Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 09:08 AM JST

PDB ID	:	6LG0
Title	:	Crystal structure of SbCGTa in complex with UDP
Authors	:	Gao, H.M.; Yun, C.H.
Deposited on	:	2019-12-04
Resolution	:	3.00 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:

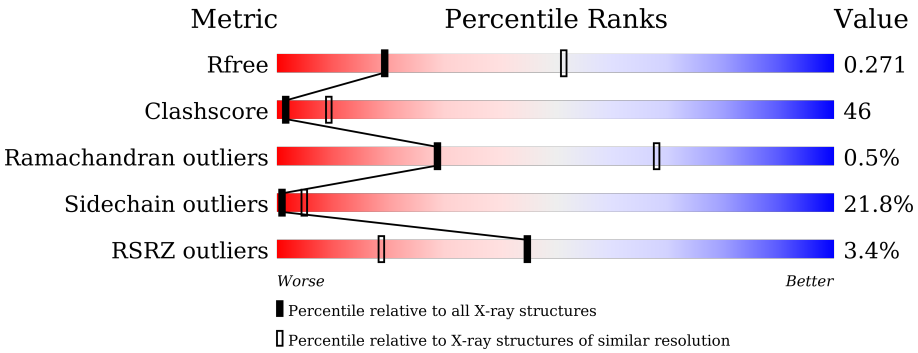
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	460	2% 55% 35% 6% ·
1	B	460	5% 52% 35% 9% ·
1	C	460	% 42% 43% 11% 5%
1	D	460	5% 43% 40% 12% 5%
1	E	460	4% 51% 37% 8% ·
1	F	460	3% 46% 42% 9% ·

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UDP	C	500	-	-	X	-
2	UDP	E	500	-	-	X	-

2 Entry composition

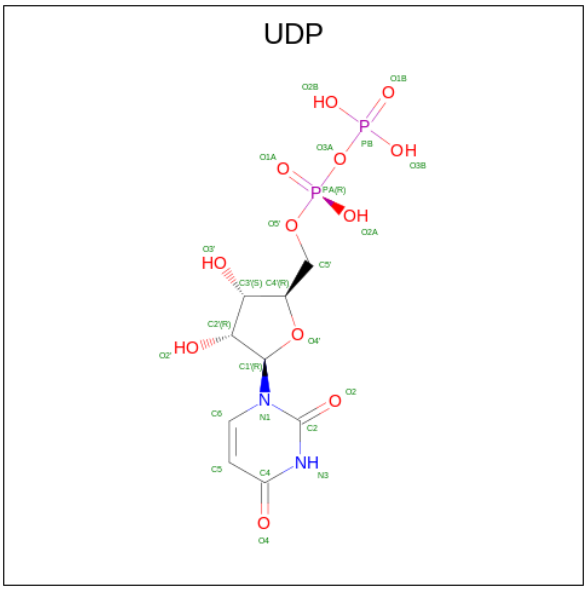
There are 3 unique types of molecules in this entry. The entry contains 19522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SbCGTa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3204	2056	539	597	12			
1	B	445	Total	C	N	O	S	0	0	1
			3198	2053	544	589	12			
1	C	439	Total	C	N	O	S	0	0	0
			3257	2091	548	603	15			
1	D	437	Total	C	N	O	S	0	0	0
			3129	2005	522	589	13			
1	E	443	Total	C	N	O	S	0	0	0
			3255	2085	547	608	15			
1	F	444	Total	C	N	O	S	0	0	0
			3319	2124	561	620	14			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is water.

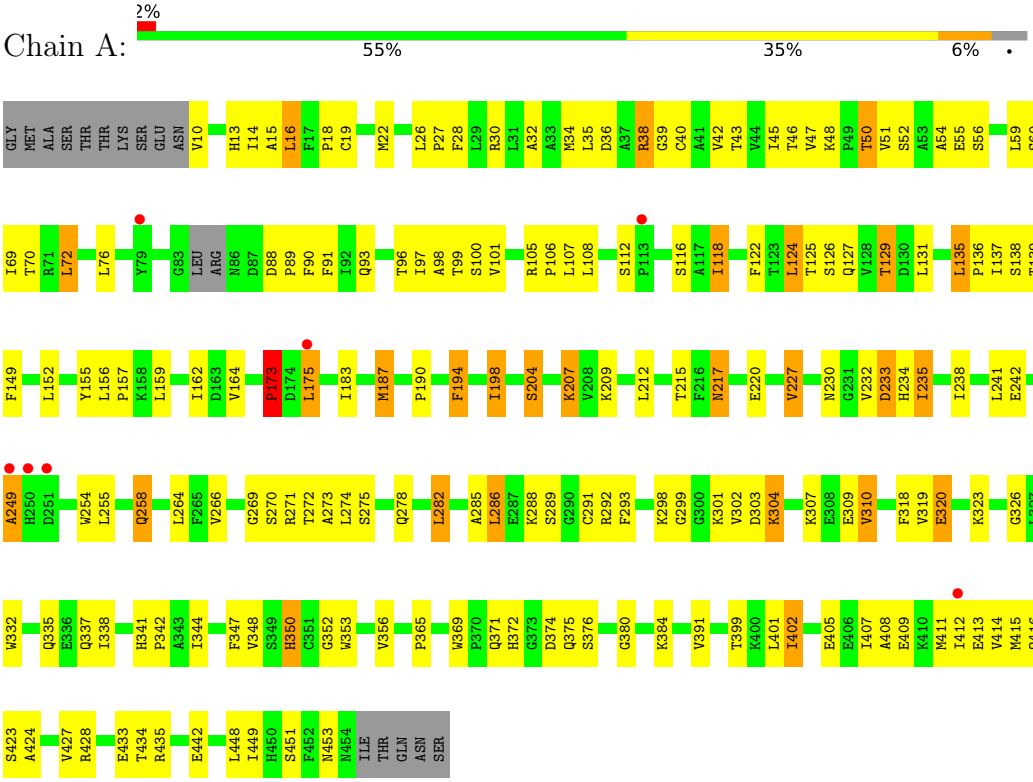
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	C	1	Total	O	0	0
			1	1		
3	D	1	Total	O	0	0
			1	1		
3	E	1	Total	O	0	0
			1	1		

