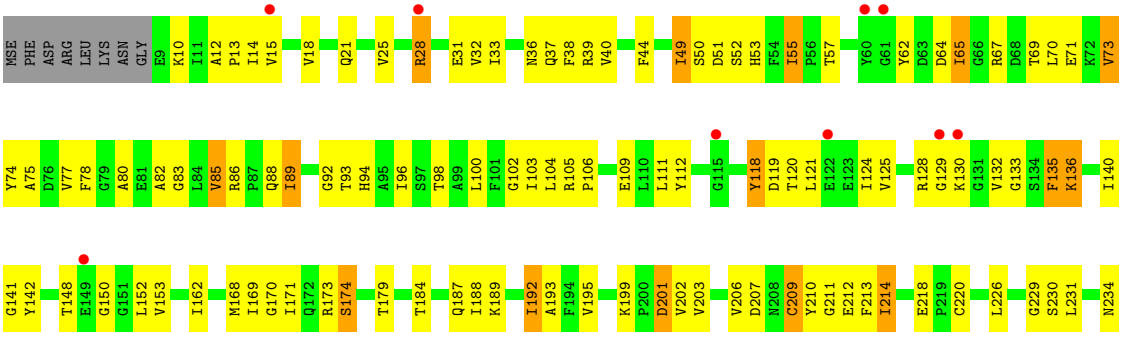
- Molecule 1: Aluminum resistance protein

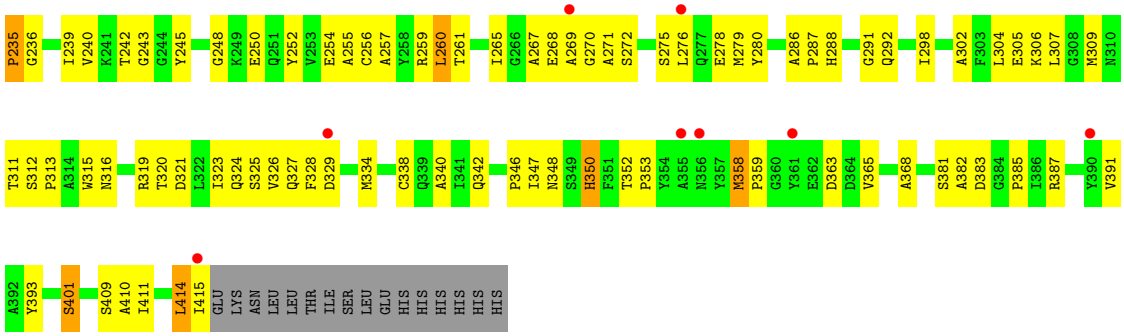
Chain A:



- Molecule 1: Aluminum resistance protein

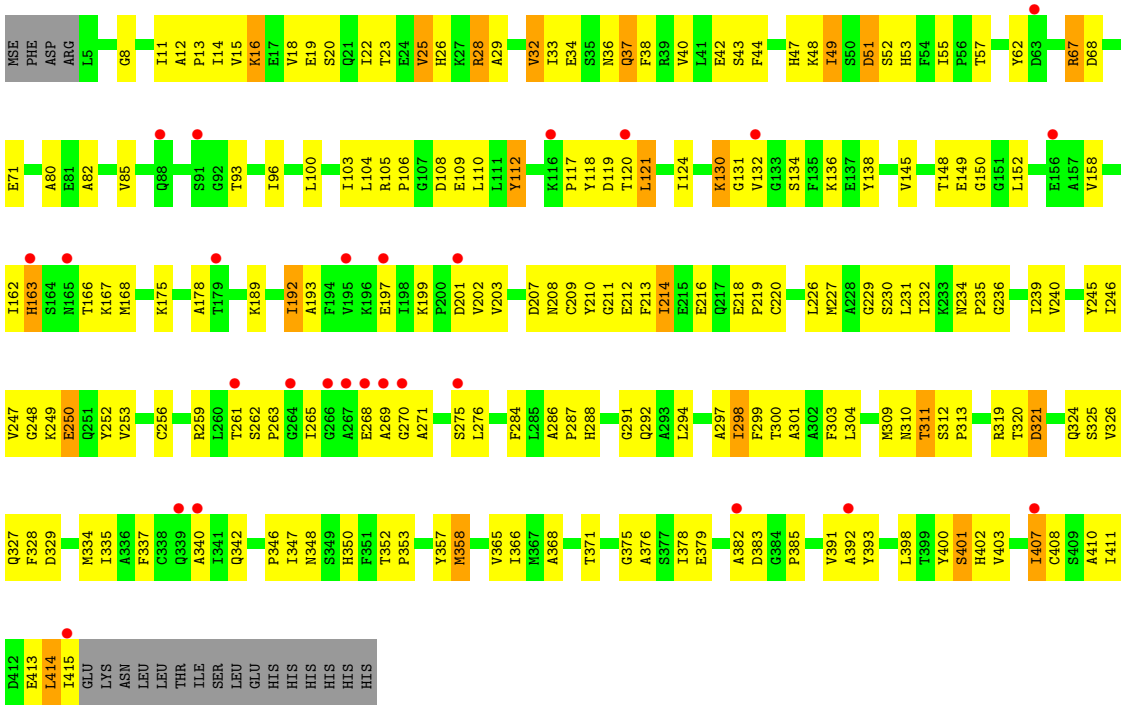
Chain B:





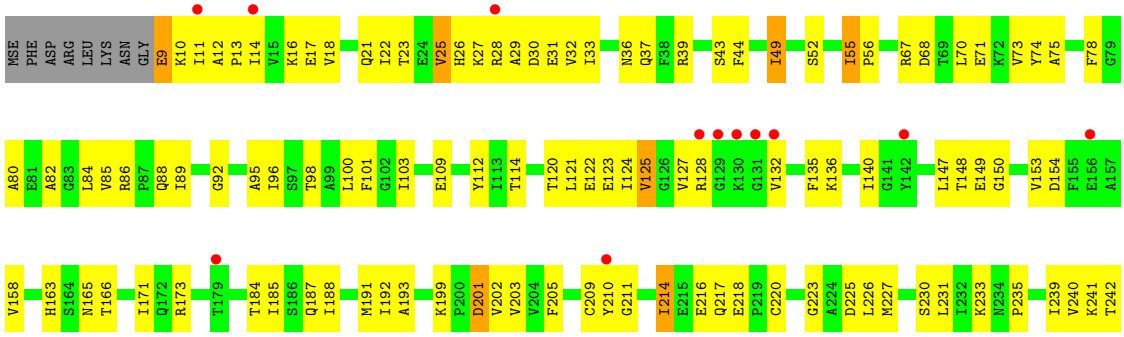
- Molecule 1: Aluminum resistance protein

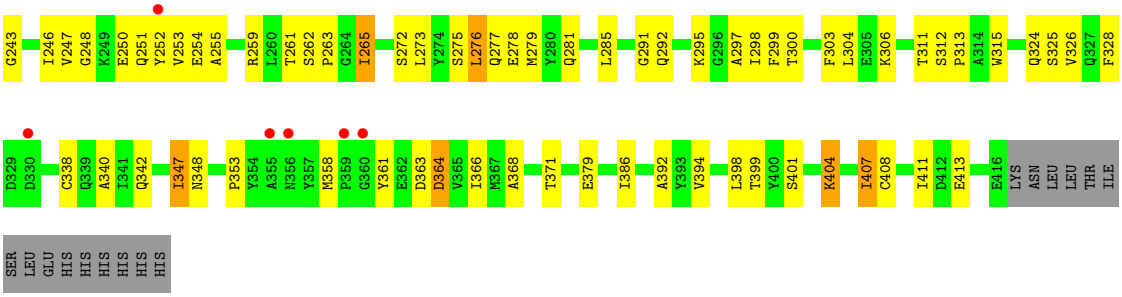
Chain C:



- Molecule 1: Aluminum resistance protein

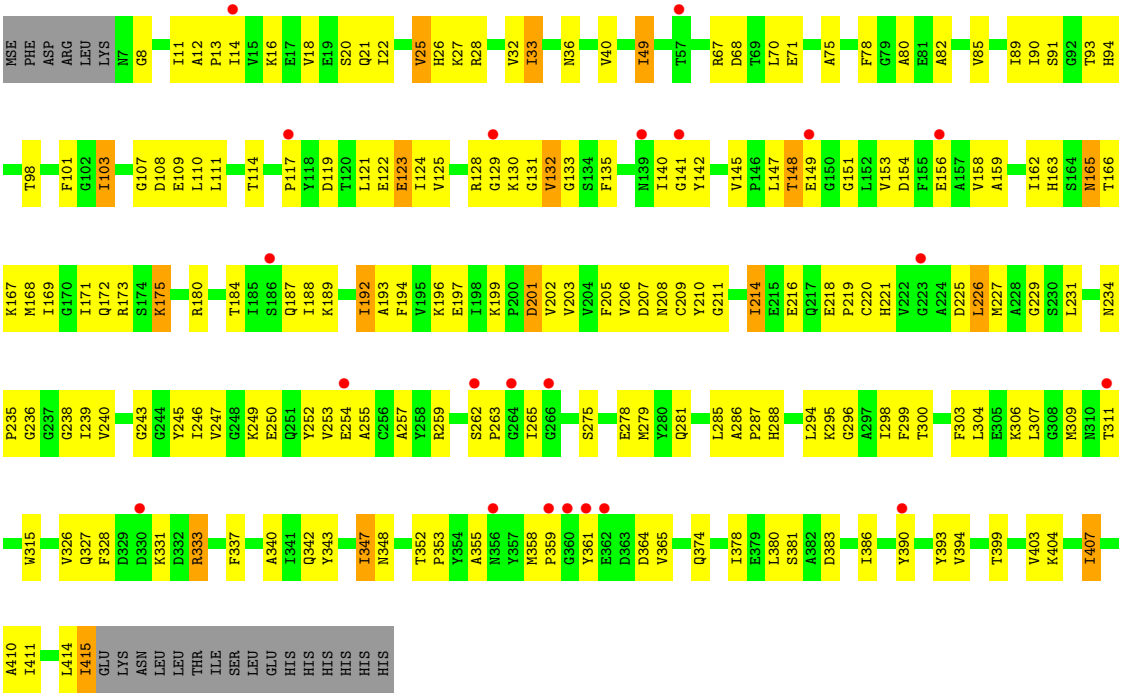
Chain D:





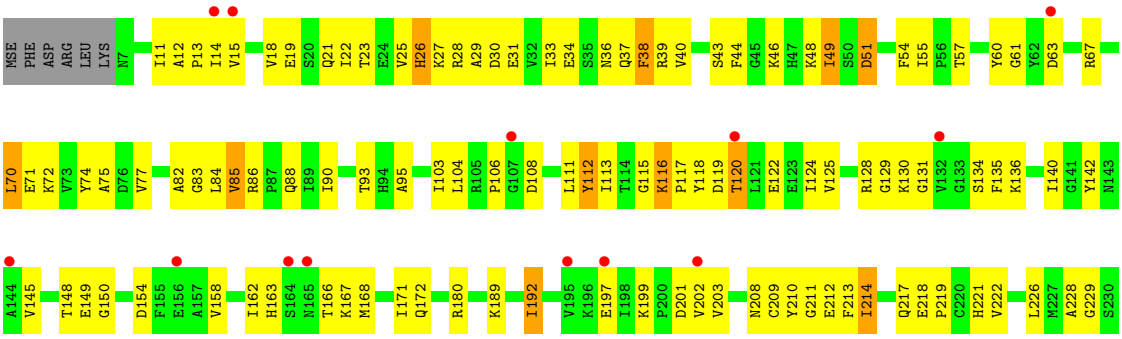
- Molecule 1: Aluminum resistance protein

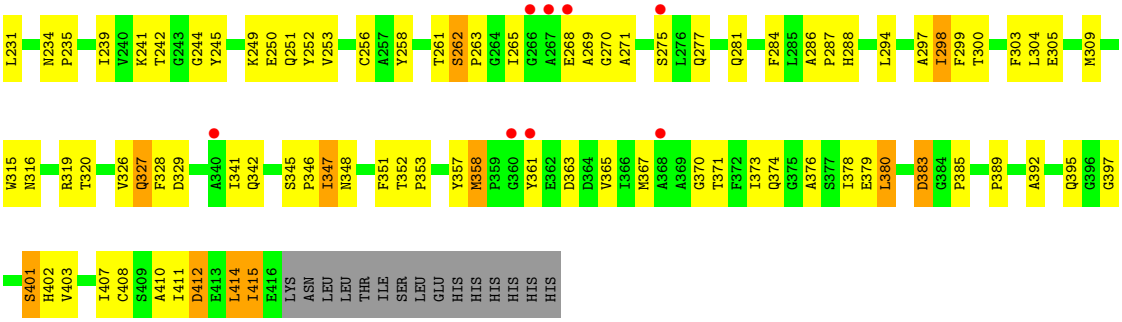
Chain E:



- Molecule 1: Aluminum resistance protein

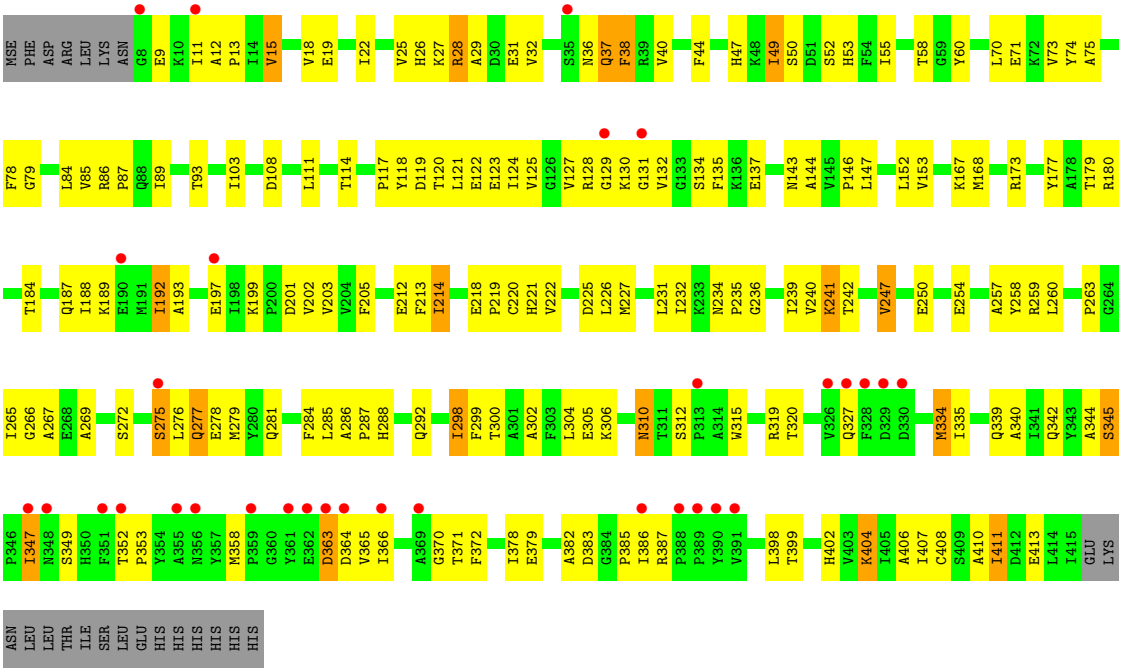
Chain F:





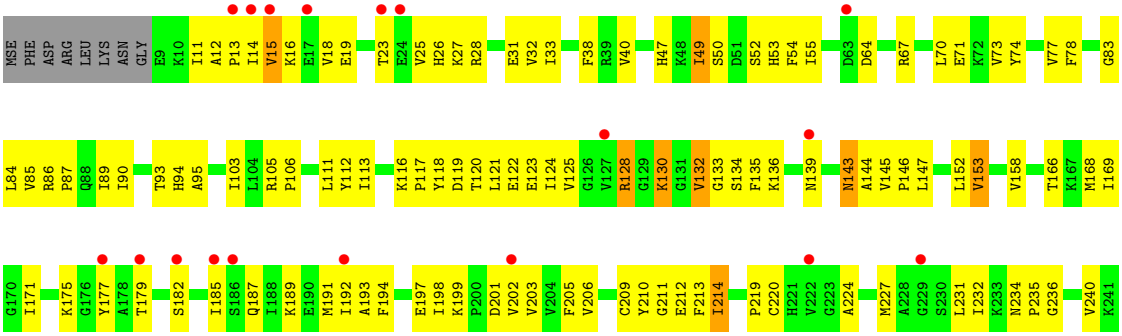
- Molecule 1: Aluminum resistance protein

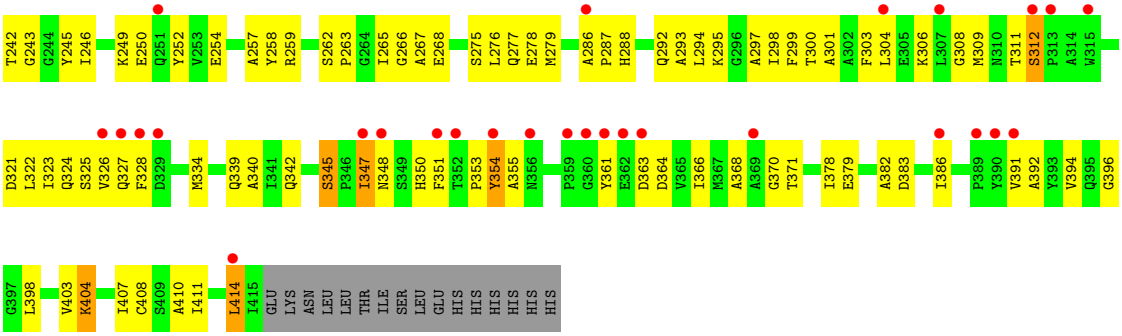
Chain G:



- Molecule 1: Aluminum resistance protein

Chain H:




T242 G243 G244 Y245 I246 K249 E250 Q251 Y252 V253 E254 A257 Y258 R259 S262 P263 G264 I265 G266 A267 E268 S275 L276 Q277 E278 M279 A286 P287 H288 Q292 A293 L294 K295 G296 A297 I298 F299 T300 A301 A302 F303 L304 E305 K306 L307 G308 M309 N310 T311 S312 P313 A314 W315
D321 L322 I323 Q324 S325 V326 Q327 F328 D329 M334 Q339 A340 I341 Q342 S345 P346 I347 N348 S349 H350 F351 T352 P353 Y354 A355 N356 P359 G360 Y361 E362 D363 D364 V365 I366 M367 A368 A369 G370 T371 I378 E379 A382 D383 I386 P389 Y390 V391 A392 Y393 V394 Q395 G396
G397 L398 V403 K404 I407 C408 S409 A410 I411 L414 I415 GLU LYS ASN LEU LEU THR ILE SER LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.41Å 144.99Å 131.97Å 90.00° 106.24° 90.00°	Depositor
Resolution (Å)	46.19 – 2.90 46.19 – 2.90	Depositor EDS
% Data completeness (in resolution range)	75.0 (46.19-2.90) 91.4 (46.19-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.274 , 0.299 0.291 , 0.319	Depositor DCC
R_{free} test set	6339 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	25070	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 28.75 % 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 1.7445e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.22	0/3213	0.36	0/4346
1	B	0.22	0/3174	0.36	0/4291
1	C	0.22	0/3185	0.37	0/4307
1	D	0.23	0/3179	0.37	0/4298
1	E	0.22	0/3179	0.36	0/4298
1	F	0.22	0/3180	0.36	0/4300
1	G	0.22	0/3164	0.37	0/4278
1	H	0.21	0/3166	0.38	0/4282
All	All	0.22	0/25440	0.37	0/34400

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 (i)

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	3151	0	3073	205	0
1	B	3112	0	3066	180	0
1	C	3123	0	3067	170	0
1	D	3117	0	3068	158	0
1	E	3117	0	3067	181	0
1	F	3118	0	3065	183	0
1	G	3102	0	3043	177	0
1	H	3104	0	3051	189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	19	0	0	1	0
2	B	16	0	0	0	0
2	C	12	0	0	2	0
2	D	24	0	0	4	0
2	E	18	0	0	3	0
2	F	18	0	0	4	0
2	G	10	0	0	1	0
2	H	9	0	0	1	0
All	All	25070	0	24500	1364	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 28.

