Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 09:14 AM EST

PDB ID	:	4XD7
Title	:	Structure of thermophilic F1-ATPase inhibited by epsilon subunit
Authors	:	SHIRAKIHARA, Y.; SHIRATORI, A.; TANIKAWA, H.; NAKASAKO, M.; YOSHIDA, M.; SUZUKI, T.
Deposited on	:	2014-12-19
Resolution	:	3.90 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:

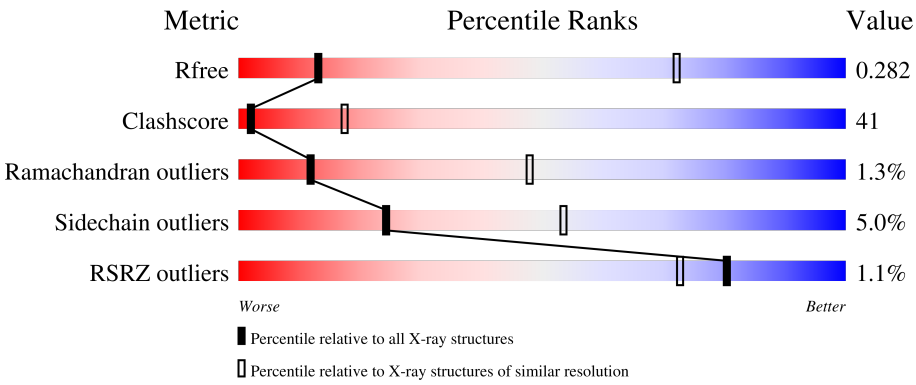
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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	502	37% 55% • 5%
1	B	502	2% 42% 40% • 16%
1	C	502	43% 48% • 5%
2	D	483	48% 47% • •
2	E	483	43% 51% • •

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Mol	Chain	Length	Quality of chain
2	F	483	2% 53% 42%
3	G	285	39% 44% 6% 11%
4	H	133	5% 45% 46% 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	700	-	-	X	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22656 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	477	3462	2189	606	658	9	0	0	0
1	B	423	2833	1786	484	554	9	0	0	0
1	C	475	3329	2109	577	634	9	1	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	SER	CYS	conflict	UNP Q5KUJ1
A	254	LYS	GLN	conflict	UNP Q5KUJ1
A	463	PHE	TRP	conflict	UNP Q5KUJ1
B	193	SER	CYS	conflict	UNP Q5KUJ1
B	254	LYS	GLN	conflict	UNP Q5KUJ1
B	463	PHE	TRP	conflict	UNP Q5KUJ1
C	193	SER	CYS	conflict	UNP Q5KUJ1
C	254	LYS	GLN	conflict	UNP Q5KUJ1
C	463	PHE	TRP	conflict	UNP Q5KUJ1

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
2	D	470	3480	2199	599	669	13	1	0	0
2	E	469	3484	2198	598	676	12	0	0	0
2	F	464	3334	2097	580	644	13	4	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	MSE	-	initiating methionine	UNP Q5KUJ3
D	-8	HIS	-	expression tag	UNP Q5KUJ3
D	-7	HIS	-	expression tag	UNP Q5KUJ3
D	-6	HIS	-	expression tag	UNP Q5KUJ3
D	-5	HIS	-	expression tag	UNP Q5KUJ3
D	-4	HIS	-	expression tag	UNP Q5KUJ3
D	-3	HIS	-	expression tag	UNP Q5KUJ3
D	-2	HIS	-	expression tag	UNP Q5KUJ3
D	-1	HIS	-	expression tag	UNP Q5KUJ3
D	0	HIS	-	expression tag	UNP Q5KUJ3
D	1	HIS	-	expression tag	UNP Q5KUJ3
E	-9	MSE	-	initiating methionine	UNP Q5KUJ3
E	-8	HIS	-	expression tag	UNP Q5KUJ3
E	-7	HIS	-	expression tag	UNP Q5KUJ3
E	-6	HIS	-	expression tag	UNP Q5KUJ3
E	-5	HIS	-	expression tag	UNP Q5KUJ3
E	-4	HIS	-	expression tag	UNP Q5KUJ3
E	-3	HIS	-	expression tag	UNP Q5KUJ3
E	-2	HIS	-	expression tag	UNP Q5KUJ3
E	-1	HIS	-	expression tag	UNP Q5KUJ3
E	0	HIS	-	expression tag	UNP Q5KUJ3
E	1	HIS	-	expression tag	UNP Q5KUJ3
F	-9	MSE	-	initiating methionine	UNP Q5KUJ3
F	-8	HIS	-	expression tag	UNP Q5KUJ3
F	-7	HIS	-	expression tag	UNP Q5KUJ3
F	-6	HIS	-	expression tag	UNP Q5KUJ3
F	-5	HIS	-	expression tag	UNP Q5KUJ3
F	-4	HIS	-	expression tag	UNP Q5KUJ3
F	-3	HIS	-	expression tag	UNP Q5KUJ3
F	-2	HIS	-	expression tag	UNP Q5KUJ3
F	-1	HIS	-	expression tag	UNP Q5KUJ3
F	0	HIS	-	expression tag	UNP Q5KUJ3
F	1	HIS	-	expression tag	UNP Q5KUJ3

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
3	G	254	1797	1142	308	339	1	7	0	0	0

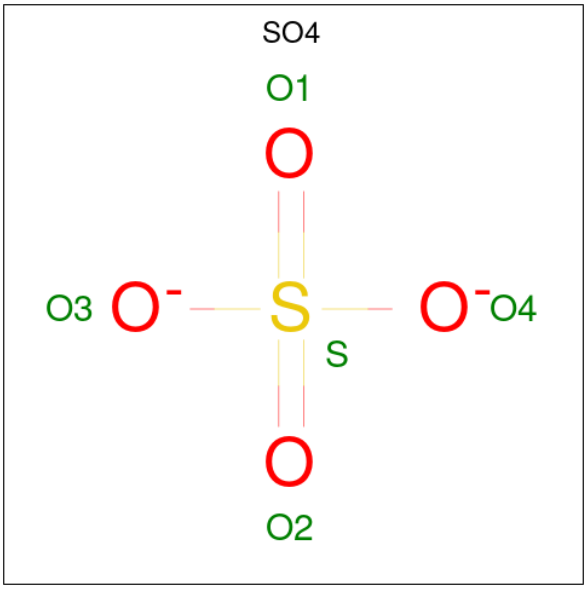
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	109	CYS	SER	conflict	UNP Q5KUJ2

- Molecule 4 is a protein called ATP synthase epsilon chain.

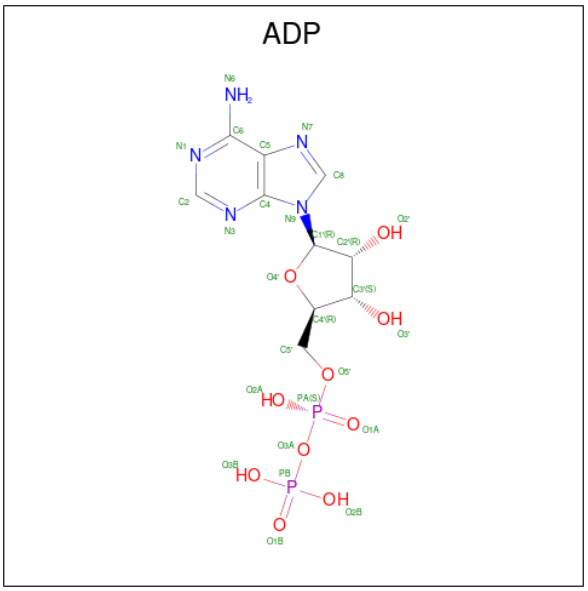
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
4	H	129	890	563	148	175	4	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	B	1	5	4	1	0	0
			Total	O	S		
5	D	1	5	4	1	0	0
			Total	O	S		
5	E	1	5	4	1	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



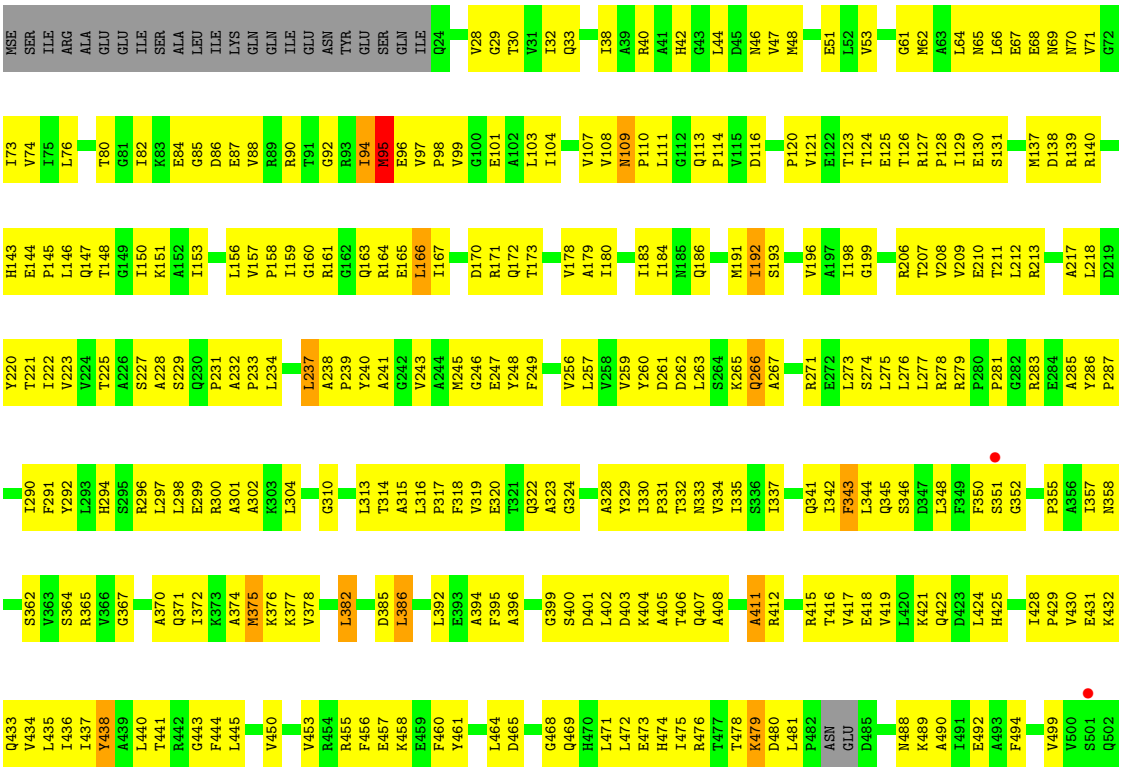
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	F	1	27	10	5	10	2	0	0

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.

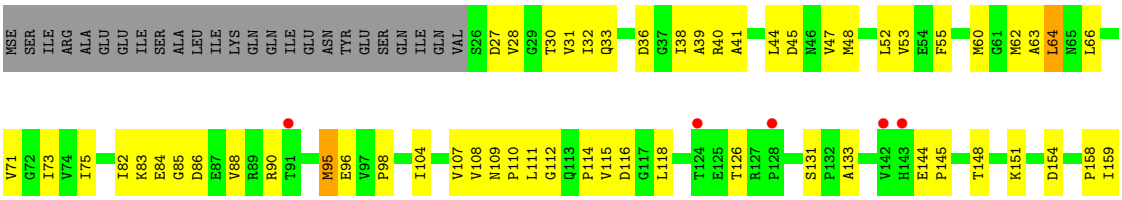
• Molecule 1: ATP synthase subunit alpha

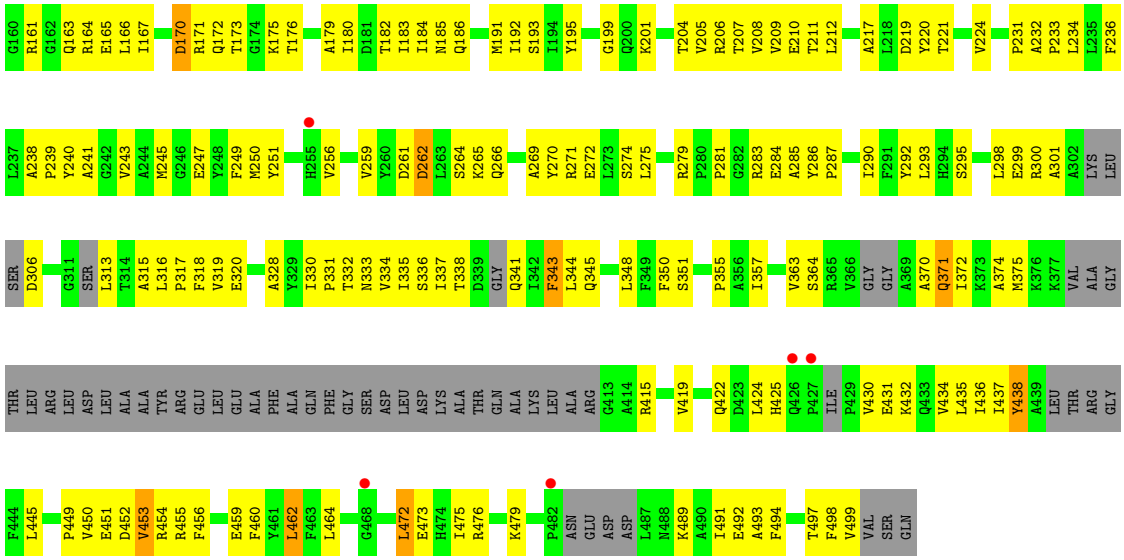
Chain A: 37% 55% • 5%



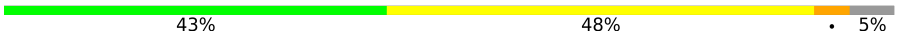
• Molecule 1: ATP synthase subunit alpha

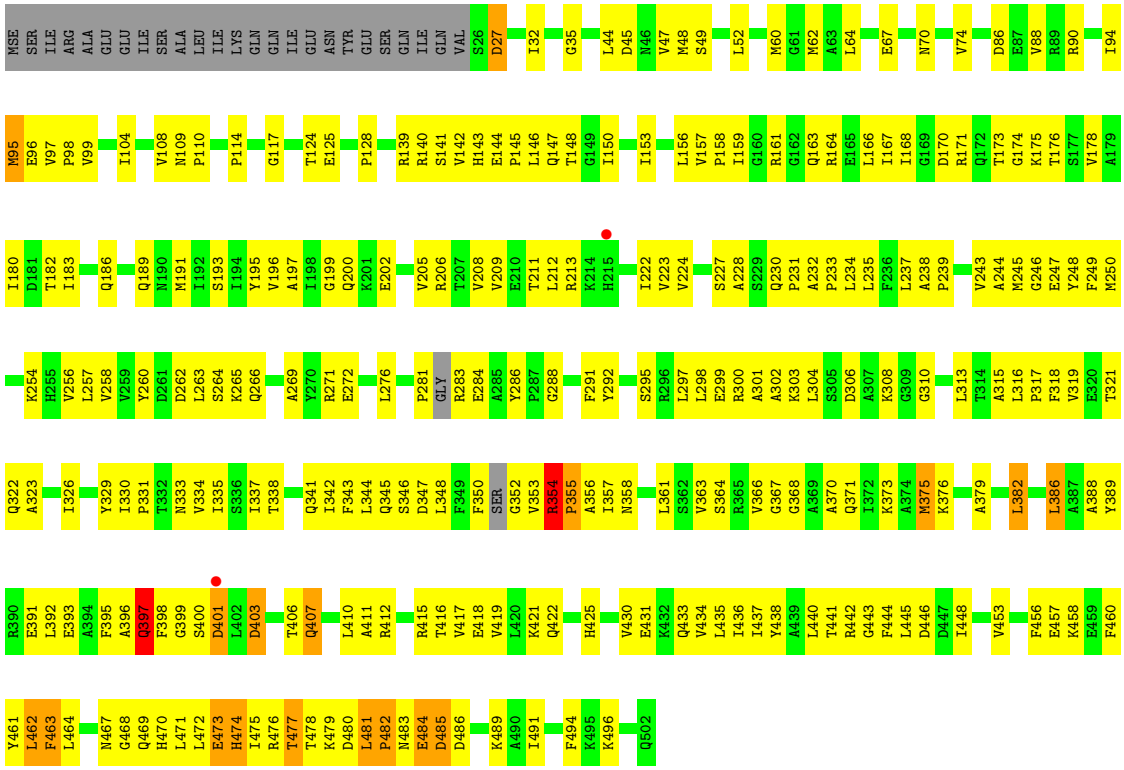
Chain B: 2% 42% 40% • 16%





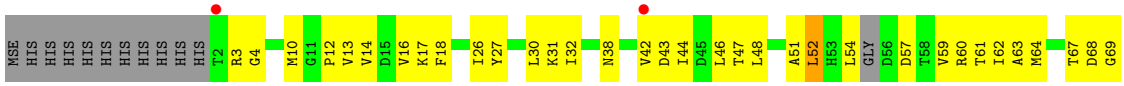
- Molecule 1: ATP synthase subunit alpha

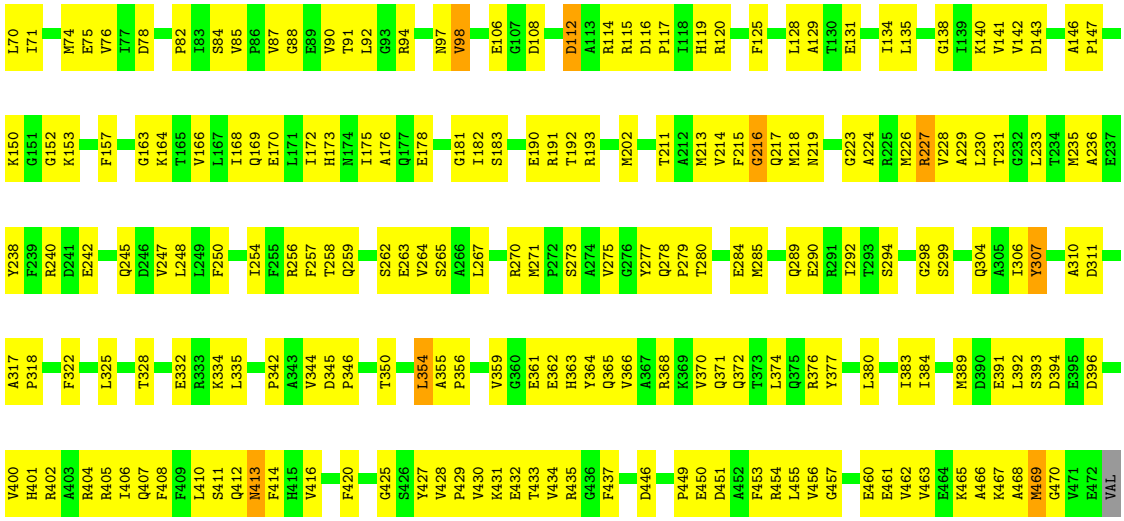
Chain C: 



- Molecule 2: ATP synthase subunit beta

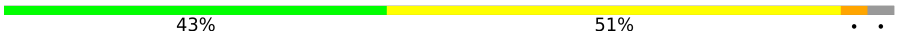
Chain D:

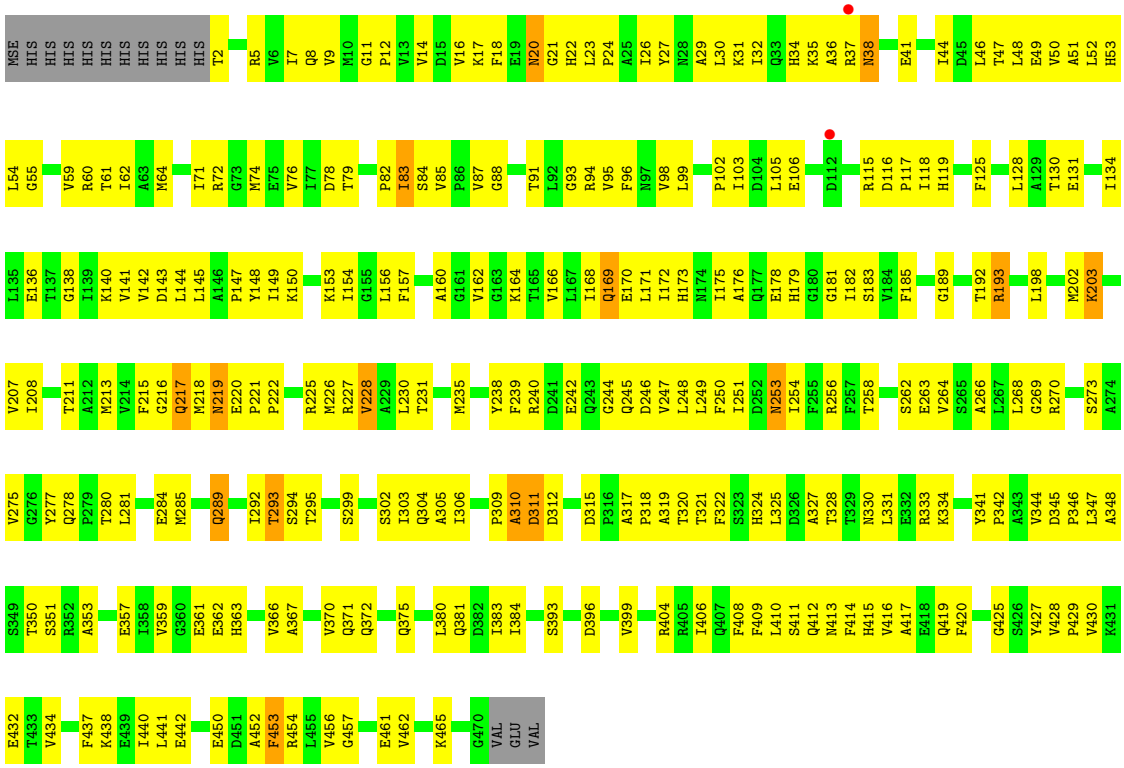




• Molecule 2: ATP synthase subunit beta

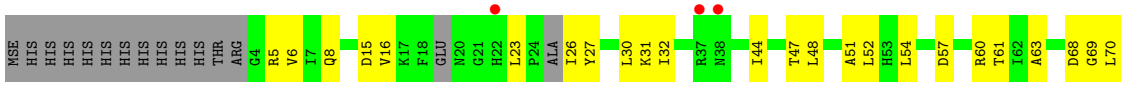
Chain E:





• Molecule 2: ATP synthase subunit beta

Chain F:



I71 R72 G73 M74 E75 V76 T79 P82 I83 S84 V85 P86 V87 V95 F96 N97 P110 D116 P117 I118 H119 R120 E126 I134 L135 E136 T137 G138 I139 K140 V141 V142 D143 L144 L145 A146 P147 Y148 I149 K150 K153 I154 G155 L156 F157 G158 V162 G163 K164 T165 V166

L167 I168 Q169 E170 L171 I172 I175 I182 F185 V188 G189 E190 R191 T192 G195 N196 Y199 H200 E201 M202 K203 D204 S205 G206 V207 I208 S209 A212 M213 V214 F215 G216 Q217 M218 P221 P222 G223 A224 R225 M226 R227 V228 A229 L230 L233 T234 M235 A236 E237 E242

Q243 GLY Q245 D246 V247 L248 L249 F250 N253 I254 F255 R256 F257 T258 Q259 A260 G261 S262 E263 V264 S265 L268 G269 R270 M271 A274 V275 Q278 M285 L288 Q289 E290 R291 I292 T293 S294 S299 I300 T301 S302 I303 Q304 A305 I306 D312 D315 P316 A317 P318 T321

F322 L325 L331 L335 Y341 P342 A343 V344 D345 P346 L347 A348 S349 T350 S351 R352 A353 L354 A355 P356 V359 Y364 Q365 V366 A367 V370 Q371 Q372 T373 L374 Q375 R376 Y377 L380 Q381 D382 I383 I384 A385 I386 M389 D390 E391 L392 S393 D396 K397 V400 H401