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.

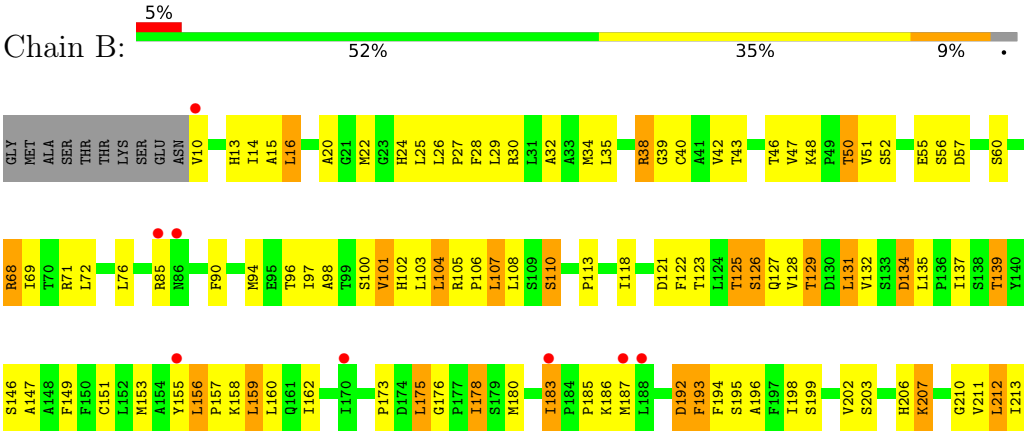
• Molecule 1: SbCGTa

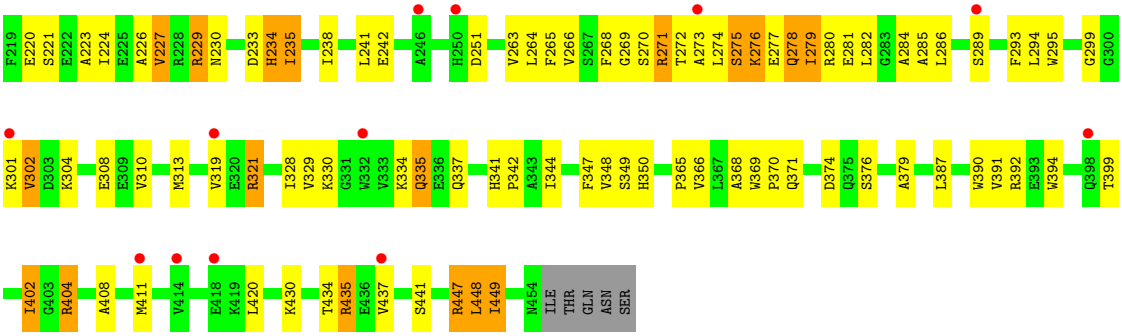
Chain A:



• Molecule 1: SbCGTa

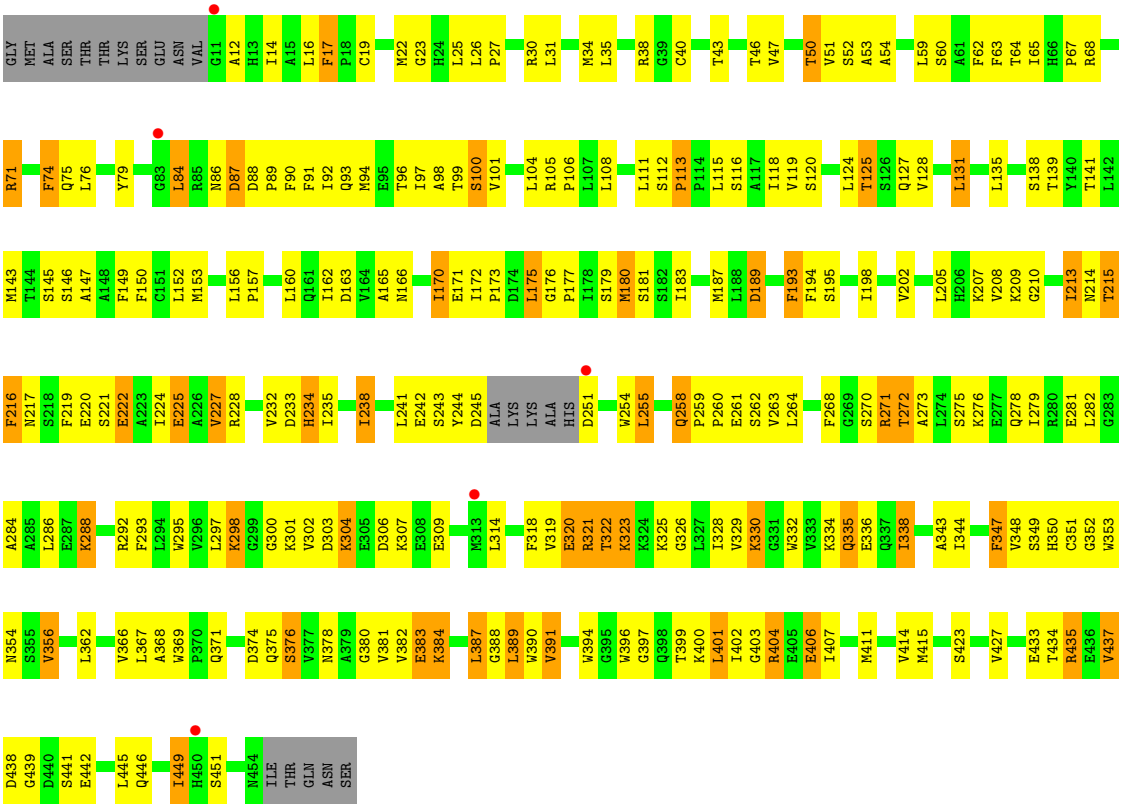
Chain B:





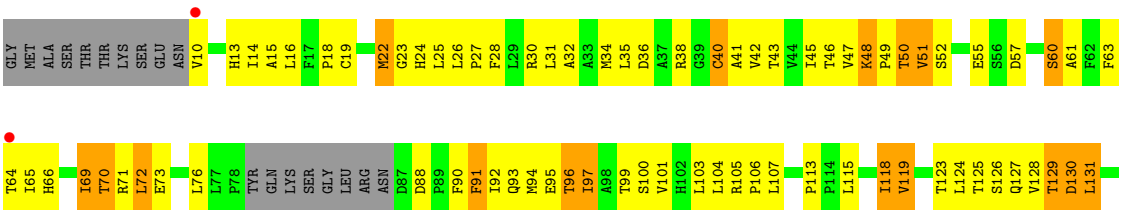
• Molecule 1: SbCGTa

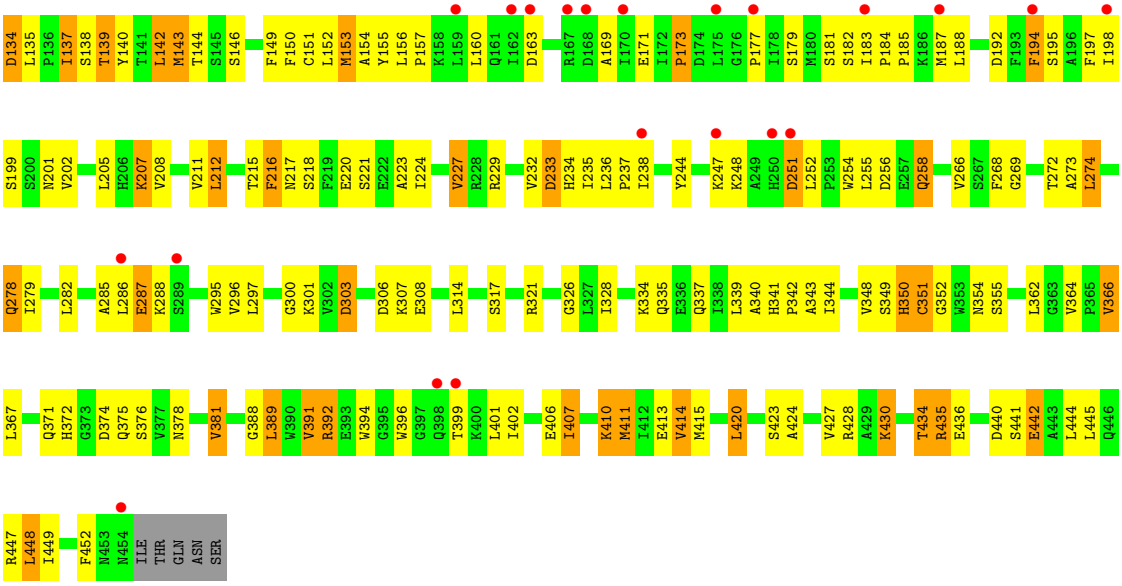
Chain C:



• Molecule 1: SbCGTa

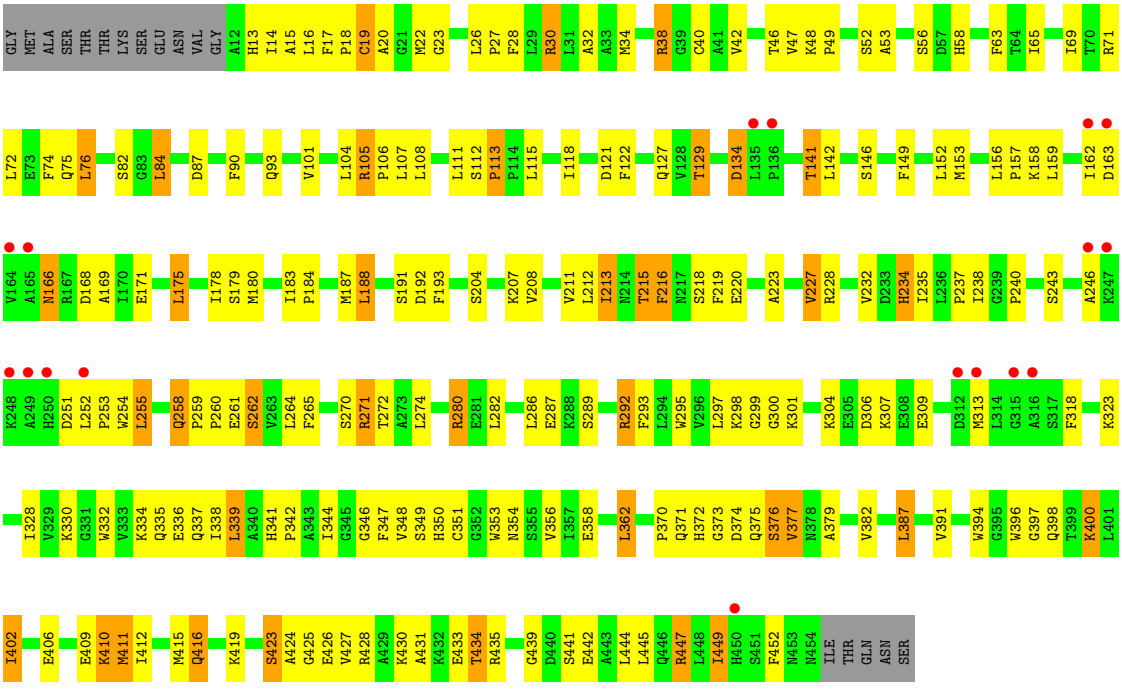
Chain D:





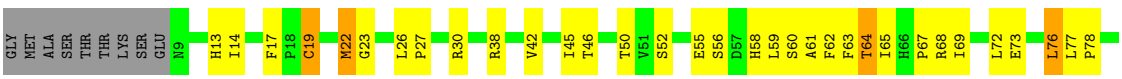
• Molecule 1: SbCGTa

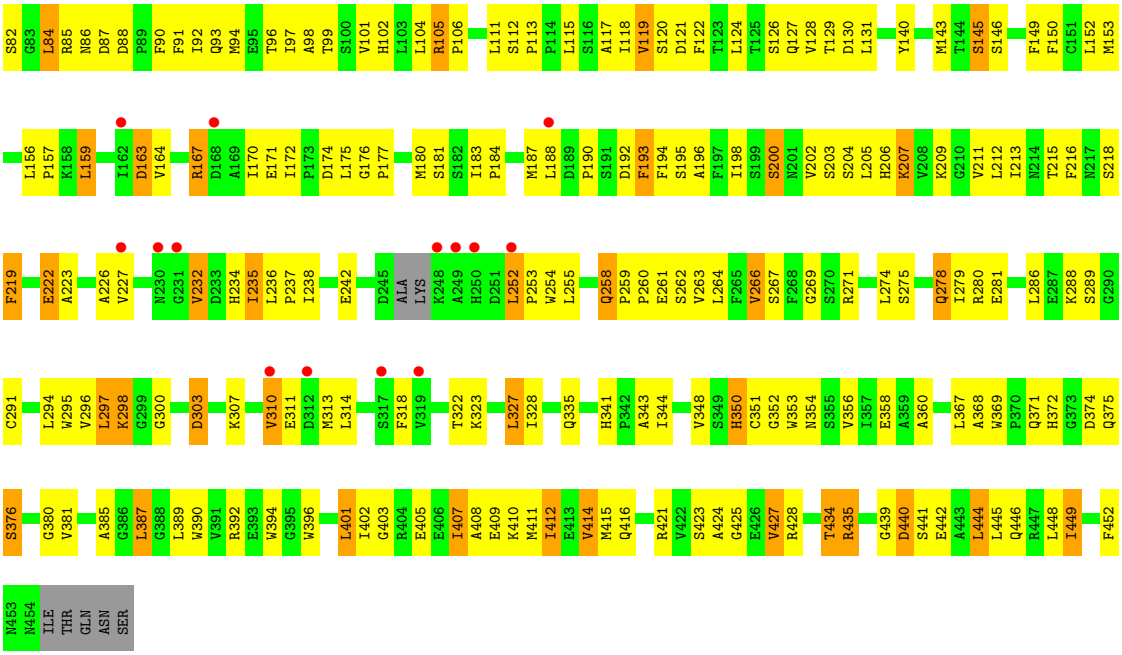
Chain E:



• Molecule 1: SbCGTa

Chain F:




S82 G83 L84 R85 N86 D87 D88 P89 F90 F91 I92 Q93 M94 E95 T96 I97 A98 T99 S100 V101 H102 L103 L104 R105 P106 L111 S112 P113 P114 L115 S116 A117 I118 V119 S120 D121 F122 T123 L124 T125 S126 Q127 V128 T129 D130 L131 Y140 M143 T144 S145 S146 F149 F150 C151 L152 M153
L156 P157 R158 L159 I162 D163 V164 R167 D168 A169 I170 E171 I172 P173 D174 L175 G176 P177 M180 S181 S182 I183 P184 M187 L188 D189 P190 S191 D192 F193 F194 S195 A196 F197 I198 S199 S200 N201 V202 S203 S204 L205 H206 K207 V208 K209 G210 V211 L212 I213 N214 T215 F216 N217 S218
F219 E222 A223 A226 V227 N230 G231 V232 D233 H234 I235 L236 P237 I238 E242 D245 ALA LYS K248 A249 H250 D251 L252 P253 W254 L255 Q258 P259 P260 E261 S262 V263 L264 F265 V266 S267 F268 G269 S270 R271 L274 S275 Q278 I279 R280 E281 L286 E287 K288 S289 G290
C291 L294 W295 V296 L297 K298 G299 G300 D303 K307 V310 E311 D312 M313 L314 S317 F318 V319 T322 K323 L327 I328 Q335 H341 P342 A343 I344 V348 S349 H350 C351 G352 W353 N354 S355 V356 I357 E358 A359 A360 L367 A368 W369 P370 Q371 H372 G373 D374 Q375
S376 G380 V381 A385 G386 L387 G388 L389 W390 V391 R392 E393 W394 G395 W396 L401 I402 G403 R404 E405 E406 I407 A408 E409 K410 M411 T412 E413 V414 M415 Q416 R421 V422 S423 A424 G425 E426 V427 R428 T434 R435 G439 D440 S441 E442 A443 L444 L445 Q446 R447 L448 I449 F452
N453 N454 ILE THR GLN ASN SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	97.32Å 171.59Å 179.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.96 – 3.00 46.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (46.96-3.00) 97.7 (46.96-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.242 , 0.271 0.242 , 0.271	Depositor DCC
R_{free} test set	2946 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 54.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	19522	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.77	0/3268	0.80	0/4441
1	B	0.63	0/3263	0.77	0/4438
1	C	0.60	0/3328	0.66	0/4522
1	D	0.55	0/3191	0.69	0/4345
1	E	0.65	0/3329	0.74	0/4532
1	F	0.61	0/3392	0.66	0/4614
All	All	0.64	0/19771	0.72	0/26892

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3204	0	3037	211	0
1	B	3198	0	3010	305	0
1	C	3257	0	3129	356	0
1	D	3129	0	2923	338	0
1	E	3255	0	3076	233	0
1	F	3319	0	3177	287	0
2	A	25	0	11	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	11	2	0
2	C	25	0	11	7	0
2	D	25	0	11	4	0
2	E	25	0	11	15	0
2	F	25	0	11	1	0
3	A	7	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
All	All	19522	0	18418	1727	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 46.