All (1364) 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:H:327:GLN:HG2	1:H:391:VAL:HG22	1.33	1.10
1:E:414:LEU:O	1:E:415:ILE:HG13	1.51	1.09
1:E:8:GLY:HA2	1:E:11:ILE:HG22	1.36	1.04
1:E:184:THR:H	1:E:187:GLN:HE21	1.03	1.02
1:B:49:ILE:HD11	1:C:346:PRO:O	1.60	1.01
1:B:53:HIS:CD2	1:B:69:THR:HG21	1.96	0.99
1:A:311:THR:HG22	1:A:326:VAL:HG12	1.44	0.97
1:D:364:ASP:HB2	1:D:386:ILE:HD12	1.44	0.96
1:A:49:ILE:HD11	1:F:346:PRO:O	1.66	0.96
1:A:199:LYS:O	1:A:202:VAL:HG22	1.67	0.94
1:B:346:PRO:O	1:C:49:ILE:HD11	1.67	0.94
1:E:49:ILE:HD13	1:E:49:ILE:O	1.68	0.94
1:B:65:ILE:O	1:B:69:THR:HG22	1.67	0.93
1:D:250:GLU:O	1:D:254:GLU:HG2	1.69	0.92
1:F:22:ILE:HB	1:F:298:ILE:HD11	1.51	0.92
1:D:122:GLU:CG	1:D:127:VAL:HG23	1.99	0.92
1:G:108:ASP:OD2	1:G:167:LYS:HD3	1.70	0.92
1:B:350:HIS:HB3	1:C:48:LYS:HG2	1.51	0.91
1:A:286:ALA:HB3	1:A:287:PRO:HD3	1.50	0.91
1:C:226:LEU:HD21	1:C:246:ILE:HG23	1.53	0.90
1:B:96:ILE:O	1:B:100:LEU:HG	1.71	0.90
1:E:8:GLY:HA2	1:E:11:ILE:CG2	2.01	0.89
1:B:148:THR:HG22	1:B:150:GLY:H	1.35	0.89
1:A:371:THR:HG23	1:A:379:GLU:CD	1.93	0.89
1:B:36:ASN:O	1:B:40:VAL:HG23	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:GLU:OE1	1:H:404:LYS:HE2	1.73	0.88
1:E:14:ILE:O	1:E:18:VAL:HG23	1.73	0.88
1:E:220:CYS:SG	1:E:227:MSE:HG2	2.14	0.88
1:D:23:THR:O	1:D:27:LYS:HG2	1.75	0.87
1:F:85:VAL:HG23	1:F:231:LEU:HD11	1.56	0.86
1:F:371:THR:HG23	1:F:379:GLU:CD	1.95	0.86
1:F:70:LEU:HD12	1:F:70:LEU:O	1.75	0.86
1:A:131:GLY:HA2	1:A:137:GLU:OE2	1.75	0.86
1:C:357:TYR:HB3	1:H:199:LYS:HD3	1.57	0.85
1:C:414:LEU:HD12	1:C:415:ILE:HG13	1.58	0.85
1:D:44:PHE:CD2	1:D:49:ILE:HD12	2.11	0.85
1:G:199:LYS:O	1:G:199:LYS:HG3	1.76	0.85
1:E:340:ALA:HB1	1:E:410:ALA:HA	1.57	0.84
1:F:168:MSE:HG3	1:F:203:VAL:HG23	1.60	0.83
1:D:199:LYS:HG2	1:D:202:VAL:HG13	1.60	0.83
1:C:148:THR:HG22	1:C:150:GLY:H	1.42	0.83
1:G:192:ILE:HD13	1:G:193:ALA:N	1.93	0.83
1:F:11:ILE:HD11	1:F:411:ILE:HG21	1.61	0.83
1:E:111:LEU:HD11	1:E:145:VAL:HG23	1.59	0.82
1:E:109:GLU:OE1	1:E:165:ASN:HB3	1.79	0.82
1:H:49:ILE:CD1	1:H:49:ILE:H	1.92	0.82
1:D:122:GLU:HG2	1:D:127:VAL:HG23	1.62	0.82
1:C:357:TYR:CB	1:H:199:LYS:HD3	2.10	0.82
1:E:199:LYS:HG2	1:E:202:VAL:HG13	1.60	0.82
1:C:209:CYS:O	1:C:210:TYR:HB2	1.80	0.81
1:D:291:GLY:O	1:D:295:LYS:HG3	1.81	0.81
1:A:346:PRO:O	1:F:49:ILE:HD11	1.81	0.81
1:B:53:HIS:HD2	1:B:69:THR:HG21	1.43	0.81
1:F:328:PHE:O	1:F:329:ASP:HB2	1.80	0.80
1:G:118:TYR:CE2	1:G:120:THR:HB	2.16	0.80
1:C:301:ALA:HA	1:C:311:THR:HG21	1.62	0.80
1:D:209:CYS:O	1:D:210:TYR:HB2	1.82	0.80
1:B:118:TYR:HE1	1:B:121:LEU:HG	1.45	0.80
1:A:304:LEU:HG	1:A:326:VAL:HG11	1.64	0.79
1:C:53:HIS:O	1:C:276:LEU:HD13	1.83	0.79
1:E:414:LEU:C	1:E:415:ILE:HG13	2.03	0.79
1:D:199:LYS:O	1:D:202:VAL:HG22	1.81	0.79
1:F:14:ILE:O	1:F:18:VAL:HG23	1.82	0.79
1:F:294:LEU:O	1:F:298:ILE:HG22	1.83	0.79
1:A:199:LYS:HG2	1:A:202:VAL:HG13	1.64	0.79
1:H:209:CYS:O	1:H:210:TYR:HB2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:257:ALA:HB1	1:H:267:ALA:HB2	1.63	0.79
1:E:159:ALA:HB2	1:E:194:PHE:HZ	1.49	0.78
1:A:33:ILE:HD11	1:A:291:GLY:HA3	1.66	0.78
1:G:258:TYR:CD1	1:G:266:GLY:HA2	2.19	0.78
1:D:211:GLY:O	1:D:214:ILE:HG23	1.83	0.78
1:H:47:HIS:HD2	1:H:73:VAL:HG22	1.49	0.78
1:A:121:LEU:O	1:A:125:VAL:HG22	1.84	0.77
1:C:299:PHE:HE2	1:C:407:ILE:HD11	1.46	0.77
1:F:148:THR:HG22	1:F:150:GLY:H	1.47	0.77
1:F:410:ALA:O	1:F:414:LEU:HD22	1.84	0.77
1:H:347:ILE:HG21	1:H:371:THR:O	1.84	0.77
1:H:403:VAL:O	1:H:407:ILE:HG12	1.85	0.77
1:A:148:THR:HG22	1:A:150:GLY:H	1.50	0.77
1:H:212:GLU:O	1:H:213:PHE:HB2	1.85	0.77
1:A:234:ASN:HA	1:A:378:ILE:HD13	1.67	0.76
1:C:8:GLY:HA2	1:C:11:ILE:HG22	1.66	0.76
1:E:184:THR:H	1:E:187:GLN:NE2	1.83	0.76
1:A:133:GLY:HA2	1:B:105:ARG:HH21	1.49	0.76
1:E:8:GLY:CA	1:E:11:ILE:HG22	2.15	0.76
1:D:263:PRO:HB2	1:H:124:ILE:HA	1.67	0.76
1:B:286:ALA:HB3	1:B:287:PRO:HD3	1.66	0.76
1:C:309:MSE:HB3	1:C:327:GLN:O	1.85	0.76
1:B:174:SER:HB2	1:B:321:ASP:OD2	1.86	0.75
1:C:208:ASN:HD22	1:C:227:MSE:HE3	1.52	0.75
1:C:214:ILE:HD11	1:C:294:LEU:HD13	1.69	0.75
1:A:80:ALA:HB3	1:A:247:VAL:HG13	1.69	0.75
1:D:122:GLU:HG3	1:D:127:VAL:HG23	1.68	0.75
1:H:342:GLN:HB2	1:H:368:ALA:HB1	1.69	0.74
1:C:340:ALA:HB2	1:C:413:GLU:OE2	1.87	0.74
1:D:220:CYS:SG	1:D:227:MSE:HG2	2.26	0.74
1:G:189:LYS:HG3	1:G:222:VAL:HB	1.69	0.74
1:E:209:CYS:O	1:E:210:TYR:HB2	1.87	0.74
1:G:199:LYS:O	1:G:202:VAL:HG22	1.86	0.74
1:A:335:ILE:O	1:A:339:GLN:HG3	1.86	0.74
1:G:118:TYR:HE2	1:G:120:THR:HB	1.51	0.74
1:H:49:ILE:H	1:H:49:ILE:HD12	1.51	0.73
1:B:365:VAL:HG12	1:B:385:PRO:HA	1.70	0.73
1:G:192:ILE:HD13	1:G:193:ALA:H	1.52	0.73
1:H:301:ALA:HA	1:H:311:THR:HG21	1.68	0.73
1:B:121:LEU:HD23	1:B:124:ILE:HD12	1.69	0.73
1:E:93:THR:HG21	1:G:265:ILE:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:THR:HG23	1:B:280:TYR:OH	1.87	0.73
1:C:327:GLN:HG3	1:C:391:VAL:HG22	1.69	0.73
1:H:15:VAL:O	1:H:19:GLU:HG3	1.88	0.73
1:A:1:MSE:HG3	1:A:2:PHE:H	1.51	0.73
1:E:342:GLN:NE2	1:E:348:ASN:O	2.22	0.73
1:E:80:ALA:HB3	1:E:247:VAL:HG22	1.71	0.73
1:G:108:ASP:OD2	1:G:167:LYS:CD	2.35	0.73
1:A:67:ARG:O	1:A:71:GLU:HG3	1.87	0.73
1:B:411:ILE:O	1:B:415:ILE:HB	1.89	0.73
1:D:78:PHE:CD1	1:D:218:GLU:HG3	2.23	0.73
1:A:214:ILE:HG13	1:A:214:ILE:O	1.89	0.72
1:B:39:ARG:HE	1:B:77:VAL:HG13	1.52	0.72
1:B:67:ARG:O	1:B:71:GLU:HG3	1.88	0.72
1:G:184:THR:H	1:G:187:GLN:NE2	1.87	0.72
1:B:311:THR:HG22	1:B:326:VAL:HG12	1.69	0.72
1:D:125:VAL:HG23	1:D:127:VAL:HG22	1.69	0.72
1:G:286:ALA:HB3	1:G:287:PRO:HD3	1.71	0.72
1:D:205:PHE:HA	1:D:226:LEU:O	1.90	0.72
1:D:14:ILE:O	1:D:18:VAL:HG23	1.90	0.72
1:E:303:PHE:HD1	1:E:407:ILE:HD11	1.55	0.71
1:F:371:THR:HG23	1:F:379:GLU:OE2	1.91	0.71
1:H:49:ILE:CD1	1:H:49:ILE:N	2.52	0.71
1:A:309:MSE:HG2	1:A:327:GLN:O	1.90	0.71
1:A:1:MSE:HB2	1:F:34:GLU:CB	2.20	0.71
1:F:57:THR:O	1:F:271:ALA:HB1	1.91	0.71
1:B:103:ILE:HD11	1:B:226:LEU:HD22	1.73	0.71
1:E:300:THR:HA	1:E:407:ILE:HD13	1.71	0.71
1:A:33:ILE:CD1	1:A:291:GLY:HA3	2.21	0.70
1:A:80:ALA:CB	1:A:247:VAL:HG13	2.21	0.70
1:H:220:CYS:SG	1:H:227:MSE:HG2	2.31	0.70
1:E:22:ILE:HG22	1:E:315:TRP:CE3	2.26	0.70
1:F:82:ALA:HB3	1:F:253:VAL:HG21	1.73	0.70
1:H:214:ILE:HG21	1:H:321:ASP:HA	1.73	0.70
1:D:128:ARG:HG3	1:D:128:ARG:HH11	1.55	0.70
1:F:253:VAL:O	1:F:256:CYS:HB2	1.92	0.70
1:B:65:ILE:O	1:B:69:THR:CG2	2.40	0.70
1:A:342:GLN:HG2	1:A:353:PRO:HD3	1.73	0.69
1:C:231:LEU:O	1:C:236:GLY:HA3	1.92	0.69
1:H:125:VAL:O	1:H:135:PHE:HB2	1.92	0.69
1:H:147:LEU:CD2	1:H:153:VAL:HA	2.22	0.69
1:F:71:GLU:HB3	1:F:83:GLY:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ILE:HG22	1:D:315:TRP:CE3	2.28	0.69
1:H:171:ILE:HB	1:H:206:VAL:HG22	1.74	0.69
1:A:371:THR:HG22	1:A:373:ILE:H	1.57	0.69
1:C:12:ALA:HB3	1:C:13:PRO:HD3	1.73	0.69
1:F:209:CYS:O	1:F:210:TYR:HB2	1.91	0.69
1:G:340:ALA:HB1	1:G:410:ALA:HA	1.74	0.69
1:F:328:PHE:HE2	1:F:392:ALA:HB3	1.57	0.69
1:A:240:VAL:HG12	1:A:278:GLU:HG3	1.75	0.69
1:C:44:PHE:CD2	1:C:49:ILE:HG13	2.28	0.69
1:C:358:MSE:HE2	1:C:358:MSE:HA	1.74	0.69
1:E:33:ILE:HD13	1:E:288:HIS:HA	1.74	0.69
1:F:357:TYR:CB	1:G:199:LYS:HD3	2.22	0.69
1:C:328:PHE:O	1:C:329:ASP:HB2	1.93	0.68
1:B:64:ASP:OD2	1:B:272:SER:HB3	1.93	0.68
1:C:347:ILE:HD11	1:C:371:THR:O	1.94	0.68
1:E:199:LYS:HD2	1:E:201:ASP:HB2	1.76	0.68
1:H:366:ILE:O	1:H:383:ASP:HA	1.93	0.68
1:G:257:ALA:HB1	1:G:267:ALA:HB2	1.75	0.68
1:H:147:LEU:HD23	1:H:153:VAL:HA	1.76	0.68
1:C:112:TYR:CD2	1:C:117:PRO:HG3	2.28	0.68
1:E:205:PHE:HA	1:E:226:LEU:O	1.94	0.68
1:B:118:TYR:CE1	1:B:121:LEU:HG	2.29	0.68
1:G:47:HIS:ND1	1:G:73:VAL:HG22	2.09	0.68
1:D:122:GLU:OE1	1:D:128:ARG:HD3	1.94	0.68
1:A:379:GLU:HG2	1:A:398:LEU:HD21	1.74	0.67
1:C:80:ALA:CB	1:C:247:VAL:HG13	2.23	0.67
1:A:101:PHE:HB3	1:A:259:ARG:HE	1.60	0.67
1:C:138:TYR:HA	1:F:106:PRO:HG2	1.76	0.67
1:F:214:ILE:HD12	1:F:294:LEU:HD13	1.75	0.67
1:B:304:LEU:HD12	1:B:309:MSE:SE	2.44	0.67
1:B:85:VAL:HG22	1:B:85:VAL:O	1.93	0.67
1:B:199:LYS:NZ	1:B:201:ASP:HB3	2.09	0.67
1:E:25:VAL:HG12	1:E:28:ARG:HH11	1.59	0.67
1:A:299:PHE:CE2	1:A:407:ILE:HD11	2.29	0.67
1:D:259:ARG:NH1	1:H:259:ARG:NH1	2.41	0.67
1:F:209:CYS:SG	1:F:229:GLY:HA2	2.35	0.67
1:B:168:MSE:HG3	1:B:203:VAL:HG23	1.76	0.67
1:E:189:LYS:O	1:E:192:ILE:HD13	1.94	0.67
1:B:12:ALA:HB3	1:B:13:PRO:HD3	1.77	0.67
1:B:121:LEU:O	1:B:125:VAL:HG22	1.95	0.67
1:D:124:ILE:HA	1:H:263:PRO:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:LYS:HG2	1:H:202:VAL:HG13	1.75	0.67
1:A:39:ARG:HH11	1:A:77:VAL:HG12	1.59	0.67
1:C:400:TYR:HB3	2:C:527:HOH:O	1.95	0.67
1:G:103:ILE:HD11	1:G:226:LEU:HD22	1.75	0.67
1:B:231:LEU:HB3	1:B:240:VAL:HG21	1.75	0.66
1:B:340:ALA:HB1	1:B:410:ALA:HA	1.75	0.66
1:H:311:THR:HG22	1:H:326:VAL:HG12	1.77	0.66
1:F:299:PHE:CD2	1:F:407:ILE:HD11	2.30	0.66
1:G:123:GLU:OE2	1:G:128:ARG:HG2	1.95	0.66
1:H:130:LYS:O	1:H:132:VAL:HG13	1.96	0.66
1:A:188:ILE:O	1:A:192:ILE:HG23	1.94	0.66
1:E:166:THR:HG22	1:E:202:VAL:CG1	2.25	0.66
1:A:1:MSE:HG3	1:A:2:PHE:N	2.11	0.66
1:G:259:ARG:HH11	1:G:259:ARG:HG3	1.60	0.66
1:D:225:ASP:HB3	1:D:252:TYR:CE2	2.31	0.65
1:E:259:ARG:NH1	1:G:259:ARG:NH1	2.45	0.65
1:H:119:ASP:O	1:H:122:GLU:HB2	1.95	0.65
1:A:1:MSE:CG	1:A:2:PHE:H	2.09	0.65
1:A:49:ILE:HD11	1:F:347:ILE:HA	1.77	0.65
1:A:71:GLU:OE2	1:A:84:LEU:HD12	1.97	0.65
1:D:311:THR:HG22	1:D:326:VAL:HG12	1.78	0.65
1:H:124:ILE:O	1:H:134:SER:HB2	1.97	0.65
1:H:199:LYS:CG	1:H:202:VAL:HG13	2.27	0.65
1:B:342:GLN:HG2	1:B:353:PRO:HD3	1.78	0.65
1:B:73:VAL:HG12	1:B:74:TYR:N	2.10	0.65
1:B:93:THR:HG21	1:B:120:THR:HG21	1.79	0.65
1:H:111:LEU:HD12	1:H:143:ASN:O	1.96	0.65
1:H:211:GLY:O	1:H:214:ILE:HG22	1.97	0.64
1:E:219:PRO:HD2	1:E:227:MSE:SE	2.48	0.64
1:G:407:ILE:HG13	1:G:408:CYS:N	2.10	0.64
1:B:199:LYS:HZ2	1:B:201:ASP:HB3	1.61	0.64
1:F:12:ALA:HB3	1:F:13:PRO:HD3	1.80	0.64
1:G:276:LEU:O	1:G:278:GLU:N	2.30	0.64
1:E:355:ALA:HB2	1:E:386:ILE:HD11	1.80	0.64
1:A:84:LEU:HD11	1:A:86:ARG:NH1	2.13	0.64
1:C:82:ALA:HB3	1:C:253:VAL:HG21	1.79	0.64
1:D:33:ILE:HD11	1:D:291:GLY:HA3	1.79	0.64
1:D:342:GLN:HG2	1:D:353:PRO:HD3	1.79	0.64
1:G:127:VAL:HG22	1:G:127:VAL:O	1.97	0.64
1:B:199:LYS:O	1:B:202:VAL:HG22	1.97	0.64
1:B:261:THR:HG21	1:B:265:ILE:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:GLU:OE1	1:D:165:ASN:HB3	1.98	0.64
1:H:249:LYS:HB2	1:H:252:TYR:CD2	2.33	0.64
1:F:29:ALA:O	1:F:33:ILE:HG13	1.97	0.64
1:F:347:ILE:HD11	1:F:371:THR:O	1.97	0.64
1:B:184:THR:OG1	1:B:187:GLN:HG3	1.98	0.64
1:D:154:ASP:O	1:D:158:VAL:HG23	1.98	0.64
1:D:265:ILE:HD11	1:H:93:THR:CG2	2.28	0.64
1:E:275:SER:O	1:E:279:MSE:HE2	1.98	0.64
1:C:218:GLU:HB3	1:C:219:PRO:HD2	1.79	0.63
1:D:199:LYS:CG	1:D:202:VAL:HG13	2.29	0.63
1:E:281:GLN:O	1:E:285:LEU:HG	1.98	0.63
1:H:199:LYS:O	1:H:202:VAL:HG22	1.98	0.63
1:E:211:GLY:O	1:E:214:ILE:HG23	1.99	0.63
1:F:108:ASP:OD2	1:F:167:LYS:HD3	1.98	0.63
1:G:12:ALA:HB3	1:G:13:PRO:HD3	1.80	0.63
1:G:212:GLU:O	1:G:213:PHE:HB2	1.97	0.63
1:H:47:HIS:CD2	1:H:73:VAL:CG2	2.82	0.63
1:A:261:THR:O	1:B:94:HIS:ND1	2.32	0.63
1:H:328:PHE:HE2	1:H:392:ALA:HB3	1.63	0.63
1:A:358:MSE:HG2	1:A:365:VAL:CG2	2.28	0.63
1:E:93:THR:CG2	1:G:265:ILE:HD11	2.28	0.63
1:E:220:CYS:SG	1:E:227:MSE:CG	2.86	0.63
1:H:47:HIS:HD2	1:H:73:VAL:CG2	2.11	0.63
1:F:70:LEU:HD12	1:F:70:LEU:C	2.18	0.63
1:H:49:ILE:N	1:H:49:ILE:HD13	2.13	0.63
1:A:12:ALA:HB3	1:A:13:PRO:HD3	1.81	0.63
1:D:262:SER:HB3	1:D:265:ILE:HD12	1.81	0.63
1:B:210:TYR:O	1:B:321:ASP:HB2	1.99	0.62
1:C:12:ALA:O	1:C:16:LYS:HB2	1.99	0.62
1:F:361:TYR:HD1	2:F:522:HOH:O	1.82	0.62
1:A:73:VAL:O	1:A:77:VAL:HG23	1.98	0.62
1:B:89:ILE:O	1:B:243:GLY:HA2	1.98	0.62
1:E:199:LYS:O	1:E:202:VAL:HG22	1.99	0.62
1:A:261:THR:O	1:B:94:HIS:CE1	2.53	0.62
1:B:184:THR:HG23	1:B:187:GLN:HE21	1.64	0.62
1:F:122:GLU:HG2	1:F:128:ARG:HB2	1.81	0.62
1:G:345:SER:HB2	1:G:370:GLY:HA3	1.80	0.62
1:C:29:ALA:O	1:C:33:ILE:HG13	1.99	0.62
1:D:89:ILE:O	1:D:243:GLY:HA2	1.98	0.62
1:D:184:THR:H	1:D:187:GLN:HE21	1.46	0.62
1:F:214:ILE:O	1:F:214:ILE:HG13	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:ASN:ND2	1:F:212:GLU:HG3	2.14	0.62
1:B:209:CYS:O	1:B:210:TYR:HB2	1.99	0.62
1:D:311:THR:CG2	1:D:326:VAL:HG12	2.29	0.62
1:G:199:LYS:HG2	1:G:202:VAL:HG13	1.81	0.62
1:H:175:LYS:HG2	1:H:182:SER:OG	1.99	0.62
1:C:85:VAL:HG13	1:C:85:VAL:O	2.00	0.62
1:C:208:ASN:HD22	1:C:227:MSE:CE	2.12	0.62
1:F:395:GLN:NE2	2:F:564:HOH:O	2.33	0.62
1:A:29:ALA:O	1:A:33:ILE:HG13	1.99	0.62
1:A:288:HIS:HE1	1:F:288:HIS:HE1	1.47	0.62
1:B:324:GLN:HE21	1:B:325:SER:H	1.48	0.62
1:G:147:LEU:HB3	1:G:152:LEU:O	2.00	0.61
1:H:203:VAL:HG23	1:H:203:VAL:O	1.99	0.61
1:E:80:ALA:HB3	1:E:247:VAL:CG2	2.30	0.61
1:H:364:ASP:HB2	1:H:386:ILE:HD12	1.82	0.61
1:E:133:GLY:O	1:G:263:PRO:HG3	2.00	0.61
1:G:103:ILE:HD12	1:G:168:MSE:CE	2.29	0.61
1:F:226:LEU:HD13	1:F:252:TYR:HB3	1.80	0.61
1:G:119:ASP:O	1:G:122:GLU:HB3	1.99	0.61
1:A:299:PHE:HE2	1:A:407:ILE:HD11	1.64	0.61
1:B:86:ARG:HB2	1:B:88:GLN:OE1	1.99	0.61
1:E:189:LYS:O	1:E:192:ILE:CD1	2.48	0.61
1:F:358:MSE:HG2	1:F:361:TYR:HD2	1.66	0.61
1:G:184:THR:H	1:G:187:GLN:HE21	1.46	0.61
1:H:74:TYR:OH	1:H:231:LEU:HD21	2.00	0.61
1:C:80:ALA:HB3	1:C:247:VAL:HG13	1.80	0.61
1:C:379:GLU:HG2	1:C:398:LEU:HD21	1.81	0.61
1:E:156:GLU:H	1:E:156:GLU:CD	2.04	0.61
1:H:111:LEU:HB3	1:H:169:ILE:HD13	1.82	0.61
1:H:145:VAL:HG11	1:H:158:VAL:HG23	1.82	0.61
1:A:211:GLY:O	1:A:214:ILE:HG23	2.01	0.61
1:D:128:ARG:HH11	1:D:128:ARG:CG	2.13	0.61
1:F:67:ARG:HD2	1:F:86:ARG:NH2	2.16	0.61
1:F:357:TYR:HB3	1:G:199:LYS:HD3	1.82	0.61
1:D:122:GLU:HG3	1:D:127:VAL:CG2	2.31	0.61
1:E:70:LEU:HD21	1:E:279:MSE:HB3	1.81	0.61
1:D:70:LEU:HD21	1:D:279:MSE:HB3	1.82	0.61
1:B:315:TRP:CZ3	1:B:316:ASN:HB3	2.36	0.60
1:B:286:ALA:HB3	1:B:287:PRO:CD	2.30	0.60
1:E:148:THR:HG22	1:E:149:GLU:OE1	2.02	0.60
1:E:342:GLN:HG2	1:E:353:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:SER:O	1:G:279:MSE:HE2	2.01	0.60
1:B:350:HIS:CB	1:C:48:LYS:HG2	2.29	0.60
1:D:122:GLU:HG2	1:D:128:ARG:HB2	1.82	0.60
1:E:89:ILE:O	1:E:243:GLY:HA2	2.00	0.60
1:F:300:THR:O	1:F:304:LEU:HD23	2.00	0.60
1:F:299:PHE:CE2	1:F:407:ILE:HD11	2.37	0.60
1:E:218:GLU:HB3	1:E:219:PRO:CD	2.32	0.60
1:D:240:VAL:HA	1:D:278:GLU:OE2	2.02	0.60
1:C:33:ILE:HD11	1:C:291:GLY:HA3	1.84	0.60
1:D:225:ASP:HB3	1:D:252:TYR:HE2	1.66	0.60
1:E:192:ILE:HD13	1:E:193:ALA:H	1.67	0.60
1:G:103:ILE:HD12	1:G:168:MSE:HE3	1.82	0.60
1:H:15:VAL:HG12	1:H:303:PHE:CE2	2.37	0.60
1:H:293:ALA:HB1	1:H:396:GLY:HA2	1.83	0.60
1:C:261:THR:OG1	1:C:262:SER:N	2.34	0.59
1:E:192:ILE:HG12	1:E:193:ALA:N	2.17	0.59
1:G:378:ILE:HG13	1:G:378:ILE:O	2.02	0.59
1:B:192:ILE:HD13	1:B:193:ALA:N	2.17	0.59
1:A:203:VAL:HG23	1:A:203:VAL:O	2.03	0.59
1:C:18:VAL:O	1:C:22:ILE:HG12	2.03	0.59
1:C:207:ASP:OD1	1:C:207:ASP:C	2.39	0.59
1:D:209:CYS:O	1:D:210:TYR:CB	2.50	0.59
1:E:108:ASP:HB3	1:E:167:LYS:HB3	1.83	0.59
1:E:166:THR:HG22	1:E:202:VAL:HG11	1.83	0.59
1:G:93:THR:OG1	1:G:120:THR:HG21	2.02	0.59
1:H:25:VAL:O	1:H:28:ARG:HB3	2.02	0.59
1:D:275:SER:HB2	2:D:599:HOH:O	2.02	0.59
1:D:297:ALA:HB1	1:D:324:GLN:HB2	1.85	0.59