R405 I406 F409 Q412 N413 F414 H415 V416 A417 E418 Q419 F420 T421 G422 Q423 P424 Y427 V430 V434 F437 G443 K444 Y445 D446 E450 D451 A452 F453 V456 G457 R458 I459 E460 E461 V462 K465 M469 G470 VAL GLU VAL

- Molecule 3: ATP synthase gamma chain

Chain G: 39% 44% 6% 11%

M1 A2 S3 L4 R5 D6 I7 R10 I11 T14 T17 I20 T21 M24 E25 M26 V27 L32 E36 A39 K40 S41 F42 V43 P44 Y45 M46 E47 K48 V52 V53 A54 N55 V56 A57 L58 GLY ALA GLY GLY ALA SER HIS PRO MSE LEU V69 P72 V73

G77 Y78 L79 V80 I81 T82 S83 D84 R85 G86 L87 A90 Y91 N92 V95 L96 V99 Y100 Q101 T102 I103 Q104 LYS R106 H107 A108 C109 P110 D111 E112 Y113 A114 I115 I116 V117 I118 G119 R120 V121 G122 L123 S124 F125 F126 R129 N130 MSE PRO V133 I134 L135 D136 I137 T138 R139 L140

P141 D142 Q143 P144 S145 I149 T156 V157 G158 L159 F160 A161 D162 GLY T164 F165 D166 E167 L168 Y171 Y172 N173 H174 Y175 A178 I179 Q180 Q181 E182 V183 R186 K187 L188 L189 P190 L191 T192 ASP LEU ALA GLU ASN LYS GLN ARG THR VAL TYR GLU PHE GLU PRO SER Q209 E210

E211 I212 L213 D214 V215 L216 L217 P218 Q219 Y220 A221 E222 S223 L224 I225 Y226 L229 L230 K233 A234 S235 E236 H237 A238 A239 R240 M241 T242 A243 M244 K245 N246 A247 T248 L254 L258 S261 Y262 R266 G280 A281 N282 A283 L284 GLN

- Molecule 4: ATP synthase epsilon chain

Chain H: 5% 45% 46% 6%

M1 K2 T3 I4 H5 V6 S7 V8 P11 E17 D18 M22 V25 K28 S29 GLY E31 I34 L35 H38 I39 P40 L41 V42 A43 P44 L45 E46 I47 K57 THR GLN TYR I61 A62 G66 F67 L68 E69 V70 R71 P72 D73 K74 V75 T76 I77 A82 E83 R84

D87 I88 D89 V90 L91 R92 A93 K94 A95 A96 K97 E98 R99 A100 E101 R102 R103 L104 Q105 S106 D109 D110 I111 D112 F113 K114 R115 A116 E117 L118 A119 L120 M124 N125 R126 L127 S128 V129 A130 E131 M132 K133

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	233.40Å 233.40Å 303.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.90 19.99 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.99-3.90) 99.7 (19.99-3.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.71Å)	Xtriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.250 , 0.282 0.251 , 0.282	Depositor DCC
R_{free} test set	2247 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	123.5	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 86.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	22656	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ADP

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	0.55	0/3496	0.75	0/4711
1	B	0.46	0/2853	0.70	0/3840
1	C	0.49	0/3367	0.74	3/4526 (0.1%)
2	D	0.50	0/3519	0.70	0/4735
2	E	0.54	0/3524	0.74	0/4751
2	F	0.45	0/3362	0.69	0/4504
3	G	0.54	0/1808	0.83	3/2435 (0.1%)
4	H	0.56	0/895	0.80	0/1202
All	All	0.51	0/22824	0.74	6/30704 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
2	D	0	2
2	F	0	1
3	G	0	1
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	484	GLU	N-CA-C	-6.31	93.97	111.00
3	G	217	LEU	CA-CB-CG	5.65	128.28	115.30
1	C	397	GLN	N-CA-C	-5.60	95.87	111.00
3	G	186	ARG	N-CA-C	-5.60	95.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	115	ILE	N-CA-C	5.53	125.93	111.00
1	C	473	GLU	N-CA-C	5.05	124.62	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	354	ARG	Peptide
1	C	401	ASP	Peptide
2	D	216	GLY	Peptide
2	D	391	GLU	Peptide
2	F	215	PHE	Peptide
3	G	188	LEU	Peptide

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	3462	0	3344	321	0
1	B	2833	0	2533	243	0
1	C	3329	0	3032	283	0
2	D	3480	0	3309	272	0
2	E	3484	0	3345	268	0
2	F	3334	0	3069	202	0
3	G	1797	0	1665	192	0
4	H	890	0	833	87	0
5	A	5	0	0	3	0
5	B	5	0	0	1	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
6	F	27	0	12	1	0
All	All	22656	0	21142	1787	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 41.