All (1727) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:HG11	1:B:97:ILE:CD1	1.35	1.50
1:D:211:VAL:C	1:D:212:LEU:HD23	1.39	1.38
1:A:47:VAL:CG1	1:A:76:LEU:HD21	1.57	1.34
1:A:407:ILE:CG2	1:A:411:MET:HE1	1.60	1.31
1:C:434:THR:CG2	1:C:441:SER:HB2	1.60	1.31
1:C:401:LEU:HD12	1:C:402:ILE:N	1.43	1.30
1:D:341:HIS:ND1	1:D:342:PRO:HD2	1.42	1.28
1:C:300:GLY:CA	1:C:307:LYS:HG2	1.63	1.26
1:C:401:LEU:HD12	1:C:401:LEU:C	1.53	1.26
1:C:27:PRO:HG3	1:C:354:ASN:ND2	1.47	1.25
1:B:212:LEU:HB3	1:B:238:ILE:CD1	1.65	1.25
1:C:27:PRO:CG	1:C:354:ASN:HD21	1.49	1.24
1:D:448:LEU:HD12	1:D:448:LEU:O	1.36	1.24
1:A:34:MET:CE	1:A:241:LEU:HD23	1.66	1.23
1:D:394:TRP:NE1	1:D:402:ILE:HD11	1.53	1.21
1:F:401:LEU:HD23	1:F:401:LEU:C	1.50	1.21
1:B:212:LEU:CB	1:B:238:ILE:HD12	1.72	1.19
1:B:47:VAL:CG2	1:B:76:LEU:HD21	1.70	1.19
1:B:156:LEU:CD1	1:B:160:LEU:HG	1.72	1.19
1:B:223:ALA:O	1:B:227:VAL:HG22	1.43	1.19
1:A:407:ILE:HG22	1:A:411:MET:CE	1.73	1.18
1:D:350:HIS:CE1	1:D:352:GLY:H	1.60	1.17
1:C:175:LEU:C	1:C:175:LEU:HD12	1.61	1.17
1:E:286:LEU:CD2	1:E:411:MET:CE	2.23	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:CG1	1:B:97:ILE:CD1	2.23	1.16
1:A:407:ILE:HG22	1:A:411:MET:HE1	1.21	1.16
1:C:138:SER:OG	1:C:209:LYS:HG3	1.44	1.15
1:D:391:VAL:HG11	1:D:394:TRP:CD1	1.82	1.15
1:C:53:ALA:HB3	1:C:304:LYS:HD3	1.24	1.15
1:B:34:MET:HE2	1:B:242:GLU:H	0.98	1.14
1:D:394:TRP:CD1	1:D:402:ILE:CD1	2.30	1.14
1:A:54:ALA:HB2	1:A:304:LYS:HE2	1.17	1.14
1:F:88:ASP:O	1:F:92:ILE:HG13	1.44	1.14
1:E:38:ARG:HH11	1:E:38:ARG:HG3	1.07	1.14
1:F:254:TRP:CD2	1:F:327:LEU:HD22	1.82	1.13
1:C:300:GLY:N	1:C:307:LYS:HG2	1.61	1.13
1:B:212:LEU:HD23	1:B:238:ILE:HD11	1.30	1.13
1:E:286:LEU:CD2	1:E:411:MET:HE2	1.76	1.12
1:B:211:VAL:C	1:B:212:LEU:HD12	1.69	1.12
1:A:47:VAL:CG1	1:A:76:LEU:CD2	2.28	1.12
1:C:227:VAL:HG11	1:C:235:ILE:HD12	1.20	1.12
1:E:169:ALA:HB1	1:E:178:ILE:O	1.48	1.11
1:F:434:THR:CG2	1:F:441:SER:HB2	1.79	1.11
1:F:434:THR:HG22	1:F:441:SER:HB2	1.31	1.11
1:B:90:PHE:O	1:B:94:MET:HG3	1.48	1.09
1:C:88:ASP:O	1:C:92:ILE:HG13	1.52	1.09
1:D:115:LEU:HB2	1:D:137:ILE:HD11	1.14	1.09
1:B:156:LEU:HD11	1:B:160:LEU:HG	1.12	1.09
1:C:213:ILE:HG23	1:C:215:THR:HG22	1.29	1.09
1:E:335:GLN:OE1	2:E:500:UDP:H2'	1.52	1.09
1:F:159:LEU:C	1:F:159:LEU:HD12	1.73	1.09
1:F:318:PHE:O	1:F:322:THR:HG23	1.53	1.09
1:C:175:LEU:HD12	1:C:175:LEU:O	1.51	1.09
1:C:300:GLY:HA3	1:C:307:LYS:HG2	1.26	1.09
1:D:389:LEU:HD21	1:D:420:LEU:CD2	1.83	1.08
1:A:407:ILE:CG2	1:A:411:MET:CE	2.30	1.08
1:C:63:PHE:CZ	1:C:71:ARG:HB2	1.88	1.08
1:B:271:ARG:HB3	1:B:301:LYS:O	1.52	1.08
1:E:447:ARG:HH11	1:E:447:ARG:CG	1.62	1.08
1:C:268:PHE:O	1:C:272:THR:HG23	1.53	1.08
1:F:278:GLN:HE21	1:F:278:GLN:CA	1.58	1.08
1:B:229:ARG:O	1:B:229:ARG:HG3	1.50	1.07
1:C:434:THR:HG22	1:C:441:SER:CB	1.85	1.07