1:D:379:GLU:HG2	1:D:398:LEU:HD21	1.84	0.59
1:A:214:ILE:HG12	1:A:320:THR:C	2.23	0.59
1:F:39:ARG:NH1	1:F:77:VAL:O	2.36	0.59
1:A:261:THR:HA	1:B:94:HIS:CE1	2.37	0.59
1:B:128:ARG:HG3	1:B:129:GLY:N	2.17	0.59
1:C:37:GLN:NE2	1:C:284:PHE:O	2.35	0.59
1:A:33:ILE:HD11	1:A:291:GLY:CA	2.33	0.59
1:C:199:LYS:O	1:C:202:VAL:HG22	2.03	0.59
1:G:342:GLN:HG2	1:G:353:PRO:HD3	1.84	0.59
1:B:192:ILE:HD13	1:B:193:ALA:H	1.67	0.59
1:H:286:ALA:HB3	1:H:287:PRO:HD3	1.85	0.59
1:F:328:PHE:O	1:F:329:ASP:CB	2.51	0.59
1:G:32:VAL:O	1:G:36:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:MSE:HE3	1:G:366:ILE:HG22	1.85	0.58
1:D:135:PHE:HB3	1:D:140:ILE:O	2.03	0.58
1:H:275:SER:O	1:H:278:GLU:HG2	2.03	0.58
1:A:133:GLY:HA2	1:B:105:ARG:NH2	2.18	0.58
1:F:341:ILE:HG23	1:F:380:LEU:HD21	1.84	0.58
1:G:231:LEU:HB3	1:G:240:VAL:HG21	1.85	0.58
1:G:259:ARG:HG3	1:G:259:ARG:NH1	2.17	0.58
1:D:347:ILE:HD12	1:D:371:THR:O	2.03	0.58
1:F:72:LYS:O	1:F:75:ALA:HB3	2.03	0.58
1:A:67:ARG:HE	1:A:86:ARG:NH2	2.01	0.58
1:F:158:VAL:O	1:F:162:ILE:HG13	2.04	0.58
1:E:168:MSE:HG3	1:E:203:VAL:HG23	1.86	0.58
1:E:214:ILE:HD13	1:E:294:LEU:HD13	1.85	0.58
1:C:259:ARG:HG3	1:C:259:ARG:HH11	1.69	0.58
1:D:303:PHE:HD2	1:D:407:ILE:HD11	1.67	0.58
1:D:347:ILE:HD11	1:D:348:ASN:HD22	1.69	0.58
1:G:11:ILE:O	1:G:15:VAL:HG13	2.03	0.58
1:G:50:SER:O	1:G:53:HIS:HB2	2.04	0.58
1:H:55:ILE:HD13	1:H:55:ILE:N	2.18	0.58
1:A:22:ILE:HD12	1:A:26:HIS:NE2	2.19	0.58
1:E:147:LEU:HD22	1:E:153:VAL:HA	1.85	0.58
1:F:19:GLU:HA	1:F:22:ILE:HG12	1.86	0.58
1:D:261:THR:O	1:H:94:HIS:CD2	2.57	0.58
1:A:286:ALA:HB3	1:A:287:PRO:CD	2.30	0.58
1:F:36:ASN:O	1:F:40:VAL:HG23	2.04	0.58
1:B:199:LYS:HG2	1:B:202:VAL:HG13	1.85	0.57
1:D:36:ASN:OD1	1:D:39:ARG:NH2	2.37	0.57
1:H:236:GLY:HA3	1:H:240:VAL:HG22	1.85	0.57
1:H:342:GLN:HG2	1:H:353:PRO:HD3	1.85	0.57
1:G:193:ALA:O	1:G:197:GLU:HG2	2.03	0.57
1:D:192:ILE:HD13	1:D:223:GLY:HA3	1.87	0.57
1:F:218:GLU:HB3	1:F:219:PRO:HD2	1.85	0.57
1:B:214:ILE:HG21	1:B:321:ASP:HA	1.86	0.57
1:G:258:TYR:CE1	1:G:266:GLY:CA	2.87	0.57
1:B:214:ILE:HD11	1:B:319:ARG:HB2	1.85	0.57
1:C:299:PHE:HE2	1:C:407:ILE:CD1	2.18	0.57
1:F:212:GLU:O	1:F:213:PHE:HB2	2.04	0.57
1:A:96:ILE:O	1:A:100:LEU:HG	2.04	0.57
1:E:36:ASN:O	1:E:40:VAL:HG23	2.03	0.57
1:G:272:SER:HB2	2:G:621:HOH:O	2.05	0.57
1:B:214:ILE:HG12	1:B:320:THR:C	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:THR:HG22	1:D:27:LYS:HE2	1.85	0.57
1:F:180:ARG:HD2	1:F:180:ARG:O	2.05	0.57
1:H:70:LEU:HD22	1:H:279:MSE:HE3	1.86	0.57
1:B:324:GLN:NE2	1:B:325:SER:H	2.03	0.57
1:F:365:VAL:HG12	1:F:385:PRO:HA	1.87	0.57
1:A:8:GLY:HA2	1:A:11:ILE:HD12	1.87	0.57
1:A:259:ARG:NH1	1:B:259:ARG:NH1	2.53	0.57
1:F:11:ILE:CD1	1:F:411:ILE:HG21	2.34	0.56
1:H:84:LEU:HD23	1:H:246:ILE:HD12	1.85	0.56
1:A:209:CYS:O	1:A:210:TYR:HB2	2.05	0.56
1:C:22:ILE:O	1:C:25:VAL:HG23	2.05	0.56
1:G:199:LYS:CG	1:G:202:VAL:HG13	2.35	0.56
1:C:43:SER:O	1:C:47:HIS:HD2	1.88	0.56
1:E:124:ILE:HA	1:G:263:PRO:HB2	1.86	0.56
1:F:95:ALA:HB1	1:F:228:ALA:HB1	1.87	0.56
1:G:36:ASN:HB2	1:G:287:PRO:HB3	1.87	0.56
1:G:124:ILE:O	1:G:134:SER:HB2	2.06	0.56
1:A:39:ARG:HE	1:A:77:VAL:HG13	1.70	0.56
1:B:288:HIS:HE1	1:C:288:HIS:HE1	1.53	0.56
1:H:144:ALA:O	1:H:146:PRO:HD3	2.06	0.56
1:H:209:CYS:O	1:H:210:TYR:CB	2.53	0.56
1:A:1:MSE:HB3	1:A:404:LYS:HZ2	1.70	0.56
1:B:103:ILE:HD12	1:B:168:MSE:CE	2.34	0.56
1:E:218:GLU:O	1:E:221:HIS:HB2	2.05	0.56
1:G:103:ILE:CD1	1:G:226:LEU:HD22	2.36	0.56
1:G:302:ALA:HB2	1:G:315:TRP:CB	2.36	0.56
1:E:355:ALA:HB2	1:E:386:ILE:CD1	2.36	0.56
1:H:210:TYR:O	1:H:321:ASP:HB2	2.05	0.56
1:E:340:ALA:CB	1:E:410:ALA:HA	2.31	0.56
1:F:397:GLY:HA3	1:F:403:VAL:CG2	2.36	0.56
1:A:103:ILE:HD11	1:A:226:LEU:CD2	2.36	0.56
1:B:312:SER:O	1:B:324:GLN:NE2	2.39	0.56
1:D:44:PHE:CE2	1:D:49:ILE:HD12	2.40	0.56
1:A:68:ASP:O	1:A:71:GLU:HB2	2.07	0.55
1:C:357:TYR:HB2	1:H:199:LYS:HD3	1.87	0.55
1:E:236:GLY:HA3	1:E:240:VAL:HG22	1.88	0.55
1:H:23:THR:O	1:H:27:LYS:HG2	2.07	0.55
1:H:152:LEU:HG	1:H:153:VAL:N	2.22	0.55
1:B:104:LEU:HD13	1:B:135:PHE:CE2	2.41	0.55
1:G:310:ASN:HB3	1:G:327:GLN:HE21	1.71	0.55
1:A:49:ILE:HD13	1:A:49:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:THR:HG22	1:D:149:GLU:N	2.22	0.55
1:E:80:ALA:CB	1:E:247:VAL:HG22	2.35	0.55
1:B:86:ARG:HH12	1:B:267:ALA:HA	1.69	0.55
1:E:114:THR:CG2	1:E:171:ILE:HG23	2.36	0.55
1:A:61:GLY:O	1:A:269:ALA:HA	2.06	0.55
1:E:358:MSE:HG2	1:E:361:TYR:CD2	2.41	0.55
1:F:249:LYS:O	1:F:253:VAL:HG23	2.07	0.55
1:H:89:ILE:O	1:H:243:GLY:HA2	2.06	0.55
1:H:123:GLU:HG3	1:H:128:ARG:HD3	1.89	0.55
1:A:67:ARG:NE	1:A:86:ARG:NH2	2.55	0.55
1:D:184:THR:H	1:D:187:GLN:NE2	2.05	0.55
1:E:199:LYS:CG	1:E:202:VAL:HG13	2.35	0.55
1:E:358:MSE:SE	1:E:365:VAL:HG21	2.57	0.55
1:H:354:TYR:N	1:H:354:TYR:CD2	2.73	0.55
1:A:365:VAL:HG12	1:A:385:PRO:HA	1.89	0.55
1:D:80:ALA:CB	1:D:247:VAL:HG22	2.37	0.55
1:D:295:LYS:O	1:D:298:ILE:HG22	2.07	0.55
1:E:355:ALA:HB1	1:E:364:ASP:HB3	1.89	0.55
1:C:232:ILE:O	1:C:376:ALA:HB1	2.07	0.55
1:C:265:ILE:O	1:C:268:GLU:HG2	2.07	0.55
1:D:11:ILE:HD11	1:D:411:ILE:HG21	1.88	0.55
1:D:340:ALA:HB2	1:D:413:GLU:OE1	2.07	0.55
1:G:128:ARG:HG3	1:G:129:GLY:N	2.21	0.55
1:G:345:SER:O	1:G:349:SER:HB3	2.07	0.55
1:H:199:LYS:O	1:H:199:LYS:HG3	2.07	0.55
1:E:225:ASP:HB3	1:E:252:TYR:CE2	2.42	0.54
1:G:79:GLY:O	1:G:220:CYS:HB3	2.07	0.54
1:G:168:MSE:HG3	1:G:203:VAL:HG23	1.89	0.54
1:E:18:VAL:HG22	1:E:306:LYS:CD	2.37	0.54
1:F:28:ARG:HH21	1:F:28:ARG:HG3	1.72	0.54
1:D:199:LYS:O	1:D:199:LYS:HG3	2.06	0.54
1:E:12:ALA:N	1:E:13:PRO:CD	2.69	0.54
1:E:343:TYR:O	1:E:343:TYR:CD2	2.61	0.54
1:F:113:ILE:HD11	1:F:171:ILE:HD11	1.90	0.54
1:F:371:THR:CG2	1:F:373:ILE:O	2.54	0.54
1:G:335:ILE:HG22	1:G:339:GLN:OE1	2.07	0.54
1:B:102:GLY:O	1:B:255:ALA:HB1	2.07	0.54
1:F:199:LYS:O	1:F:202:VAL:HG22	2.06	0.54
1:F:367:MSE:HG2	1:F:383:ASP:HB2	1.89	0.54
1:H:47:HIS:CD2	1:H:73:VAL:HG23	2.41	0.54
1:A:1:MSE:SE	1:A:404:LYS:HD3	2.57	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HD12	1:B:270:GLY:N	2.22	0.54
1:D:82:ALA:O	1:D:247:VAL:HG23	2.07	0.54
1:E:91:SER:HB2	1:G:60:TYR:HE1	1.72	0.54
1:E:231:LEU:O	1:E:236:GLY:HA3	2.06	0.54
1:F:93:THR:HG21	1:F:120:THR:HG21	1.89	0.54
1:D:276:LEU:HB2	2:D:618:HOH:O	2.06	0.54
1:F:358:MSE:SE	1:F:365:VAL:HG21	2.58	0.54
1:H:40:VAL:HA	1:H:77:VAL:HG21	1.89	0.54
1:H:210:TYR:CD2	1:H:323:ILE:HD11	2.42	0.54
1:A:229:GLY:HA3	1:A:245:TYR:CE1	2.42	0.54
1:C:401:SER:O	1:C:402:HIS:C	2.46	0.54
1:G:111:LEU:HD12	1:G:143:ASN:O	2.08	0.54
1:G:173:ARG:NH1	1:G:219:PRO:HD3	2.22	0.54
1:A:52:SER:O	1:A:55:ILE:HG12	2.07	0.54
1:D:239:ILE:HG22	1:D:278:GLU:HB2	1.89	0.54
1:F:357:TYR:HB2	1:G:199:LYS:HD3	1.89	0.54
1:H:293:ALA:HB3	1:H:322:LEU:HD13	1.89	0.54
1:H:371:THR:HG22	1:H:379:GLU:HB2	1.88	0.54
1:C:132:VAL:HB	1:F:258:TYR:CE2	2.43	0.54
1:C:192:ILE:HD13	1:C:193:ALA:N	2.23	0.54
1:D:9:GLU:OE2	1:D:11:ILE:HG22	2.07	0.54
1:A:241:LYS:O	1:A:242:THR:HB	2.07	0.53
1:C:105:ARG:HB3	1:C:106:PRO:HD2	1.90	0.53
1:C:382:ALA:HA	1:C:393:TYR:O	2.08	0.53
1:D:132:VAL:HG23	1:H:263:PRO:HB3	1.89	0.53
1:H:295:LYS:O	1:H:298:ILE:HB	2.09	0.53
1:D:25:VAL:HG12	1:D:28:ARG:HH11	1.73	0.53
1:E:75:ALA:HA	1:E:247:VAL:HG21	1.90	0.53
1:E:98:THR:HB	1:E:246:ILE:HD11	1.90	0.53
1:E:122:GLU:HB3	1:E:128:ARG:HB2	1.90	0.53
1:A:329:ASP:HA	1:A:389:PRO:O	2.08	0.53
1:B:174:SER:CB	1:B:321:ASP:OD2	2.55	0.53
1:C:18:VAL:HG21	1:C:303:PHE:HD1	1.72	0.53
1:A:358:MSE:HG2	1:A:365:VAL:HG21	1.89	0.53
1:C:286:ALA:HB3	1:C:287:PRO:HD3	1.89	0.53
1:E:226:LEU:HD21	1:E:246:ILE:CG2	2.39	0.53
1:A:64:ASP:OD2	1:A:272:SER:HB3	2.08	0.53
1:C:378:ILE:O	1:C:378:ILE:HG13	2.07	0.53
1:E:18:VAL:HG22	1:E:306:LYS:HD2	1.90	0.53
1:E:214:ILE:HD13	1:E:294:LEU:CD1	2.38	0.53
1:G:203:VAL:HG23	1:G:203:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:THR:CG2	1:D:171:ILE:HG23	2.37	0.53
1:H:49:ILE:HD13	1:H:49:ILE:O	2.08	0.53
1:A:7:ASN:O	1:A:9:GLU:N	2.39	0.53
1:A:229:GLY:HA3	1:A:245:TYR:HE1	1.74	0.53
1:B:288:HIS:O	1:B:292:GLN:HG2	2.08	0.53
1:C:52:SER:O	1:C:55:ILE:HG12	2.09	0.53
1:C:62:TYR:HE1	1:C:269:ALA:HB2	1.74	0.53
1:E:229:GLY:HA3	1:E:245:TYR:CE1	2.44	0.53
1:F:214:ILE:HD11	1:F:319:ARG:HB3	1.91	0.53
1:F:389:PRO:HA	2:F:573:HOH:O	2.08	0.53
1:H:121:LEU:HD23	1:H:124:ILE:HD12	1.91	0.53
1:C:49:ILE:O	1:C:49:ILE:HD13	2.09	0.53
1:E:171:ILE:HB	1:E:206:VAL:HG22	1.90	0.53
1:E:331:LYS:HB2	1:E:390:TYR:CE1	2.44	0.53
1:G:299:PHE:CE2	1:G:404:LYS:HA	2.44	0.53
1:A:103:ILE:HD11	1:A:226:LEU:HD22	1.91	0.53
1:C:340:ALA:HB2	1:C:413:GLU:CD	2.29	0.53
1:F:122:GLU:HG2	1:F:128:ARG:CB	2.39	0.53
1:A:84:LEU:N	1:A:246:ILE:O	2.42	0.52
1:F:371:THR:HG22	1:F:373:ILE:O	2.09	0.52
1:G:123:GLU:HG2	1:G:128:ARG:HG2	1.91	0.52
1:B:226:LEU:HD12	1:B:248:GLY:HA3	1.91	0.52
1:B:229:GLY:HA3	1:B:245:TYR:CE1	2.44	0.52
1:D:75:ALA:HA	1:D:247:VAL:HG21	1.91	0.52
1:H:414:LEU:HD22	1:H:414:LEU:H	1.75	0.52
1:C:415:ILE:HG23	2:C:540:HOH:O	2.09	0.52
1:E:218:GLU:HB3	1:E:219:PRO:HD2	1.91	0.52
1:F:128:ARG:HG3	1:F:129:GLY:N	2.24	0.52
1:F:212:GLU:OE2	1:F:245:TYR:OH	2.25	0.52
1:G:276:LEU:O	1:G:277:GLN:C	2.46	0.52
1:B:257:ALA:HB1	1:B:267:ALA:HB2	1.91	0.52
1:B:410:ALA:O	1:B:414:LEU:HG	2.09	0.52
1:C:132:VAL:HB	1:F:258:TYR:CD2	2.44	0.52
1:C:365:VAL:HG12	1:C:385:PRO:HA	1.92	0.52
1:E:188:ILE:O	1:E:192:ILE:HG23	2.10	0.52
1:B:136:LYS:O	1:B:136:LYS:HE2	2.10	0.52
1:C:263:PRO:HB2	1:F:124:ILE:HA	1.91	0.52
1:F:44:PHE:CA	1:F:49:ILE:HD12	2.40	0.52
1:H:304:LEU:HD21	1:H:411:ILE:HD11	1.91	0.52
1:H:308:GLY:O	1:H:309:MSE:HG3	2.10	0.52
1:B:340:ALA:CB	1:B:410:ALA:HA	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:ALA:O	1:B:383:ASP:HB3	2.09	0.52
1:C:226:LEU:CD2	1:C:246:ILE:HG23	2.33	0.52
1:E:414:LEU:C	1:E:415:ILE:CG1	2.76	0.52
1:G:258:TYR:CD1	1:G:266:GLY:CA	2.91	0.52
1:H:340:ALA:HB1	1:H:410:ALA:HA	1.90	0.52
1:A:78:PHE:HB3	1:A:227:MSE:HE2	1.91	0.52
1:B:71:GLU:HB3	1:B:83:GLY:O	2.10	0.52
1:C:234:ASN:HB2	1:C:235:PRO:HD3	1.90	0.52
1:D:80:ALA:HB3	1:D:247:VAL:CG2	2.39	0.52
1:G:219:PRO:O	1:G:222:VAL:HG22	2.09	0.52
1:H:301:ALA:CA	1:H:311:THR:HG21	2.37	0.52
1:H:327:GLN:HG2	1:H:391:VAL:CG2	2.24	0.52
1:E:303:PHE:CD1	1:E:407:ILE:HD11	2.41	0.52
1:G:302:ALA:HB2	1:G:315:TRP:HB3	1.91	0.52
1:E:135:PHE:HB3	1:E:140:ILE:O	2.10	0.52
1:E:250:GLU:O	1:E:254:GLU:HG2	2.09	0.52
1:E:259:ARG:NH1	1:G:259:ARG:HH12	2.07	0.52
1:E:347:ILE:O	1:E:347:ILE:HG13	2.07	0.52
1:B:39:ARG:HH11	1:B:213:PHE:HE1	1.58	0.52
1:B:52:SER:O	1:B:55:ILE:HG12	2.10	0.52
1:C:211:GLY:O	1:C:214:ILE:HG22	2.08	0.52
1:D:49:ILE:HD13	1:D:49:ILE:O	2.09	0.52
1:E:117:PRO:HB2	1:E:121:LEU:HD12	1.91	0.52
1:A:358:MSE:HG2	1:A:365:VAL:HG22	1.91	0.51
1:D:88:GLN:HE21	1:H:90:ILE:HG22	1.75	0.51
1:E:71:GLU:HG2	1:E:85:VAL:H	1.75	0.51
1:E:238:GLY:HA2	1:E:378:ILE:HG21	1.91	0.51
1:E:358:MSE:HE2	1:E:359:PRO:HD2	1.92	0.51
1:H:350:HIS:ND1	1:H:350:HIS:N	2.58	0.51
1:B:226:LEU:HD21	1:B:256:CYS:SG	2.50	0.51
1:E:166:THR:HG22	1:E:202:VAL:HG12	1.92	0.51
1:F:128:ARG:HG3	1:F:128:ARG:HH11	1.74	0.51
1:G:340:ALA:CB	1:G:410:ALA:HA	2.40	0.51
1:H:84:LEU:O	1:H:246:ILE:N	2.40	0.51
1:C:40:VAL:HG11	1:C:284:PHE:HA	1.91	0.51
1:C:312:SER:HA	1:C:313:PRO:C	2.31	0.51
1:F:48:LYS:NZ	1:H:130:LYS:HA	2.25	0.51
1:F:345:SER:CB	1:F:370:GLY:HA3	2.41	0.51
1:A:183:PHE:O	1:A:320:THR:HG21	2.11	0.51
1:A:262:SER:HB3	1:A:265:ILE:HD12	1.92	0.51
1:A:347:ILE:HD11	1:A:371:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:TYR:O	1:D:255:ALA:HB3	2.10	0.51
1:D:67:ARG:HD2	1:D:86:ARG:CZ	2.40	0.51
1:E:166:THR:O	1:E:202:VAL:HG12	2.09	0.51
1:D:328:PHE:HE2	1:D:392:ALA:HB3	1.75	0.51
1:G:345:SER:CB	1:G:370:GLY:HA3	2.41	0.51
1:G:379:GLU:HG2	1:G:398:LEU:HD11	1.92	0.51
1:B:70:LEU:HD13	1:B:280:TYR:CE1	2.46	0.51
1:C:105:ARG:HB3	1:C:106:PRO:CD	2.41	0.51
1:C:328:PHE:HE2	1:C:392:ALA:HB3	1.75	0.51
1:A:229:GLY:N	1:A:245:TYR:CE1	2.79	0.51
1:A:229:GLY:CA	1:A:245:TYR:CE1	2.93	0.51
1:B:14:ILE:O	1:B:18:VAL:HG23	2.11	0.51
1:B:414:LEU:C	1:B:414:LEU:CD1	2.79	0.51
1:C:212:GLU:OE1	1:C:234:ASN:HB2	2.10	0.51
1:E:303:PHE:O	1:E:307:LEU:HD12	2.11	0.51
1:F:103:ILE:HG21	1:F:203:VAL:HG21	1.91	0.51
1:B:168:MSE:HG3	1:B:203:VAL:CG2	2.39	0.51
1:B:214:ILE:HD11	1:B:319:ARG:CB	2.41	0.51
1:D:80:ALA:HB3	1:D:247:VAL:HG22	1.92	0.51
1:D:192:ILE:HG13	1:D:193:ALA:H	1.75	0.51
1:F:118:TYR:HE2	1:F:120:THR:HB	1.76	0.51
1:F:211:GLY:O	1:F:214:ILE:HG23	2.10	0.51
1:B:327:GLN:HG2	1:B:391:VAL:HG22	1.93	0.50
1:C:342:GLN:HB2	1:C:368:ALA:HB1	1.93	0.50
1:D:148:THR:C	1:D:150:GLY:H	2.15	0.50
1:H:105:ARG:HB3	1:H:106:PRO:HD2	1.93	0.50
1:H:192:ILE:HD12	1:H:193:ALA:N	2.26	0.50
1:H:288:HIS:CE1	1:H:292:GLN:NE2	2.79	0.50
1:H:386:ILE:HG22	1:H:386:ILE:O	2.10	0.50
1:A:119:ASP:O	1:A:122:GLU:HB2	2.10	0.50
1:A:214:ILE:HG12	1:A:320:THR:O	2.11	0.50
1:A:338:CYS:O	1:A:368:ALA:HB2	2.11	0.50
1:B:49:ILE:CD1	1:C:346:PRO:O	2.48	0.50
1:B:82:ALA:HB2	1:B:250:GLU:HA	1.93	0.50
1:C:209:CYS:O	1:C:210:TYR:CB	2.54	0.50
1:D:28:ARG:HA	1:D:31:GLU:HB2	1.93	0.50
1:D:166:THR:HG22	1:D:202:VAL:CG1	2.40	0.50
1:D:272:SER:HB2	2:D:599:HOH:O	2.12	0.50
1:G:15:VAL:O	1:G:19:GLU:HG3	2.11	0.50
1:H:245:TYR:O	1:H:246:ILE:HG13	2.12	0.50
1:A:85:VAL:HG23	1:A:231:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLN:O	1:A:191:MSE:HB2	2.11	0.50
1:B:12:ALA:O	1:B:15:VAL:HG22	2.11	0.50
1:B:254:GLU:O	1:B:257:ALA:HB3	2.11	0.50
1:C:214:ILE:HD11	1:C:294:LEU:CD1	2.41	0.50
1:D:275:SER:O	1:D:279:MSE:HE2	2.12	0.50
1:E:167:LYS:O	1:E:167:LYS:HG3	2.11	0.50
1:E:184:THR:N	1:E:187:GLN:HE21	1.88	0.50
1:E:239:ILE:CG2	1:E:278:GLU:HB2	2.41	0.50
1:E:259:ARG:CZ	1:G:259:ARG:CZ	2.89	0.50
1:C:167:LYS:O	1:C:203:VAL:HG12	2.11	0.50
1:D:71:GLU:HA	1:D:85:VAL:HG12	1.94	0.50
1:F:154:ASP:O	1:F:158:VAL:HG23	2.12	0.50
1:G:55:ILE:HD13	1:G:55:ILE:N	2.26	0.50
1:G:184:THR:HG23	1:G:187:GLN:NE2	2.26	0.50
1:G:199:LYS:C	1:G:201:ASP:H	2.15	0.50
1:H:378:ILE:HG13	1:H:378:ILE:O	2.12	0.50
1:C:49:ILE:N	1:C:49:ILE:CD1	2.74	0.50
1:C:189:LYS:O	1:C:192:ILE:HD13	2.12	0.50
1:E:407:ILE:O	1:E:411:ILE:HD12	2.11	0.50
1:F:54:PHE:CD2	1:F:277:GLN:HG3	2.46	0.50
1:A:214:ILE:HD12	1:A:294:LEU:HD13	1.94	0.50
1:D:96:ILE:O	1:D:100:LEU:HG	2.10	0.50
1:D:281:GLN:O	1:D:285:LEU:HG	2.11	0.50
1:F:86:ARG:HB2	1:F:88:GLN:OE1	2.11	0.50
1:H:257:ALA:CB	1:H:267:ALA:HB2	2.39	0.50
1:A:199:LYS:C	1:A:201:ASP:H	2.14	0.50
1:E:296:GLY:O	1:E:299:PHE:HB3	2.11	0.50
1:G:27:LYS:O	1:G:31:GLU:HG3	2.11	0.50
1:G:40:VAL:HG12	1:G:44:PHE:CE1	2.46	0.50
1:G:232:ILE:CG2	1:G:242:THR:HA	2.42	0.50
1:A:70:LEU:HD21	1:A:279:MSE:HB3	1.93	0.50
1:A:110:LEU:CD1	1:A:168:MSE:HG2	2.42	0.50
1:F:71:GLU:OE2	1:F:84:LEU:HD12	2.12	0.50
1:F:231:LEU:HD12	1:F:244:GLY:N	2.27	0.50
1:E:101:PHE:HE2	1:E:124:ILE:HG23	1.76	0.50
1:E:114:THR:HG21	1:E:172:GLN:H	1.77	0.50
1:F:19:GLU:HA	1:F:22:ILE:CG1	2.42	0.50
1:G:250:GLU:O	1:G:254:GLU:HG2	2.12	0.50
1:C:232:ILE:HG13	1:C:376:ALA:HA	1.94	0.49
1:C:411:ILE:HG23	1:C:415:ILE:HD12	1.93	0.49
1:E:163:HIS:HD2	1:E:165:ASN:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:203:VAL:HG12	1:E:252:TYR:CZ	2.47	0.49
1:E:337:PHE:CE1	1:E:394:VAL:HG21	2.47	0.49