All (1787) 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:C:262:ASP:H	1:C:318:PHE:HB2	1.05	1.13
1:A:404:LYS:HG3	1:A:405:ALA:H	1.06	1.11
4:H:129:VAL:HG13	4:H:132:MSE:HA	1.33	1.09
2:F:139:ILE:HA	2:F:412:GLN:NE2	1.69	1.07
1:A:32:ILE:HG22	1:A:33:GLN:HG3	1.40	1.04
3:G:189:LEU:H	3:G:190:PRO:CD	1.71	1.02
2:D:31:LYS:HD2	2:D:47:THR:HG22	1.38	1.02
1:C:419:VAL:HG21	1:C:440:LEU:HD13	1.38	1.01
1:B:62:MSE:HE3	1:B:95:MSE:HG3	1.43	1.01
2:F:139:ILE:HA	2:F:412:GLN:HE22	0.86	1.01
4:H:38:HIS:CE1	4:H:41:LEU:HD23	1.96	1.00
1:C:109:ASN:HB2	1:C:110:PRO:HD2	1.43	1.00
1:A:145:PRO:HB3	1:A:370:ALA:O	1.61	1.00
1:B:109:ASN:HB2	1:B:110:PRO:HD2	1.42	1.00
1:C:319:VAL:HG21	1:C:334:VAL:HG11	1.42	0.99
1:A:196:VAL:HG12	1:A:198:ILE:HD11	1.45	0.99
1:B:64:LEU:HD21	1:B:279:ARG:NH2	1.76	0.98
3:G:82:THR:HG22	3:G:83:SER:H	1.27	0.98
2:F:190:GLU:HG3	2:F:191:ARG:H	1.25	0.98
1:A:262:ASP:H	1:A:318:PHE:HB2	1.24	0.97
3:G:82:THR:HG21	3:G:92:ASN:OD1	1.64	0.97
2:E:38:ASN:HD21	2:E:41:GLU:HG3	1.29	0.97
2:D:10:MSE:HB2	2:D:13:VAL:CG1	1.95	0.96
2:D:143:ASP:HB3	2:D:430:VAL:HG22	1.46	0.96
2:F:139:ILE:CA	2:F:412:GLN:HE22	1.78	0.96
1:A:239:PRO:HG2	1:A:266:GLN:HE21	1.29	0.96
1:B:472:LEU:O	1:B:475:ILE:HG22	1.65	0.95
1:A:404:LYS:HG3	1:A:405:ALA:N	1.82	0.95
1:A:233:PRO:HG3	1:A:273:LEU:HD12	1.46	0.94
2:D:271:MSE:HE2	3:G:281:ALA:HB1	1.46	0.94
2:F:253:ASN:H	2:F:305:ALA:HB3	1.31	0.94
1:B:27:ASP:O	1:B:44:LEU:HD23	1.65	0.94
1:C:476:ARG:O	1:C:479:LYS:HG3	1.68	0.94
2:F:6:VAL:HG22	2:F:16:VAL:HG22	1.50	0.94
3:G:173:ASN:OD1	3:G:183:VAL:HG22	1.67	0.93
3:G:189:LEU:N	3:G:190:PRO:CD	2.29	0.93
2:D:10:MSE:HB2	2:D:13:VAL:HG13	1.49	0.93
2:D:216:GLY:HA3	2:D:228:VAL:HG21	1.49	0.93
1:A:104:ILE:HD13	1:A:222:ILE:HD11	1.50	0.92
2:F:31:LYS:HG3	2:F:47:THR:HG22	1.51	0.92
1:A:419:VAL:HG21	1:A:440:LEU:HD13	1.51	0.91
2:D:383:ILE:H	2:D:383:ILE:HD12	1.33	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:154:ILE:HD12	2:F:303:ILE:HG12	1.50	0.91
1:A:148:THR:HG22	1:A:150:ILE:HG13	1.53	0.91
1:A:319:VAL:HG21	1:A:334:VAL:HG11	1.51	0.91
2:F:147:PRO:HG2	2:F:353:ALA:HB3	1.53	0.91
2:E:53:HIS:CD2	2:E:59:VAL:HG12	2.06	0.90
2:F:199:TYR:HD2	2:F:200:HIS:CE1	1.89	0.90
1:C:481:LEU:CB	1:C:482:PRO:HD2	2.01	0.90
1:B:64:LEU:HD21	1:B:279:ARG:HH22	1.32	0.90
1:C:443:GLY:HA2	1:C:446:ASP:OD2	1.72	0.89
1:B:319:VAL:HG21	1:B:334:VAL:HG11	1.54	0.89
1:A:170:ASP:O	1:A:173:THR:HG23	1.73	0.89
2:E:328:THR:HG23	2:E:350:THR:H	1.37	0.89
1:A:198:ILE:HG21	1:A:266:GLN:HB2	1.53	0.88
2:E:181:GLY:HA2	2:E:245:GLN:NE2	1.89	0.88
2:F:168:ILE:HD11	2:F:305:ALA:HB2	1.56	0.88
2:E:289:GLN:HE21	2:E:289:GLN:HA	1.38	0.88
1:B:52:LEU:HD21	1:B:60:MSE:HB3	1.55	0.87
3:G:179:ILE:HD13	3:G:242:THR:HB	1.56	0.87
1:A:440:LEU:HB3	1:A:445:LEU:HD13	1.55	0.87
2:D:193:ARG:HB3	2:D:193:ARG:HH11	1.39	0.86
2:E:408:PHE:CE1	2:E:454:ARG:HD2	2.11	0.86
1:C:262:ASP:N	1:C:318:PHE:HB2	1.89	0.86
2:D:71:ILE:H	2:D:74:MSE:SE	2.10	0.85
2:E:94:ARG:NH1	2:E:106:GLU:HB2	1.90	0.85
3:G:112:GLU:CD	3:G:113:TYR:H	1.80	0.84
3:G:179:ILE:HD13	3:G:242:THR:CB	2.07	0.84
1:B:166:LEU:HB2	1:B:338:THR:HG21	1.58	0.84
1:B:176:THR:O	1:B:180:ILE:HG12	1.77	0.84
1:C:477:THR:HG23	1:C:478:THR:H	1.42	0.84
1:C:146:LEU:HG	1:C:191:MSE:HE2	1.59	0.84
2:E:62:ILE:HD11	2:E:268:LEU:HD21	1.58	0.84
2:F:453:PHE:CD1	2:F:462:VAL:HG11	2.13	0.84
4:H:132:MSE:O	4:H:133:LYS:HG3	1.78	0.84
1:A:109:ASN:HB2	1:A:110:PRO:HD2	1.60	0.83
1:C:96:GLU:HB3	1:C:128:PRO:HA	1.59	0.83
1:A:42:HIS:CA	1:A:42:HIS:CG	2.61	0.83
2:D:181:GLY:HA2	2:D:245:GLN:OE1	1.77	0.83
2:D:405:ARG:HD3	2:D:453:PHE:CZ	2.14	0.83
1:B:107:VAL:HB	1:B:116:ASP:HB3	1.59	0.83
2:F:223:GLY:O	2:F:226:MSE:HB2	1.78	0.83
1:C:444:PHE:CG	1:C:444:PHE:CA	2.62	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:99:VAL:HG11	3:G:126:PHE:CZ	2.13	0.82
3:G:10:ARG:HD2	4:H:129:VAL:HA	1.61	0.82
2:F:415:HIS:CA	2:F:415:HIS:CG	2.62	0.82
2:E:289:GLN:HG3	2:E:324:HIS:CG	2.14	0.82
2:F:96:PHE:CG	2:F:96:PHE:CA	2.62	0.82
1:B:53:VAL:HG21	1:B:73:ILE:CD1	2.09	0.82
2:D:401:HIS:CD2	2:D:405:ARG:HH12	1.98	0.82
2:D:383:ILE:HD12	2:D:383:ILE:N	1.95	0.81
1:B:199:GLY:HA3	1:B:265:LYS:HD3	1.62	0.81
2:E:181:GLY:HA2	2:E:245:GLN:HE21	1.42	0.81
1:A:243:VAL:CG1	1:A:260:TYR:OH	2.29	0.81
1:C:476:ARG:O	1:C:479:LYS:CG	2.28	0.81
2:D:414:PHE:CG	2:D:414:PHE:CA	2.63	0.81
2:E:315:ASP:O	2:E:318:PRO:HD2	1.80	0.81
1:A:395:PHE:CE2	3:G:26:MSE:HE1	2.14	0.81
2:D:64:MSE:HE1	2:D:227:ARG:HB2	1.61	0.81
2:E:53:HIS:HD2	2:E:59:VAL:HG12	1.41	0.81
1:C:412:ARG:O	1:C:416:THR:HG23	1.79	0.81
3:G:82:THR:CG2	3:G:92:ASN:OD1	2.28	0.81
1:C:425:HIS:CA	1:C:425:HIS:CG	2.64	0.81
1:C:475:ILE:O	1:C:479:LYS:HA	1.80	0.81
1:C:355:PRO:O	1:C:357:ILE:HG12	1.81	0.80
2:D:141:VAL:HG11	2:D:344:VAL:HB	1.63	0.80
3:G:10:ARG:CD	4:H:129:VAL:HA	2.11	0.80
2:D:10:MSE:O	2:D:13:VAL:HG12	1.81	0.80
1:B:370:ALA:O	1:B:371:GLN:O	2.00	0.79
2:D:31:LYS:CD	2:D:47:THR:HG22	2.12	0.79
3:G:78:TYR:CD1	3:G:171:TYR:CE1	2.69	0.79
4:H:127:LEU:O	4:H:129:VAL:N	2.16	0.79
1:A:376:LYS:CD	1:A:376:LYS:CB	2.59	0.79
2:D:271:MSE:HE2	3:G:281:ALA:CB	2.12	0.79
2:E:216:GLY:HA3	2:E:228:VAL:HG21	1.64	0.79
3:G:1:MSE:HG2	3:G:2:ALA:H	1.48	0.79
1:A:239:PRO:HG2	1:A:266:GLN:NE2	1.98	0.79
1:B:350:PHE:CD1	1:B:350:PHE:CB	2.66	0.79
1:C:231:PRO:HG2	1:C:234:LEU:HG	1.65	0.79
2:E:46:LEU:HD21	2:E:48:LEU:HD21	1.65	0.79
1:C:391:GLU:O	1:C:391:GLU:HG2	1.82	0.79
1:A:172:GLN:N	5:A:700:SO4:O4	2.15	0.78
1:B:453:VAL:O	1:B:456:PHE:HB3	1.81	0.78
2:E:143:ASP:HB3	2:E:430:VAL:HG22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:428:VAL:HG23	2:E:432:GLU:HB2	1.66	0.78
4:H:8:VAL:HG22	4:H:77:ILE:HB	1.64	0.78
1:B:53:VAL:HG21	1:B:73:ILE:HD12	1.65	0.78
1:A:488:ASN:O	1:A:492:GLU:HG2	1.83	0.78
2:F:315:ASP:O	2:F:318:PRO:HD2	1.82	0.78
1:A:375:MSE:HG2	1:A:434:VAL:HG12	1.66	0.78
1:B:161:ARG:HH12	1:B:191:MSE:HG3	1.48	0.78
2:F:233:LEU:HD23	2:F:291:ARG:HD2	1.64	0.78
4:H:129:VAL:HG13	4:H:132:MSE:CA	2.13	0.78
2:D:193:ARG:HB3	2:D:193:ARG:NH1	1.98	0.78
4:H:38:HIS:HE1	4:H:41:LEU:HD23	1.48	0.78
1:C:382:LEU:HG	1:C:437:ILE:HD11	1.64	0.78
2:D:262:SER:HB3	2:D:278:GLN:OE1	1.84	0.78
2:D:258:THR:HG21	2:D:285:MSE:HE2	1.66	0.78
1:C:431:GLU:HG2	1:C:473:GLU:HG2	1.64	0.78
1:C:230:GLN:HB3	1:C:234:LEU:HD12	1.67	0.77
2:E:85:VAL:HG12	2:E:99:LEU:O	1.84	0.77
2:E:253:ASN:H	2:E:305:ALA:HB3	1.48	0.77
1:C:140:ARG:CZ	1:C:143:HIS:NE2	2.47	0.77
2:D:175:ILE:HG13	2:D:248:LEU:HD11	1.66	0.77
2:E:141:VAL:HG22	2:E:410:LEU:HB3	1.67	0.77
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.65	0.77
1:C:460:PHE:CA	1:C:460:PHE:CG	2.68	0.77
3:G:78:TYR:HD1	3:G:171:TYR:CE1	2.02	0.77
1:B:195:TYR:CE1	1:B:259:VAL:HG11	2.20	0.77
1:C:95:MSE:HE2	1:C:96:GLU:H	1.50	0.77
1:C:263:LEU:CD1	1:C:317:PRO:HB3	2.15	0.76
2:F:8:GLN:HB2	2:F:15:ASP:HB2	1.67	0.76
1:C:250:MSE:HG2	1:C:304:LEU:HD11	1.64	0.76
1:A:416:THR:HA	1:A:440:LEU:CD1	2.15	0.76
1:B:262:ASP:H	1:B:318:PHE:HB2	1.48	0.76
2:F:51:ALA:O	2:F:52:LEU:HD23	1.85	0.76
1:A:53:VAL:CG1	1:A:88:VAL:HG12	2.15	0.76
1:B:64:LEU:CD2	1:B:279:ARG:NH2	2.48	0.76
2:D:3:ARG:CD	2:D:3:ARG:CZ	2.64	0.76
1:A:65:ASN:ND2	1:A:277:LEU:HB3	2.01	0.75
4:H:130:ALA:HB3	4:H:133:LYS:CE	2.16	0.75
2:D:140:LYS:CG	2:D:140:LYS:CA	2.65	0.75
2:D:153:LYS:N	2:D:153:LYS:HD2	2.02	0.75
1:A:29:GLY:HA3	1:A:42:HIS:O	1.86	0.75
2:D:377:TYR:CE1	2:D:400:VAL:HG13	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:383:ILE:H	2:D:383:ILE:CD1	1.99	0.75
2:D:404:ARG:HD3	2:D:450:GLU:OE2	1.87	0.75
3:G:10:ARG:HD2	4:H:128:SER:O	1.87	0.75
2:E:348:ALA:O	2:E:350:THR:HG23	1.87	0.74
1:C:288:GLY:O	2:D:263:GLU:HG3	1.86	0.74
1:B:372:ILE:O	1:B:479:LYS:O	2.05	0.74
1:C:243:VAL:CG1	1:C:260:TYR:OH	2.35	0.74
3:G:78:TYR:HE1	3:G:171:TYR:HH	1.34	0.74
1:B:108:VAL:HG12	1:B:114:PRO:HA	1.68	0.74
2:D:178:GLU:HG3	2:D:427:TYR:CE2	2.23	0.74
3:G:87:LEU:HD23	3:G:244:MSE:HE1	1.70	0.74
1:B:39:ALA:O	1:B:73:ILE:HG22	1.87	0.74
2:D:271:MSE:CE	3:G:281:ALA:HB1	2.16	0.74
2:D:401:HIS:CE1	2:D:405:ARG:HH12	2.06	0.74
2:F:401:HIS:HD2	2:F:405:ARG:NH2	1.84	0.74
3:G:82:THR:HG22	3:G:83:SER:N	2.03	0.74
4:H:91:LEU:O	4:H:94:LYS:N	2.21	0.74
1:B:83:LYS:CD	1:B:83:LYS:CB	2.65	0.73
1:C:395:PHE:O	1:C:397:GLN:HG3	1.88	0.73
2:E:162:VAL:HG11	2:E:331:LEU:HB3	1.70	0.73
1:A:480:ASP:O	1:A:481:LEU:HD23	1.86	0.73
1:B:53:VAL:CG2	1:B:73:ILE:HD11	2.18	0.73
2:F:87:VAL:HG21	2:F:116:ASP:OD2	1.88	0.73
1:C:262:ASP:H	1:C:318:PHE:CB	1.95	0.73
1:C:434:VAL:HA	1:C:437:ILE:HG22	1.70	0.73
2:D:431:LYS:CD	2:D:431:LYS:CB	2.66	0.73
2:D:26:ILE:O	2:D:27:TYR:HB2	1.86	0.73
2:F:212:ALA:HB1	2:F:235:MSE:HE3	1.68	0.73
1:C:27:ASP:O	1:C:90:ARG:HG3	1.89	0.73
1:C:166:LEU:HB2	1:C:338:THR:HG21	1.69	0.73
2:E:428:VAL:HG23	2:E:432:GLU:CB	2.19	0.73
1:A:243:VAL:HG12	1:A:260:TYR:OH	1.89	0.73
2:E:240:ARG:HD2	2:E:295:THR:HG23	1.71	0.73
2:F:405:ARG:CB	2:F:405:ARG:CD	2.66	0.73
1:A:186:GLN:OE1	1:A:191:MSE:HG3	1.89	0.73
1:C:104:ILE:HD13	1:C:222:ILE:HD11	1.71	0.73
1:A:372:ILE:HD12	1:A:375:MSE:H	1.54	0.73
2:E:262:SER:HB3	2:E:278:GLN:OE1	1.89	0.73
2:E:318:PRO:HB2	2:E:322:PHE:CE1	2.24	0.73
1:A:231:PRO:HD2	1:A:234:LEU:HD12	1.71	0.72
1:B:271:ARG:CD	1:B:271:ARG:CB	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:VAL:HG11	1:C:248:TYR:HB2	1.71	0.72
1:C:474:HIS:HA	1:C:477:THR:HG22	1.71	0.72
2:D:466:ALA:O	2:D:469:MSE:N	2.22	0.72
2:E:419:GLN:CA	2:E:419:GLN:CG	2.67	0.72
2:D:202:MSE:HE2	2:D:211:THR:HG21	1.69	0.72
2:E:14:VAL:O	2:E:61:THR:HG22	1.89	0.72
1:B:472:LEU:HD23	1:B:473:GLU:N	2.05	0.72
1:C:263:LEU:HD11	1:C:317:PRO:HB3	1.71	0.72
2:F:192:THR:OG1	2:F:217:GLN:HG3	1.88	0.72
2:D:254:ILE:HD12	2:D:304:GLN:NE2	2.04	0.72
2:F:443:GLY:HA2	2:F:446:ASP:OD1	1.90	0.72
1:A:450:VAL:HA	1:A:453:VAL:HG23	1.70	0.72
1:C:144:GLU:CG	1:C:144:GLU:CA	2.66	0.72
3:G:53:VAL:HG22	3:G:216:LEU:HD13	1.70	0.72
2:D:226:MSE:HG2	2:D:227:ARG:HH11	1.53	0.72
2:E:94:ARG:CB	2:E:94:ARG:CD	2.68	0.72
4:H:125:ASN:C	4:H:127:LEU:H	1.93	0.72
1:C:166:LEU:HD22	1:C:334:VAL:HG22	1.71	0.72
2:E:294:SER:HA	2:E:299:SER:HA	1.71	0.72
2:D:342:PRO:HG3	2:D:414:PHE:CZ	2.25	0.71
2:E:138:GLY:HA3	2:E:427:TYR:CD1	2.25	0.71
2:E:342:PRO:HG3	2:E:414:PHE:CZ	2.25	0.71
3:G:20:ILE:HD13	4:H:119:ALA:HB1	1.69	0.71
3:G:36:GLU:HA	3:G:39:ALA:HB3	1.71	0.71
1:A:161:ARG:HH12	1:A:191:MSE:HG2	1.56	0.71
1:C:156:LEU:O	1:C:158:PRO:HD3	1.90	0.71
1:C:235:LEU:H	1:C:235:LEU:HD12	1.55	0.71
1:A:32:ILE:O	1:A:84:GLU:HG2	1.90	0.71
1:B:195:TYR:HD1	1:B:259:VAL:HB	1.56	0.71
1:C:308:LYS:CE	1:C:308:LYS:CG	2.68	0.71
1:C:345:GLN:O	1:C:356:ALA:HB1	1.91	0.71
1:A:32:ILE:CG2	1:A:33:GLN:HG3	2.19	0.71
1:C:238:ALA:HB3	1:C:239:PRO:HD3	1.72	0.71
2:F:306:ILE:HD13	2:F:321:THR:HG21	1.71	0.71
3:G:96:LEU:CD2	3:G:125:PHE:HB3	2.20	0.71
2:F:72:ARG:CG	2:F:72:ARG:CA	2.69	0.71
3:G:4:LEU:HD21	3:G:262:TYR:CE1	2.26	0.71
1:C:96:GLU:CB	1:C:128:PRO:HA	2.20	0.70
2:D:411:SER:HB2	2:D:455:LEU:HD23	1.72	0.70
3:G:87:LEU:HD23	3:G:244:MSE:CE	2.20	0.70
1:A:62:MSE:CE	1:A:95:MSE:HB2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:GLN:HG2	1:A:164:ARG:N	2.06	0.70
2:E:35:LYS:CA	2:E:36:ALA:N	2.54	0.70
3:G:112:GLU:CD	3:G:113:TYR:N	2.44	0.70
4:H:83:GLU:OE1	4:H:95:ALA:CB	2.38	0.70
1:A:121:VAL:O	1:A:121:VAL:HG23	1.91	0.70
1:A:167:ILE:HD11	1:A:318:PHE:CE2	2.26	0.70
1:A:109:ASN:C	1:A:109:ASN:HD22	1.93	0.70
1:A:196:VAL:CG1	1:A:198:ILE:HD11	2.20	0.70
1:B:161:ARG:HH12	1:B:191:MSE:CG	2.04	0.70
2:E:31:LYS:HD2	2:E:47:THR:HG22	1.74	0.70
1:B:372:ILE:HD11	1:B:434:VAL:HG11	1.72	0.70
2:E:182:ILE:O	2:E:247:VAL:HG13	1.92	0.70
1:B:44:LEU:O	1:B:47:VAL:HG22	1.90	0.70
2:E:277:TYR:CE2	2:E:317:ALA:HB2	2.26	0.70
2:E:408:PHE:HE1	2:E:454:ARG:HD2	1.56	0.70
1:C:271:ARG:HD3	1:C:286:TYR:CD2	2.27	0.70
1:C:52:LEU:HG	1:C:60:MSE:HE3	1.73	0.70
1:A:345:GLN:HG2	1:A:358:ASN:HB2	1.73	0.69
1:C:458:LYS:CB	1:C:458:LYS:CD	2.70	0.69
2:E:258:THR:CG2	2:E:285:MSE:HE2	2.21	0.69
3:G:80:VAL:CG1	3:G:117:VAL:HG22	2.22	0.69
1:B:330:ILE:HB	1:B:331:PRO:HD3	1.73	0.69
2:E:141:VAL:HG11	2:E:344:VAL:HB	1.74	0.69
1:B:145:PRO:HB3	1:B:370:ALA:O	1.91	0.69
1:B:328:ALA:HB3	1:B:331:PRO:HG2	1.73	0.69
2:D:384:ILE:HG23	2:D:389:MSE:SE	2.41	0.69
2:D:457:GLY:HA3	2:D:461:GLU:OE2	1.92	0.69
1:C:167:ILE:HG22	1:C:342:ILE:HB	1.72	0.69
3:G:52:VAL:HG13	4:H:42:VAL:HG11	1.73	0.69
1:B:163:GLN:HG2	1:B:164:ARG:N	2.08	0.69
1:C:463:PHE:O	1:C:467:ASN:HB2	1.92	0.69
2:D:256:ARG:NH1	2:D:259:GLN:HE22	1.90	0.69
3:G:86:GLY:O	3:G:240:ARG:NH1	2.26	0.69
1:A:196:VAL:HG12	1:A:198:ILE:CD1	2.21	0.69
1:C:419:VAL:CG2	1:C:440:LEU:HD13	2.18	0.69
2:F:253:ASN:HA	2:F:305:ALA:O	1.92	0.69
2:D:401:HIS:CE1	2:D:446:ASP:HB3	2.28	0.69
2:F:171:LEU:HD13	2:F:303:ILE:HD13	1.75	0.69
2:F:172:ILE:HD11	2:F:185:PHE:CE2	2.28	0.69
1:A:148:THR:HG21	1:A:153:ILE:HD12	1.73	0.69
2:E:147:PRO:HB2	2:E:353:ALA:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:179:ILE:HD13	3:G:242:THR:OG1	1.93	0.69
2:D:214:VAL:HG12	2:D:228:VAL:HG13	1.74	0.68
2:E:46:LEU:CD2	2:E:48:LEU:HD21	2.23	0.68
2:F:249:LEU:HD23	2:F:292:ILE:HG23	1.75	0.68
2:F:23:LEU:HD21	2:F:57:ASP:HA	1.75	0.68
2:F:48:LEU:HB3	2:F:61:THR:HB	1.73	0.68
2:F:139:ILE:HD12	2:F:414:PHE:HE1	1.58	0.68
1:C:375:MSE:SE	1:C:379:ALA:HB2	2.44	0.68
2:D:214:VAL:CG1	2:D:228:VAL:HG13	2.23	0.68
2:D:377:TYR:HD1	2:D:400:VAL:HG22	1.58	0.68
1:B:241:ALA:O	1:B:245:MSE:HG3	1.93	0.68
1:C:249:PHE:HB3	1:C:254:LYS:HB2	1.74	0.68
2:E:381:GLN:O	2:E:384:ILE:HG22	1.94	0.68
2:D:318:PRO:O	2:D:322:PHE:HD1	1.77	0.68
1:A:110:PRO:HG2	1:A:234:LEU:HD22	1.74	0.68
1:A:382:LEU:HG	1:A:437:ILE:HD11	1.74	0.68
1:C:436:ILE:CB	1:C:461:TYR:OH	2.41	0.68
2:D:27:TYR:O	2:D:82:PRO:HB3	1.94	0.68
2:F:120:ARG:O	2:F:291:ARG:NH2	2.22	0.68
1:A:301:ALA:HB1	1:A:313:LEU:O	1.92	0.68
1:C:330:ILE:HB	1:C:331:PRO:HD3	1.76	0.68
2:E:253:ASN:HA	2:E:305:ALA:O	1.93	0.68
2:F:456:VAL:HG21	2:F:462:VAL:HG22	1.74	0.68
1:C:445:LEU:HD21	1:C:453:VAL:HG22	1.76	0.67
2:D:31:LYS:NZ	2:D:47:THR:CG2	2.57	0.67
2:D:182:ILE:HG23	2:D:183:SER:N	2.08	0.67
1:C:434:VAL:HA	1:C:437:ILE:CG2	2.24	0.67
1:C:231:PRO:HD2	1:C:234:LEU:HD12	1.75	0.67
1:A:163:GLN:HG2	1:A:164:ARG:H	1.60	0.67
2:D:98:VAL:HG21	2:D:224:ALA:HB1	1.77	0.67
2:D:435:ARG:CD	2:D:435:ARG:CB	2.73	0.67
1:B:53:VAL:CG2	1:B:73:ILE:CD1	2.73	0.67
1:B:52:LEU:HG	1:B:95:MSE:HE3	1.77	0.67
2:F:450:GLU:CA	2:F:450:GLU:CG	2.72	0.67
2:D:88:GLY:HA2	2:D:238:TYR:CE2	2.30	0.67
3:G:161:ALA:O	3:G:164:THR:HB	1.94	0.67
2:D:401:HIS:CE1	2:D:446:ASP:O	2.47	0.67
4:H:132:MSE:O	4:H:133:LYS:CG	2.43	0.67
1:A:53:VAL:HG11	1:A:88:VAL:HG12	1.75	0.67
3:G:254:LEU:O	3:G:258:LEU:HG	1.95	0.67
1:A:435:LEU:O	1:A:438:TYR:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HB3	1:B:47:VAL:CG1	2.25	0.67
1:B:193:SER:HB2	1:B:221:THR:OG1	1.96	0.66
2:F:275:VAL:O	2:F:275:VAL:HG12	1.95	0.66
1:B:182:THR:O	1:B:186:GLN:HG2	1.95	0.66
1:B:209:VAL:HG11	2:E:125:PHE:HZ	1.59	0.66
2:F:370:VAL:HG13	2:F:406:ILE:HG21	1.77	0.66
1:C:388:ALA:O	1:C:392:LEU:N	2.28	0.66
2:E:48:LEU:HD13	2:E:61:THR:HG21	1.77	0.66
2:E:168:ILE:HG23	2:E:250:PHE:CE2	2.30	0.66
1:A:395:PHE:CD2	3:G:26:MSE:HE1	2.30	0.66
1:B:430:VAL:O	1:B:434:VAL:HG13	1.95	0.66
2:F:190:GLU:HG3	2:F:191:ARG:N	2.07	0.66
1:A:438:TYR:O	1:A:441:THR:HG22	1.96	0.66
1:C:191:MSE:HE3	1:C:257:LEU:HD12	1.78	0.66
2:D:62:ILE:HD13	2:D:226:MSE:HE1	1.78	0.66
2:D:116:ASP:HB3	2:D:117:PRO:HD2	1.77	0.66
4:H:111:ILE:O	4:H:115:ARG:HG3	1.96	0.66
1:C:199:GLY:O	1:C:228:ALA:HB2	1.95	0.66
1:B:434:VAL:O	1:B:437:ILE:HG22	1.96	0.66
1:C:300:ARG:CD	1:C:300:ARG:CB	2.74	0.66
2:F:155:GLY:HA3	2:F:325:LEU:HD13	1.78	0.66
2:F:199:TYR:CD2	2:F:200:HIS:CE1	2.80	0.66
2:F:372:GLN:OE1	2:F:376:ARG:NH2	2.29	0.66
1:A:404:LYS:HB3	1:A:406:THR:OG1	1.96	0.66
1:C:174:GLY:O	1:C:178:VAL:HG23	1.96	0.66
1:A:419:VAL:CG2	1:A:440:LEU:HD13	2.24	0.66
1:B:343:PHE:HD2	1:B:344:LEU:N	1.93	0.66
1:C:62:MSE:HE3	1:C:95:MSE:HG3	1.78	0.65
2:D:168:ILE:HG23	2:D:250:PHE:CD2	2.31	0.65
2:D:190:GLU:HA	2:D:218:MSE:HE3	1.78	0.65
1:A:210:GLU:O	1:A:213:ARG:N	2.30	0.65
1:C:350:PHE:CE2	2:F:347:LEU:O	2.49	0.65
1:A:90:ARG:CB	1:A:90:ARG:NE	2.59	0.65
1:C:186:GLN:OE1	1:C:191:MSE:HG3	1.97	0.65
1:B:243:VAL:O	1:B:247:GLU:HG3	1.97	0.65
2:F:137:THR:HG21	2:F:148:TYR:CD2	2.32	0.65
2:D:226:MSE:HG2	2:D:227:ARG:NH1	2.11	0.65
2:E:208:ILE:HA	2:E:211:THR:HG22	1.77	0.65
3:G:174:HIS:CG	3:G:175:TYR:H	2.15	0.65
1:A:137:MSE:HG3	2:E:105:LEU:HG	1.78	0.65
1:B:167:ILE:HD12	1:B:318:PHE:HE2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:PHE:HD1	1:C:463:PHE:H	1.44	0.65
2:D:150:LYS:CD	2:D:150:LYS:CB	2.75	0.65
2:F:396:ASP:O	2:F:400:VAL:HG23	1.96	0.65
1:B:207:THR:O	1:B:211:THR:HG23	1.96	0.65
1:C:257:LEU:HD23	1:C:257:LEU:C	2.17	0.65
2:D:216:GLY:CA	2:D:228:VAL:HG21	2.23	0.65
2:E:430:VAL:O	2:E:434:VAL:HG23	1.96	0.65
1:C:301:ALA:HB1	1:C:313:LEU:O	1.96	0.65
2:D:392:LEU:O	2:D:394:ASP:N	2.30	0.65
1:C:474:HIS:O	1:C:474:HIS:HD2	1.81	0.64
1:A:38:ILE:CD1	1:A:74:VAL:HG12	2.27	0.64
2:F:260:ALA:HA	2:F:263:GLU:OE2	1.97	0.64
3:G:179:ILE:CD1	3:G:242:THR:HB	2.27	0.64
1:A:233:PRO:CG	1:A:273:LEU:HD12	2.26	0.64
1:B:75:ILE:HD13	1:B:82:ILE:HD12	1.78	0.64
1:C:474:HIS:C	1:C:474:HIS:CD2	2.70	0.64
2:E:17:LYS:CA	2:E:18:PHE:N	2.60	0.64
2:F:135:LEU:HD12	2:F:150:LYS:HG2	1.79	0.64
2:F:142:VAL:HG13	2:F:146:ALA:O	1.97	0.64
2:F:453:PHE:CE1	2:F:462:VAL:HG11	2.31	0.64
1:A:416:THR:HA	1:A:440:LEU:HD12	1.78	0.64
1:B:261:ASP:HA	1:B:318:PHE:CD1	2.32	0.64
1:C:416:THR:HA	1:C:440:LEU:CD1	2.28	0.64
1:C:445:LEU:O	1:C:445:LEU:HD23	1.97	0.64
2:F:376:ARG:O	2:F:380:LEU:HG	1.96	0.64
3:G:103:ILE:O	3:G:107:HIS:HB3	1.96	0.64
1:A:87:GLU:CG	1:A:87:GLU:CA	2.76	0.64
1:A:146:LEU:HD12	1:A:314:THR:HG21	1.80	0.64
1:C:491:ILE:O	1:C:494:PHE:HB2	1.98	0.64
2:D:64:MSE:CE	2:D:227:ARG:HB2	2.28	0.64
2:D:277:TYR:CE2	2:D:317:ALA:HB2	2.33	0.64
1:A:104:ILE:HD11	1:A:249:PHE:CZ	2.33	0.64
1:A:213:ARG:HD2	1:A:218:LEU:HD12	1.79	0.64
1:B:435:LEU:O	1:B:438:TYR:HB3	1.98	0.64
1:C:371:GLN:HB3	1:C:375:MSE:HB3	1.80	0.64
2:D:120:ARG:CG	2:D:120:ARG:NE	2.60	0.64
2:E:251:ILE:HD12	2:E:304:GLN:HE21	1.63	0.64
1:C:139:ARG:NH1	2:D:192:THR:HB	2.12	0.64
2:D:335:LEU:HD11	2:D:345:ASP:HA	1.80	0.64
3:G:43:VAL:N	3:G:44:PRO:HD2	2.13	0.64
1:A:44:LEU:HB3	1:A:47:VAL:CG1	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:38:ASN:ND2	2:E:41:GLU:HG3	2.10	0.64
2:E:173:HIS:CD2	2:E:415:HIS:ND1	2.66	0.64
1:B:144:GLU:CA	1:B:144:GLU:CG	2.76	0.64
1:C:482:PRO:C	1:C:484:GLU:H	2.00	0.64
1:A:296:ARG:HA	2:E:219:ASN:HB2	1.79	0.63
2:E:94:ARG:HH11	2:E:106:GLU:HB2	1.64	0.63
2:F:354:LEU:O	2:F:364:TYR:HD2	1.80	0.63
2:F:382:ASP:OD1	4:H:128:SER:HB2	1.98	0.63
1:C:208:VAL:O	1:C:212:LEU:HG	1.98	0.63
2:F:6:VAL:CG2	2:F:16:VAL:HG22	2.27	0.63
2:F:294:SER:HB2	2:F:299:SER:HA	1.80	0.63
1:A:198:ILE:HD12	1:A:198:ILE:N	2.13	0.63
1:B:301:ALA:HB2	1:B:313:LEU:HD22	1.80	0.63
2:D:92:LEU:HD21	2:D:182:ILE:CG1	2.29	0.63
2:D:213:MSE:HE2	2:D:215:PHE:CZ	2.33	0.63
2:D:247:VAL:HG12	2:D:248:LEU:N	2.14	0.63
3:G:24:MSE:HE3	3:G:244:MSE:HE3	1.80	0.63
3:G:114:ALA:C	3:G:115:ILE:HG13	2.18	0.63
1:A:392:LEU:O	1:A:394:ALA:N	2.30	0.63
2:D:182:ILE:CG2	2:D:183:SER:N	2.61	0.63
2:F:354:LEU:O	2:F:364:TYR:CD2	2.52	0.63
1:B:55:PHE:CZ	1:B:73:ILE:HD13	2.33	0.63
1:C:232:ALA:HA	1:C:235:LEU:HD13	1.79	0.63
3:G:78:TYR:HD1	3:G:171:TYR:HE1	1.43	0.63
1:A:304:LEU:O	1:A:310:GLY:HA2	1.98	0.63
2:D:362:GLU:O	2:D:366:VAL:HG23	1.99	0.63
1:B:39:ALA:O	1:B:73:ILE:CG2	2.47	0.63
1:C:260:TYR:HB2	1:C:317:PRO:HA	1.80	0.63
1:C:448:ILE:HD12	1:C:456:PHE:CD1	2.33	0.63
1:C:438:TYR:HE1	1:C:489:LYS:HB3	1.63	0.62
2:D:294:SER:HB3	2:D:299:SER:HB2	1.81	0.62
3:G:159:LEU:HD11	3:G:221:ALA:HB3	1.79	0.62
1:C:463:PHE:N	1:C:463:PHE:CD1	2.65	0.62
2:F:430:VAL:O	2:F:434:VAL:HG23	1.99	0.62
1:C:315:ALA:C	1:C:317:PRO:HD3	2.19	0.62