1:C:434:THR:HG22	1:C:441:SER:HB2	1.08	1.06
1:E:38:ARG:HH11	1:E:38:ARG:CG	1.68	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:CG2	1:B:76:LEU:CD2	2.33	1.05
1:D:424:ALA:O	1:D:427:VAL:HG12	1.54	1.05
1:C:63:PHE:CE1	1:C:71:ARG:HB2	1.91	1.05
1:C:434:THR:CG2	1:C:441:SER:CB	2.35	1.05
1:D:184:PRO:HD2	1:D:187:MET:HE3	1.13	1.05
1:B:47:VAL:HG21	1:B:76:LEU:CD2	1.84	1.05
1:B:224:ILE:O	1:B:227:VAL:HG23	1.56	1.04
1:D:394:TRP:CE2	1:D:402:ILE:HD11	1.92	1.04
1:D:76:LEU:HD13	1:D:96:THR:HG21	1.40	1.04
1:A:173:PRO:HB2	1:A:230:ASN:HD21	1.19	1.04
1:B:47:VAL:HG11	1:B:97:ILE:HD13	1.09	1.04
1:C:162:ILE:HD12	1:C:163:ASP:H	1.22	1.04
1:C:54:ALA:H	1:C:304:LYS:HD2	1.23	1.03
1:B:76:LEU:HD13	1:B:96:THR:HG22	1.39	1.03
1:C:298:LYS:HB2	1:C:298:LYS:NZ	1.72	1.03
1:C:387:LEU:HD23	1:C:387:LEU:O	1.58	1.03
1:E:16:LEU:HD22	1:E:32:ALA:HB2	1.37	1.03
1:A:60:SER:O	1:A:64:THR:HG23	1.57	1.02
1:B:34:MET:HE2	1:B:242:GLU:N	1.74	1.02
1:D:115:LEU:HB2	1:D:137:ILE:CD1	1.89	1.02
1:D:212:LEU:HD23	1:D:212:LEU:N	1.65	1.02
1:E:286:LEU:HD23	1:E:411:MET:CE	1.90	1.02
1:F:348:VAL:HG22	1:F:367:LEU:HD23	1.41	1.02
1:C:84:LEU:HD22	1:C:84:LEU:H	1.22	1.02
1:E:286:LEU:HD21	1:E:411:MET:CE	1.88	1.02
1:E:346:GLY:HA3	1:E:415:MET:HE3	1.38	1.02
1:F:235:ILE:O	1:F:236:LEU:HD23	1.59	1.02
1:A:424:ALA:O	1:A:427:VAL:HG12	1.59	1.02
1:D:378:ASN:O	1:D:381:VAL:HG23	1.60	1.02
1:B:34:MET:HE1	1:B:241:LEU:HA	1.41	1.02
1:C:50:THR:HG21	1:C:52:SER:O	1.59	1.02
1:C:74:PHE:CZ	1:C:104:LEU:HG	1.95	1.02
1:D:184:PRO:HD2	1:D:187:MET:CE	1.88	1.02
1:D:448:LEU:HD12	1:D:448:LEU:C	1.75	1.01
1:E:49:PRO:HD2	1:E:76:LEU:HD21	1.42	1.01
1:A:47:VAL:HG11	1:A:76:LEU:CD2	1.89	1.01
1:A:411:MET:O	1:A:414:VAL:HG12	1.61	1.01
1:C:101:VAL:HG21	1:C:127:GLN:HB3	1.41	1.01
1:B:76:LEU:HD13	1:B:96:THR:CG2	1.90	1.01
1:C:138:SER:HG	1:C:209:LYS:HG3	1.25	1.01
1:E:447:ARG:HH11	1:E:447:ARG:HG2	0.87	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:LEU:HD23	1:F:411:MET:SD	2.00	1.01
1:A:16:LEU:CD1	1:A:32:ALA:HB2	1.90	1.00
1:D:211:VAL:C	1:D:212:LEU:CD2	2.30	0.99
1:E:169:ALA:HB2	1:E:179:SER:HA	1.40	0.99
1:B:42:VAL:CG1	1:B:69:ILE:HG12	1.91	0.99
1:F:112:SER:HB3	1:F:113:PRO:HD3	1.38	0.99
1:F:401:LEU:C	1:F:401:LEU:CD2	2.30	0.99
1:A:341:HIS:ND1	1:A:342:PRO:HD2	1.77	0.99
1:D:341:HIS:CG	1:D:342:PRO:HD2	1.97	0.99
1:D:350:HIS:CE1	1:D:352:GLY:N	2.30	0.99
1:B:22:MET:CE	1:B:25:LEU:HD23	1.92	0.99
1:F:278:GLN:HA	1:F:278:GLN:NE2	1.74	0.99
1:A:16:LEU:HD11	1:A:32:ALA:CB	1.92	0.99
1:B:271:ARG:HG2	1:B:271:ARG:HH11	1.22	0.99
1:B:126:SER:O	1:B:129:THR:HG22	1.62	0.99
1:F:61:ALA:O	1:F:64:THR:HG22	1.63	0.99
1:B:47:VAL:HG11	1:B:97:ILE:HD11	1.40	0.99
1:F:159:LEU:HD12	1:F:159:LEU:O	1.61	0.99
1:C:175:LEU:C	1:C:175:LEU:CD1	2.30	0.99
1:F:171:GLU:CG	1:F:177:PRO:HB3	1.91	0.99
1:C:401:LEU:C	1:C:401:LEU:CD1	2.30	0.98
1:C:300:GLY:HA3	1:C:307:LYS:CG	1.93	0.98