1:A:67:ARG:NH1	1:A:270:GLY:O	2.45	0.49
1:A:250:GLU:O	1:A:254:GLU:HG2	2.13	0.49
1:C:145:VAL:HG21	1:C:158:VAL:HA	1.94	0.49
1:E:159:ALA:HB2	1:E:194:PHE:CZ	2.39	0.49
1:C:342:GLN:NE2	1:C:348:ASN:O	2.46	0.49
1:D:85:VAL:HG23	1:D:231:LEU:HD11	1.94	0.49
1:G:70:LEU:O	1:G:70:LEU:HG	2.12	0.49
1:A:78:PHE:HB3	1:A:227:MSE:CE	2.42	0.49
1:A:167:LYS:O	1:A:203:VAL:HG22	2.12	0.49
1:B:121:LEU:CD2	1:B:124:ILE:HD12	2.40	0.49
1:C:8:GLY:HA2	1:C:11:ILE:CG2	2.39	0.49
1:C:214:ILE:HG21	1:C:320:THR:O	2.12	0.49
1:E:91:SER:HB2	1:G:60:TYR:CE1	2.48	0.49
1:C:100:LEU:HD11	1:C:121:LEU:HD21	1.95	0.49
1:C:214:ILE:HG21	1:C:320:THR:C	2.32	0.49
1:C:249:LYS:HB2	1:C:252:TYR:CD2	2.48	0.49
1:D:128:ARG:CG	1:D:128:ARG:NH1	2.73	0.49
1:G:180:ARG:HD2	1:G:180:ARG:O	2.13	0.49
1:H:212:GLU:HB2	1:H:234:ASN:HB2	1.93	0.49
1:B:103:ILE:HD11	1:B:226:LEU:CD2	2.43	0.49
1:C:299:PHE:CE2	1:C:407:ILE:HD11	2.36	0.49
1:E:156:GLU:CD	1:E:156:GLU:N	2.66	0.49
1:E:263:PRO:HB2	1:G:124:ILE:HA	1.95	0.49
1:E:263:PRO:HG2	1:G:124:ILE:HA	1.94	0.49
1:F:44:PHE:HA	1:F:49:ILE:HD12	1.94	0.49
1:G:258:TYR:CE1	1:G:266:GLY:HA3	2.47	0.49
1:A:218:GLU:O	1:A:221:HIS:HB2	2.12	0.49
1:B:358:MSE:HE2	1:B:359:PRO:HD2	1.94	0.49
1:D:251:GLN:HG2	1:D:252:TYR:N	2.26	0.49
1:E:265:ILE:HD11	1:G:93:THR:CG2	2.42	0.49
1:H:231:LEU:O	1:H:240:VAL:CG2	2.61	0.49
1:H:379:GLU:HG2	1:H:398:LEU:HD21	1.93	0.49
1:B:234:ASN:C	1:B:236:GLY:H	2.16	0.49
1:B:347:ILE:O	1:B:348:ASN:HB2	2.12	0.49
1:C:93:THR:HG21	1:C:120:THR:HG21	1.95	0.49
1:D:71:GLU:HG2	1:D:85:VAL:H	1.77	0.49
1:F:38:PHE:HD1	1:F:38:PHE:O	1.95	0.49
1:G:25:VAL:HB	1:G:298:ILE:HD12	1.93	0.49
1:A:374:GLN:OE1	1:B:62:TYR:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LYS:O	1:C:253:VAL:HG23	2.12	0.49
1:D:358:MSE:HG2	1:D:361:TYR:HE2	1.77	0.49
1:F:212:GLU:OE1	1:F:234:ASN:HB2	2.13	0.49
1:F:345:SER:HB3	1:F:346:PRO:HD2	1.95	0.49
1:F:411:ILE:HA	1:F:414:LEU:HD23	1.95	0.49
1:G:239:ILE:HD13	1:G:281:GLN:HG2	1.93	0.49
1:H:18:VAL:HG21	1:H:303:PHE:HD2	1.77	0.49
1:A:192:ILE:O	1:A:196:LYS:HG2	2.13	0.49
1:E:82:ALA:HB3	1:E:253:VAL:HG21	1.94	0.49
1:G:344:ALA:HB1	1:G:406:ALA:HA	1.95	0.49
1:H:12:ALA:C	1:H:14:ILE:H	2.16	0.49
1:H:275:SER:O	1:H:276:LEU:C	2.51	0.49
1:B:44:PHE:CB	1:B:49:ILE:HD12	2.44	0.48
1:F:67:ARG:HD2	1:F:86:ARG:CZ	2.42	0.48
1:G:40:VAL:HG11	1:G:284:PHE:HA	1.94	0.48
1:G:52:SER:HA	1:G:55:ILE:HD11	1.93	0.48
1:A:55:ILE:HD12	1:C:55:ILE:CG2	2.42	0.48
1:F:15:VAL:HG13	1:F:303:PHE:CE2	2.48	0.48
1:H:345:SER:CB	1:H:370:GLY:HA3	2.43	0.48
1:A:1:MSE:HE2	1:A:3:ASP:OD1	2.12	0.48
1:A:111:LEU:HB3	1:A:169:ILE:HD13	1.95	0.48
1:A:345:SER:HB3	1:A:346:PRO:HD2	1.96	0.48
1:C:199:LYS:HE2	1:C:201:ASP:HB3	1.93	0.48
1:F:93:THR:HG21	1:F:120:THR:CG2	2.43	0.48
1:D:11:ILE:HD11	1:D:411:ILE:CG2	2.43	0.48
1:D:71:GLU:OE2	1:D:84:LEU:HD12	2.13	0.48
1:G:25:VAL:O	1:G:28:ARG:HG2	2.13	0.48
1:D:358:MSE:HG2	1:D:361:TYR:CE2	2.49	0.48
1:E:192:ILE:CG1	1:E:193:ALA:N	2.75	0.48
1:E:259:ARG:HD2	1:E:259:ARG:O	2.14	0.48
2:E:600:HOH:O	1:G:265:ILE:HD13	2.13	0.48
1:F:118:TYR:CE2	1:F:120:THR:HB	2.48	0.48
1:G:74:TYR:O	1:G:78:PHE:HB2	2.13	0.48
1:A:328:PHE:O	1:A:329:ASP:HB2	2.12	0.48
1:G:227:MSE:HG3	1:G:247:VAL:HG12	1.94	0.48
1:H:118:TYR:HE2	1:H:120:THR:HB	1.79	0.48
1:B:212:GLU:HA	1:B:218:GLU:OE1	2.14	0.48
1:C:14:ILE:O	1:C:18:VAL:HG23	2.14	0.48
1:C:335:ILE:HG23	1:C:366:ILE:HD13	1.94	0.48
1:C:358:MSE:HA	1:C:358:MSE:CE	2.41	0.48
1:C:410:ALA:O	1:C:414:LEU:HG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:298:ILE:HG23	1:E:315:TRP:HB2	1.95	0.48
1:F:376:ALA:O	1:F:379:GLU:HG3	2.14	0.48
1:G:9:GLU:HB3	1:G:11:ILE:HG22	1.96	0.48
1:G:40:VAL:HG21	1:G:287:PRO:HG2	1.96	0.48
1:G:188:ILE:O	1:G:192:ILE:HG23	2.12	0.48
1:H:203:VAL:O	1:H:203:VAL:CG2	2.61	0.48
1:A:234:ASN:C	1:A:236:GLY:H	2.17	0.48
1:C:226:LEU:HD11	1:C:256:CYS:SG	2.53	0.48
1:E:85:VAL:O	1:E:85:VAL:HG13	2.12	0.48
1:E:225:ASP:HA	1:E:249:LYS:HG3	1.96	0.48
1:G:26:HIS:CD2	1:G:298:ILE:HD13	2.49	0.48
1:A:49:ILE:HA	1:A:53:HIS:CE1	2.49	0.48
1:B:171:ILE:HB	1:B:206:VAL:HG13	1.96	0.48
1:B:312:SER:HA	1:B:313:PRO:C	2.33	0.48
1:C:49:ILE:HD13	1:C:49:ILE:N	2.28	0.48
1:C:208:ASN:OD1	1:C:208:ASN:O	2.31	0.48
1:E:328:PHE:HB3	1:E:333:ARG:CG	2.44	0.48
1:F:115:GLY:O	1:F:117:PRO:HD3	2.14	0.48
1:F:189:LYS:HB2	1:F:222:VAL:HB	1.96	0.48
1:F:300:THR:O	1:F:304:LEU:HB2	2.14	0.48
1:H:339:GLN:HG2	1:H:353:PRO:O	2.14	0.48
1:C:212:GLU:O	1:C:213:PHE:HB2	2.13	0.48
1:E:33:ILE:HG12	2:E:511:HOH:O	2.14	0.48
1:G:52:SER:HA	1:G:55:ILE:CD1	2.43	0.48
1:B:103:ILE:CD1	1:B:226:LEU:HD22	2.43	0.47
1:C:236:GLY:O	1:C:239:ILE:HG22	2.14	0.47
1:D:114:THR:HG23	1:D:171:ILE:HA	1.96	0.47
1:F:342:GLN:NE2	1:F:348:ASN:O	2.47	0.47
1:H:67:ARG:NE	1:H:86:ARG:NH2	2.62	0.47
1:A:103:ILE:CD1	1:A:226:LEU:HD22	2.44	0.47
1:A:239:ILE:HG22	1:A:278:GLU:HB2	1.96	0.47
1:A:371:THR:CG2	1:A:379:GLU:CD	2.76	0.47
1:B:135:PHE:HD1	1:B:135:PHE:H	1.62	0.47
1:D:241:LYS:O	1:D:242:THR:HB	2.14	0.47
1:F:358:MSE:HE2	1:F:365:VAL:HG11	1.95	0.47
1:G:28:ARG:HA	1:G:31:GLU:HG3	1.96	0.47
1:A:67:ARG:NE	1:A:86:ARG:HH21	2.12	0.47
1:A:378:ILE:HG13	1:A:378:ILE:O	2.15	0.47
1:D:88:GLN:NE2	1:H:90:ILE:HG22	2.29	0.47
1:E:90:ILE:HG13	1:E:94:HIS:HB2	1.96	0.47
1:E:380:LEU:HD13	1:E:403:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:GLU:CD	1:F:86:ARG:HH21	2.17	0.47
1:A:1:MSE:HG2	1:A:404:LYS:NZ	2.29	0.47
1:C:121:LEU:HA	1:C:124:ILE:HD12	1.95	0.47
1:F:30:ASP:O	1:F:31:GLU:C	2.53	0.47
1:G:28:ARG:HG3	1:G:29:ALA:N	2.29	0.47
1:B:103:ILE:HD12	1:B:168:MSE:HE3	1.96	0.47
1:D:292:GLN:HE22	1:D:295:LYS:NZ	2.12	0.47
1:E:27:LYS:HD2	1:E:27:LYS:N	2.29	0.47
1:E:374:GLN:HB3	1:G:58:THR:O	2.14	0.47
1:F:28:ARG:HG3	1:F:28:ARG:NH2	2.29	0.47
1:G:36:ASN:O	1:G:37:GLN:C	2.52	0.47
1:G:49:ILE:HA	1:G:53:HIS:CE1	2.49	0.47
1:G:199:LYS:O	1:G:201:ASP:N	2.47	0.47
1:G:199:LYS:HD2	1:G:201:ASP:HB3	1.95	0.47
1:H:26:HIS:C	1:H:28:ARG:N	2.68	0.47
1:A:67:ARG:CD	1:A:86:ARG:HH21	2.28	0.47
1:C:166:THR:O	1:C:199:LYS:NZ	2.48	0.47
1:E:101:PHE:CE2	1:E:124:ILE:HG23	2.49	0.47
1:E:172:GLN:HA	1:E:207:ASP:HB3	1.96	0.47
1:F:29:ALA:HB1	1:F:294:LEU:HD23	1.96	0.47
1:A:36:ASN:O	1:A:40:VAL:HG23	2.15	0.47
1:A:50:SER:O	1:A:53:HIS:HB2	2.15	0.47
1:A:78:PHE:CD1	1:A:218:GLU:HG3	2.49	0.47
1:A:218:GLU:HB3	1:A:219:PRO:HD2	1.97	0.47
1:A:347:ILE:HD13	1:A:347:ILE:O	2.15	0.47
1:A:371:THR:HG23	1:A:379:GLU:OE2	2.13	0.47
1:A:371:THR:CG2	1:A:379:GLU:OE2	2.63	0.47
1:B:207:ASP:OD1	1:B:207:ASP:C	2.53	0.47
1:B:288:HIS:CE1	1:C:288:HIS:HE1	2.32	0.47
1:C:15:VAL:O	1:C:19:GLU:HG3	2.15	0.47
1:D:166:THR:HG22	1:D:202:VAL:HG11	1.97	0.47
1:D:239:ILE:CG2	1:D:278:GLU:HB2	2.45	0.47
1:F:214:ILE:HD12	1:F:294:LEU:CD1	2.44	0.47
1:F:309:MSE:HG2	1:F:327:GLN:O	2.14	0.47
1:F:373:ILE:HB	1:F:376:ALA:HB2	1.96	0.47
1:G:214:ILE:HG12	1:G:320:THR:O	2.14	0.47
1:H:64:ASP:OD2	1:H:67:ARG:HB2	2.14	0.47
1:H:234:ASN:HB2	1:H:235:PRO:HD3	1.96	0.47
1:A:127:VAL:O	1:A:127:VAL:HG22	2.14	0.47
1:B:44:PHE:CD2	1:B:49:ILE:CD1	2.98	0.47
1:D:124:ILE:HG12	1:H:262:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:GLY:H	1:D:253:VAL:CG2	2.28	0.47
1:H:71:GLU:HB3	1:H:83:GLY:O	2.15	0.47
1:H:334:MSE:HE3	1:H:392:ALA:HB2	1.96	0.47
1:A:210:TYR:CD2	1:A:323:ILE:HD11	2.49	0.47
1:D:231:LEU:HA	1:D:235:PRO:HG2	1.97	0.47
1:H:28:ARG:O	1:H:31:GLU:HB2	2.15	0.47
1:H:50:SER:O	1:H:53:HIS:HB2	2.15	0.47
1:H:67:ARG:NE	1:H:86:ARG:HH22	2.13	0.47
1:A:49:ILE:CD1	1:F:347:ILE:HA	2.44	0.47
1:A:123:GLU:HG3	1:A:128:ARG:HB3	1.97	0.47
1:A:261:THR:OG1	1:A:262:SER:N	2.47	0.47
1:B:28:ARG:O	1:B:31:GLU:HB2	2.15	0.47
1:B:62:TYR:CE1	1:B:269:ALA:HB2	2.49	0.47
1:B:214:ILE:HD11	1:B:319:ARG:O	2.14	0.47
1:D:347:ILE:HG12	1:D:348:ASN:N	2.30	0.47
1:F:167:LYS:O	1:F:203:VAL:HG22	2.15	0.47
1:A:288:HIS:O	1:A:292:GLN:HG2	2.15	0.46
1:B:70:LEU:HD13	1:B:280:TYR:CD1	2.50	0.46
1:G:220:CYS:SG	1:G:227:MSE:HG2	2.55	0.46
1:G:371:THR:HG22	1:G:379:GLU:HB2	1.97	0.46
1:H:122:GLU:OE1	1:H:128:ARG:HB2	2.15	0.46
1:H:407:ILE:O	1:H:411:ILE:HD12	2.15	0.46
1:A:276:LEU:HD23	1:A:279:MSE:CE	2.44	0.46
1:B:214:ILE:HD11	1:B:319:ARG:C	2.36	0.46
1:B:259:ARG:HD2	1:B:259:ARG:O	2.15	0.46
1:E:125:VAL:HG12	1:E:135:PHE:CE2	2.50	0.46
1:E:163:HIS:HB3	2:E:550:HOH:O	2.15	0.46
1:F:88:GLN:O	1:F:90:ILE:HG23	2.16	0.46
1:G:127:VAL:O	1:G:127:VAL:CG2	2.61	0.46
1:H:245:TYR:C	1:H:246:ILE:HG13	2.34	0.46
1:C:218:GLU:HB3	1:C:219:PRO:CD	2.44	0.46
1:D:29:ALA:O	1:D:32:VAL:HG22	2.16	0.46
1:E:225:ASP:HB3	1:E:252:TYR:HE2	1.78	0.46
1:F:111:LEU:HD23	1:F:162:ILE:HG12	1.98	0.46
1:G:125:VAL:O	1:G:135:PHE:HB2	2.16	0.46
1:H:147:LEU:HD22	1:H:153:VAL:HA	1.97	0.46
1:A:97:SER:O	1:A:98:THR:C	2.54	0.46
1:A:199:LYS:O	1:A:202:VAL:CG2	2.52	0.46
1:A:249:LYS:O	1:A:251:GLN:N	2.48	0.46
1:C:226:LEU:HD23	1:C:227:MSE:N	2.30	0.46
1:D:12:ALA:N	1:D:13:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:GLU:O	1:D:21:GLN:HB2	2.16	0.46
1:E:147:LEU:HD13	1:E:151:GLY:O	2.15	0.46
1:F:125:VAL:HG12	1:F:135:PHE:CE2	2.51	0.46
1:G:103:ILE:HG21	1:G:203:VAL:HG21	1.96	0.46
1:B:234:ASN:O	1:B:236:GLY:N	2.48	0.46
1:B:363:ASP:HB2	1:B:387:ARG:NH1	2.30	0.46
1:C:234:ASN:HB2	1:C:235:PRO:CD	2.46	0.46
1:C:310:ASN:HB2	1:C:327:GLN:HB2	1.97	0.46
1:E:303:PHE:HD1	1:E:407:ILE:CD1	2.25	0.46
1:G:78:PHE:O	1:G:220:CYS:HB2	2.15	0.46
1:H:87:PRO:C	1:H:89:ILE:H	2.18	0.46
1:A:352:THR:HG21	1:H:130:LYS:HZ1	1.81	0.46
1:E:67:ARG:O	1:E:71:GLU:HG3	2.16	0.46
1:E:252:TYR:O	1:E:255:ALA:HB3	2.16	0.46
1:G:18:VAL:HG12	1:G:22:ILE:HD13	1.96	0.46
1:H:27:LYS:O	1:H:31:GLU:HG3	2.16	0.46
1:A:205:PHE:HD1	1:A:226:LEU:HB3	1.80	0.46
1:F:286:ALA:HB3	1:F:287:PRO:HD3	1.97	0.46
1:A:114:THR:HA	1:A:147:LEU:HD21	1.97	0.46
1:A:118:TYR:HB3	1:A:172:GLN:HE22	1.80	0.46
1:A:120:THR:HG22	1:A:120:THR:O	2.15	0.46
1:D:82:ALA:O	1:D:253:VAL:HG21	2.16	0.46
1:B:173:ARG:HG3	1:B:188:ILE:HD11	1.97	0.46
1:C:226:LEU:HD21	1:C:246:ILE:CG2	2.35	0.46
1:C:231:LEU:HB3	1:C:240:VAL:HG21	1.98	0.46
1:D:52:SER:O	1:D:55:ILE:HG13	2.16	0.46
1:D:163:HIS:HD2	1:D:165:ASN:H	1.62	0.46
1:E:189:LYS:HA	1:E:192:ILE:CD1	2.46	0.46
1:E:299:PHE:HE2	1:E:407:ILE:HG12	1.81	0.46
1:E:299:PHE:CE2	1:E:407:ILE:HG12	2.51	0.46
1:F:347:ILE:O	1:F:347:ILE:HG13	2.16	0.46
1:G:79:GLY:HA3	1:G:221:HIS:CD2	2.51	0.46
1:A:12:ALA:N	1:A:13:PRO:CD	2.79	0.46
1:B:39:ARG:HE	1:B:77:VAL:CG1	2.22	0.46
1:B:276:LEU:HD23	1:B:279:MSE:HE3	1.97	0.46
1:C:105:ARG:O	1:C:108:ASP:HB2	2.16	0.46
1:D:98:THR:HB	1:D:246:ILE:HD11	1.97	0.46
1:E:71:GLU:HA	1:E:85:VAL:HG12	1.97	0.46
1:A:148:THR:HG22	1:A:149:GLU:N	2.30	0.45
1:B:324:GLN:HE21	1:B:325:SER:N	2.12	0.45
1:C:324:GLN:HE21	1:C:325:SER:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:MSE:HE2	1:E:245:TYR:HE2	1.82	0.45
1:G:205:PHE:HA	1:G:226:LEU:O	2.16	0.45
1:A:192:ILE:HD11	1:A:222:VAL:O	2.16	0.45
1:C:403:VAL:O	1:C:407:ILE:HG23	2.16	0.45
1:D:263:PRO:CB	1:H:124:ILE:HA	2.43	0.45
1:A:234:ASN:O	1:A:236:GLY:N	2.50	0.45
1:B:199:LYS:HE3	1:B:202:VAL:HG13	1.98	0.45
1:B:239:ILE:HG22	1:B:278:GLU:HB2	1.98	0.45
1:D:26:HIS:CD2	1:D:298:ILE:HG21	2.51	0.45
1:D:101:PHE:CE2	1:D:124:ILE:HG23	2.51	0.45
1:E:147:LEU:CD2	1:E:153:VAL:HA	2.46	0.45
1:F:18:VAL:O	1:F:22:ILE:HG12	2.16	0.45
1:H:118:TYR:CE2	1:H:120:THR:HB	2.51	0.45
1:B:18:VAL:HG13	1:B:302:ALA:HB1	1.98	0.45
1:C:229:GLY:HA3	1:C:245:TYR:CE1	2.51	0.45
1:D:199:LYS:HG3	1:D:202:VAL:H	1.81	0.45
1:E:123:GLU:HA	1:E:129:GLY:H	1.81	0.45
1:F:37:GLN:NE2	1:F:284:PHE:CE1	2.84	0.45
1:G:117:PRO:HB2	1:G:121:LEU:HD12	1.98	0.45
1:A:122:GLU:HB3	1:A:128:ARG:HB2	1.98	0.45
1:A:347:ILE:O	1:A:348:ASN:HB2	2.15	0.45
1:B:121:LEU:HD23	1:B:121:LEU:HA	1.82	0.45
1:B:348:ASN:HA	1:B:350:HIS:CE1	2.50	0.45
1:C:168:MSE:HG3	1:C:203:VAL:HG13	1.98	0.45
1:D:23:THR:CG2	1:D:27:LYS:HE2	2.47	0.45
1:H:53:HIS:O	1:H:276:LEU:HD13	2.16	0.45
1:H:74:TYR:O	1:H:78:PHE:HB2	2.15	0.45
1:H:249:LYS:O	1:H:250:GLU:C	2.55	0.45
1:B:214:ILE:O	1:B:214:ILE:HG13	2.10	0.45
1:D:199:LYS:HE2	1:D:201:ASP:HB3	1.98	0.45
1:D:299:PHE:O	1:D:300:THR:C	2.54	0.45
1:E:234:ASN:HB2	1:E:235:PRO:HD3	1.99	0.45
1:E:309:MSE:HG2	1:E:327:GLN:O	2.15	0.45
1:F:112:TYR:CE2	1:F:117:PRO:HB3	2.51	0.45
1:F:119:ASP:O	1:F:122:GLU:CB	2.64	0.45
1:F:189:LYS:O	1:F:192:ILE:HD13	2.17	0.45
1:H:231:LEU:HB2	1:H:243:GLY:C	2.37	0.45
1:A:1:MSE:HG2	1:A:404:LYS:HZ3	1.80	0.45
1:C:57:THR:O	1:C:271:ALA:HB1	2.16	0.45
1:C:340:ALA:HB1	1:C:410:ALA:HA	1.99	0.45
1:D:17:GLU:HB3	1:D:306:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:MSE:HE3	1:F:361:TYR:CE2	2.52	0.45
1:G:214:ILE:HD11	1:G:320:THR:N	2.32	0.45
1:H:103:ILE:HD11	1:H:252:TYR:HB3	1.99	0.45
1:A:296:GLY:CA	1:A:403:VAL:HG11	2.47	0.45
1:B:189:LYS:O	1:B:192:ILE:HD13	2.17	0.45
1:C:124:ILE:HA	1:F:263:PRO:HB2	1.99	0.45
1:D:132:VAL:HG12	1:H:258:TYR:CE2	2.52	0.45
1:D:192:ILE:HG13	1:D:193:ALA:N	2.32	0.45
1:E:11:ILE:CG2	1:E:12:ALA:N	2.79	0.45
1:E:103:ILE:HG21	1:E:203:VAL:HG21	1.98	0.45
1:H:366:ILE:O	1:H:366:ILE:HG23	2.17	0.45
1:H:368:ALA:N	1:H:382:ALA:O	2.47	0.45
1:A:319:ARG:NH2	1:A:324:GLN:OE1	2.50	0.45
1:B:135:PHE:CD1	1:B:135:PHE:N	2.84	0.45
1:C:109:GLU:OE1	1:C:163:HIS:NE2	2.50	0.45
1:D:298:ILE:CG2	1:D:299:PHE:N	2.80	0.45
1:H:119:ASP:O	1:H:122:GLU:CB	2.64	0.45
1:H:404:LYS:O	1:H:408:CYS:HB2	2.17	0.45
1:A:210:TYR:O	1:A:321:ASP:HB2	2.17	0.45
1:A:402:HIS:O	1:A:406:ALA:HB2	2.16	0.45
1:B:92:GLY:O	1:B:96:ILE:HG13	2.17	0.45
1:D:135:PHE:O	1:D:136:LYS:C	2.55	0.45
1:D:338:CYS:O	1:D:368:ALA:HB2	2.16	0.45
1:E:154:ASP:O	1:E:158:VAL:HG23	2.16	0.45
1:G:114:THR:HA	1:G:147:LEU:HD21	1.99	0.45
1:H:185:ILE:HD11	1:H:219:PRO:HD3	1.99	0.45
1:H:236:GLY:CA	1:H:240:VAL:HG22	2.47	0.45
1:A:181:PRO:HB2	2:A:568:HOH:O	2.17	0.44
1:B:86:ARG:HH12	1:B:267:ALA:CA	2.30	0.44
1:E:110:LEU:O	1:E:142:TYR:HA	2.17	0.44
1:A:268:GLU:H	1:A:268:GLU:HG2	1.50	0.44
1:C:337:PHE:CD2	1:C:410:ALA:HB1	2.52	0.44
1:E:199:LYS:O	1:E:199:LYS:HG3	2.17	0.44
1:F:23:THR:O	1:F:27:LYS:HE2	2.16	0.44
1:F:48:LYS:HZ1	1:H:130:LYS:HA	1.81	0.44
1:G:236:GLY:HA3	1:G:240:VAL:HG22	1.99	0.44
1:H:12:ALA:N	1:H:13:PRO:CD	2.80	0.44
1:H:139:ASN:N	1:H:139:ASN:ND2	2.65	0.44
1:A:184:THR:HG23	1:A:187:GLN:OE1	2.17	0.44
1:A:347:ILE:CD1	1:A:371:THR:O	2.66	0.44
1:B:382:ALA:HA	1:B:393:TYR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:CYS:SG	1:C:227:MSE:SE	3.26	0.44
1:F:203:VAL:HG23	1:F:203:VAL:O	2.17	0.44
1:A:109:GLU:HG2	1:A:141:GLY:HA3	1.99	0.44
1:B:363:ASP:HB2	1:B:387:ARG:HH12	1.81	0.44
1:C:36:ASN:ND2	1:C:213:PHE:O	2.51	0.44
1:F:30:ASP:HA	1:F:33:ILE:HD12	1.99	0.44
1:F:131:GLY:HA2	1:F:134:SER:HB3	1.99	0.44
1:G:347:ILE:HD12	1:G:371:THR:O	2.18	0.44
1:B:44:PHE:HB3	1:B:49:ILE:HD12	1.98	0.44
1:B:323:ILE:N	1:B:323:ILE:HD13	2.33	0.44
1:C:294:LEU:HD11	1:C:319:ARG:HG3	1.98	0.44
1:E:166:THR:HG21	1:E:169:ILE:HD11	2.00	0.44
1:F:34:GLU:O	1:F:38:PHE:HB2	2.17	0.44
1:F:61:GLY:HA3	1:F:270:GLY:O	2.17	0.44
1:H:299:PHE:HD2	1:H:407:ILE:HD11	1.82	0.44
1:A:71:GLU:OE2	1:A:84:LEU:HA	2.18	0.44
1:A:85:VAL:O	1:A:85:VAL:HG22	2.17	0.44
1:A:372:PHE:HE2	1:F:284:PHE:CD2	2.35	0.44
1:B:78:PHE:O	1:B:220:CYS:HB2	2.17	0.44
1:F:49:ILE:HD13	1:F:49:ILE:N	2.33	0.44