2:E:453:PHE:HD1	2:E:453:PHE:H	1.46	0.62
4:H:106:SER:HB2	4:H:109:ASP:OD2	1.99	0.62
2:D:191:ARG:HH11	2:D:191:ARG:HG3	1.64	0.62
2:F:294:SER:HB3	2:F:300:ILE:H	1.64	0.62
2:D:10:MSE:O	2:D:13:VAL:CG1	2.47	0.62
2:F:383:ILE:HA	4:H:124:MSE:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASP:HA	2:E:125:PHE:HD2	1.64	0.62
1:C:363:VAL:CG1	1:C:364:SER:N	2.62	0.62
1:C:463:PHE:HD1	1:C:463:PHE:N	1.97	0.62
1:C:481:LEU:CB	1:C:482:PRO:CD	2.75	0.62
2:D:131:GLU:CB	2:D:131:GLU:CD	2.68	0.62
2:E:26:ILE:HA	2:E:50:VAL:CG1	2.30	0.62
1:A:499:VAL:HG22	1:A:499:VAL:O	1.99	0.62
2:E:34:HIS:CB	2:E:74:MSE:HE3	2.29	0.62
2:E:134:ILE:HG13	2:E:148:TYR:O	2.00	0.62
2:E:240:ARG:O	2:E:244:GLY:HA2	1.99	0.62
2:E:250:PHE:CE2	2:E:303:ILE:HD12	2.34	0.62
2:F:227:ARG:HD2	2:F:230:LEU:HD12	1.81	0.62
4:H:127:LEU:C	4:H:129:VAL:H	2.01	0.62
1:B:47:VAL:HG12	1:B:90:ARG:HG3	1.82	0.62
1:C:388:ALA:HB1	1:C:392:LEU:HD13	1.82	0.62
1:C:448:ILE:HD12	1:C:456:PHE:CE1	2.35	0.62
1:A:90:ARG:HH21	1:A:92:GLY:HA2	1.63	0.61
1:C:163:GLN:HG2	1:C:164:ARG:N	2.15	0.61
2:E:193:ARG:HB3	2:E:193:ARG:HH11	1.65	0.61
3:G:99:VAL:HG11	3:G:126:PHE:CE2	2.35	0.61
1:A:465:ASP:CG	1:A:465:ASP:CA	2.68	0.61
1:C:363:VAL:HG12	1:C:364:SER:N	2.12	0.61
2:E:51:ALA:O	2:E:52:LEU:HD23	2.00	0.61
3:G:114:ALA:C	3:G:115:ILE:CG1	2.68	0.61
1:C:354:ARG:O	1:C:355:PRO:C	2.38	0.61
1:C:438:TYR:HE2	1:C:442:ARG:CD	2.12	0.61
2:E:278:GLN:HG3	2:E:284:GLU:OE1	2.00	0.61
1:A:104:ILE:HD13	1:A:222:ILE:CD1	2.28	0.61
2:E:183:SER:O	2:E:211:THR:HA	1.99	0.61
2:F:373:THR:HG22	2:F:376:ARG:NH1	2.15	0.61
1:A:232:ALA:HB3	1:A:233:PRO:HD3	1.83	0.61
1:C:140:ARG:NH2	1:C:143:HIS:NE2	2.49	0.61
1:C:392:LEU:O	1:C:395:PHE:HB2	2.00	0.61
2:E:372:GLN:CB	2:E:372:GLN:CD	2.69	0.61
1:A:179:ALA:HB2	1:A:318:PHE:HZ	1.64	0.61
1:A:206:ARG:NH1	2:D:125:PHE:O	2.34	0.61
2:F:196:ASN:OD1	2:F:200:HIS:CE1	2.54	0.61
1:A:67:GLU:HA	2:E:8:GLN:HG2	1.82	0.61
2:D:258:THR:CG2	2:D:285:MSE:HE2	2.29	0.61
2:F:139:ILE:HD12	2:F:414:PHE:CE1	2.35	0.61
3:G:219:GLN:OE1	4:H:66:GLY:HA2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:MSE:HE3	1:A:95:MSE:HB2	1.82	0.61
1:A:206:ARG:HD2	2:D:128:LEU:HB2	1.82	0.61
1:A:209:VAL:HG11	2:D:125:PHE:HZ	1.66	0.61
1:B:30:THR:O	1:B:41:ALA:HB1	1.99	0.61
1:B:33:GLN:OE1	1:B:40:ARG:CZ	2.49	0.61
1:A:457:GLU:CA	1:A:457:GLU:CG	2.79	0.61
1:C:395:PHE:O	1:C:397:GLN:N	2.33	0.61
2:F:26:ILE:HG22	2:F:27:TYR:CD1	2.36	0.61
1:A:209:VAL:HA	1:A:212:LEU:HD12	1.83	0.61
2:E:153:LYS:N	2:E:153:LYS:HD2	2.16	0.61
2:E:115:ARG:HG3	2:E:115:ARG:HH11	1.65	0.60
1:C:67:GLU:CB	1:C:67:GLU:CD	2.69	0.60
1:C:474:HIS:HA	1:C:477:THR:CG2	2.31	0.60
2:F:147:PRO:HD2	2:F:351:SER:HB3	1.82	0.60
3:G:53:VAL:O	3:G:53:VAL:HG12	2.00	0.60
3:G:96:LEU:HG	3:G:126:PHE:HE1	1.66	0.60
1:C:347:ASP:O	1:C:348:LEU:HD23	2.01	0.60
1:A:139:ARG:NH1	1:A:302:ALA:HB2	2.16	0.60
2:F:148:TYR:CD2	2:F:154:ILE:HD13	2.37	0.60
3:G:212:ILE:HG12	4:H:44:PRO:HD3	1.82	0.60
4:H:45:LEU:HB2	4:H:66:GLY:O	2.00	0.60
1:A:124:THR:HG23	1:A:125:GLU:HG3	1.83	0.60
1:B:131:SER:HB3	1:B:300:ARG:HH21	1.67	0.60
1:B:195:TYR:CD1	1:B:259:VAL:HG11	2.37	0.60
1:B:275:LEU:HD21	1:B:281:PRO:HB3	1.82	0.60
2:E:157:PHE:HZ	2:E:322:PHE:HE2	1.50	0.60
2:D:166:VAL:HG13	2:D:416:VAL:HG23	1.84	0.60
2:E:47:THR:O	2:E:48:LEU:HD23	2.01	0.60
2:E:289:GLN:HA	2:E:289:GLN:NE2	2.14	0.60
2:F:195:GLY:HA2	2:F:215:PHE:HE2	1.65	0.60
1:A:345:GLN:CB	1:A:348:LEU:HD23	2.31	0.60
1:A:434:VAL:HA	1:A:437:ILE:HG22	1.83	0.60
2:E:34:HIS:HB3	2:E:74:MSE:HE3	1.82	0.60
1:B:44:LEU:HB3	1:B:47:VAL:HG13	1.83	0.60
1:B:195:TYR:HE1	1:B:259:VAL:HG11	1.63	0.60
1:B:497:THR:C	1:B:499:VAL:H	2.05	0.60
2:E:289:GLN:HG3	2:E:324:HIS:CD2	2.35	0.60
2:E:318:PRO:HB2	2:E:322:PHE:HE1	1.66	0.60
1:B:262:ASP:H	1:B:318:PHE:CB	2.15	0.60
1:C:232:ALA:HB3	1:C:233:PRO:HD3	1.83	0.60
2:D:202:MSE:CE	2:D:211:THR:HG21	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:407:GLN:HA	2:D:410:LEU:HD12	1.84	0.60
2:E:138:GLY:HA3	2:E:427:TYR:CE1	2.37	0.60
1:A:109:ASN:HD21	1:A:113:GLN:H	1.49	0.60
4:H:7:SER:HA	4:H:17:GLU:HG3	1.84	0.60
2:E:453:PHE:N	2:E:453:PHE:CD1	2.70	0.59
2:F:26:ILE:O	2:F:27:TYR:HB2	2.02	0.59
1:B:84:GLU:OE1	2:E:55:GLY:HA2	2.02	0.59
1:B:208:VAL:O	1:B:212:LEU:HG	2.02	0.59
1:A:159:ILE:HA	1:A:163:GLN:OE1	2.02	0.59
1:A:239:PRO:HG2	1:A:266:GLN:HG3	1.84	0.59
1:A:404:LYS:CG	1:A:405:ALA:H	1.93	0.59
2:D:54:LEU:HD11	2:D:60:ARG:NE	2.17	0.59
2:E:413:ASN:CB	2:E:425:GLY:HA2	2.33	0.59
1:A:386:LEU:HD13	1:A:386:LEU:O	2.01	0.59
1:B:151:LYS:HB2	1:B:151:LYS:HZ3	1.66	0.59
1:C:205:VAL:O	1:C:209:VAL:HG12	2.02	0.59
2:D:84:SER:HB3	2:D:115:ARG:O	2.02	0.59
4:H:41:LEU:C	4:H:41:LEU:HD12	2.22	0.59
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.83	0.59
1:A:156:LEU:HD21	1:A:382:LEU:HD12	1.85	0.59
2:F:213:MSE:HB3	2:F:215:PHE:HE1	1.68	0.59
3:G:179:ILE:HD12	3:G:238:ALA:C	2.23	0.59
4:H:89:ASP:O	4:H:91:LEU:N	2.36	0.59
1:C:373:LYS:HB2	1:C:480:ASP:CB	2.33	0.59
2:E:134:ILE:HD12	2:E:147:PRO:HB3	1.85	0.59
2:F:248:LEU:HD23	2:F:301:THR:HB	1.84	0.59
3:G:10:ARG:HD3	4:H:130:ALA:H	1.66	0.59
1:B:284:GLU:O	1:B:285:ALA:HB3	2.03	0.59
1:C:418:GLU:O	1:C:421:LYS:HB2	2.02	0.59
2:E:370:VAL:HG13	2:E:406:ILE:HG21	1.84	0.59
1:A:355:PRO:HB2	1:A:357:ILE:HG12	1.85	0.59
2:D:328:THR:HG22	2:D:350:THR:OG1	2.03	0.59
2:F:401:HIS:CD2	2:F:405:ARG:NH2	2.67	0.59
3:G:87:LEU:CD2	3:G:244:MSE:HE1	2.32	0.59
1:C:263:LEU:HD12	1:C:317:PRO:HB3	1.85	0.59
2:D:230:LEU:O	2:D:233:LEU:HB3	2.02	0.59
3:G:226:TYR:CZ	3:G:230:LEU:HD21	2.37	0.59
1:B:292:TYR:HA	1:B:295:SER:OG	2.02	0.59
1:C:62:MSE:HE3	1:C:95:MSE:CG	2.33	0.59
2:D:85:VAL:HG11	2:D:231:THR:HG23	1.85	0.59
2:D:401:HIS:HE1	2:D:446:ASP:O	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:289:GLN:O	2:F:292:ILE:N	2.35	0.59
1:A:48:MSE:HG2	2:E:71:ILE:HD11	1.83	0.58
1:B:195:TYR:HD1	1:B:259:VAL:CB	2.15	0.58
3:G:72:PRO:CG	3:G:166:ASP:OD2	2.51	0.58
4:H:22:MSE:HB2	4:H:35:LEU:HD23	1.85	0.58
4:H:125:ASN:O	4:H:127:LEU:N	2.36	0.58
1:A:151:LYS:HA	1:A:433:GLN:OE1	2.02	0.58
1:C:202:GLU:OE1	1:C:227:SER:HB2	2.03	0.58
1:C:416:THR:HG22	1:C:440:LEU:CD1	2.33	0.58
2:D:98:VAL:HG11	2:D:224:ALA:HA	1.86	0.58
2:F:212:ALA:HB1	2:F:235:MSE:CE	2.33	0.58
3:G:78:TYR:HE1	3:G:171:TYR:OH	1.85	0.58
3:G:96:LEU:HD21	3:G:125:PHE:HB3	1.83	0.58
1:A:74:VAL:HG11	1:A:273:LEU:HD21	1.86	0.58
1:C:438:TYR:O	1:C:441:THR:HG22	2.03	0.58
2:E:29:ALA:HB2	2:E:83:ILE:H	1.68	0.58
2:F:288:LEU:O	2:F:288:LEU:HG	2.03	0.58
4:H:129:VAL:HG22	4:H:132:MSE:SE	2.53	0.58
1:C:482:PRO:HB3	1:C:485:ASP:O	2.03	0.58
1:C:484:GLU:O	1:C:485:ASP:C	2.41	0.58
1:C:485:ASP:CG	1:C:486:ASP:H	2.07	0.58
2:D:175:ILE:HG13	2:D:248:LEU:CD1	2.32	0.58
1:A:101:GLU:CG	1:A:101:GLU:CA	2.81	0.58
1:A:108:VAL:HG12	1:A:114:PRO:HA	1.84	0.58
1:A:294:HIS:O	1:A:298:LEU:HD13	2.03	0.58
1:A:403:ASP:O	1:A:407:GLN:HG3	2.04	0.58
1:B:167:ILE:HD11	1:B:316:LEU:HB3	1.85	0.58
1:C:148:THR:HG23	1:C:182:THR:OG1	2.01	0.58
2:E:44:ILE:HG13	2:E:74:MSE:HE1	1.85	0.58
2:D:48:LEU:HD13	2:D:61:THR:OG1	2.04	0.58
3:G:174:HIS:CG	3:G:175:TYR:N	2.72	0.58
2:E:306:ILE:CD1	2:E:325:LEU:HD11	2.34	0.58
2:F:172:ILE:HD11	2:F:185:PHE:HE2	1.68	0.58
3:G:96:LEU:HD23	3:G:125:PHE:HB3	1.86	0.58
1:A:167:ILE:HD11	1:A:318:PHE:CZ	2.38	0.58
2:D:354:LEU:O	2:D:354:LEU:HD22	2.04	0.58
3:G:118:ILE:HA	3:G:138:THR:HB	1.84	0.58
1:B:55:PHE:CE1	1:B:73:ILE:HD11	2.38	0.58
1:B:96:GLU:HB3	1:B:126:THR:HG22	1.86	0.58
2:D:307:TYR:HD2	2:D:307:TYR:O	1.87	0.58
1:A:372:ILE:HD12	1:A:372:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:452:ALA:O	2:E:465:LYS:HD3	2.04	0.58
1:A:489:LYS:HA	1:A:492:GLU:HB2	1.86	0.57
1:B:492:GLU:CA	1:B:493:ALA:N	2.67	0.57
1:C:333:ASN:O	1:C:337:ILE:HG13	2.03	0.57
2:E:328:THR:CG2	2:E:350:THR:OG1	2.52	0.57
4:H:97:LYS:O	4:H:100:ALA:N	2.33	0.57
1:B:107:VAL:HG12	1:B:115:VAL:CG2	2.34	0.57
2:D:254:ILE:O	2:D:254:ILE:HG12	2.03	0.57
3:G:3:SER:HB2	3:G:6:ASP:CB	2.34	0.57
1:B:64:LEU:CD2	1:B:279:ARG:HH21	2.17	0.57
1:C:407:GLN:HA	1:C:410:LEU:HD12	1.86	0.57
2:D:456:VAL:HG21	2:D:462:VAL:HG22	1.86	0.57
2:F:207:VAL:O	2:F:209:SER:N	2.36	0.57
2:F:237:GLU:OE1	2:F:291:ARG:HD3	2.04	0.57
1:A:143:HIS:ND1	1:A:144:GLU:N	2.51	0.57
1:B:55:PHE:CD2	1:B:82:ILE:HD13	2.39	0.57
1:B:452:ASP:O	1:B:455:ARG:HB2	2.03	0.57
2:E:24:PRO:HB3	2:E:78:ASP:OD1	2.04	0.57
2:E:48:LEU:CD1	2:E:61:THR:HG21	2.34	0.57
2:E:413:ASN:HB3	2:E:425:GLY:HA2	1.86	0.57
2:F:364:TYR:O	2:F:367:ALA:HB3	2.05	0.57
3:G:225:ILE:HD12	3:G:226:TYR:N	2.18	0.57
1:A:65:ASN:HD22	1:A:277:LEU:HB3	1.69	0.57
1:B:163:GLN:HG2	1:B:164:ARG:H	1.70	0.57
1:C:434:VAL:CA	1:C:437:ILE:HG22	2.35	0.57
2:D:213:MSE:HE2	2:D:215:PHE:CE1	2.38	0.57
2:E:341:TYR:HA	2:E:342:PRO:C	2.25	0.57
3:G:100:TYR:HD1	3:G:129:ARG:HD2	1.70	0.57
1:A:104:ILE:HA	1:A:222:ILE:CD1	2.34	0.57
1:A:172:GLN:CA	5:A:700:SO4:O4	2.53	0.57
1:A:233:PRO:HG3	1:A:273:LEU:CD1	2.30	0.57
1:A:297:LEU:HG	1:A:298:LEU:HD12	1.87	0.57
2:E:366:VAL:HG13	2:E:441:LEU:HD12	1.85	0.57
3:G:109:CYS:N	3:G:110:PRO:CD	2.67	0.57
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.85	0.57
3:G:216:LEU:HG	4:H:67:PHE:CE1	2.39	0.57
2:D:310:ALA:O	2:D:311:ASP:C	2.43	0.57
3:G:1:MSE:HG2	3:G:2:ALA:N	2.16	0.57
1:C:170:ASP:O	1:C:173:THR:HG23	2.05	0.57
1:C:354:ARG:CB	1:C:355:PRO:CD	2.83	0.57
3:G:1:MSE:CG	3:G:2:ALA:H	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:PRO:HB3	1:B:238:ALA:HA	1.86	0.57
1:C:345:GLN:O	1:C:356:ALA:CB	2.52	0.57
2:D:135:LEU:HB2	2:D:150:LYS:CB	2.34	0.57
2:D:342:PRO:HG3	2:D:414:PHE:CE1	2.40	0.57
2:E:62:ILE:CD1	2:E:268:LEU:HD21	2.33	0.57
1:A:109:ASN:ND2	1:A:113:GLN:H	2.03	0.56
1:B:133:ALA:CB	1:B:300:ARG:HA	2.35	0.56
1:B:231:PRO:HB2	1:B:233:PRO:HD2	1.86	0.56
1:C:48:MSE:HB3	2:D:69:GLY:HA2	1.86	0.56
3:G:83:SER:HB3	3:G:236:GLU:CD	2.25	0.56
3:G:87:LEU:N	3:G:87:LEU:HD12	2.19	0.56
3:G:133:VAL:O	3:G:133:VAL:HG12	2.05	0.56
1:B:133:ALA:HB2	1:B:300:ARG:HA	1.86	0.56
1:B:206:ARG:HA	1:B:209:VAL:HG12	1.87	0.56
2:F:83:ILE:HD12	2:F:118:ILE:HD11	1.86	0.56
1:B:98:PRO:HG2	1:B:112:GLY:HA3	1.87	0.56
1:B:432:LYS:O	1:B:436:ILE:HD13	2.05	0.56
1:B:445:LEU:HD21	1:B:453:VAL:HG22	1.86	0.56
1:C:191:MSE:CE	1:C:257:LEU:HB2	2.35	0.56
1:C:485:ASP:N	1:C:485:ASP:OD1	2.38	0.56
2:D:463:VAL:O	2:D:466:ALA:HB3	2.05	0.56
1:A:97:VAL:O	1:A:126:THR:HG23	2.04	0.56
1:A:267:ALA:HB2	1:A:294:HIS:CE1	2.41	0.56
1:B:109:ASN:HB2	1:B:110:PRO:CD	2.24	0.56
1:B:210:GLU:OE1	2:E:130:THR:OG1	2.24	0.56
1:A:401:ASP:O	1:A:402:LEU:C	2.44	0.56
1:A:488:ASN:C	1:A:492:GLU:HG2	2.25	0.56
2:F:384:ILE:HD12	2:F:392:LEU:HD11	1.86	0.56
1:C:109:ASN:HB2	1:C:110:PRO:CD	2.27	0.56
2:D:94:ARG:NH1	2:D:106:GLU:HB2	2.21	0.56
2:D:178:GLU:HG3	2:D:427:TYR:CD2	2.40	0.56
2:E:64:MSE:HE1	2:E:227:ARG:HB2	1.87	0.56
1:B:148:THR:HG23	1:B:182:THR:OG1	2.05	0.56
1:B:232:ALA:HB3	1:B:233:PRO:HD3	1.88	0.56
1:C:148:THR:HA	1:C:182:THR:HG23	1.87	0.56
1:C:292:TYR:HA	1:C:295:SER:OG	2.06	0.56
2:E:26:ILE:HA	2:E:50:VAL:HG12	1.88	0.56
2:E:48:LEU:HD13	2:E:61:THR:CG2	2.35	0.56
2:F:265:SER:HB2	2:F:278:GLN:HB3	1.87	0.56
1:A:145:PRO:HA	1:A:160:GLY:HA2	1.87	0.56
1:A:159:ILE:HD11	1:A:165:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:PHE:CE1	1:B:73:ILE:CD1	2.89	0.56
1:B:337:ILE:HA	2:F:218:MSE:HE1	1.87	0.56
2:D:14:VAL:HB	2:D:61:THR:OG1	2.05	0.56
2:D:46:LEU:HD11	2:D:63:ALA:HB1	1.88	0.56
2:F:353:ALA:O	2:F:359:VAL:HG13	2.05	0.56
1:A:274:SER:OG	1:A:279:ARG:HD2	2.05	0.56
1:A:450:VAL:HA	1:A:453:VAL:CG2	2.36	0.56
1:C:283:ARG:HD2	1:C:329:TYR:CD1	2.41	0.56
1:C:386:LEU:O	1:C:386:LEU:HD13	2.05	0.56
1:C:477:THR:HG23	1:C:478:THR:N	2.19	0.56
2:D:275:VAL:O	2:D:275:VAL:HG12	2.06	0.56
2:F:253:ASN:HB3	2:F:256:ARG:HG2	1.87	0.56
4:H:127:LEU:C	4:H:129:VAL:N	2.53	0.56
1:A:66:LEU:HD23	1:A:71:VAL:HG13	1.88	0.56
2:D:91:THR:HG21	2:D:235:MSE:HE2	1.88	0.56
2:D:401:HIS:CD2	2:D:405:ARG:NH1	2.71	0.56
2:E:37:ARG:HG2	2:E:41:GLU:OE1	2.06	0.56
2:F:6:VAL:HG23	2:F:76:VAL:CG2	2.36	0.56
2:F:71:ILE:H	2:F:74:MSE:SE	2.39	0.56
2:F:237:GLU:OE2	2:F:291:ARG:HG3	2.06	0.56
2:F:384:ILE:CD1	2:F:392:LEU:HD11	2.35	0.56
4:H:25:VAL:HG21	4:H:68:LEU:HD22	1.86	0.56
1:B:193:SER:O	1:B:221:THR:HA	2.06	0.55
1:B:262:ASP:OD2	1:B:265:LYS:HG3	2.06	0.55
1:C:145:PRO:HB3	1:C:370:ALA:O	2.06	0.55
3:G:4:LEU:HD21	3:G:262:TYR:HE1	1.70	0.55
3:G:112:GLU:CG	3:G:113:TYR:H	2.20	0.55
1:A:412:ARG:O	1:A:416:THR:HG23	2.06	0.55
1:B:179:ALA:O	1:B:183:ILE:HG13	2.06	0.55
2:D:223:GLY:HA2	2:D:226:MSE:HE2	1.87	0.55
3:G:143:GLN:O	3:G:145:SER:N	2.39	0.55
4:H:28:LYS:O	4:H:29:SER:HB2	2.06	0.55
1:A:158:PRO:HD2	1:A:364:SER:HB3	1.89	0.55
1:B:110:PRO:HG2	1:B:234:LEU:HD22	1.88	0.55
1:C:243:VAL:HG12	1:C:260:TYR:OH	2.07	0.55
1:C:335:ILE:HG23	1:C:341:GLN:OE1	2.06	0.55
2:E:93:GLY:HA2	2:E:208:ILE:HG12	1.88	0.55
3:G:36:GLU:O	3:G:39:ALA:N	2.39	0.55
3:G:85:ARG:H	3:G:85:ARG:HD2	1.71	0.55
1:A:396:ALA:O	1:A:399:GLY:N	2.39	0.55
2:D:182:ILE:O	2:D:247:VAL:HG13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:137:THR:HG22	2:F:175:ILE:HD11	1.88	0.55
3:G:24:MSE:SE	4:H:116:ALA:HB1	2.56	0.55
3:G:36:GLU:O	3:G:40:LYS:N	2.40	0.55
3:G:109:CYS:N	3:G:110:PRO:HD3	2.22	0.55
3:G:123:LEU:HD23	3:G:123:LEU:O	2.06	0.55
1:B:62:MSE:CE	1:B:95:MSE:HG3	2.28	0.55
1:C:395:PHE:O	1:C:397:GLN:CG	2.54	0.55
2:D:413:ASN:HB2	2:D:425:GLY:HA2	1.86	0.55
3:G:142:ASP:O	3:G:143:GLN:HB2	2.05	0.55
2:D:191:ARG:H	2:D:218:MSE:HE3	1.70	0.55
4:H:129:VAL:CG2	4:H:132:MSE:SE	3.04	0.55
1:A:319:VAL:CG2	1:A:334:VAL:HG11	2.33	0.55
1:B:107:VAL:O	1:B:115:VAL:HG22	2.06	0.55
1:B:171:ARG:HB2	1:B:320:GLU:OE2	2.07	0.55
1:C:140:ARG:NH1	1:C:306:ASP:OD1	2.40	0.55
2:D:224:ALA:O	2:D:228:VAL:HG23	2.06	0.55
2:E:94:ARG:HH12	2:E:106:GLU:HB2	1.67	0.55
2:E:275:VAL:O	2:E:275:VAL:HG12	2.06	0.55
2:F:393:SER:O	2:F:397:LYS:HG3	2.07	0.55
1:A:206:ARG:HD3	2:D:129:ALA:O	2.06	0.55
1:B:240:TYR:OH	1:B:293:LEU:HD12	2.07	0.55
2:D:152:GLY:C	2:D:153:LYS:HD2	2.27	0.55
2:E:202:MSE:HE2	2:E:207:VAL:HG23	1.89	0.55
1:A:51:GLU:OE2	1:A:90:ARG:NE	2.40	0.54
1:B:159:ILE:HA	1:B:163:GLN:OE1	2.07	0.54
2:D:262:SER:CB	2:D:278:GLN:OE1	2.53	0.54
2:D:453:PHE:CD2	2:D:462:VAL:HG11	2.42	0.54
3:G:181:GLN:HE22	3:G:239:ALA:HB2	1.72	0.54
1:C:322:GLN:O	1:C:323:ALA:HB3	2.07	0.54
2:E:366:VAL:O	2:E:370:VAL:HG23	2.07	0.54
1:B:452:ASP:O	1:B:456:PHE:N	2.38	0.54
2:D:91:THR:CG2	2:D:235:MSE:HE2	2.38	0.54
2:F:48:LEU:HD13	2:F:61:THR:OG1	2.07	0.54
1:C:99:VAL:HG13	1:C:245:MSE:HA	1.90	0.54
1:C:197:ALA:HB1	1:C:200:GLN:HB2	1.90	0.54
2:E:277:TYR:CZ	2:E:317:ALA:HB2	2.42	0.54
2:F:341:TYR:HA	2:F:342:PRO:C	2.27	0.54
2:F:355:ALA:O	2:F:359:VAL:HG22	2.08	0.54
3:G:21:THR:HG21	3:G:248:THR:N	2.22	0.54
1:A:150:ILE:HD12	1:A:153:ILE:HD12	1.88	0.54
1:A:161:ARG:HH12	1:A:191:MSE:CG	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLU:O	1:A:434:VAL:HG22	2.08	0.54
2:D:176:ALA:HA	2:D:181:GLY:H	1.73	0.54
2:E:203:LYS:NZ	2:E:203:LYS:HB3	2.22	0.54
2:F:386:ILE:HB	4:H:124:MSE:CE	2.37	0.54
1:A:212:LEU:HB3	1:A:217:ALA:HB3	1.89	0.54
2:F:271:MSE:HE1	3:G:283:ALA:HB2	1.88	0.54
2:F:344:VAL:O	2:F:346:PRO:HD3	2.07	0.54
3:G:40:LYS:HG3	3:G:41:SER:N	2.21	0.54
3:G:52:VAL:HG22	4:H:69:GLU:HG2	1.89	0.54
3:G:87:LEU:CD2	3:G:244:MSE:CE	2.85	0.54
1:C:104:ILE:HD13	1:C:222:ILE:CD1	2.37	0.54
2:D:31:LYS:HD2	2:D:47:THR:CG2	2.24	0.54
1:A:206:ARG:O	1:A:209:VAL:HG12	2.08	0.54
1:A:455:ARG:NH2	1:A:458:LYS:HZ2	2.05	0.54
2:D:67:THR:HB	2:D:70:LEU:HD12	1.89	0.54
2:E:35:LYS:O	2:E:36:ALA:N	2.41	0.54
2:E:322:PHE:HD2	2:E:325:LEU:HD12	1.73	0.54
2:F:95:VAL:HA	2:F:213:MSE:O	2.08	0.54
3:G:143:GLN:O	3:G:144:PRO:C	2.44	0.54
1:A:262:ASP:N	1:A:318:PHE:HB2	2.08	0.54
1:B:204:THR:O	1:B:208:VAL:HG23	2.08	0.54
2:D:17:LYS:HG3	2:D:57:ASP:O	2.07	0.54
2:D:430:VAL:O	2:D:434:VAL:HG23	2.08	0.54
4:H:125:ASN:C	4:H:127:LEU:N	2.58	0.54
1:B:195:TYR:CD1	1:B:259:VAL:CG1	2.90	0.53
1:B:239:PRO:HG2	1:B:266:GLN:CD	2.28	0.53
1:C:124:THR:HG23	1:C:125:GLU:H	1.73	0.53
1:C:371:GLN:HB3	1:C:375:MSE:CB	2.38	0.53
1:C:481:LEU:O	1:C:483:ASN:N	2.41	0.53
2:D:191:ARG:HG3	2:D:191:ARG:NH1	2.23	0.53
2:E:262:SER:HA	2:E:278:GLN:HB3	1.91	0.53
3:G:84:ASP:N	3:G:84:ASP:OD1	2.41	0.53
1:B:171:ARG:O	1:B:172:GLN:HB3	2.08	0.53
2:F:268:LEU:CD1	2:F:270:ARG:CZ	2.86	0.53
1:B:250:MSE:HE2	1:B:251:TYR:CD1	2.43	0.53
2:E:32:ILE:HG12	2:E:76:VAL:HG22	1.89	0.53
2:F:345:ASP:HB3	2:F:348:ALA:HB3	1.90	0.53
2:F:356:PRO:HD3	2:F:364:TYR:CE2	2.43	0.53
1:B:238:ALA:HB3	1:B:239:PRO:HD3	1.89	0.53
2:E:17:LYS:O	2:E:18:PHE:N	2.41	0.53
2:F:85:VAL:O	2:F:87:VAL:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:175:TYR:CE1	3:G:178:ALA:O	2.61	0.53
4:H:46:GLU:HG3	4:H:47:ILE:N	2.23	0.53
3:G:40:LYS:O	3:G:42:PHE:N	2.41	0.53
3:G:78:TYR:CD1	3:G:171:TYR:HE1	2.20	0.53
1:B:175:LYS:CE	5:B:700:SO4:O4	2.56	0.53
1:B:452:ASP:HA	1:B:455:ARG:HB2	1.91	0.53
1:B:497:THR:C	1:B:499:VAL:N	2.60	0.53
1:B:44:LEU:O	2:F:72:ARG:NH2	2.41	0.53
1:C:354:ARG:O	1:C:356:ALA:N	2.42	0.53
2:D:168:ILE:O	2:D:172:ILE:HG13	2.09	0.53
2:F:383:ILE:HA	4:H:124:MSE:CE	2.38	0.53
4:H:4:ILE:O	4:H:4:ILE:HG23	2.09	0.53
1:C:258:VAL:CG2	1:C:313:LEU:HD21	2.38	0.53
1:C:281:PRO:HG2	3:G:280:GLY:HA2	1.89	0.53
2:D:322:PHE:HA	2:D:325:LEU:HD12	1.90	0.53
2:E:7:ILE:O	2:E:72:ARG:HG2	2.09	0.53
2:E:128:LEU:HA	2:E:295:THR:HA	1.90	0.53
2:E:345:ASP:OD1	2:E:348:ALA:N	2.38	0.53
1:C:468:GLY:O	1:C:470:HIS:N	2.42	0.53
3:G:42:PHE:CZ	3:G:46:MSE:HE2	2.44	0.53
1:B:131:SER:HB3	1:B:300:ARG:NH2	2.24	0.53
1:C:144:GLU:O	1:C:161:ARG:HG3	2.09	0.53
1:C:163:GLN:HG2	1:C:164:ARG:H	1.74	0.53
2:D:140:LYS:HE2	2:D:457:GLY:O	2.08	0.53
1:A:104:ILE:HA	1:A:222:ILE:HD13	1.89	0.52
1:B:492:GLU:O	1:B:493:ALA:N	2.42	0.52
2:D:277:TYR:HE2	2:D:317:ALA:HB2	1.72	0.52
2:E:2:THR:HB	2:E:22:HIS:CE1	2.44	0.52
2:E:51:ALA:HB3	2:E:60:ARG:O	2.09	0.52
3:G:114:ALA:HB3	3:G:165:PHE:HE1	1.73	0.52
1:A:38:ILE:HG13	1:A:276:LEU:HB3	1.91	0.52
2:D:361:GLU:O	2:D:365:GLN:N	2.41	0.52
2:D:410:LEU:HD23	2:D:437:PHE:CZ	2.45	0.52
2:F:356:PRO:HD3	2:F:364:TYR:CD2	2.44	0.52
4:H:97:LYS:O	4:H:99:ARG:N	2.43	0.52
1:B:472:LEU:O	1:B:475:ILE:CG2	2.49	0.52
1:C:346:SER:C	1:C:348:LEU:H	2.13	0.52
2:D:401:HIS:CG	2:D:405:ARG:HH12	2.27	0.52
2:D:404:ARG:CD	2:D:450:GLU:OE2	2.57	0.52
1:B:453:VAL:O	1:B:456:PHE:CB	2.55	0.52
1:C:197:ALA:HB1	1:C:200:GLN:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:LEU:HD11	1:C:453:VAL:HG13	1.92	0.52
2:E:149:ILE:HD12	2:E:149:ILE:N	2.24	0.52
4:H:41:LEU:HD12	4:H:42:VAL:N	2.25	0.52
1:A:103:LEU:HB3	1:A:222:ILE:HD12	1.91	0.52
1:A:151:LYS:NZ	1:A:422:GLN:HB2	2.24	0.52
1:B:108:VAL:HG12	1:B:114:PRO:CA	2.38	0.52
1:C:161:ARG:HH22	1:C:189:GLN:HB3	1.74	0.52
3:G:20:ILE:CD1	4:H:119:ALA:HB1	2.38	0.52
3:G:56:VAL:HG21	3:G:211:GLU:OE2	2.08	0.52
1:A:166:LEU:HD12	1:A:167:ILE:N	2.25	0.52
1:A:291:PHE:HB3	2:E:263:GLU:OE1	2.09	0.52
1:C:176:THR:O	1:C:180:ILE:HG12	2.08	0.52
2:D:134:ILE:HG12	2:D:135:LEU:N	2.23	0.52
2:D:247:VAL:HG12	2:D:248:LEU:H	1.75	0.52
3:G:25:GLU:CD	3:G:245:LYS:HD3	2.30	0.52
3:G:139:ARG:C	3:G:141:PRO:HD3	2.29	0.52
1:A:64:LEU:HD12	1:A:273:LEU:HD21	1.91	0.52
1:A:150:ILE:HA	1:A:422:GLN:OE1	2.10	0.52
1:C:222:ILE:HG22	1:C:223:VAL:H	1.75	0.52
2:D:370:VAL:HG13	2:D:406:ILE:HG21	1.92	0.52
2:F:30:LEU:HD12	2:F:61:THR:HG21	1.90	0.52
2:F:221:PRO:HB2	2:F:222:PRO:HD2	1.92	0.52
3:G:221:ALA:O	3:G:225:ILE:HG13	2.10	0.52
1:C:416:THR:HG22	1:C:440:LEU:HD11	1.91	0.52
1:C:444:PHE:CA	1:C:444:PHE:CD2	2.93	0.52
2:E:87:VAL:HG21	2:E:116:ASP:OD2	2.10	0.52
3:G:72:PRO:HG2	3:G:166:ASP:OD2	2.09	0.52
3:G:80:VAL:HG11	3:G:117:VAL:HG22	1.92	0.52
1:B:52:LEU:CG	1:B:95:MSE:HE3	2.40	0.52
1:C:400:SER:O	1:C:401:ASP:C	2.47	0.52
1:C:496:LYS:N	1:C:496:LYS:HD2	2.25	0.52
2:D:94:ARG:HH11	2:D:106:GLU:HB2	1.74	0.52
2:E:150:LYS:HD2	2:E:246:ASP:OD1	2.10	0.52