1:G:177:TYR:N	1:G:177:TYR:CD2	2.85	0.44
1:H:52:SER:C	1:H:54:PHE:H	2.19	0.44
1:H:71:GLU:HB3	1:H:83:GLY:C	2.38	0.44
1:H:288:HIS:O	1:H:292:GLN:HG2	2.17	0.44
1:H:414:LEU:H	1:H:414:LEU:HD13	1.82	0.44
1:A:78:PHE:O	1:A:220:CYS:HB2	2.18	0.44
1:A:107:GLY:O	1:A:165:ASN:OD1	2.36	0.44
1:B:338:CYS:O	1:B:368:ALA:HB2	2.18	0.44
1:D:55:ILE:HA	1:D:56:PRO:HD3	1.89	0.44
1:D:70:LEU:HD21	1:D:279:MSE:CB	2.48	0.44
1:F:265:ILE:HG23	1:F:269:ALA:HB3	1.99	0.44
1:F:342:GLN:HG2	1:F:353:PRO:HD3	1.99	0.44
1:G:119:ASP:O	1:G:122:GLU:N	2.50	0.44
1:B:125:VAL:HG21	1:B:142:TYR:CE2	2.52	0.44
1:B:385:PRO:HB2	1:B:387:ARG:CZ	2.48	0.44
1:C:67:ARG:NH1	1:C:270:GLY:O	2.50	0.44
1:E:239:ILE:HG22	1:E:278:GLU:HB2	1.99	0.44
1:H:78:PHE:CD2	1:H:227:MSE:HE2	2.53	0.44
1:H:250:GLU:O	1:H:254:GLU:HG2	2.17	0.44
1:A:257:ALA:HB1	1:A:267:ALA:HB2	2.00	0.44
1:B:88:GLN:H	1:B:88:GLN:CD	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:HG2	1:B:141:GLY:HA3	2.00	0.44
1:B:328:PHE:O	1:B:329:ASP:HB2	2.18	0.44
1:C:100:LEU:CD1	1:C:121:LEU:HD21	2.48	0.44
1:D:188:ILE:O	1:D:192:ILE:HG23	2.18	0.44
1:D:404:LYS:O	1:D:408:CYS:HB2	2.18	0.44
1:F:70:LEU:C	1:F:70:LEU:CD1	2.85	0.44
1:F:412:ASP:O	1:F:415:ILE:HG23	2.17	0.44
1:G:399:THR:OG1	1:G:402:HIS:HB2	2.17	0.44
1:A:372:PHE:CZ	1:F:281:GLN:HA	2.53	0.43
1:B:104:LEU:HD22	1:B:140:ILE:CG2	2.48	0.43
1:B:188:ILE:O	1:B:192:ILE:HG23	2.18	0.43
1:B:307:LEU:HD13	1:B:411:ILE:HG12	1.99	0.43
1:C:414:LEU:HD12	1:C:415:ILE:H	1.83	0.43
1:E:108:ASP:HB3	1:E:167:LYS:CB	2.48	0.43
1:E:263:PRO:HD2	1:G:124:ILE:HG23	2.00	0.43
1:E:365:VAL:HG23	1:E:365:VAL:O	2.18	0.43
1:G:29:ALA:O	1:G:32:VAL:HG22	2.18	0.43
1:G:192:ILE:CD1	1:G:193:ALA:N	2.75	0.43
1:G:241:LYS:HD3	1:G:241:LYS:N	2.33	0.43
1:G:254:GLU:HA	1:G:254:GLU:OE2	2.18	0.43
1:G:347:ILE:HG21	1:G:372:PHE:HA	2.00	0.43
1:H:299:PHE:CD2	1:H:407:ILE:HD11	2.52	0.43
1:H:311:THR:HB	1:H:324:GLN:HE22	1.84	0.43
1:A:86:ARG:NH1	1:A:267:ALA:O	2.51	0.43
1:C:375:GLY:HA3	1:F:60:TYR:CE2	2.53	0.43
1:D:233:LYS:C	1:D:235:PRO:HD2	2.39	0.43
1:E:236:GLY:CA	1:E:240:VAL:HG22	2.48	0.43
1:F:172:GLN:HB3	2:F:542:HOH:O	2.18	0.43
1:F:241:LYS:HG2	1:F:373:ILE:HD12	1.99	0.43
1:G:49:ILE:HD13	1:G:49:ILE:N	2.33	0.43
1:H:232:ILE:CG2	1:H:242:THR:HA	2.48	0.43
1:A:203:VAL:O	1:A:203:VAL:CG2	2.66	0.43
1:B:82:ALA:CB	1:B:250:GLU:HA	2.47	0.43
1:B:214:ILE:HG12	1:B:321:ASP:N	2.33	0.43
1:C:96:ILE:O	1:C:100:LEU:HG	2.18	0.43
1:C:131:GLY:HA2	1:C:134:SER:OG	2.17	0.43
1:E:131:GLY:O	1:E:133:GLY:N	2.51	0.43
1:F:108:ASP:CG	1:F:167:LYS:HD3	2.38	0.43
1:G:267:ALA:C	1:G:269:ALA:H	2.21	0.43
1:H:128:ARG:HH21	1:H:128:ARG:CG	2.31	0.43
1:H:145:VAL:HG11	1:H:158:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ILE:H	1:B:65:ILE:HG12	1.64	0.43
1:B:203:VAL:HG12	1:B:252:TYR:CZ	2.53	0.43
1:C:118:TYR:O	1:C:119:ASP:C	2.56	0.43
1:D:92:GLY:N	1:D:230:SER:HB2	2.34	0.43
1:E:295:LYS:HB2	1:E:295:LYS:HE3	1.74	0.43
1:H:258:TYR:CD1	1:H:266:GLY:HA2	2.53	0.43
1:H:300:THR:OG1	1:H:407:ILE:HD13	2.18	0.43
1:A:34:GLU:HA	1:F:401:SER:OG	2.19	0.43
1:B:105:ARG:HB3	1:B:106:PRO:HD2	1.99	0.43
1:C:104:LEU:HD11	1:C:110:LEU:HB2	2.00	0.43
1:C:226:LEU:HD12	1:C:252:TYR:HB3	2.01	0.43
1:D:32:VAL:CG2	1:D:33:ILE:N	2.81	0.43
1:D:312:SER:O	1:D:325:SER:N	2.44	0.43
1:G:131:GLY:C	1:G:137:GLU:OE2	2.56	0.43
1:A:171:ILE:HB	1:A:206:VAL:HG22	2.00	0.43
1:A:212:GLU:O	1:A:213:PHE:HB2	2.18	0.43
1:E:254:GLU:O	1:E:257:ALA:HB3	2.19	0.43
1:G:75:ALA:HA	1:G:247:VAL:HG21	2.00	0.43
1:A:49:ILE:CD1	1:F:346:PRO:O	2.53	0.43
1:B:103:ILE:HG21	1:B:203:VAL:HG21	2.00	0.43
1:B:135:PHE:HD1	1:B:135:PHE:N	2.16	0.43
1:F:297:ALA:O	1:F:300:THR:N	2.52	0.43
1:G:70:LEU:HD21	1:G:279:MSE:HB3	2.00	0.43
1:A:249:LYS:O	1:A:250:GLU:C	2.56	0.43
1:A:284:PHE:HZ	1:F:402:HIS:CD2	2.36	0.43
1:B:307:LEU:CD1	1:B:411:ILE:HG12	2.49	0.43
1:B:328:PHE:CD2	1:B:334:MSE:HA	2.53	0.43
1:C:32:VAL:HB	1:C:216:GLU:HG2	2.01	0.43
1:C:337:PHE:HB2	1:C:414:LEU:HD21	2.01	0.43
1:F:135:PHE:HB3	1:F:140:ILE:O	2.19	0.43
1:G:52:SER:O	1:G:55:ILE:HG12	2.18	0.43
1:H:212:GLU:HB2	1:H:234:ASN:CB	2.49	0.43
1:H:347:ILE:CG2	1:H:371:THR:O	2.61	0.43
1:B:86:ARG:H	1:B:89:ILE:HD12	1.84	0.43
1:B:327:GLN:CG	1:B:391:VAL:HG22	2.49	0.43
1:C:29:ALA:HB1	1:C:294:LEU:HD23	2.00	0.43
1:C:209:CYS:SG	1:C:229:GLY:HA2	2.59	0.43
1:D:33:ILE:O	1:D:37:GLN:HB2	2.19	0.43
1:D:259:ARG:CZ	1:H:259:ARG:CZ	2.96	0.43
1:E:49:ILE:HD13	1:E:49:ILE:C	2.31	0.43
1:E:107:GLY:O	1:E:165:ASN:OD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:THR:O	1:F:202:VAL:HG12	2.18	0.43
1:F:217:GLN:OE1	1:F:221:HIS:HB3	2.18	0.43
1:F:218:GLU:HB3	1:F:219:PRO:CD	2.49	0.43
1:G:214:ILE:HD11	1:G:319:ARG:C	2.39	0.43
1:G:342:GLN:O	1:G:342:GLN:HG3	2.19	0.43
1:G:382:ALA:O	1:G:383:ASP:HB3	2.18	0.43
1:B:242:THR:OG1	1:B:243:GLY:N	2.52	0.43
1:C:28:ARG:HG2	1:C:28:ARG:HH21	1.84	0.43
1:D:30:ASP:OD1	1:D:295:LYS:HD3	2.19	0.43
1:F:44:PHE:HB3	1:F:49:ILE:HD11	1.99	0.43
1:H:220:CYS:HA	1:H:224:ALA:HB3	2.01	0.43
1:A:86:ARG:HB2	1:A:88:GLN:OE1	2.19	0.42
1:A:194:PHE:CE2	1:A:198:ILE:HD11	2.54	0.42
1:A:233:LYS:HB3	1:A:234:ASN:H	1.67	0.42
1:C:292:GLN:HB3	1:C:400:TYR:N	2.34	0.42
1:D:26:HIS:NE2	1:D:298:ILE:HG21	2.34	0.42
1:D:171:ILE:HD13	1:D:191:MSE:SE	2.70	0.42
1:D:407:ILE:O	1:D:411:ILE:HD12	2.18	0.42
1:E:11:ILE:HG23	1:E:12:ALA:N	2.33	0.42
1:E:194:PHE:O	1:E:197:GLU:N	2.49	0.42
1:E:383:ASP:O	1:E:393:TYR:N	2.41	0.42
1:F:371:THR:HG21	1:F:373:ILE:O	2.18	0.42
1:G:218:GLU:N	1:G:221:HIS:ND1	2.62	0.42
1:G:288:HIS:CE1	1:G:292:GLN:NE2	2.87	0.42
1:H:189:LYS:O	1:H:192:ILE:HG13	2.19	0.42
1:A:357:TYR:O	1:A:359:PRO:HD3	2.20	0.42
1:B:162:ILE:HD11	1:B:195:VAL:HG12	2.01	0.42
1:D:25:VAL:HA	1:D:28:ARG:HG2	2.01	0.42
1:D:312:SER:HA	1:D:313:PRO:C	2.39	0.42
1:F:36:ASN:OD1	1:F:39:ARG:NH2	2.50	0.42
1:G:288:HIS:CE1	1:G:292:GLN:HE21	2.36	0.42
1:H:113:ILE:HG22	1:H:158:VAL:HG22	2.00	0.42
1:H:294:LEU:HB2	1:H:322:LEU:CD2	2.49	0.42
1:B:103:ILE:HD12	1:B:168:MSE:HE1	2.02	0.42
1:C:214:ILE:HD12	1:C:321:ASP:N	2.34	0.42
1:D:147:LEU:HD22	1:D:153:VAL:HA	2.01	0.42
1:H:312:SER:O	1:H:325:SER:N	2.51	0.42
1:A:115:GLY:HA2	1:A:145:VAL:O	2.19	0.42
1:B:10:LYS:O	1:B:13:PRO:HD2	2.20	0.42
1:B:128:ARG:HG3	1:B:129:GLY:H	1.85	0.42
1:C:303:PHE:HE2	1:C:411:ILE:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ARG:O	1:D:71:GLU:HG3	2.20	0.42
1:E:286:ALA:HB3	1:E:287:PRO:HD3	2.02	0.42
1:G:75:ALA:HA	1:G:247:VAL:CG2	2.49	0.42
1:G:411:ILE:C	1:G:413:GLU:H	2.20	0.42
1:H:214:ILE:HD13	1:H:214:ILE:O	2.19	0.42
1:A:44:PHE:HD2	1:F:346:PRO:O	2.03	0.42
1:A:130:LYS:HG2	1:A:131:GLY:H	1.83	0.42
1:C:130:LYS:O	1:C:130:LYS:HD3	2.20	0.42
1:E:265:ILE:HD11	1:G:93:THR:HG22	2.01	0.42
1:G:177:TYR:N	1:G:177:TYR:HD2	2.17	0.42
1:G:300:THR:O	1:G:304:LEU:HD23	2.19	0.42
1:A:102:GLY:O	1:A:255:ALA:HB1	2.20	0.42
1:B:33:ILE:HD11	1:B:291:GLY:HA3	2.02	0.42
1:B:111:LEU:HB3	1:B:169:ILE:HD13	2.02	0.42
1:B:226:LEU:HD13	1:B:252:TYR:HB2	2.01	0.42
1:C:42:GLU:HA	1:C:42:GLU:OE1	2.18	0.42
1:D:265:ILE:HD11	1:H:93:THR:HG21	2.00	0.42
1:E:90:ILE:HG13	1:E:91:SER:N	2.34	0.42
1:E:175:LYS:HB3	1:E:180:ARG:O	2.19	0.42
1:F:115:GLY:HA2	1:F:145:VAL:O	2.19	0.42
1:F:119:ASP:O	1:F:122:GLU:HB3	2.20	0.42
1:F:249:LYS:O	1:F:250:GLU:C	2.57	0.42
1:H:55:ILE:HD13	1:H:55:ILE:H	1.85	0.42
1:H:177:TYR:N	1:H:177:TYR:CD2	2.88	0.42
1:A:103:ILE:CD1	1:A:226:LEU:CD2	2.97	0.42
1:C:297:ALA:O	1:C:298:ILE:C	2.58	0.42
1:D:398:LEU:HG	2:D:534:HOH:O	2.19	0.42
1:E:109:GLU:HG3	1:E:141:GLY:HA3	2.01	0.42
1:E:111:LEU:HD11	1:E:145:VAL:CG2	2.40	0.42
1:E:173:ARG:HD3	1:E:208:ASN:OD1	2.20	0.42
1:F:130:LYS:O	1:F:131:GLY:C	2.58	0.42
1:H:199:LYS:HG3	1:H:202:VAL:HG13	1.98	0.42
1:H:300:THR:HG21	1:H:394:VAL:CG1	2.50	0.42
1:A:231:LEU:O	1:A:240:VAL:CG2	2.67	0.42
1:E:355:ALA:CB	1:E:386:ILE:CD1	2.98	0.42
1:F:22:ILE:HD12	1:F:26:HIS:CE1	2.54	0.42
1:F:234:ASN:HB2	1:F:235:PRO:HD3	2.01	0.42
1:G:234:ASN:HA	1:G:378:ILE:HD13	2.02	0.42
1:G:334:MSE:HE2	1:G:386:ILE:HG12	2.02	0.42
1:H:139:ASN:N	1:H:139:ASN:HD22	2.16	0.42
1:C:80:ALA:HB1	1:C:248:GLY:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:LYS:O	1:C:250:GLU:C	2.58	0.42
1:F:55:ILE:HD13	1:F:55:ILE:N	2.35	0.42
1:H:171:ILE:HG23	1:H:191:MSE:SE	2.69	0.42
1:H:354:TYR:HB2	1:H:355:ALA:H	1.65	0.42
1:A:175:LYS:O	1:A:178:ALA:HB3	2.20	0.42
1:D:92:GLY:CA	1:D:230:SER:HB2	2.50	0.42
1:G:108:ASP:OD2	1:G:167:LYS:HD2	2.19	0.42
1:B:57:THR:O	1:B:271:ALA:HB1	2.20	0.41
1:B:286:ALA:CB	1:B:287:PRO:CD	2.97	0.41
1:C:158:VAL:O	1:C:162:ILE:HG13	2.20	0.41
1:D:173:ARG:NH1	1:D:185:ILE:HD11	2.34	0.41
1:A:37:GLN:HA	1:A:37:GLN:HE21	1.85	0.41
1:B:21:GLN:NE2	1:B:306:LYS:HE2	2.36	0.41
1:B:170:GLY:C	1:B:171:ILE:HG13	2.40	0.41
1:C:148:THR:HG22	1:C:149:GLU:N	2.35	0.41
1:F:51:ASP:HA	1:F:54:PHE:CE2	2.55	0.41
1:F:104:LEU:HB3	1:F:140:ILE:HD13	2.02	0.41
1:F:116:LYS:HE2	1:F:116:LYS:HB3	1.77	0.41
1:G:364:ASP:HB2	1:G:386:ILE:HD12	2.02	0.41
1:H:116:LYS:HA	1:H:117:PRO:HD3	1.91	0.41
1:A:110:LEU:HD12	1:A:168:MSE:HG2	2.02	0.41
1:A:358:MSE:HG3	1:A:365:VAL:HG11	2.01	0.41
1:B:401:SER:OG	1:C:34:GLU:HA	2.20	0.41
1:C:175:LYS:O	1:C:178:ALA:HB3	2.21	0.41
1:C:259:ARG:HG3	1:C:259:ARG:NH1	2.34	0.41
1:D:122:GLU:CG	1:D:128:ARG:HB2	2.47	0.41
1:F:347:ILE:O	1:F:348:ASN:HB2	2.20	0.41
1:F:401:SER:O	1:F:402:HIS:C	2.58	0.41
1:G:18:VAL:O	1:G:22:ILE:HG12	2.20	0.41
1:G:121:LEU:HA	1:G:124:ILE:HD12	2.02	0.41
1:H:26:HIS:C	1:H:28:ARG:H	2.22	0.41
1:H:276:LEU:O	1:H:277:GLN:C	2.59	0.41
1:A:286:ALA:O	1:A:288:HIS:N	2.54	0.41
1:A:299:PHE:CD2	1:A:407:ILE:HD11	2.56	0.41
1:B:276:LEU:HD23	1:B:279:MSE:CE	2.50	0.41
1:C:300:THR:HG23	1:C:304:LEU:HD23	2.01	0.41
1:C:342:GLN:HG2	1:C:353:PRO:HD3	2.02	0.41
1:C:350:HIS:ND1	1:C:350:HIS:N	2.65	0.41
1:D:265:ILE:HD11	1:H:93:THR:HG22	2.03	0.41
1:F:54:PHE:CE2	1:F:277:GLN:HG3	2.55	0.41
1:F:71:GLU:OE2	1:F:86:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:TYR:HD2	1:F:120:THR:HG1	1.60	0.41
1:F:315:TRP:CZ3	1:F:316:ASN:HB3	2.54	0.41
1:H:12:ALA:HB3	1:H:13:PRO:HD3	2.02	0.41
1:H:118:TYR:O	1:H:119:ASP:C	2.59	0.41
1:H:166:THR:O	1:H:202:VAL:HG12	2.20	0.41
1:A:110:LEU:O	1:A:142:TYR:HA	2.20	0.41
1:A:194:PHE:CZ	1:A:198:ILE:HD11	2.55	0.41
1:B:321:ASP:C	1:B:321:ASP:OD1	2.59	0.41
1:C:145:VAL:HG11	1:C:158:VAL:HG23	2.03	0.41
1:E:119:ASP:O	1:E:121:LEU:N	2.54	0.41
1:F:18:VAL:HG21	1:F:303:PHE:HD2	1.85	0.41
1:A:259:ARG:HH12	1:B:259:ARG:NH1	2.18	0.41
1:A:315:TRP:CZ3	1:A:316:ASN:HB3	2.55	0.41
1:F:407:ILE:HG13	1:F:408:CYS:N	2.34	0.41
1:G:71:GLU:OE2	1:G:86:ARG:NH2	2.41	0.41
1:G:84:LEU:HD21	1:G:260:LEU:HD22	2.03	0.41
1:H:78:PHE:HD2	1:H:227:MSE:HE2	1.85	0.41
1:H:89:ILE:HG21	1:H:95:ALA:HB2	2.02	0.41
1:H:119:ASP:OD2	1:H:361:TYR:HE1	2.03	0.41
1:A:293:ALA:HB2	1:A:397:GLY:O	2.21	0.41
1:C:11:ILE:O	1:C:15:VAL:HG22	2.21	0.41
1:D:364:ASP:OD1	1:D:364:ASP:N	2.52	0.41
1:G:363:ASP:OD1	1:G:387:ARG:HD3	2.20	0.41
1:H:220:CYS:HB2	1:H:227:MSE:SE	2.71	0.41
1:H:297:ALA:HA	2:H:585:HOH:O	2.20	0.41
1:B:211:GLY:O	1:B:214:ILE:HG23	2.21	0.41
1:B:350:HIS:CD2	1:C:48:LYS:HB3	2.56	0.41
1:C:199:LYS:HD3	1:C:202:VAL:HG13	2.03	0.41
1:E:309:MSE:HB3	1:E:327:GLN:O	2.21	0.41
1:A:88:GLN:H	1:A:88:GLN:CD	2.24	0.41
1:A:105:ARG:HH21	1:B:133:GLY:HA2	1.85	0.41
1:C:163:HIS:ND1	1:C:163:HIS:N	2.68	0.41
1:C:234:ASN:HA	1:C:378:ILE:HD13	2.03	0.41
1:C:347:ILE:CD1	1:C:371:THR:O	2.64	0.41
1:D:43:SER:OG	1:D:73:VAL:HG13	2.21	0.41
1:D:89:ILE:HG21	1:D:95:ALA:HB2	2.01	0.41
1:D:185:ILE:HG13	1:D:217:GLN:O	2.20	0.41
1:E:78:PHE:CD1	1:E:218:GLU:HG3	2.56	0.41
1:E:158:VAL:O	1:E:162:ILE:HG13	2.21	0.41
1:F:18:VAL:HG21	1:F:303:PHE:CD2	2.55	0.41
1:F:61:GLY:HA3	1:F:270:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:THR:HG22	1:F:149:GLU:N	2.35	0.41
1:G:87:PRO:C	1:G:89:ILE:H	2.24	0.41
1:G:119:ASP:O	1:G:120:THR:C	2.60	0.41
1:G:218:GLU:H	1:G:221:HIS:CE1	2.38	0.41
1:H:347:ILE:HD13	1:H:348:ASN:CG	2.42	0.41
1:H:348:ASN:OD1	1:H:351:PHE:CE2	2.74	0.41
1:A:70:LEU:CD2	1:A:279:MSE:HE3	2.50	0.41
1:A:234:ASN:HB2	1:A:235:PRO:HD3	2.02	0.41
1:A:241:LYS:H	1:A:241:LYS:HG2	1.64	0.41
1:B:98:THR:HG21	1:B:260:LEU:HD12	2.02	0.41
1:B:298:ILE:HG13	1:B:315:TRP:HB2	2.02	0.41
1:C:407:ILE:HD13	1:C:408:CYS:H	1.86	0.41
1:E:194:PHE:O	1:E:196:LYS:N	2.54	0.41
1:G:234:ASN:N	1:G:235:PRO:CD	2.83	0.41
1:H:135:PHE:O	1:H:136:LYS:C	2.58	0.41
1:A:70:LEU:HD13	1:A:280:TYR:CD1	2.56	0.40
1:A:199:LYS:C	1:A:201:ASP:N	2.75	0.40
1:A:253:VAL:O	1:A:256:CYS:HB2	2.21	0.40
1:C:68:ASP:O	1:C:71:GLU:HB2	2.22	0.40
1:D:125:VAL:HG12	1:D:135:PHE:CE2	2.56	0.40
1:E:22:ILE:CD1	1:E:26:HIS:CE1	3.04	0.40
1:E:214:ILE:HD12	1:E:214:ILE:O	2.21	0.40
1:E:247:VAL:HG13	1:E:247:VAL:O	2.21	0.40
1:G:111:LEU:HA	1:G:143:ASN:O	2.22	0.40
1:G:121:LEU:O	1:G:122:GLU:C	2.60	0.40
1:G:203:VAL:HA	1:G:225:ASP:OD2	2.21	0.40
1:A:1:MSE:CB	1:F:34:GLU:CB	2.97	0.40
1:A:40:VAL:HG11	1:A:284:PHE:HA	2.02	0.40
1:A:348:ASN:C	1:A:350:HIS:H	2.25	0.40
1:B:173:ARG:NH2	1:B:320:THR:O	2.54	0.40
1:B:234:ASN:N	1:B:235:PRO:HD2	2.36	0.40
1:D:67:ARG:HD2	1:D:86:ARG:NH2	2.36	0.40
1:D:148:THR:CG2	1:D:149:GLU:N	2.84	0.40
1:D:263:PRO:HG3	1:H:133:GLY:O	2.21	0.40
1:E:236:GLY:HA3	1:E:240:VAL:CG2	2.49	0.40
1:F:82:ALA:HB3	1:F:253:VAL:CG2	2.48	0.40
1:F:189:LYS:HG3	1:F:222:VAL:HB	2.03	0.40
1:F:234:ASN:HA	1:F:378:ILE:HD13	2.03	0.40
1:H:11:ILE:O	1:H:15:VAL:HG13	2.21	0.40
1:A:327:GLN:HE21	1:A:327:GLN:HB2	1.66	0.40
1:B:174:SER:HA	1:B:321:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:ASP:HA	1:D:33:ILE:HD12	2.04	0.40
1:E:21:GLN:HE21	1:E:21:GLN:HB3	1.70	0.40
1:F:212:GLU:OE1	1:F:235:PRO:HD3	2.20	0.40
1:G:144:ALA:O	1:G:146:PRO:HD3	2.21	0.40
1:H:52:SER:O	1:H:55:ILE:HG12	2.21	0.40
1:A:113:ILE:HA	1:A:145:VAL:HB	2.03	0.40
1:A:236:GLY:O	1:A:282:GLY:HA3	2.22	0.40
1:A:286:ALA:CB	1:A:287:PRO:HD3	2.34	0.40
1:B:75:ALA:O	1:B:80:ALA:N	2.47	0.40
1:B:312:SER:O	1:B:325:SER:N	2.53	0.40
1:C:51:ASP:OD2	1:C:51:ASP:N	2.38	0.40
1:C:112:TYR:CG	1:C:117:PRO:HG3	2.55	0.40
1:D:226:LEU:HD11	1:D:246:ILE:HG22	2.03	0.40
1:E:259:ARG:CZ	1:G:259:ARG:NH1	2.84	0.40
1:E:311:THR:HB	1:E:326:VAL:HG12	2.03	0.40
1:F:85:VAL:O	1:F:85:VAL:HG22	2.21	0.40
1:G:36:ASN:O	1:G:38:PHE:N	2.55	0.40
1:G:258:TYR:HD1	1:G:266:GLY:HA2	1.82	0.40
1:G:365:VAL:HA	1:G:385:PRO:HA	2.03	0.40
1:A:2:PHE:C	1:A:4:ARG:H	2.23	0.40
1:A:209:CYS:O	1:A:210:TYR:CB	2.69	0.40
1:C:249:LYS:HB2	1:C:252:TYR:HD2	1.87	0.40
1:D:18:VAL:O	1:D:21:GLN:HB3	2.21	0.40
1:F:261:THR:OG1	1:F:262:SER:N	2.52	0.40
1:G:188:ILE:O	1:G:192:ILE:CG2	2.69	0.40
1:G:239:ILE:HD11	1:G:285:LEU:HD12	2.03	0.40
1:H:168:MSE:HE2	1:H:205:PHE:HB2	2.04	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	414/431 (96%)	356 (86%)	53 (13%)	5 (1%)	13	40
1	B	405/431 (94%)	347 (86%)	56 (14%)	2 (0%)	29	61
1	C	409/431 (95%)	361 (88%)	45 (11%)	3 (1%)	22	54
1	D	406/431 (94%)	350 (86%)	55 (14%)	1 (0%)	47	78
1	E	407/431 (94%)	361 (89%)	45 (11%)	1 (0%)	47	78
1	F	408/431 (95%)	356 (87%)	51 (12%)	1 (0%)	47	78
1	G	406/431 (94%)	344 (85%)	60 (15%)	2 (0%)	29	61
1	H	405/431 (94%)	335 (83%)	65 (16%)	5 (1%)	13	40
All	All	3260/3448 (94%)	2810 (86%)	430 (13%)	20 (1%)	25	58