2:F:237:GLU:OE2	2:F:291:ARG:CG	2.58	0.52
3:G:103:ILE:HG22	3:G:104:GLN:N	2.24	0.52
2:D:32:ILE:HD11	2:D:76:VAL:HG22	1.92	0.52
2:F:258:THR:OG1	2:F:285:MSE:HE2	2.10	0.52
3:G:20:ILE:HD13	4:H:119:ALA:CB	2.39	0.52
1:A:139:ARG:NH1	1:A:302:ALA:CB	2.73	0.51
1:A:180:ILE:O	1:A:184:ILE:HG13	2.10	0.51
1:A:275:LEU:HD21	1:A:281:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLN:O	1:A:376:LYS:HE3	2.10	0.51
1:B:272:GLU:CD	2:E:280:THR:HA	2.30	0.51
1:C:354:ARG:CB	1:C:355:PRO:HD3	2.40	0.51
1:C:431:GLU:HB3	1:C:472:LEU:O	2.10	0.51
2:D:457:GLY:HA3	2:D:461:GLU:CD	2.30	0.51
2:F:227:ARG:CD	2:F:230:LEU:HD12	2.41	0.51
3:G:216:LEU:HG	4:H:67:PHE:CZ	2.45	0.51
1:B:372:ILE:HD11	1:B:434:VAL:CG1	2.40	0.51
1:B:434:VAL:C	1:B:437:ILE:HG22	2.30	0.51
1:C:209:VAL:HA	1:C:212:LEU:HD12	1.91	0.51
2:D:138:GLY:HA2	2:D:428:VAL:O	2.10	0.51
2:E:144:LEU:CD1	2:E:367:ALA:HB2	2.40	0.51
2:E:145:LEU:HD22	2:E:371:GLN:CG	2.40	0.51
2:E:238:TYR:CE1	2:E:242:GLU:HG2	2.46	0.51
2:F:32:ILE:HG12	2:F:76:VAL:HG22	1.92	0.51
1:A:207:THR:O	1:A:211:THR:HG22	2.10	0.51
1:B:345:GLN:HB2	1:B:348:LEU:HB2	1.93	0.51
1:A:283:ARG:HH22	2:E:275:VAL:HG12	1.76	0.51
2:D:307:TYR:C	2:D:307:TYR:CD2	2.84	0.51
2:F:140:LYS:N	2:F:412:GLN:OE1	2.44	0.51
1:A:131:SER:HB3	1:A:300:ARG:NH2	2.25	0.51
1:B:328:ALA:HB3	1:B:331:PRO:CG	2.41	0.51
1:C:206:ARG:HA	1:C:209:VAL:HG12	1.93	0.51
1:B:170:ASP:O	1:B:173:THR:HG23	2.10	0.51
2:D:377:TYR:HE1	2:D:400:VAL:HG13	1.73	0.51
2:D:401:HIS:NE2	2:D:405:ARG:NH2	2.57	0.51
2:E:347:LEU:HD13	2:E:375:GLN:OE1	2.10	0.51
3:G:72:PRO:HG2	3:G:73:VAL:H	1.75	0.51
1:A:400:SER:OG	1:A:400:SER:CA	2.58	0.51
1:C:183:ILE:HG23	1:C:193:SER:OG	2.11	0.51
1:C:262:ASP:OD2	1:C:264:SER:HB2	2.11	0.51
2:D:30:LEU:HD23	2:D:78:ASP:HA	1.92	0.51
2:E:48:LEU:HB3	2:E:61:THR:OG1	2.10	0.51
2:E:370:VAL:HG21	2:E:437:PHE:HD2	1.75	0.51
1:A:415:ARG:O	1:A:418:GLU:HB2	2.11	0.51
1:C:474:HIS:CA	1:C:477:THR:HG22	2.40	0.51
2:F:225:ARG:HA	2:F:228:VAL:HG22	1.92	0.51
1:A:103:LEU:HD21	1:A:245:MSE:HE2	1.93	0.51
2:E:254:ILE:O	2:E:254:ILE:HG12	2.11	0.51
2:E:415:HIS:HD2	2:E:425:GLY:HA3	1.75	0.51
3:G:175:TYR:HE1	3:G:178:ALA:O	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:62:ALA:O	4:H:82:ALA:HA	2.11	0.51
1:A:109:ASN:C	1:A:109:ASN:ND2	2.63	0.51
1:A:331:PRO:O	1:A:335:ILE:HG13	2.10	0.51
1:B:195:TYR:CE1	1:B:259:VAL:CG1	2.93	0.51
1:B:491:ILE:O	1:B:494:PHE:N	2.33	0.51
1:C:32:ILE:HG22	1:C:32:ILE:O	2.10	0.51
2:E:96:PHE:CG	2:E:235:MSE:HE1	2.45	0.51
2:F:48:LEU:HD23	2:F:63:ALA:HA	1.91	0.51
1:A:345:GLN:HB3	1:A:348:LEU:HD23	1.92	0.50
1:B:161:ARG:NH1	1:B:191:MSE:SE	2.94	0.50
1:B:299:GLU:OE1	2:F:192:THR:HB	2.11	0.50
1:C:250:MSE:HG2	1:C:304:LEU:CD1	2.39	0.50
1:C:335:ILE:C	1:C:337:ILE:H	2.14	0.50
1:C:368:GLY:O	1:C:376:LYS:HE2	2.11	0.50
1:C:415:ARG:HG2	1:C:445:LEU:HD22	1.93	0.50
1:C:445:LEU:HG	1:C:456:PHE:CD1	2.47	0.50
1:C:474:HIS:O	1:C:474:HIS:CD2	2.63	0.50
2:D:4:GLY:O	2:D:76:VAL:N	2.38	0.50
2:D:429:PRO:HG2	2:D:432:GLU:HG2	1.92	0.50
1:A:172:GLN:HA	5:A:700:SO4:O4	2.10	0.50
1:B:66:LEU:HD23	1:B:71:VAL:HG13	1.92	0.50
1:B:161:ARG:HH12	1:B:191:MSE:SE	2.44	0.50
1:C:476:ARG:O	1:C:479:LYS:HG2	2.09	0.50
2:D:166:VAL:HG11	2:D:414:PHE:HD1	1.76	0.50
1:A:157:VAL:HG21	1:A:362:SER:HB3	1.94	0.50
2:E:84:SER:HA	2:E:116:ASP:O	2.11	0.50
2:E:172:ILE:HD12	2:E:202:MSE:CE	2.41	0.50
2:E:189:GLY:O	2:E:218:MSE:HE3	2.11	0.50
2:F:195:GLY:HA2	2:F:215:PHE:CE2	2.46	0.50
1:A:44:LEU:HD22	1:A:47:VAL:CG1	2.42	0.50
1:C:235:LEU:H	1:C:235:LEU:CD1	2.24	0.50
2:D:262:SER:CA	2:D:278:GLN:OE1	2.60	0.50
2:F:261:GLY:O	2:F:264:VAL:HG22	2.11	0.50
3:G:21:THR:HG21	3:G:247:ALA:HB3	1.92	0.50
4:H:6:VAL:HG12	4:H:18:ASP:O	2.10	0.50
1:C:74:VAL:CG1	1:C:233:PRO:HB3	2.41	0.50
1:C:460:PHE:CE2	1:C:464:LEU:HD11	2.46	0.50
2:D:153:LYS:N	2:D:153:LYS:CD	2.74	0.50
2:D:178:GLU:HG3	2:D:427:TYR:CZ	2.46	0.50
2:D:190:GLU:C	2:D:217:GLN:HE22	2.14	0.50
2:E:315:ASP:C	2:E:318:PRO:HD2	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:458:ARG:HG3	2:F:461:GLU:HG3	1.93	0.50
3:G:96:LEU:HG	3:G:126:PHE:CE1	2.44	0.50
2:D:30:LEU:HB3	2:D:76:VAL:CG1	2.40	0.50
2:D:31:LYS:HZ3	2:D:47:THR:CG2	2.24	0.50
2:E:130:THR:HG23	2:E:131:GLU:N	2.27	0.50
2:F:44:ILE:HG21	2:F:70:LEU:HD21	1.93	0.50
1:A:292:TYR:CE2	1:A:296:ARG:HD3	2.47	0.50
1:A:365:ARG:C	1:A:367:GLY:H	2.14	0.50
1:B:33:GLN:OE1	1:B:40:ARG:NH2	2.45	0.50
2:E:309:PRO:O	2:E:311:ASP:N	2.45	0.50
1:A:151:LYS:HE3	1:A:428:ILE:HD12	1.94	0.50
1:A:455:ARG:NH2	1:A:458:LYS:NZ	2.60	0.50
2:D:31:LYS:CE	2:D:47:THR:HG22	2.41	0.50
3:G:77:GLY:HA3	3:G:165:PHE:CZ	2.47	0.50
4:H:39:ILE:HD12	4:H:39:ILE:O	2.12	0.50
2:F:71:ILE:HG22	2:F:72:ARG:N	2.27	0.50
3:G:102:THR:O	3:G:107:HIS:HB2	2.12	0.50
3:G:242:THR:O	3:G:245:LYS:N	2.28	0.50
1:B:44:LEU:HB3	1:B:47:VAL:HG11	1.93	0.49
1:B:453:VAL:HG12	1:B:454:ARG:N	2.27	0.49
1:C:257:LEU:HD23	1:C:258:VAL:N	2.27	0.49
2:D:264:VAL:O	2:D:267:LEU:N	2.45	0.49
2:D:289:GLN:NE2	2:D:292:ILE:HD12	2.27	0.49
2:E:26:ILE:O	2:E:27:TYR:HB2	2.11	0.49
2:E:414:PHE:O	2:E:417:ALA:HB3	2.12	0.49
2:F:5:ARG:HA	2:F:74:MSE:O	2.12	0.49
1:C:208:VAL:O	1:C:211:THR:HG22	2.12	0.49
2:E:226:MSE:HE3	2:E:227:ARG:NE	2.26	0.49
2:F:190:GLU:CG	2:F:191:ARG:H	2.05	0.49
3:G:96:LEU:CD2	3:G:125:PHE:CB	2.90	0.49
1:A:145:PRO:O	1:A:161:ARG:HG3	2.12	0.49
2:D:413:ASN:N	2:D:413:ASN:OD1	2.45	0.49
2:E:440:ILE:HD11	2:E:453:PHE:CD2	2.46	0.49
3:G:100:TYR:CD1	3:G:129:ARG:HD2	2.47	0.49
1:B:262:ASP:OD2	1:B:264:SER:HB2	2.13	0.49
2:F:290:GLU:O	2:F:293:THR:HG22	2.12	0.49
1:C:243:VAL:HG23	1:C:244:ALA:N	2.28	0.49
1:C:398:PHE:N	1:C:398:PHE:CD1	2.80	0.49
1:C:431:GLU:O	1:C:434:VAL:HG22	2.12	0.49
2:E:94:ARG:NH1	2:E:106:GLU:CB	2.70	0.49
2:E:428:VAL:HG23	2:E:432:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:96:LEU:HD23	3:G:125:PHE:CB	2.42	0.49
1:B:167:ILE:HD12	1:B:318:PHE:CE2	2.44	0.49
1:C:397:GLN:O	1:C:398:PHE:C	2.51	0.49
2:F:458:ARG:HH11	2:F:460:GLU:HB2	1.76	0.49
3:G:95:VAL:HG23	3:G:96:LEU:N	2.27	0.49
1:A:241:ALA:O	1:A:245:MSE:HG3	2.13	0.49
1:B:206:ARG:O	1:B:209:VAL:HG12	2.12	0.49
2:D:414:PHE:CA	2:D:414:PHE:CD2	2.95	0.49
2:E:277:TYR:HD2	2:E:281:LEU:HD22	1.78	0.49
1:A:444:PHE:HE1	1:A:490:ALA:HA	1.77	0.49
1:B:270:TYR:CD2	1:B:293:LEU:HD22	2.48	0.49
1:B:492:GLU:CA	1:B:492:GLU:O	2.60	0.49
2:D:332:GLU:HG3	2:D:334:LYS:H	1.78	0.49
2:E:359:VAL:HB	2:E:363:HIS:HB3	1.95	0.49
2:E:362:GLU:HG3	2:E:434:VAL:HG11	1.95	0.49
1:A:94:ILE:O	1:A:95:MSE:C	2.51	0.49
1:A:206:ARG:HA	1:A:209:VAL:HG12	1.95	0.49
1:A:372:ILE:HB	1:A:479:LYS:HB3	1.93	0.49
1:A:151:LYS:NZ	1:A:151:LYS:HB2	2.28	0.49
1:B:295:SER:O	1:B:299:GLU:HB2	2.12	0.49
1:C:95:MSE:HE2	1:C:96:GLU:N	2.22	0.49
1:C:171:ARG:HD3	2:F:322:PHE:HB3	1.94	0.49
2:F:31:LYS:HD3	2:F:79:THR:CG2	2.43	0.49
2:F:188:VAL:HG13	2:F:228:VAL:HG23	1.95	0.49
2:F:250:PHE:HE1	2:F:303:ILE:HD12	1.76	0.49
2:F:397:LYS:NZ	2:F:397:LYS:HB3	2.28	0.49
2:F:465:LYS:O	2:F:469:MSE:HG2	2.13	0.49
1:A:408:ALA:O	1:A:411:ALA:HB3	2.12	0.48
1:B:355:PRO:HB2	1:B:357:ILE:HG12	1.95	0.48
1:C:95:MSE:SE	1:C:237:LEU:HD21	2.63	0.48
1:C:153:ILE:O	1:C:157:VAL:O	2.30	0.48
2:D:138:GLY:HA3	2:D:427:TYR:CD1	2.48	0.48
2:D:401:HIS:NE2	2:D:405:ARG:NH1	2.55	0.48
2:E:450:GLU:C	2:E:452:ALA:H	2.16	0.48
4:H:102:ARG:HH11	4:H:102:ARG:HG3	1.78	0.48
1:C:139:ARG:CZ	1:C:302:ALA:HB2	2.42	0.48
2:E:412:GLN:HG2	2:E:413:ASN:N	2.28	0.48
2:F:140:LYS:H	2:F:412:GLN:CD	2.17	0.48
2:F:445:TYR:HB3	2:F:453:PHE:HZ	1.77	0.48
1:B:164:ARG:HH12	1:B:299:GLU:CD	2.16	0.48
1:C:196:VAL:HG13	1:C:224:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:SER:C	1:C:348:LEU:N	2.66	0.48
2:D:54:LEU:HD11	2:D:60:ARG:HE	1.78	0.48
2:E:258:THR:HG23	2:E:285:MSE:HE2	1.94	0.48
2:F:135:LEU:HD23	2:F:135:LEU:C	2.33	0.48
1:A:341:GLN:CD	1:A:341:GLN:N	2.67	0.48
1:A:385:ASP:OD2	1:A:412:ARG:HD2	2.14	0.48
1:B:159:ILE:HG23	1:B:163:GLN:OE1	2.13	0.48
1:B:217:ALA:HA	1:B:220:TYR:CE2	2.49	0.48
1:B:450:VAL:O	1:B:451:GLU:C	2.50	0.48
2:D:13:VAL:HG21	2:D:60:ARG:HD3	1.95	0.48
2:D:31:LYS:HZ3	2:D:47:THR:HG21	1.77	0.48
2:D:51:ALA:O	2:D:52:LEU:HD23	2.12	0.48
2:E:29:ALA:HB3	2:E:79:THR:OG1	2.13	0.48
2:E:82:PRO:HG2	2:E:117:PRO:HB2	1.95	0.48
2:E:309:PRO:HG2	2:E:318:PRO:HD3	1.95	0.48
2:F:348:ALA:O	2:F:350:THR:HG23	2.13	0.48
1:C:64:LEU:CD1	1:C:74:VAL:HG21	2.44	0.48
1:C:117:GLY:HA3	2:F:126:GLU:OE2	2.14	0.48
1:C:440:LEU:HD23	1:C:441:THR:H	1.78	0.48
2:D:16:VAL:HB	2:D:59:VAL:HG23	1.96	0.48
2:D:172:ILE:HD12	2:D:202:MSE:HE3	1.96	0.48
2:E:273:SER:HB3	2:E:277:TYR:O	2.14	0.48
2:F:156:LEU:HD13	2:F:167:LEU:HD23	1.94	0.48
1:A:30:THR:CG2	1:A:85:GLY:HA2	2.43	0.48
1:A:298:LEU:HD12	1:A:298:LEU:N	2.28	0.48
1:B:456:PHE:CE2	1:B:460:PHE:HB2	2.49	0.48
2:D:30:LEU:HB3	2:D:76:VAL:HG12	1.94	0.48
2:E:342:PRO:HB2	2:E:344:VAL:HG23	1.94	0.48
2:E:410:LEU:HD23	2:E:437:PHE:HZ	1.79	0.48
2:F:366:VAL:O	2:F:370:VAL:HG23	2.13	0.48
4:H:22:MSE:HG3	4:H:34:ILE:O	2.13	0.48
1:A:46:ASN:HB3	1:A:90:ARG:NH1	2.29	0.48
1:A:424:LEU:HD23	1:A:425:HIS:CG	2.49	0.48
2:D:64:MSE:HE3	2:D:224:ALA:HA	1.94	0.48
2:E:231:THR:O	2:E:235:MSE:HG3	2.13	0.48
1:C:161:ARG:HH12	1:C:191:MSE:HG2	1.78	0.48
1:C:197:ALA:HB1	1:C:200:GLN:CG	2.44	0.48
2:D:191:ARG:N	2:D:218:MSE:HE3	2.29	0.48
2:E:456:VAL:HG21	2:E:462:VAL:HG22	1.95	0.48
3:G:14:THR:OG1	3:G:254:LEU:HD23	2.14	0.48
4:H:104:LEU:C	4:H:106:SER:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:MSE:O	1:A:73:ILE:HG23	2.14	0.48
1:A:350:PHE:C	1:A:352:GLY:H	2.17	0.48
1:C:326:ILE:HD11	1:C:343:PHE:CZ	2.49	0.48
2:D:119:HIS:HE1	2:D:227:ARG:NH2	2.12	0.48
2:E:53:HIS:CD2	2:E:59:VAL:CG1	2.88	0.48
2:F:163:GLY:HA2	6:F:600:ADP:O2A	2.14	0.48
2:F:253:ASN:N	2:F:305:ALA:HB3	2.13	0.48
3:G:42:PHE:HD1	4:H:11:PRO:HA	1.79	0.48
3:G:78:TYR:CE1	3:G:171:TYR:OH	2.65	0.48
1:A:286:TYR:CD2	1:A:290:ILE:HG12	2.49	0.48
1:A:299:GLU:HG3	2:E:219:ASN:HB3	1.95	0.48
2:D:240:ARG:HG3	2:D:299:SER:N	2.28	0.48
2:E:130:THR:HG23	2:E:131:GLU:H	1.79	0.48
2:E:408:PHE:O	2:E:411:SER:OG	2.28	0.48
2:F:6:VAL:HG23	2:F:76:VAL:HG21	1.96	0.48
3:G:80:VAL:HG21	3:G:99:VAL:HG21	1.95	0.48
4:H:89:ASP:C	4:H:91:LEU:N	2.67	0.48
1:A:432:LYS:O	1:A:461:TYR:HE2	1.97	0.47
1:C:440:LEU:HD23	1:C:441:THR:N	2.29	0.47
2:E:292:ILE:O	2:E:293:THR:HG23	2.13	0.47
2:F:144:LEU:HD21	2:F:370:VAL:HG21	1.95	0.47
3:G:80:VAL:O	3:G:80:VAL:HG13	2.14	0.47
3:G:85:ARG:HB3	4:H:113:PHE:CE2	2.49	0.47
1:A:109:ASN:ND2	1:A:111:LEU:H	2.11	0.47
1:A:167:ILE:O	1:A:167:ILE:HG13	2.13	0.47
1:C:35:GLY:HA3	2:F:52:LEU:HD22	1.95	0.47
4:H:68:LEU:HG	4:H:70:VAL:HG23	1.94	0.47
4:H:88:ILE:HG23	4:H:90:VAL:N	2.28	0.47
1:A:38:ILE:HD11	1:A:74:VAL:HG12	1.95	0.47
1:A:48:MSE:HA	2:E:71:ILE:HG12	1.95	0.47
1:A:99:VAL:HG21	1:A:127:ARG:CB	2.45	0.47
1:A:146:LEU:HD21	1:A:257:LEU:HD12	1.96	0.47
1:A:429:PRO:HG2	1:A:432:LYS:HG2	1.96	0.47
1:C:292:TYR:HB2	2:D:263:GLU:OE2	2.14	0.47
2:D:377:TYR:CD1	2:D:400:VAL:HG22	2.44	0.47
2:E:49:GLU:N	2:E:61:THR:OG1	2.46	0.47
2:E:88:GLY:HA2	2:E:238:TYR:CE2	2.48	0.47
2:E:162:VAL:CG1	2:E:331:LEU:HB3	2.42	0.47
2:F:418:GLU:O	2:F:422:GLY:N	2.47	0.47
1:A:53:VAL:HG12	1:A:88:VAL:HG12	1.94	0.47
1:B:217:ALA:HA	1:B:220:TYR:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:VAL:HA	1:B:453:VAL:HG23	1.96	0.47
1:C:108:VAL:HA	1:C:114:PRO:HA	1.96	0.47
1:C:167:ILE:HD11	1:C:318:PHE:CE2	2.49	0.47
1:C:345:GLN:HB3	1:C:347:ASP:HB3	1.97	0.47
1:C:382:LEU:CG	1:C:437:ILE:HD11	2.42	0.47
2:D:355:ALA:HB1	2:D:356:PRO:HD2	1.97	0.47
2:E:118:ILE:HG13	2:E:119:HIS:N	2.29	0.47
2:E:380:LEU:HA	2:E:383:ILE:HG22	1.96	0.47
2:E:429:PRO:HG2	2:E:432:GLU:HG2	1.96	0.47
2:F:54:LEU:HD21	2:F:60:ARG:HB2	1.97	0.47
2:F:249:LEU:HD23	2:F:292:ILE:CG2	2.42	0.47
3:G:46:MSE:CE	3:G:223:SER:O	2.62	0.47
1:A:64:LEU:CD1	1:A:273:LEU:HD21	2.45	0.47
1:A:99:VAL:CG1	1:A:248:TYR:HB2	2.45	0.47
1:C:269:ALA:O	1:C:272:GLU:HB3	2.14	0.47
1:C:313:LEU:C	1:C:313:LEU:HD23	2.35	0.47
1:C:344:LEU:HA	1:C:356:ALA:O	2.13	0.47
2:D:318:PRO:O	2:D:322:PHE:CD1	2.65	0.47
2:E:140:LYS:HG2	2:E:428:VAL:HG11	1.94	0.47
2:F:145:LEU:HD22	2:F:371:GLN:HG3	1.96	0.47
4:H:93:ALA:O	4:H:97:LYS:N	2.48	0.47
1:C:199:GLY:HA3	1:C:265:LYS:HD3	1.95	0.47
2:D:214:VAL:HG12	2:D:228:VAL:CG1	2.44	0.47
2:D:307:TYR:O	2:D:307:TYR:CD2	2.65	0.47
2:E:361:GLU:O	2:E:362:GLU:C	2.51	0.47
2:F:172:ILE:HD11	2:F:185:PHE:CD2	2.49	0.47
1:A:96:GLU:CB	1:A:128:PRO:HA	2.45	0.47
1:A:375:MSE:HG2	1:A:434:VAL:CG1	2.41	0.47
1:B:55:PHE:CZ	1:B:73:ILE:CD1	2.97	0.47
1:B:165:GLU:OE2	1:B:341:GLN:N	2.48	0.47
1:B:449:PRO:O	1:B:453:VAL:HG23	2.15	0.47
1:C:44:LEU:O	1:C:47:VAL:HG22	2.14	0.47
1:C:430:VAL:HA	1:C:433:GLN:HE21	1.79	0.47
2:D:280:THR:HG23	2:D:284:GLU:CD	2.35	0.47
2:E:17:LYS:CA	2:E:17:LYS:O	2.62	0.47
2:E:156:LEU:HD21	2:E:164:LYS:CG	2.44	0.47
2:E:277:TYR:CD2	2:E:281:LEU:HD22	2.50	0.47
2:E:285:MSE:HG2	2:E:320:THR:HG22	1.97	0.47
2:F:222:PRO:O	2:F:226:MSE:HG2	2.15	0.47
1:A:249:PHE:HB2	1:A:256:VAL:CG2	2.45	0.47
1:B:40:ARG:HA	1:B:71:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ALA:HB1	1:B:313:LEU:O	2.15	0.47
1:C:48:MSE:SE	2:D:42:VAL:HG23	2.65	0.47
2:D:4:GLY:O	2:D:75:GLU:HA	2.15	0.47
3:G:80:VAL:HG13	3:G:117:VAL:HG13	1.97	0.47
1:A:480:ASP:O	1:A:481:LEU:CD2	2.62	0.47
1:B:31:VAL:HB	1:B:85:GLY:H	1.80	0.47
1:C:140:ARG:NH1	1:C:306:ASP:OD2	2.48	0.47
1:C:142:VAL:O	1:C:142:VAL:HG23	2.14	0.47
1:C:222:ILE:HG22	1:C:223:VAL:N	2.30	0.47
2:D:157:PHE:HE1	2:D:306:ILE:HB	1.79	0.47
1:A:126:THR:HG22	1:A:127:ARG:N	2.30	0.46
1:C:291:PHE:CZ	2:D:256:ARG:NH1	2.84	0.46
2:F:44:ILE:HG21	2:F:70:LEU:CD2	2.45	0.46
2:F:233:LEU:CD2	2:F:291:ARG:HD2	2.39	0.46
3:G:32:LEU:HD21	3:G:238:ALA:HB2	1.96	0.46
3:G:157:VAL:O	3:G:161:ALA:HB2	2.15	0.46
4:H:110:ASP:OD1	4:H:114:LYS:HE3	2.15	0.46
1:A:434:VAL:CA	1:A:437:ILE:HG22	2.45	0.46
1:A:474:HIS:CE1	1:A:478:THR:HG21	2.50	0.46
1:B:66:LEU:CD2	1:B:71:VAL:HG13	2.45	0.46
1:C:235:LEU:HD12	1:C:235:LEU:N	2.28	0.46
2:D:265:SER:OG	2:D:270:ARG:HB2	2.15	0.46
1:A:32:ILE:HG22	1:A:33:GLN:CG	2.28	0.46
1:A:62:MSE:CE	1:A:95:MSE:CB	2.90	0.46
1:A:80:THR:C	1:A:82:ILE:H	2.17	0.46
1:A:271:ARG:HD2	1:A:285:ALA:HB3	1.98	0.46
1:A:322:GLN:C	1:A:324:GLY:H	2.19	0.46
1:B:166:LEU:HD11	1:B:319:VAL:HG23	1.97	0.46
1:B:337:ILE:HG12	2:F:218:MSE:SE	2.66	0.46
2:E:162:VAL:O	2:E:162:VAL:HG12	2.16	0.46
2:E:266:ALA:O	2:E:269:GLY:N	2.40	0.46
1:A:283:ARG:HD2	1:A:329:TYR:CD1	2.51	0.46
1:B:116:ASP:HA	2:E:125:PHE:CD2	2.47	0.46
1:B:171:ARG:O	1:B:172:GLN:CB	2.63	0.46
1:B:262:ASP:C	1:B:264:SER:N	2.67	0.46
1:C:124:THR:HG23	1:C:125:GLU:N	2.29	0.46
2:D:264:VAL:O	2:D:265:SER:C	2.54	0.46
2:D:317:ALA:HB3	2:D:318:PRO:CD	2.45	0.46
2:D:411:SER:O	2:D:412:GLN:HB2	2.15	0.46
2:E:95:VAL:O	2:E:102:PRO:HA	2.15	0.46
2:E:310:ALA:O	2:E:312:ASP:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:89:ASP:C	4:H:91:LEU:H	2.17	0.46
1:A:95:MSE:SE	1:A:237:LEU:HD21	2.66	0.46
1:A:210:GLU:O	1:A:213:ARG:HB3	2.15	0.46
1:A:298:LEU:N	1:A:298:LEU:CD1	2.78	0.46
1:C:97:VAL:HB	1:C:98:PRO:HD2	1.98	0.46
1:C:482:PRO:C	1:C:484:GLU:N	2.68	0.46
2:F:290:GLU:O	2:F:293:THR:CG2	2.63	0.46
3:G:165:PHE:CD2	3:G:168:LEU:HD21	2.51	0.46
1:A:170:ASP:O	1:A:173:THR:CG2	2.54	0.46
1:C:195:TYR:O	1:C:223:VAL:HA	2.16	0.46
1:C:316:LEU:N	1:C:317:PRO:HD3	2.30	0.46
3:G:179:ILE:HD12	3:G:238:ALA:O	2.16	0.46
4:H:83:GLU:O	4:H:84:ARG:C	2.53	0.46
1:A:103:LEU:CD1	1:A:123:THR:HG21	2.46	0.46
1:A:292:TYR:O	1:A:296:ARG:HG2	2.15	0.46
1:B:231:PRO:HD2	1:B:234:LEU:HD12	1.98	0.46
2:D:64:MSE:HE3	2:D:98:VAL:HG11	1.98	0.46
2:D:98:VAL:HG21	2:D:224:ALA:CB	2.45	0.46
2:D:402:ARG:O	2:D:406:ILE:HG13	2.15	0.46
2:E:289:GLN:NE2	2:E:289:GLN:CA	2.77	0.46
2:F:83:ILE:HB	2:F:118:ILE:CD1	2.46	0.46
2:F:409:PHE:HD2	2:F:437:PHE:CE1	2.34	0.46
1:A:144:GLU:HG2	1:A:161:ARG:HD2	1.98	0.46
1:A:243:VAL:HG11	1:A:260:TYR:OH	2.13	0.46
1:A:468:GLY:O	1:A:471:LEU:N	2.48	0.46
1:B:286:TYR:CD2	1:B:290:ILE:HG12	2.51	0.46
1:C:388:ALA:O	1:C:391:GLU:N	2.48	0.46
1:C:446:ASP:C	1:C:448:ILE:H	2.19	0.46
2:D:294:SER:HB3	2:D:299:SER:CB	2.44	0.46
2:D:451:ASP:OD1	2:D:454:ARG:NH1	2.45	0.46
2:F:294:SER:CB	2:F:299:SER:HA	2.46	0.46
3:G:114:ALA:O	3:G:115:ILE:HG12	2.16	0.46
4:H:98:GLU:O	4:H:102:ARG:HD2	2.15	0.46
1:A:62:MSE:HE3	1:A:95:MSE:CG	2.45	0.46
1:A:148:THR:CG2	1:A:150:ILE:HG13	2.37	0.46
1:A:330:ILE:HB	1:A:331:PRO:HD3	1.97	0.46
1:A:333:ASN:O	1:A:337:ILE:HG13	2.15	0.46
1:C:257:LEU:C	1:C:257:LEU:CD2	2.83	0.46
1:C:343:PHE:CD2	1:C:344:LEU:N	2.84	0.46
1:C:435:LEU:O	1:C:438:TYR:HB3	2.15	0.46
1:C:446:ASP:C	1:C:448:ILE:N	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:GLY:HA3	2:E:12:PRO:HD2	1.70	0.46
3:G:101:GLN:O	3:G:103:ILE:N	2.49	0.46
3:G:118:ILE:N	3:G:118:ILE:HD12	2.31	0.46
1:A:40:ARG:CZ	1:A:40:ARG:CG	2.94	0.46
1:A:262:ASP:OD1	1:A:265:LYS:CD	2.64	0.46
1:C:62:MSE:HE3	1:C:95:MSE:HB2	1.98	0.46
1:C:230:GLN:HB3	1:C:231:PRO:HD2	1.98	0.46
1:C:335:ILE:C	1:C:337:ILE:N	2.70	0.46
2:E:145:LEU:HD13	2:E:346:PRO:O	2.15	0.46
2:E:258:THR:HG21	2:E:285:MSE:HE2	1.96	0.46
3:G:219:GLN:HE22	4:H:66:GLY:CA	2.29	0.46
1:A:455:ARG:CZ	1:A:458:LYS:HZ2	2.29	0.45
1:A:479:LYS:HD2	1:A:479:LYS:N	2.30	0.45
1:B:199:GLY:CA	1:B:265:LYS:HD3	2.41	0.45
1:B:262:ASP:C	1:B:264:SER:H	2.18	0.45
2:D:429:PRO:HG2	2:D:432:GLU:CG	2.46	0.45
2:E:169:GLN:CG	2:E:207:VAL:HG21	2.46	0.45
2:E:318:PRO:O	2:E:321:THR:N	2.49	0.45
2:F:134:ILE:HG22	2:F:135:LEU:N	2.32	0.45
3:G:43:VAL:N	3:G:44:PRO:CD	2.79	0.45
1:A:276:LEU:C	1:A:278:ARG:H	2.17	0.45
1:A:350:PHE:HE2	2:D:350:THR:HG21	1.81	0.45
2:E:46:LEU:HG	2:E:47:THR:N	2.31	0.45
3:G:42:PHE:HZ	3:G:46:MSE:HE2	1.82	0.45
3:G:83:SER:HB3	3:G:236:GLU:OE1	2.16	0.45
1:A:435:LEU:HD13	1:A:464:LEU:HD13	1.98	0.45
1:B:201:LYS:O	1:B:205:VAL:HG23	2.16	0.45
1:B:372:ILE:HG13	1:B:374:ALA:H	1.81	0.45
1:C:303:LYS:NZ	1:C:310:GLY:O	2.49	0.45
1:B:283:ARG:HG2	1:B:284:GLU:N	2.30	0.45
1:B:489:LYS:O	1:B:493:ALA:N	2.50	0.45
2:D:401:HIS:HE1	2:D:446:ASP:HB3	1.75	0.45
2:F:221:PRO:CB	2:F:222:PRO:HD2	2.47	0.45
3:G:123:LEU:HD23	3:G:123:LEU:C	2.37	0.45
4:H:5:HIS:O	4:H:74:LYS:HA	2.16	0.45
2:D:141:VAL:HG11	2:D:344:VAL:CB	2.42	0.45
2:F:188:VAL:HG13	2:F:228:VAL:CG2	2.45	0.45
3:G:142:ASP:O	3:G:143:GLN:CB	2.65	0.45
1:A:139:ARG:NE	2:E:192:THR:HG21	2.31	0.45
1:A:472:LEU:O	1:A:475:ILE:HB	2.16	0.45
1:B:96:GLU:OE1	1:B:126:THR:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:HD21	1:C:88:VAL:O	2.16	0.45
1:C:147:GLN:OE1	1:C:430:VAL:HG22	2.16	0.45
2:E:168:ILE:HG23	2:E:250:PHE:CD2	2.52	0.45
2:F:191:ARG:HA	2:F:218:MSE:HE3	1.98	0.45
2:F:391:GLU:CD	3:G:87:LEU:CD1	2.85	0.45
1:A:147:GLN:OE1	1:A:430:VAL:HG22	2.17	0.45
1:A:157:VAL:HG11	1:A:342:ILE:HG12	1.98	0.45
1:A:440:LEU:HA	1:A:445:LEU:CB	2.46	0.45
1:A:469:GLN:O	1:A:473:GLU:HG2	2.16	0.45
1:B:104:ILE:HG21	1:B:219:ASP:O	2.17	0.45
1:B:438:TYR:C	1:B:438:TYR:CD2	2.89	0.45
2:D:240:ARG:HG3	2:D:298:GLY:HA3	1.98	0.45
2:E:239:PHE:HB2	2:E:247:VAL:HG21	1.98	0.45
2:F:166:VAL:HG13	2:F:416:VAL:HG23	1.99	0.45
1:A:110:PRO:HB3	1:A:238:ALA:HA	1.99	0.45
1:B:295:SER:HA	1:B:337:ILE:HD13	1.98	0.45
2:D:112:ASP:OD1	2:D:112:ASP:N	2.48	0.45
1:A:278:ARG:CZ	3:G:284:LEU:HD13	2.47	0.45
1:C:417:VAL:HG23	1:C:418:GLU:N	2.32	0.45
2:D:396:ASP:O	2:D:400:VAL:HG23	2.16	0.45
3:G:80:VAL:CG2	3:G:99:VAL:HG21	2.47	0.45
1:B:195:TYR:CD1	1:B:259:VAL:HB	2.44	0.45
2:D:51:ALA:C	2:D:52:LEU:HD23	2.37	0.45
3:G:110:PRO:HG2	3:G:112:GLU:HB3	1.98	0.45
1:A:445:LEU:HD21	1:A:453:VAL:HG13	1.98	0.44
1:C:168:ILE:HD11	1:C:321:THR:CG2	2.46	0.44
1:C:246:GLY:O	1:C:256:VAL:HG21	2.17	0.44
1:C:482:PRO:O	1:C:484:GLU:N	2.48	0.44
2:D:248:LEU:HB3	2:D:250:PHE:CE1	2.52	0.44
2:E:30:LEU:HB2	2:E:48:LEU:HB2	1.98	0.44
2:E:170:GLU:HG2	2:E:414:PHE:CE2	2.52	0.44
2:F:222:PRO:HB2	2:F:264:VAL:HG13	1.98	0.44
3:G:5:ARG:CB	3:G:5:ARG:NE	2.79	0.44
1:A:377:LYS:CG	1:A:378:VAL:H	2.29	0.44
1:B:236:PHE:HE1	1:B:293:LEU:CD1	2.29	0.44
2:F:145:LEU:HD22	2:F:371:GLN:CG	2.48	0.44
2:F:158:GLY:O	2:F:164:LYS:HD3	2.18	0.44
2:F:169:GLN:HB3	2:F:416:VAL:HG11	2.00	0.44
1:A:74:VAL:HG23	1:A:74:VAL:O	2.17	0.44
1:A:246:GLY:O	1:A:247:GLU:C	2.56	0.44
1:A:416:THR:HG22	1:A:440:LEU:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:VAL:HB	1:B:112:GLY:C	2.37	0.44
1:B:179:ALA:HB1	1:B:259:VAL:HG21	2.00	0.44
1:B:452:ASP:C	1:B:455:ARG:HB2	2.38	0.44
1:C:431:GLU:HG2	1:C:473:GLU:CG	2.42	0.44
1:C:445:LEU:CD2	1:C:453:VAL:HG22	2.46	0.44
2:D:30:LEU:CD2	2:D:78:ASP:HA	2.47	0.44
2:E:144:LEU:HD11	2:E:367:ALA:HB2	1.99	0.44
2:F:202:MSE:HE3	2:F:207:VAL:HG23	2.00	0.44
4:H:132:MSE:O	4:H:133:LYS:CB	2.64	0.44
1:A:151:LYS:HZ1	1:A:422:GLN:HB2	1.82	0.44
1:A:179:ALA:HB1	1:A:259:VAL:HG11	1.98	0.44
1:B:262:ASP:N	1:B:318:PHE:HB2	2.24	0.44
1:B:450:VAL:O	1:B:453:VAL:HB	2.17	0.44
1:C:343:PHE:HD2	1:C:344:LEU:N	2.15	0.44
1:C:343:PHE:HD1	1:C:361:LEU:HD12	1.82	0.44
2:E:2:THR:HB	2:E:22:HIS:HE1	1.80	0.44
2:E:141:VAL:HG23	2:E:410:LEU:O	2.18	0.44
2:E:457:GLY:HA3	2:E:461:GLU:OE2	2.17	0.44
3:G:220:TYR:O	3:G:224:LEU:HD12	2.18	0.44
1:A:429:PRO:HB2	1:A:431:GLU:OE1	2.18	0.44
1:A:440:LEU:HA	1:A:445:LEU:HB3	1.98	0.44
1:C:334:VAL:O	1:C:338:THR:HG23	2.17	0.44
2:D:31:LYS:HZ2	2:D:47:THR:CG2	2.29	0.44
2:E:16:VAL:CG1	2:E:18:PHE:CE1	3.01	0.44
2:E:185:PHE:CE2	2:E:198:LEU:CD2	3.00	0.44
2:E:249:LEU:O	2:E:302:SER:HA	2.17	0.44
2:F:148:TYR:CD2	2:F:154:ILE:CD1	3.00	0.44
2:F:274:ALA:O	2:F:275:VAL:HB	2.18	0.44
3:G:96:LEU:HD11	3:G:122:GLY:HA2	1.99	0.44
1:A:68:GLU:HG3	1:A:69:ASN:N	2.33	0.44
1:A:396:ALA:C	1:A:399:GLY:H	2.21	0.44
1:A:405:ALA:O	1:A:408:ALA:N	2.44	0.44
1:A:445:LEU:HD23	1:A:445:LEU:O	2.17	0.44
1:B:166:LEU:HB3	1:B:341:GLN:HB3	1.99	0.44
2:E:213:MSE:HE2	2:E:215:PHE:CZ	2.53	0.44
2:E:270:ARG:HG3	2:E:270:ARG:HH11	1.81	0.44
2:F:6:VAL:HA	2:F:16:VAL:HA	1.99	0.44
2:F:30:LEU:HB3	2:F:76:VAL:CG1	2.47	0.44
2:F:190:GLU:OE2	2:F:191:ARG:NH1	2.51	0.44
2:F:275:VAL:O	2:F:275:VAL:CG1	2.64	0.44
2:F:391:GLU:OE1	3:G:87:LEU:HD11	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:21:THR:CG2	3:G:247:ALA:HB3	2.47	0.44
1:A:157:VAL:O	1:A:157:VAL:HG12	2.18	0.44
1:C:403:ASP:O	1:C:406:THR:OG1	2.36	0.44
2:E:47:THR:C	2:E:48:LEU:HD23	2.38	0.44
1:A:129:ILE:HG23	1:A:240:TYR:HB3	2.00	0.44
1:A:275:LEU:HD12	2:D:279:PRO:HB3	1.99	0.44
1:B:154:ASP:C	1:B:375:MSE:HE3	2.38	0.44
1:C:239:PRO:HG2	1:C:266:GLN:NE2	2.33	0.44
1:C:345:GLN:NE2	1:C:358:ASN:HD22	2.16	0.44
1:C:397:GLN:C	1:C:399:GLY:N	2.69	0.44
2:D:27:TYR:O	2:D:82:PRO:CB	2.63	0.44
2:E:20:ASN:O	2:E:21:GLY:C	2.56	0.44
2:E:35:LYS:CA	2:E:35:LYS:O	2.66	0.44
2:E:91:THR:HA	2:E:96:PHE:HZ	1.82	0.44
2:F:353:ALA:O	2:F:355:ALA:N	2.51	0.44
3:G:24:MSE:CE	4:H:116:ALA:HB1	2.47	0.44
3:G:166:ASP:OD1	3:G:167:GLU:CB	2.66	0.44
1:A:292:TYR:CD1	2:E:221:PRO:HA	2.53	0.44
1:A:355:PRO:HB2	1:A:357:ILE:CG1	2.47	0.44
1:B:32:ILE:CG1	1:B:41:ALA:HA	2.48	0.44
1:C:434:VAL:C	1:C:437:ILE:HG22	2.38	0.44
2:D:87:VAL:HG22	2:D:114:ARG:O	2.18	0.44
2:D:140:LYS:CG	2:D:428:VAL:HG11	2.48	0.44
2:D:146:ALA:N	2:D:147:PRO:HD3	2.33	0.44
2:D:214:VAL:HG11	2:D:228:VAL:HG13	1.98	0.44
2:D:294:SER:HA	2:D:299:SER:HA	1.99	0.44
2:E:250:PHE:CZ	2:E:303:ILE:HD12	2.53	0.44
1:B:274:SER:OG	1:B:287:PRO:HG3	2.18	0.43
1:B:424:LEU:O	1:B:425:HIS:HB2	2.18	0.43
1:C:62:MSE:CE	1:C:95:MSE:HB2	2.48	0.43
2:D:166:VAL:HG13	2:D:416:VAL:CG2	2.48	0.43
2:D:247:VAL:CG1	2:D:248:LEU:N	2.80	0.43
2:D:317:ALA:HB3	2:D:318:PRO:HD3	1.99	0.43
2:D:453:PHE:CD1	2:D:453:PHE:N	2.86	0.43
2:E:289:GLN:HE21	2:E:289:GLN:CA	2.09	0.43
3:G:77:GLY:O	3:G:168:LEU:HA	2.17	0.43
3:G:162:ASP:OD2	3:G:189:LEU:HD11	2.18	0.43
1:A:114:PRO:HG3	1:A:120:PRO:HA	2.01	0.43
1:A:322:GLN:O	1:A:323:ALA:HB3	2.18	0.43
1:A:431:GLU:CG	1:A:476:ARG:CG	2.95	0.43
1:B:158:PRO:HB2	1:B:370:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ILE:C	1:B:493:ALA:N	2.72	0.43
2:D:254:ILE:O	2:D:257:PHE:HB3	2.18	0.43
2:D:328:THR:HG23	2:D:328:THR:O	2.18	0.43
2:D:354:LEU:HD22	2:D:364:TYR:HD1	1.83	0.43
2:E:14:VAL:O	2:E:61:THR:CG2	2.63	0.43
2:E:156:LEU:HD21	2:E:164:LYS:HG2	1.99	0.43
2:E:370:VAL:HG22	2:E:441:LEU:HD11	1.99	0.43
3:G:262:TYR:O	3:G:266:ARG:N	2.47	0.43
1:A:53:VAL:HG11	1:A:88:VAL:CG1	2.47	0.43
1:A:329:TYR:O	1:A:332:THR:OG1	2.30	0.43
1:B:331:PRO:O	1:B:335:ILE:HG13	2.18	0.43
1:B:453:VAL:O	1:B:456:PHE:N	2.52	0.43
1:C:49:SER:OG	2:D:68:ASP:HA	2.18	0.43
2:D:43:ASP:O	2:D:44:ILE:HD13	2.18	0.43
2:D:405:ARG:NH2	2:D:446:ASP:O	2.51	0.43
1:B:363:VAL:HG22	1:B:364:SER:N	2.33	0.43
1:C:52:LEU:HD22	1:C:95:MSE:HE3	2.01	0.43
1:C:297:LEU:HG	1:C:298:LEU:HD12	1.99	0.43
2:D:16:VAL:HG22	2:D:76:VAL:HG21	2.00	0.43
2:D:359:VAL:HG11	2:D:363:HIS:CE1	2.54	0.43
2:E:34:HIS:CE1	2:E:35:LYS:O	2.72	0.43
2:E:219:ASN:C	2:E:219:ASN:HD22	2.21	0.43
3:G:217:LEU:N	3:G:218:PRO:HD2	2.34	0.43
1:A:104:ILE:HA	1:A:222:ILE:HD11	2.01	0.43
1:A:460:PHE:O	1:A:464:LEU:HG	2.18	0.43
1:B:96:GLU:HB3	1:B:126:THR:CG2	2.47	0.43
1:B:261:ASP:O	1:B:262:ASP:CB	2.65	0.43
1:B:434:VAL:HA	1:B:437:ILE:HG22	2.01	0.43
3:G:96:LEU:CG	3:G:126:PHE:HE1	2.31	0.43
1:A:101:GLU:CG	1:A:101:GLU:N	2.82	0.43
1:A:103:LEU:CD2	1:A:245:MSE:HE2	2.49	0.43
1:A:298:LEU:HD22	1:A:337:ILE:HG21	2.00	0.43
1:B:298:LEU:HD21	1:B:317:PRO:HG2	2.01	0.43
1:B:330:ILE:O	1:B:333:ASN:HB2	2.19	0.43
2:D:172:ILE:HG23	2:D:183:SER:OG	2.19	0.43
2:D:380:LEU:HA	2:D:383:ILE:HD13	2.01	0.43
2:E:173:HIS:NE2	2:E:415:HIS:ND1	2.66	0.43
1:A:399:GLY:O	1:A:402:LEU:N	2.52	0.43
1:B:48:MSE:HB3	2:F:69:GLY:HA2	2.01	0.43
1:B:348:LEU:HA	1:B:351:SER:OG	2.18	0.43
1:C:44:LEU:HB3	1:C:47:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:368:ARG:O	2:D:372:GLN:HG3	2.19	0.43
2:E:309:PRO:O	2:E:310:ALA:C	2.54	0.43
4:H:39:ILE:HD12	4:H:39:ILE:C	2.38	0.43
1:A:110:PRO:CG	1:A:234:LEU:HD22	2.48	0.43
1:A:328:ALA:O	1:A:332:THR:HG23	2.17	0.43
1:A:350:PHE:C	1:A:352:GLY:N	2.71	0.43
1:B:459:GLU:O	1:B:462:LEU:N	2.51	0.43
1:C:158:PRO:HG2	1:C:367:GLY:HA2	2.00	0.43
1:C:163:GLN:HG3	1:C:366:VAL:HG21	1.99	0.43
1:C:457:GLU:O	1:C:458:LYS:C	2.57	0.43
2:E:166:VAL:HG13	2:E:416:VAL:CG2	2.48	0.43
2:E:292:ILE:HD13	2:E:302:SER:HB2	1.99	0.43
2:E:440:ILE:HD11	2:E:453:PHE:CE2	2.54	0.43
2:F:138:GLY:HA3	2:F:427:TYR:CD1	2.53	0.43
2:F:373:THR:HG22	2:F:376:ARG:HH11	1.81	0.43
2:F:391:GLU:CD	3:G:87:LEU:HD11	2.38	0.43
4:H:115:ARG:O	4:H:118:LEU:HB3	2.19	0.43
1:A:38:ILE:HD13	1:A:74:VAL:HA	2.00	0.43
1:A:443:GLY:C	1:A:445:LEU:H	2.21	0.43
1:B:45:ASP:HA	2:F:72:ARG:NH2	2.34	0.43
1:B:460:PHE:O	1:B:464:LEU:HG	2.18	0.43
1:B:475:ILE:HG23	1:B:476:ARG:N	2.33	0.43
1:C:94:ILE:O	1:C:95:MSE:C	2.57	0.43
2:D:172:ILE:HG23	2:D:183:SER:CB	2.49	0.43
2:E:30:LEU:HB3	2:E:76:VAL:CG1	2.49	0.43
2:E:315:ASP:O	2:E:318:PRO:CD	2.58	0.43
2:F:225:ARG:HA	2:F:228:VAL:CG2	2.48	0.43
3:G:53:VAL:HG22	3:G:216:LEU:CD1	2.46	0.43
3:G:156:THR:HG23	3:G:160:PHE:CE1	2.53	0.43
4:H:91:LEU:O	4:H:92:ARG:C	2.55	0.43
1:A:150:ILE:CD1	1:A:178:VAL:HG13	2.49	0.43
1:B:33:GLN:CD	1:B:40:ARG:NH2	2.73	0.43
1:B:450:VAL:HA	1:B:453:VAL:CG2	2.49	0.43
1:C:243:VAL:HG13	1:C:260:TYR:OH	2.16	0.43
1:C:352:GLY:O	1:C:353:VAL:C	2.56	0.43
1:C:435:LEU:HD21	1:C:475:ILE:HD11	2.01	0.43
3:G:25:GLU:OE2	3:G:245:LYS:HD3	2.18	0.43
3:G:52:VAL:C	3:G:54:ALA:H	2.22	0.43
3:G:80:VAL:HG11	3:G:126:PHE:CZ	2.54	0.43
1:A:294:HIS:O	1:A:297:LEU:HB3	2.19	0.42
1:A:343:PHE:HD2	1:A:344:LEU:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:VAL:O	1:A:421:LYS:HG3	2.19	0.42
1:A:431:GLU:H	1:A:431:GLU:CD	2.22	0.42
1:A:434:VAL:O	1:A:438:TYR:HB2	2.19	0.42
1:C:373:LYS:HD3	1:C:376:LYS:HD2	2.00	0.42
2:D:405:ARG:CD	2:D:453:PHE:CZ	2.97	0.42
2:D:460:GLU:O	2:D:463:VAL:HB	2.18	0.42
2:E:38:ASN:HD22	2:E:38:ASN:C	2.21	0.42
2:F:346:PRO:HB2	2:F:374:LEU:HD13	2.01	0.42
1:A:66:LEU:O	2:E:8:GLN:HA	2.19	0.42
1:B:195:TYR:HD1	1:B:259:VAL:CG1	2.31	0.42
1:B:240:TYR:O	1:B:243:VAL:HG22	2.19	0.42
2:D:168:ILE:HG23	2:D:250:PHE:CE2	2.53	0.42
2:D:370:VAL:HG13	2:D:406:ILE:CG2	2.48	0.42
2:D:406:ILE:O	2:D:410:LEU:HG	2.18	0.42
2:E:96:PHE:CD1	2:E:235:MSE:HE1	2.54	0.42
2:E:408:PHE:CD1	2:E:454:ARG:HB2	2.53	0.42
2:E:410:LEU:HD23	2:E:437:PHE:CZ	2.54	0.42
3:G:90:ALA:O	3:G:91:TYR:C	2.58	0.42
3:G:235:SER:O	3:G:236:GLU:C	2.57	0.42
3:G:258:LEU:HA	3:G:261:SER:OG	2.19	0.42
1:A:365:ARG:C	1:A:367:GLY:N	2.73	0.42
1:B:55:PHE:HE1	1:B:73:ILE:HD11	1.80	0.42
1:B:334:VAL:O	1:B:338:THR:HG23	2.20	0.42
1:C:416:THR:HA	1:C:440:LEU:HD12	1.99	0.42
2:D:170:GLU:HG2	2:D:414:PHE:CE2	2.54	0.42
2:F:312:ASP:HA	3:G:1:MSE:HB2	2.00	0.42
3:G:236:GLU:O	3:G:237:HIS:C	2.57	0.42
1:A:61:GLY:HA2	1:A:76:LEU:HG	2.01	0.42
1:A:239:PRO:CG	1:A:266:GLN:HG3	2.46	0.42
1:B:185:ASN:O	1:B:185:ASN:ND2	2.53	0.42
1:B:298:LEU:HD11	1:B:317:PRO:HG3	2.02	0.42
1:C:150:ILE:HA	1:C:422:GLN:OE1	2.19	0.42
2:D:342:PRO:HB2	2:D:344:VAL:HG23	2.02	0.42
2:D:371:GLN:O	2:D:374:LEU:HB2	2.19	0.42
2:D:392:LEU:C	2:D:394:ASP:N	2.73	0.42
2:D:467:LYS:O	2:D:470:GLY:N	2.51	0.42
2:E:5:ARG:HA	2:E:74:MSE:O	2.20	0.42
2:E:103:ILE:HD11	2:E:215:PHE:HD1	1.85	0.42
2:E:157:PHE:HB2	2:E:330:ASN:HD22	1.84	0.42
2:E:409:PHE:HD2	2:E:437:PHE:CE1	2.37	0.42
2:E:409:PHE:CD2	2:E:437:PHE:CE1	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:381:GLN:HA	2:F:384:ILE:HG12	2.01	0.42
2:F:384:ILE:HD13	2:F:384:ILE:N	2.35	0.42
3:G:156:THR:HG23	3:G:160:PHE:CD1	2.54	0.42
1:A:95:MSE:SE	1:A:237:LEU:CD2	3.16	0.42
1:A:192:ILE:HA	1:A:220:TYR:HB2	2.01	0.42
1:C:288:GLY:C	2:D:263:GLU:HG3	2.38	0.42
2:D:466:ALA:HA	2:D:469:MSE:HG2	2.01	0.42
3:G:7:ILE:O	3:G:11:ILE:HG13	2.19	0.42
3:G:10:ARG:HD3	4:H:129:VAL:HA	1.94	0.42
3:G:229:LEU:O	3:G:230:LEU:C	2.58	0.42
1:A:151:LYS:HE3	1:A:428:ILE:CD1	2.49	0.42
1:A:229:SER:HB3	2:D:290:GLU:CB	2.50	0.42
1:A:416:THR:HG22	1:A:440:LEU:HD12	2.01	0.42
1:B:233:PRO:O	1:B:236:PHE:HB3	2.20	0.42
1:B:343:PHE:CD2	1:B:344:LEU:N	2.79	0.42
2:D:163:GLY:O	2:D:164:LYS:C	2.57	0.42
2:D:256:ARG:HH11	2:D:259:GLN:HE22	1.67	0.42
2:E:154:ILE:HG13	2:E:327:ALA:HB3	2.02	0.42
3:G:52:VAL:CG2	4:H:69:GLU:HG2	2.49	0.42
3:G:116:ILE:HG23	3:G:136:ASP:HB2	2.02	0.42
1:A:99:VAL:HG21	1:A:127:ARG:HB2	2.02	0.42
1:A:193:SER:O	1:A:221:THR:HA	2.19	0.42
1:A:208:VAL:HA	1:A:211:THR:HG22	2.02	0.42
1:B:180:ILE:HG23	1:B:212:LEU:HD21	2.02	0.42
1:B:315:ALA:C	1:B:317:PRO:HD3	2.40	0.42
2:D:362:GLU:O	2:D:366:VAL:CG2	2.66	0.42
4:H:83:GLU:OE1	4:H:95:ALA:HB1	2.19	0.42
1:A:129:ILE:HG22	1:A:130:GLU:N	2.35	0.42
1:A:315:ALA:C	1:A:317:PRO:HD3	2.40	0.42
1:B:415:ARG:O	1:B:419:VAL:HG23	2.19	0.42
1:B:497:THR:O	1:B:499:VAL:N	2.53	0.42
2:E:147:PRO:HD2	2:E:351:SER:HB3	2.00	0.42
2:F:170:GLU:OE2	2:F:414:PHE:HA	2.20	0.42
3:G:112:GLU:CG	3:G:113:TYR:N	2.83	0.42
3:G:120:ARG:O	3:G:123:LEU:N	2.53	0.42
1:B:195:TYR:HA	1:B:259:VAL:HB	2.01	0.42
1:C:435:LEU:HD13	1:C:464:LEU:HD13	2.01	0.42
2:D:97:ASN:O	2:D:98:VAL:C	2.58	0.42
2:E:171:LEU:HD13	2:E:303:ILE:HD13	2.02	0.42
2:F:144:LEU:HD22	2:F:437:PHE:CD2	2.55	0.42
3:G:233:LYS:HD3	3:G:236:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ILE:HA	1:C:163:GLN:OE1	2.20	0.42
1:C:407:GLN:HA	1:C:410:LEU:HB2	2.01	0.42
2:D:18:PHE:N	2:D:18:PHE:CD1	2.87	0.42
2:E:175:ILE:HG13	2:E:248:LEU:HD11	2.01	0.42
2:E:270:ARG:HG3	2:E:270:ARG:NH1	2.35	0.42
2:E:285:MSE:HG3	2:E:324:HIS:CD2	2.55	0.42
2:E:328:THR:CG2	2:E:350:THR:H	2.19	0.42
2:F:30:LEU:O	2:F:47:THR:HA	2.20	0.42
2:F:162:VAL:CG1	2:F:331:LEU:HB3	2.49	0.42
3:G:212:ILE:H	3:G:212:ILE:HD12	1.84	0.42
4:H:28:LYS:O	4:H:29:SER:CB	2.68	0.42
4:H:130:ALA:O	4:H:132:MSE:O	2.37	0.42
1:A:319:VAL:HG11	1:A:331:PRO:HA	2.02	0.41
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.83	0.41
1:B:452:ASP:CA	1:B:455:ARG:HB2	2.50	0.41
1:C:157:VAL:HG13	1:C:364:SER:HB2	2.02	0.41
2:D:26:ILE:O	2:D:27:TYR:CB	2.62	0.41
2:D:335:LEU:HD11	2:D:346:PRO:HD3	2.02	0.41
2:E:227:ARG:HD2	2:E:230:LEU:HD12	2.01	0.41
2:F:195:GLY:CA	2:F:215:PHE:HE2	2.31	0.41
3:G:212:ILE:O	3:G:214:ASP:N	2.53	0.41
4:H:90:VAL:O	4:H:90:VAL:HG12	2.20	0.41
1:A:240:TYR:O	1:A:243:VAL:HG22	2.20	0.41
1:A:286:TYR:HA	1:A:287:PRO:HD3	1.92	0.41
1:B:62:MSE:HE3	1:B:95:MSE:CG	2.31	0.41
1:B:165:GLU:OE2	1:B:341:GLN:CA	2.68	0.41
2:D:190:GLU:C	2:D:217:GLN:NE2	2.73	0.41
2:D:322:PHE:HA	2:D:325:LEU:CD1	2.49	0.41
2:F:377:TYR:HE1	2:F:400:VAL:HG13	1.85	0.41
3:G:181:GLN:NE2	3:G:239:ALA:HB2	2.34	0.41
1:B:453:VAL:O	1:B:454:ARG:C	2.58	0.41
2:D:392:LEU:C	2:D:394:ASP:H	2.24	0.41
2:E:396:ASP:O	2:E:399:VAL:HB	2.19	0.41
2:F:182:ILE:O	2:F:247:VAL:HG13	2.21	0.41
2:F:317:ALA:HB3	2:F:318:PRO:HD3	2.00	0.41
1:A:355:PRO:HB2	1:A:357:ILE:CD1	2.50	0.41
1:A:434:VAL:HA	1:A:437:ILE:CG2	2.47	0.41
1:B:28:VAL:O	1:B:28:VAL:HG13	2.20	0.41
1:C:139:ARG:NH2	1:C:299:GLU:O	2.54	0.41
1:C:463:PHE:O	1:C:467:ASN:O	2.39	0.41
2:E:148:TYR:CE1	2:E:154:ILE:HG12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:222:PRO:HB2	2:E:264:VAL:HG22	2.02	0.41
2:E:438:LYS:O	2:E:442:GLU:HG3	2.20	0.41
2:F:148:TYR:CG	2:F:154:ILE:CD1	3.04	0.41
2:F:265:SER:CB	2:F:278:GLN:HB3	2.51	0.41
2:F:354:LEU:HD23	2:F:354:LEU:HA	1.77	0.41
1:A:62:MSE:HE3	1:A:95:MSE:CB	2.47	0.41
1:A:263:LEU:HD12	1:A:317:PRO:HB3	2.03	0.41
1:A:319:VAL:HG21	1:A:334:VAL:CG1	2.35	0.41
1:B:108:VAL:O	1:B:224:VAL:HA	2.20	0.41
1:B:109:ASN:OD1	1:B:111:LEU:HB2	2.20	0.41
1:B:328:ALA:O	1:B:332:THR:HG23	2.20	0.41
1:C:175:LYS:HB3	1:C:318:PHE:CE1	2.55	0.41
2:D:404:ARG:O	2:D:408:PHE:HB2	2.20	0.41
2:D:449:PRO:O	2:D:450:GLU:C	2.58	0.41
2:E:84:SER:HB3	2:E:115:ARG:HB3	2.02	0.41
2:E:217:GLN:O	2:E:220:GLU:CG	2.68	0.41
2:E:334:LYS:CE	2:E:334:LYS:HA	2.50	0.41
1:A:179:ALA:O	1:A:183:ILE:HG13	2.21	0.41
1:A:257:LEU:HD21	1:A:316:LEU:HD12	2.02	0.41
1:B:333:ASN:O	1:B:336:SER:OG	2.35	0.41
1:C:474:HIS:C	1:C:476:ARG:N	2.72	0.41
2:E:7:ILE:HG22	2:E:8:GLN:HG3	2.02	0.41
2:F:185:PHE:CD2	2:F:250:PHE:HB2	2.56	0.41
3:G:81:ILE:HD13	3:G:229:LEU:HD22	2.02	0.41
4:H:101:GLU:HA	4:H:104:LEU:HD12	2.02	0.41
1:A:95:MSE:HG3	1:A:237:LEU:HD21	2.02	0.41
1:A:343:PHE:C	1:A:343:PHE:CD2	2.94	0.41
1:B:232:ALA:N	1:B:233:PRO:CD	2.83	0.41
1:C:373:LYS:HB2	1:C:480:ASP:CA	2.51	0.41
1:C:462:LEU:HD13	1:C:462:LEU:HA	1.83	0.41
2:D:12:PRO:HG2	2:D:267:LEU:CD1	2.50	0.41
2:D:376:ARG:O	2:D:380:LEU:HG	2.21	0.41
2:E:318:PRO:HG2	2:E:319:ALA:N	2.36	0.41
3:G:95:VAL:CG2	3:G:96:LEU:N	2.84	0.41
1:A:171:ARG:NE	1:A:320:GLU:OE2	2.54	0.41
1:A:322:GLN:C	1:A:324:GLY:N	2.73	0.41
1:B:44:LEU:HD21	1:B:88:VAL:O	2.20	0.41
1:B:151:LYS:HZ1	1:B:422:GLN:CB	2.34	0.41
1:B:209:VAL:HG11	2:E:125:PHE:CZ	2.48	0.41
1:C:146:LEU:HD23	1:C:146:LEU:C	2.41	0.41
1:C:266:GLN:O	1:C:269:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:ALA:O	2:D:233:LEU:HB2	2.20	0.41
2:D:342:PRO:CG	2:D:414:PHE:CZ	3.01	0.41
2:D:433:THR:O	2:D:437:PHE:HD1	2.04	0.41
2:E:136:GLU:HB3	2:E:179:HIS:HE2	1.86	0.41
2:E:144:LEU:HD12	2:E:367:ALA:HB2	2.02	0.41
2:E:328:THR:HG23	2:E:350:THR:N	2.20	0.41
3:G:72:PRO:HG3	3:G:166:ASP:OD2	2.21	0.41
3:G:129:ARG:O	3:G:130:ASN:CB	2.69	0.41
1:A:65:ASN:O	1:A:71:VAL:HA	2.20	0.41
1:A:377:LYS:CG	1:A:378:VAL:N	2.84	0.41
1:A:431:GLU:HB3	1:A:472:LEU:HB2	2.03	0.41
1:A:436:ILE:O	1:A:440:LEU:HD22	2.21	0.41
1:A:453:VAL:O	1:A:456:PHE:HB3	2.21	0.41
1:B:33:GLN:HG2	2:E:54:LEU:O	2.21	0.41
1:B:36:ASP:C	1:B:38:ILE:H	2.23	0.41
1:C:209:VAL:O	1:C:213:ARG:HG3	2.20	0.41
1:C:395:PHE:O	1:C:396:ALA:C	2.55	0.41
2:D:10:MSE:CB	2:D:13:VAL:HG13	2.36	0.41
2:D:88:GLY:C	2:D:90:VAL:H	2.24	0.41
2:D:233:LEU:O	2:D:236:ALA:N	2.54	0.41
2:D:465:LYS:O	2:D:468:ALA:HB3	2.21	0.41
2:E:9:VAL:HG13	2:E:14:VAL:HG22	2.01	0.41
2:E:95:VAL:HG12	2:E:103:ILE:CG1	2.51	0.41
2:E:157:PHE:HB2	2:E:330:ASN:ND2	2.36	0.41
2:E:216:GLY:O	2:E:225:ARG:HG2	2.21	0.41
2:F:416:VAL:HG23	2:F:416:VAL:O	2.21	0.41
3:G:21:THR:HB	3:G:248:THR:OG1	2.21	0.41
3:G:48:LYS:HD2	4:H:69:GLU:HG3	2.02	0.41
3:G:101:GLN:C	3:G:103:ILE:H	2.25	0.41
3:G:140:LEU:N	3:G:141:PRO:HD3	2.36	0.41
1:A:471:LEU:HD21	1:A:489:LYS:CG	2.50	0.41
1:B:265:LYS:O	1:B:269:ALA:HB2	2.21	0.41
1:B:301:ALA:CB	1:B:313:LEU:HD22	2.49	0.41
1:C:197:ALA:HB1	1:C:200:GLN:CB	2.50	0.41
2:D:213:MSE:HE2	2:D:215:PHE:HZ	1.80	0.41
2:D:256:ARG:HH11	2:D:259:GLN:NE2	2.17	0.41
2:D:404:ARG:NH1	2:D:408:PHE:CE2	2.89	0.41
2:E:87:VAL:O	2:E:87:VAL:HG23	2.21	0.41
3:G:25:GLU:HG3	3:G:245:LYS:HG3	2.03	0.41
3:G:46:MSE:HE1	3:G:223:SER:C	2.41	0.41
4:H:6:VAL:HG13	4:H:6:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:129:VAL:CG1	4:H:132:MSE:HA	2.24	0.41
1:A:62:MSE:CE	1:A:95:MSE:HG3	2.52	0.40
1:A:121:VAL:O	1:A:121:VAL:CG2	2.63	0.40
1:A:431:GLU:CG	1:A:476:ARG:HG3	2.51	0.40
1:B:62:MSE:HG2	1:B:63:ALA:N	2.36	0.40
1:B:249:PHE:HB2	1:B:256:VAL:CG2	2.51	0.40
2:D:32:ILE:CD1	2:D:76:VAL:HG22	2.50	0.40
2:D:170:GLU:O	2:D:173:HIS:HB3	2.21	0.40
2:E:176:ALA:HA	2:E:181:GLY:H	1.86	0.40
2:F:401:HIS:HD2	2:F:405:ARG:HH21	1.64	0.40
3:G:78:TYR:CE1	3:G:171:TYR:CE1	3.07	0.40
3:G:164:THR:O	3:G:164:THR:HG22	2.21	0.40
1:A:95:MSE:SE	1:A:129:ILE:HD12	2.71	0.40
1:A:209:VAL:HG23	1:A:223:VAL:HG21	2.01	0.40
1:A:372:ILE:HD13	1:A:374:ALA:HB3	2.04	0.40
1:A:430:VAL:O	1:A:431:GLU:C	2.58	0.40
1:B:206:ARG:O	1:B:209:VAL:N	2.55	0.40
1:C:272:GLU:O	1:C:276:LEU:HD23	2.22	0.40
1:C:326:ILE:O	1:C:326:ILE:HG22	2.21	0.40
2:D:115:ARG:HG2	2:D:115:ARG:HH11	1.87	0.40
2:D:359:VAL:HB	2:D:363:HIS:ND1	2.36	0.40
2:E:91:THR:HA	2:E:96:PHE:CZ	2.56	0.40
2:E:450:GLU:O	2:E:452:ALA:N	2.54	0.40
2:F:253:ASN:C	2:F:255:PHE:N	2.75	0.40
3:G:114:ALA:HB3	3:G:165:PHE:CE1	2.54	0.40
4:H:104:LEU:C	4:H:106:SER:N	2.75	0.40
4:H:126:ARG:O	4:H:127:LEU:C	2.59	0.40
1:C:99:VAL:CG1	1:C:245:MSE:HA	2.51	0.40
1:C:145:PRO:HB2	1:C:147:GLN:HE21	1.87	0.40
1:C:186:GLN:HB3	1:C:191:MSE:HB2	2.02	0.40
1:C:243:VAL:O	1:C:247:GLU:N	2.45	0.40
1:C:412:ARG:HA	1:C:415:ARG:HB2	2.03	0.40
2:D:256:ARG:NH1	2:D:259:GLN:NE2	2.62	0.40
2:E:453:PHE:CD2	2:E:462:VAL:HG11	2.56	0.40
2:F:153:LYS:NZ	2:F:289:GLN:HB3	2.37	0.40
2:F:335:LEU:HB2	2:F:343:ALA:HB1	2.02	0.40
3:G:14:THR:O	3:G:17:THR:HB	2.22	0.40
3:G:24:MSE:HA	3:G:27:VAL:HB	2.03	0.40
3:G:92:ASN:O	3:G:95:VAL:HG22	2.21	0.40
4:H:129:VAL:O	4:H:129:VAL:HG12	2.21	0.40
1:A:382:LEU:CG	1:A:437:ILE:HD11	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ASP:OD2	1:A:481:LEU:N	2.55	0.40
1:B:241:ALA:O	1:B:245:MSE:HE3	2.20	0.40
1:C:389:TYR:O	1:C:393:GLU:HB2	2.20	0.40
2:D:317:ALA:N	2:D:318:PRO:HD2	2.36	0.40
2:E:98:VAL:HG13	2:E:228:VAL:HA	2.03	0.40
2:E:226:MSE:HE3	2:E:227:ARG:CZ	2.50	0.40
2:E:246:ASP:HA	2:E:299:SER:O	2.20	0.40
2:E:370:VAL:CG1	2:E:406:ILE:HG21	2.50	0.40
2:E:404:ARG:O	2:E:408:PHE:HD2	2.03	0.40
2:E:428:VAL:CG2	2:E:432:GLU:HB2	2.44	0.40
4:H:22:MSE:HB2	4:H:35:LEU:CD2	2.50	0.40
1:A:166:LEU:HD12	1:A:166:LEU:C	2.41	0.40
1:A:199:GLY:O	1:A:228:ALA:HB2	2.21	0.40
1:A:261:ASP:O	1:A:262:ASP:HB3	2.22	0.40
1:B:184:ILE:HA	1:B:220:TYR:OH	2.22	0.40
1:B:192:ILE:HA	1:B:220:TYR:O	2.22	0.40
1:B:445:LEU:HG	1:B:456:PHE:CD1	2.56	0.40
1:C:284:GLU:HG2	1:C:284:GLU:O	2.22	0.40
2:D:88:GLY:C	2:D:90:VAL:N	2.75	0.40
2:E:160:ALA:HB3	2:E:333:ARG:NH2	2.37	0.40
2:E:178:GLU:HG3	2:E:427:TYR:CE2	2.57	0.40
2:F:250:PHE:CE1	2:F:303:ILE:HD12	2.54	0.40
2:F:384:ILE:HG23	2:F:389:MSE:CG	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	473/502 (94%)	429 (91%)	42 (9%)	2 (0%)	34 71
1	B	403/502 (80%)	357 (89%)	42 (10%)	4 (1%)	15 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	469/502 (93%)	411 (88%)	51 (11%)	7 (2%)	10	45
2	D	466/483 (96%)	414 (89%)	50 (11%)	2 (0%)	34	71
2	E	463/483 (96%)	418 (90%)	39 (8%)	6 (1%)	12	48
2	F	456/483 (94%)	406 (89%)	46 (10%)	4 (1%)	17	54
3	G	242/285 (85%)	193 (80%)	38 (16%)	11 (4%)	2	25
4	H	123/133 (92%)	108 (88%)	12 (10%)	3 (2%)	6	37
All	All	3095/3373 (92%)	2736 (88%)	320 (10%)	39 (1%)	12	48