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	265	ILE
1	A	166	THR
1	A	351	PHE
1	B	89	ILE
1	C	67	ARG
1	E	132	VAL
1	A	97	SER
1	F	374	GLN
1	G	37	GLN
1	G	277	GLN
1	H	194	PHE
1	A	118	TYR
1	D	265	ILE
1	H	198	ILE
1	A	226	LEU
1	C	250	GLU
1	H	132	VAL
1	C	298	ILE
1	H	33	ILE
1	B	235	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	325/340 (96%)	285 (88%)	40 (12%)	4	14
1	B	326/340 (96%)	287 (88%)	39 (12%)	5	15
1	C	324/340 (95%)	291 (90%)	33 (10%)	7	22
1	D	326/340 (96%)	295 (90%)	31 (10%)	8	26
1	E	325/340 (96%)	296 (91%)	29 (9%)	9	29
1	F	324/340 (95%)	280 (86%)	44 (14%)	3	11
1	G	322/340 (95%)	295 (92%)	27 (8%)	11	31
1	H	324/340 (95%)	299 (92%)	25 (8%)	13	35
All	All	2596/2720 (95%)	2328 (90%)	268 (10%)	7	22

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	32	VAL
1	A	37	GLN
1	A	38	PHE
1	A	49	ILE
1	A	51	ASP
1	A	81	GLU
1	A	85	VAL
1	A	86	ARG
1	A	112	TYR
1	A	116	LYS
1	A	121	LEU
1	A	128	ARG
1	A	136	LYS
1	A	137	GLU
1	A	153	VAL
1	A	174	SER
1	A	179	THR
1	A	190	GLU
1	A	192	ILE
1	A	197	GLU
1	A	201	ASP
1	A	202	VAL
1	A	214	ILE