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	GLN
1	C	354	ARG
2	D	393	SER
2	E	311	ASP
3	G	143	GLN
1	C	355	PRO
1	C	469	GLN
2	E	20	ASN
2	E	83	ILE
2	F	275	VAL
3	G	190	PRO
4	H	126	ARG
1	C	485	ASP
3	G	72	PRO
3	G	167	GLU
3	G	213	LEU
4	H	90	VAL
4	H	128	SER
1	A	95	MSE
1	C	482	PRO
3	G	102	THR
1	A	411	ALA
1	B	431	GLU
1	B	498	PHE
1	C	411	ALA
1	C	481	LEU
2	E	310	ALA
2	E	393	SER
2	F	424	PRO

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Mol	Chain	Res	Type
3	G	189	LEU
2	F	354	LEU
3	G	149	ILE
2	D	142	VAL
1	B	453	VAL
2	F	82	PRO
3	G	11	ILE
3	G	53	VAL
3	G	73	VAL
2	E	142	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/402 (83%)	309 (93%)	23 (7%)	15	45
1	B	242/402 (60%)	232 (96%)	10 (4%)	30	58
1	C	291/402 (72%)	274 (94%)	17 (6%)	20	50
2	D	333/385 (86%)	318 (96%)	15 (4%)	27	56
2	E	349/385 (91%)	334 (96%)	15 (4%)	29	57
2	F	309/385 (80%)	301 (97%)	8 (3%)	46	68
3	G	157/231 (68%)	148 (94%)	9 (6%)	20	50
4	H	78/104 (75%)	71 (91%)	7 (9%)	9	36
All	All	2091/2696 (78%)	1987 (95%)	104 (5%)	24	53