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Mol	Chain	Res	Type
1	A	216	GLU
1	A	230	SER
1	A	241	LYS
1	A	247	VAL
1	A	268	GLU
1	A	275	SER
1	A	304	LEU
1	A	305	GLU
1	A	306	LYS
1	A	347	ILE
1	A	352	THR
1	A	357	TYR
1	A	358	MSE
1	A	395	GLN
1	A	401	SER
1	A	407	ILE
1	B	25	VAL
1	B	28	ARG
1	B	32	VAL
1	B	37	GLN
1	B	38	PHE
1	B	49	ILE
1	B	50	SER
1	B	51	ASP
1	B	55	ILE
1	B	65	ILE
1	B	73	VAL
1	B	85	VAL
1	B	112	TYR
1	B	118	TYR
1	B	119	ASP
1	B	130	LYS
1	B	132	VAL
1	B	135	PHE
1	B	136	LYS
1	B	152	LEU
1	B	153	VAL
1	B	174	SER
1	B	179	THR
1	B	192	ILE
1	B	201	ASP
1	B	209	CYS

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Mol	Chain	Res	Type
1	B	214	ILE
1	B	230	SER
1	B	260	LEU
1	B	268	GLU
1	B	275	SER
1	B	305	GLU
1	B	350	HIS
1	B	352	THR
1	B	358	MSE
1	B	381	SER
1	B	401	SER
1	B	409	SER
1	B	414	LEU
1	C	16	LYS
1	C	20	SER
1	C	23	THR
1	C	25	VAL
1	C	26	HIS
1	C	28	ARG
1	C	32	VAL
1	C	37	GLN
1	C	38	PHE
1	C	49	ILE
1	C	51	ASP
1	C	103	ILE
1	C	112	TYR
1	C	121	LEU
1	C	130	LYS
1	C	136	LYS
1	C	152	LEU
1	C	163	HIS
1	C	192	ILE
1	C	197	GLU
1	C	214	ILE
1	C	230	SER
1	C	275	SER
1	C	311	THR
1	C	321	ASP
1	C	326	VAL
1	C	334	MSE
1	C	352	THR
1	C	358	MSE

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Mol	Chain	Res	Type
1	C	383	ASP
1	C	401	SER
1	C	407	ILE
1	C	414	LEU
1	D	9	GLU
1	D	10	LYS
1	D	16	LYS
1	D	25	VAL
1	D	49	ILE
1	D	55	ILE
1	D	68	ASP
1	D	74	TYR
1	D	103	ILE
1	D	112	TYR
1	D	120	THR
1	D	121	LEU
1	D	123	GLU
1	D	125	VAL
1	D	201	ASP
1	D	203	VAL
1	D	214	ILE
1	D	216	GLU
1	D	273	LEU
1	D	276	LEU
1	D	277	GLN
1	D	304	LEU
1	D	347	ILE
1	D	363	ASP
1	D	364	ASP
1	D	366	ILE
1	D	394	VAL
1	D	399	THR
1	D	401	SER
1	D	404	LYS
1	D	407	ILE
1	E	16	LYS
1	E	20	SER
1	E	25	VAL
1	E	32	VAL
1	E	33	ILE
1	E	49	ILE
1	E	68	ASP

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Mol	Chain	Res	Type
1	E	103	ILE
1	E	123	GLU
1	E	130	LYS
1	E	132	VAL
1	E	148	THR
1	E	165	ASN
1	E	175	LYS
1	E	192	ILE
1	E	201	ASP
1	E	214	ILE
1	E	216	GLU
1	E	226	LEU
1	E	262	SER
1	E	304	LEU
1	E	333	ARG
1	E	347	ILE
1	E	352	THR
1	E	381	SER
1	E	399	THR
1	E	404	LYS
1	E	407	ILE
1	E	415	ILE
1	F	21	GLN
1	F	25	VAL
1	F	26	HIS
1	F	38	PHE
1	F	43	SER
1	F	46	LYS
1	F	49	ILE
1	F	51	ASP
1	F	63	ASP
1	F	70	LEU
1	F	74	TYR
1	F	85	VAL
1	F	112	TYR
1	F	116	LYS
1	F	120	THR
1	F	136	LYS
1	F	142	TYR
1	F	163	HIS
1	F	192	ILE
1	F	197	GLU

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Mol	Chain	Res	Type
1	F	201	ASP
1	F	214	ILE
1	F	239	ILE
1	F	242	THR
1	F	251	GLN
1	F	262	SER
1	F	268	GLU
1	F	275	SER
1	F	298	ILE
1	F	305	GLU
1	F	320	THR
1	F	326	VAL
1	F	327	GLN
1	F	347	ILE
1	F	351	PHE
1	F	352	THR
1	F	358	MSE
1	F	363	ASP
1	F	380	LEU
1	F	383	ASP
1	F	401	SER
1	F	412	ASP
1	F	414	LEU
1	F	415	ILE
1	G	15	VAL
1	G	28	ARG
1	G	38	PHE
1	G	49	ILE
1	G	85	VAL
1	G	130	LYS
1	G	132	VAL
1	G	153	VAL
1	G	179	THR
1	G	192	ILE
1	G	214	ILE
1	G	241	LYS
1	G	247	VAL
1	G	275	SER
1	G	298	ILE
1	G	305	GLU
1	G	306	LYS
1	G	310	ASN

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Mol	Chain	Res	Type
1	G	312	SER
1	G	334	MSE
1	G	345	SER
1	G	347	ILE
1	G	352	THR
1	G	358	MSE
1	G	363	ASP
1	G	404	LYS
1	G	411	ILE
1	H	15	VAL
1	H	16	LYS
1	H	32	VAL
1	H	38	PHE
1	H	49	ILE
1	H	85	VAL
1	H	112	TYR
1	H	128	ARG
1	H	130	LYS
1	H	143	ASN
1	H	153	VAL
1	H	179	THR
1	H	187	GLN
1	H	197	GLU
1	H	201	ASP
1	H	214	ILE
1	H	268	GLU
1	H	306	LYS
1	H	312	SER
1	H	345	SER
1	H	347	ILE
1	H	354	TYR
1	H	363	ASP
1	H	404	LYS
1	H	414	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	37	GLN
1	A	277	GLN
1	A	288	HIS

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Mol	Chain	Res	Type
1	A	327	GLN
1	B	21	GLN
1	B	94	HIS
1	B	139	ASN
1	B	187	GLN
1	B	288	HIS
1	B	324	GLN
1	C	47	HIS
1	C	139	ASN
1	C	187	GLN
1	C	310	ASN
1	C	356	ASN
1	D	21	GLN
1	D	37	GLN
1	D	139	ASN
1	D	163	HIS
1	D	187	GLN
1	D	292	GLN
1	D	324	GLN
1	D	348	ASN
1	E	21	GLN
1	E	139	ASN
1	E	187	GLN
1	F	21	GLN
1	F	94	HIS
1	F	139	ASN
1	F	327	GLN
1	G	21	GLN
1	G	187	GLN
1	G	217	GLN
1	G	310	ASN
1	G	327	GLN
1	H	21	GLN
1	H	47	HIS
1	H	139	ASN
1	H	187	GLN
1	H	217	GLN
1	H	288	HIS
1	H	292	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	407/431 (94%)	0.58	23 (5%)	23	19	15, 33, 51, 62	0
1	B	399/431 (92%)	0.52	17 (4%)	35	31	14, 30, 50, 66	0
1	C	403/431 (93%)	0.63	27 (6%)	17	13	15, 32, 55, 69	0
1	D	400/431 (92%)	0.51	18 (4%)	33	29	10, 28, 57, 71	0
1	E	401/431 (93%)	0.53	22 (5%)	25	21	8, 29, 56, 67	0
1	F	402/431 (93%)	0.53	21 (5%)	27	23	14, 30, 53, 64	0
1	G	400/431 (92%)	0.71	32 (8%)	12	9	17, 36, 71, 84	0
1	H	399/431 (92%)	0.83	46 (11%)	4	3	20, 37, 67, 81	0
All	All	3211/3448 (93%)	0.60	206 (6%)	19	15	8, 32, 60, 84	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	360	GLY	12.6
1	D	359	PRO	10.7
1	E	360	GLY	7.3
1	H	362	GLU	6.2
1	G	362	GLU	6.0
1	E	359	PRO	5.9
1	E	129	GLY	5.4
1	F	267	ALA	5.1
1	G	386	ILE	5.1
1	D	129	GLY	5.0
1	F	360	GLY	4.9
1	G	389	PRO	4.8
1	C	267	ALA	4.7
1	C	415	ILE	4.6
1	H	360	GLY	4.5
1	B	130	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	G	363	ASP	4.3
1	D	130	LYS	4.2
1	E	361	TYR	4.2
1	F	132	VAL	4.0
1	C	340	ALA	4.0
1	H	414	LEU	3.9
1	H	328	PHE	3.9
1	F	165	ASN	3.7
1	B	356	ASN	3.7
1	A	361	TYR	3.7
1	H	386	ILE	3.7
1	H	14	ILE	3.6
1	H	186	SER	3.6
1	D	128	ARG	3.6
1	H	347	ILE	3.5
1	D	330	ASP	3.5
1	D	14	ILE	3.5
1	C	197	GLU	3.5
1	H	359	PRO	3.4
1	C	261	THR	3.4
1	H	389	PRO	3.4
1	H	329	ASP	3.4
1	G	352	THR	3.3
1	G	131	GLY	3.3
1	C	88	GLN	3.3
1	E	356	ASN	3.3
1	F	15	VAL	3.2
1	C	266	GLY	3.2
1	E	311	THR	3.2
1	F	63	ASP	3.2
1	G	348	ASN	3.2
1	B	61	GLY	3.2
1	B	149	GLU	3.2
1	C	268	GLU	3.2
1	B	129	GLY	3.1
1	H	139	ASN	3.1
1	A	204	VAL	3.1
1	G	347	ILE	3.1
1	B	15	VAL	3.1
1	G	351	PHE	3.1
1	C	132	VAL	3.1
1	D	131	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	361	TYR	3.1
1	G	326	VAL	3.0
1	A	318	PRO	3.0
1	D	156	GLU	3.0
1	C	156	GLU	3.0
1	B	415	ILE	3.0
1	A	390	TYR	3.0
1	G	328	PHE	3.0
1	C	165	ASN	3.0
1	G	390	TYR	2.9
1	F	266	GLY	2.9
1	H	251	GLN	2.9
1	H	23	THR	2.9
1	H	179	THR	2.9
1	E	390	TYR	2.9
1	H	354	TYR	2.9
1	G	388	PRO	2.9
1	F	14	ILE	2.8
1	F	268	GLU	2.8
1	A	118	TYR	2.8
1	G	129	GLY	2.8
1	A	221	HIS	2.8
1	D	252	TYR	2.8
1	C	382	ALA	2.7
1	G	190	GLU	2.7
1	F	144	ALA	2.7
1	B	390	TYR	2.7
1	H	390	TYR	2.7
1	E	14	ILE	2.7
1	F	156	GLU	2.7
1	F	197	GLU	2.7
1	F	120	THR	2.7
1	H	352	THR	2.7
1	H	361	TYR	2.7
1	C	91	SER	2.7
1	H	182	SER	2.6
1	H	304	LEU	2.6
1	F	275	SER	2.6
1	G	275	SER	2.6
1	D	142	TYR	2.6
1	B	28	ARG	2.6
1	A	152	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	307	LEU	2.6
1	G	329	ASP	2.6
1	E	139	ASN	2.6
1	A	130	LYS	2.6
1	G	364	ASP	2.6
1	D	356	ASN	2.6
1	E	266	GLY	2.6
1	G	359	PRO	2.5
1	D	179	THR	2.5
1	C	201	ASP	2.5
1	H	286	ALA	2.5
1	C	116	LYS	2.5
1	H	391	VAL	2.5
1	C	163	HIS	2.5
1	H	13	PRO	2.5
1	C	275	SER	2.5
1	F	195	VAL	2.5
1	H	17	GLU	2.5
1	H	63	ASP	2.5
1	H	369	ALA	2.5
1	A	202	VAL	2.5
1	E	156	GLU	2.5
1	C	269	ALA	2.5
1	G	361	TYR	2.5
1	H	24	GLU	2.4
1	H	177	TYR	2.4
1	E	223	GLY	2.4
1	F	202	VAL	2.4
1	G	327	GLN	2.4
1	A	124	ILE	2.4
1	F	368	ALA	2.4
1	A	139	ASN	2.4
1	B	269	ALA	2.4
1	F	164	SER	2.4
1	A	192	ILE	2.4
1	E	186	SER	2.3
1	E	254	GLU	2.3
1	G	391	VAL	2.3
1	H	222	VAL	2.3
1	A	84	LEU	2.3
1	D	28	ARG	2.3
1	G	356	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	330	ASP	2.3
1	H	363	ASP	2.3
1	B	355	ALA	2.3
1	F	107	GLY	2.3
1	H	327	GLN	2.3
1	E	117	PRO	2.3
1	G	355	ALA	2.3
1	D	132	VAL	2.3
1	H	315	TRP	2.3
1	G	197	GLU	2.3
1	B	115	GLY	2.2
1	A	122	GLU	2.2
1	A	264	GLY	2.2
1	C	392	ALA	2.2
1	E	264	GLY	2.2
1	G	8	GLY	2.2
1	C	339	GLN	2.2
1	A	149	GLU	2.2
1	C	264	GLY	2.2
1	H	229	GLY	2.2
1	D	11	ILE	2.2
1	G	35	SER	2.2
1	G	366	ILE	2.2
1	A	120	THR	2.2
1	D	355	ALA	2.2
1	A	184	THR	2.2
1	E	149	GLU	2.2
1	A	203	VAL	2.2
1	B	329	ASP	2.1
1	F	340	ALA	2.1
1	G	313	PRO	2.1
1	E	262	SER	2.1
1	E	362	GLU	2.1
1	H	356	ASN	2.1
1	H	15	VAL	2.1
1	D	210	TYR	2.1
1	C	63	ASP	2.1
1	H	348	ASN	2.1
1	H	313	PRO	2.1
1	C	195	VAL	2.1
1	A	308	GLY	2.1
1	C	270	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	60	TYR	2.1
1	H	185	ILE	2.1
1	E	57	THR	2.1
1	B	122	GLU	2.1
1	B	276	LEU	2.1
1	H	312	SER	2.1
1	A	386	ILE	2.1
1	C	120	THR	2.1
1	C	407	ILE	2.1
1	A	28	ARG	2.0
1	C	179	THR	2.0
1	E	141	GLY	2.0
1	A	391	VAL	2.0
1	H	127	VAL	2.0
1	E	330	ASP	2.0
1	G	369	ALA	2.0
1	H	326	VAL	2.0
1	G	11	ILE	2.0
1	H	192	ILE	2.0
1	F	361	TYR	2.0
1	H	202	VAL	2.0
1	H	351	PHE	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.