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	70	ASN
1	A	86	ASP
1	A	94	ILE
1	A	95	MSE

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Mol	Chain	Res	Type
1	A	109	ASN
1	A	138	ASP
1	A	140	ARG
1	A	166	LEU
1	A	192	ILE
1	A	225	THR
1	A	227	SER
1	A	237	LEU
1	A	266	GLN
1	A	343	PHE
1	A	346	SER
1	A	351	SER
1	A	375	MSE
1	A	382	LEU
1	A	386	LEU
1	A	438	TYR
1	A	479	LYS
1	A	494	PHE
1	B	64	LEU
1	B	86	ASP
1	B	95	MSE
1	B	170	ASP
1	B	262	ASP
1	B	306	ASP
1	B	343	PHE
1	B	438	TYR
1	B	462	LEU
1	B	472	LEU
1	C	27	ASP
1	C	45	ASP
1	C	70	ASN
1	C	86	ASP
1	C	95	MSE
1	C	141	SER
1	C	375	MSE
1	C	382	LEU
1	C	386	LEU
1	C	397	GLN
1	C	403	ASP
1	C	407	GLN
1	C	462	LEU
1	C	463	PHE

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Mol	Chain	Res	Type
1	C	471	LEU
1	C	474	HIS
1	C	477	THR
2	D	38	ASN
2	D	52	LEU
2	D	98	VAL
2	D	108	ASP
2	D	112	ASP
2	D	169	GLN
2	D	219	ASN
2	D	227	ARG
2	D	242	GLU
2	D	273	SER
2	D	307	TYR
2	D	354	LEU
2	D	413	ASN
2	D	420	PHE
2	D	469	MSE
2	E	23	LEU
2	E	38	ASN
2	E	169	GLN
2	E	193	ARG
2	E	203	LYS
2	E	217	GLN
2	E	219	ASN
2	E	228	VAL
2	E	253	ASN
2	E	256	ARG
2	E	289	GLN
2	E	293	THR
2	E	357	GLU
2	E	420	PHE
2	E	453	PHE
2	F	68	ASP
2	F	97	ASN
2	F	204	ASP
2	F	246	ASP
2	F	278	GLN
2	F	384	ILE
2	F	412	GLN
2	F	451	ASP
3	G	4	LEU

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Mol	Chain	Res	Type
3	G	82	THR
3	G	84	ASP
3	G	96	LEU
3	G	135	LEU
3	G	143	GLN
3	G	165	PHE
3	G	212	ILE
3	G	244	MSE
4	H	18	ASP
4	H	41	LEU
4	H	45	LEU
4	H	87	ASP
4	H	88	ILE
4	H	120	LEU
4	H	127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	109	ASN
1	A	113	GLN
1	A	266	GLN
1	A	433	GLN
1	C	345	GLN
1	C	433	GLN
1	C	474	HIS
2	D	289	GLN
2	D	304	GLN
2	E	22	HIS
2	E	38	ASN
2	E	245	GLN
2	E	289	GLN
2	E	304	GLN
2	E	324	HIS
2	F	200	HIS
2	F	401	HIS

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)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	B	700	-	4,4,4	0.18	0	6,6,6	0.20	0
6	ADP	F	600	-	24,29,29	1.03	2 (8%)	29,45,45	1.43	4 (13%)
5	SO4	D	700	-	4,4,4	0.16	0	6,6,6	0.18	0
5	SO4	E	700	-	4,4,4	0.16	0	6,6,6	0.20	0
5	SO4	A	700	-	4,4,4	0.18	0	6,6,6	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	F	600	-	-	8/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	600	ADP	C5-C4	2.63	1.47	1.40
6	F	600	ADP	C2-N3	2.02	1.35	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	600	ADP	C3'-C2'-C1'	3.69	106.53	100.98
6	F	600	ADP	N3-C2-N1	-3.17	123.72	128.68
6	F	600	ADP	PA-O3A-PB	-3.05	122.35	132.83
6	F	600	ADP	C4-C5-N7	-2.07	107.24	109.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	600	ADP	PA-O3A-PB-O2B
6	F	600	ADP	PA-O3A-PB-O3B
6	F	600	ADP	C5'-O5'-PA-O2A
6	F	600	ADP	C5'-O5'-PA-O3A
6	F	600	ADP	O4'-C4'-C5'-O5'
6	F	600	ADP	C3'-C4'-C5'-O5'
6	F	600	ADP	C5'-O5'-PA-O1A
6	F	600	ADP	PA-O3A-PB-O1B

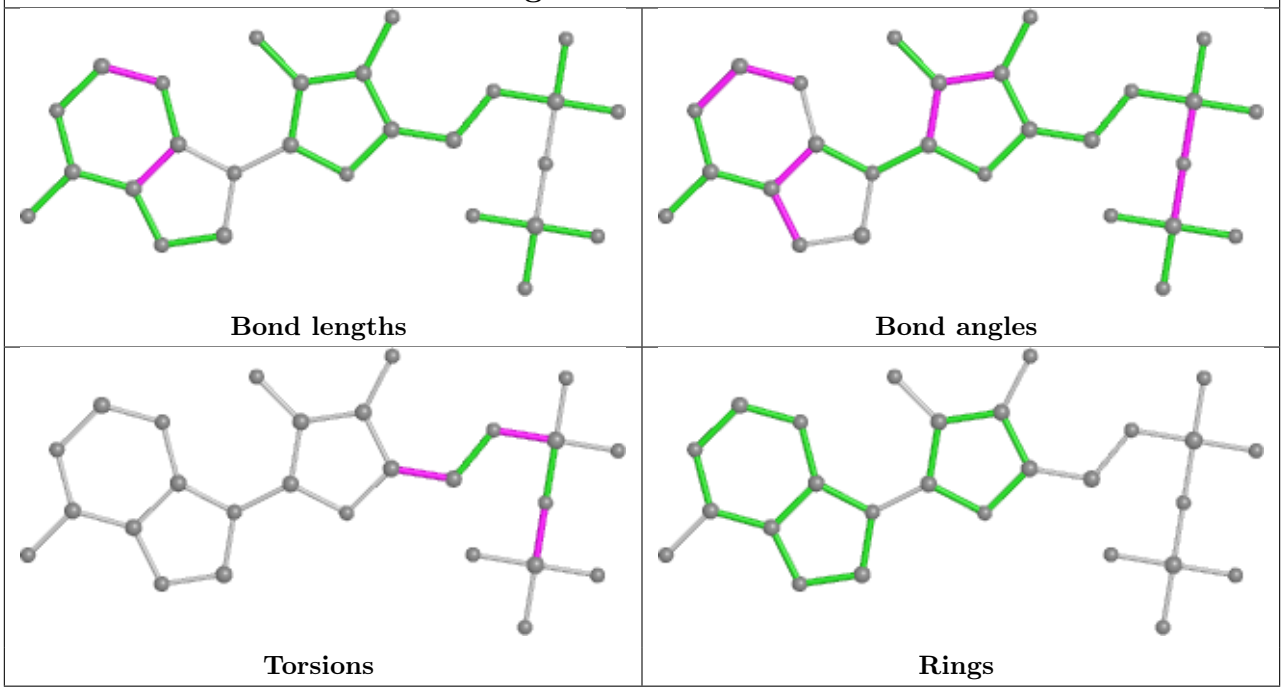
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	700	SO4	1	0
6	F	600	ADP	1	0
5	A	700	SO4	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP F 600



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	468/502 (93%)	-0.55	2 (0%)	92	87	63, 97, 156, 240	0
1	B	414/502 (82%)	-0.21	10 (2%)	59	48	92, 129, 236, 263	0
1	C	466/502 (92%)	-0.39	2 (0%)	92	87	86, 124, 177, 215	0
2	D	457/483 (94%)	-0.35	2 (0%)	92	87	70, 107, 165, 212	0
2	E	456/483 (94%)	-0.39	2 (0%)	92	87	71, 103, 155, 210	0
2	F	451/483 (93%)	-0.22	9 (1%)	65	55	95, 137, 164, 211	0
3	G	247/285 (86%)	-0.25	1 (0%)	92	87	80, 134, 182, 199	0
4	H	125/133 (93%)	0.05	7 (5%)	24	19	114, 143, 168, 191	0
All	All	3084/3373 (91%)	-0.33	35 (1%)	80	73	63, 119, 180, 263	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	243	GLN	5.7
2	D	2	THR	4.0
4	H	76	THR	4.0
2	F	420	PHE	3.8
1	B	142	VAL	3.5
2	E	112	ASP	3.1
2	F	38	ASN	3.1
4	H	3	THR	2.8
1	B	143	HIS	2.7
3	G	160	PHE	2.6
1	B	482	PRO	2.6
1	B	255	HIS	2.6
1	C	401	ASP	2.5
1	C	215	HIS	2.5
1	B	128	PRO	2.5
2	F	37	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	42	VAL	2.3
1	B	427	PRO	2.3
2	E	37	ARG	2.3
1	B	468	GLY	2.3
4	H	72	PRO	2.2
1	B	91	THR	2.2
2	F	22	HIS	2.2
1	A	351	SER	2.2
2	F	206	GLY	2.2
1	B	426	GLN	2.2
1	A	501	SER	2.1
4	H	29	SER	2.1
4	H	2	LYS	2.1
1	B	124	THR	2.1
4	H	84	ARG	2.1
2	F	242	GLU	2.1
4	H	130	ALA	2.1
2	F	245	GLN	2.0
2	F	110	PRO	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)

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, 95th 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
5	SO4	B	700	5/5	0.58	0.39	187,190,191,194	0
5	SO4	E	700	5/5	0.75	0.35	185,189,190,191	0
6	ADP	F	600	27/27	0.78	0.34	173,198,203,203	0
5	SO4	A	700	5/5	0.79	0.49	184,186,190,192	0

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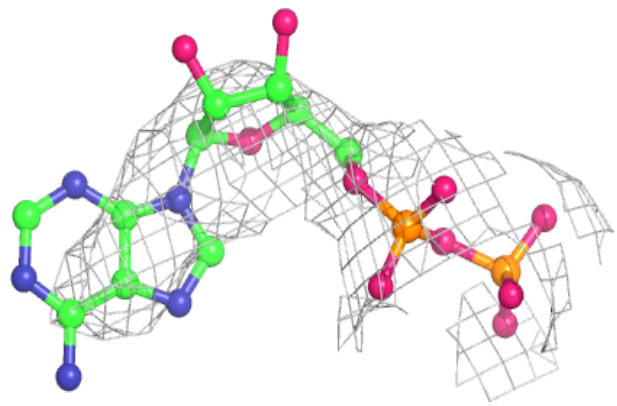
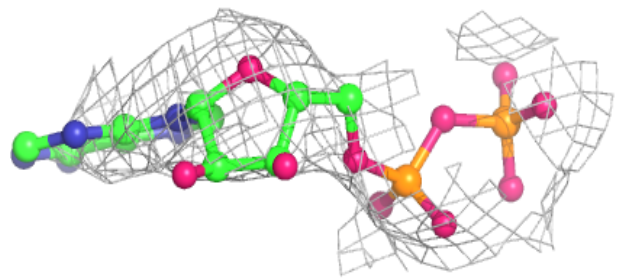
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	D	700	5/5	0.83	0.25	190,192,193,194	0

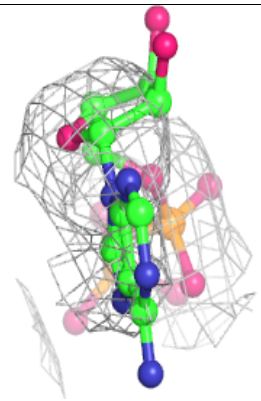
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP F 600:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.