1:D:394:TRP:CD1	1:D:402:ILE:HD12	1.96	0.98
1:B:47:VAL:HG21	1:B:76:LEU:HD21	0.98	0.98
1:F:120:SER:OG	1:F:128:VAL:HG11	1.62	0.98
1:C:278:GLN:NE2	1:C:369:TRP:CH2	2.31	0.98
1:F:401:LEU:HD23	1:F:402:ILE:N	1.79	0.97
1:F:434:THR:CG2	1:F:441:SER:CB	2.41	0.97
1:E:286:LEU:HD21	1:E:411:MET:HE2	1.46	0.97
1:B:263:VAL:HG22	1:B:344:ILE:HD12	1.42	0.97
1:C:353:TRP:HA	1:C:356:VAL:CG2	1.95	0.97
1:E:286:LEU:HD23	1:E:411:MET:HE2	1.43	0.97
1:D:105:ARG:HG2	1:D:131:LEU:HD11	1.47	0.96
1:F:235:ILE:C	1:F:236:LEU:HD23	1.85	0.96
1:A:47:VAL:HG11	1:A:76:LEU:HD21	0.97	0.96
1:F:403:GLY:O	1:F:407:ILE:HG13	1.66	0.96
1:D:389:LEU:CD2	1:D:420:LEU:CD2	2.42	0.96
1:F:254:TRP:CE3	1:F:327:LEU:CD2	2.48	0.96
1:D:202:VAL:O	1:D:205:LEU:HB2	1.65	0.96
1:E:424:ALA:O	1:E:427:VAL:HG12	1.66	0.96
1:A:254:TRP:O	1:A:258:GLN:HG2	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HD11	1:B:160:LEU:CG	1.95	0.95
1:B:212:LEU:HD12	1:B:212:LEU:N	1.75	0.95
1:E:354:ASN:O	1:E:358:GLU:HG3	1.65	0.95
1:B:276:LYS:NZ	1:B:280:ARG:HH21	1.65	0.95
1:A:341:HIS:ND1	1:A:342:PRO:CD	2.30	0.95
1:B:213:ILE:HG23	1:B:215:THR:HG22	1.46	0.95
1:B:289:SER:HB3	1:B:411:MET:CE	1.95	0.95
1:F:278:GLN:HE21	1:F:278:GLN:HA	1.26	0.95
1:D:394:TRP:NE1	1:D:402:ILE:CD1	2.30	0.95
1:A:16:LEU:HD11	1:A:32:ALA:HB2	0.97	0.95
1:B:212:LEU:N	1:B:212:LEU:CD1	2.30	0.95
1:D:295:TRP:HB3	1:D:328:ILE:HD12	1.46	0.95
1:B:47:VAL:CG1	1:B:97:ILE:HD11	1.90	0.95
1:D:391:VAL:HG11	1:D:394:TRP:NE1	1.81	0.94
1:C:401:LEU:CD1	1:C:402:ILE:N	2.30	0.94
1:D:126:SER:O	1:D:129:THR:HG22	1.67	0.94
1:D:184:PRO:CD	1:D:187:MET:HE3	1.97	0.94
1:E:286:LEU:CD2	1:E:411:MET:HE1	1.95	0.94
1:E:447:ARG:HG2	1:E:447:ARG:NH1	1.66	0.94
1:F:434:THR:CG2	1:F:441:SER:H	1.81	0.94
1:C:213:ILE:CG2	1:C:215:THR:HG22	1.97	0.94
1:D:184:PRO:CD	1:D:187:MET:CE	2.46	0.94
1:F:278:GLN:CA	1:F:278:GLN:NE2	2.30	0.94
1:E:358:GLU:O	1:E:362:LEU:HD12	1.68	0.93
1:B:434:THR:CG2	1:B:441:SER:HB2	1.97	0.93
1:C:300:GLY:H	1:C:307:LYS:CG	1.82	0.92
1:D:367:LEU:HD12	1:D:389:LEU:O	1.69	0.92
1:F:254:TRP:CD2	1:F:327:LEU:CD2	2.52	0.92
1:A:350:HIS:CD2	1:A:352:GLY:H	1.87	0.92
1:F:26:LEU:O	1:F:30:ARG:HG3	1.69	0.92
1:A:54:ALA:CB	1:A:304:LYS:HE2	2.00	0.92
1:F:242:GLU:OE1	1:F:435:ARG:HD2	1.70	0.92
1:A:34:MET:HE1	1:A:241:LEU:HD23	1.52	0.91
1:F:238:ILE:O	1:F:238:ILE:HG22	1.70	0.91
1:C:50:THR:HG23	1:C:52:SER:H	1.31	0.91
1:C:403:GLY:O	1:C:407:ILE:HG13	1.71	0.91
1:F:434:THR:HG21	1:F:441:SER:CB	1.99	0.91
1:B:52:SER:OG	1:B:55:GLU:HG3	1.69	0.91
1:D:76:LEU:HD13	1:D:96:THR:CG2	2.00	0.91
1:B:22:MET:HE3	1:B:25:LEU:HD23	1.50	0.90
1:E:90:PHE:CE2	1:E:271:ARG:HB3	2.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:PRO:HG2	1:D:187:MET:HE2	1.53	0.90
1:D:24:HIS:O	1:D:27:PRO:HG2	1.72	0.90
1:F:86:ASN:ND2	1:F:92:ILE:HG12	1.86	0.89
1:B:155:TYR:CE1	1:B:159:LEU:HB2	2.07	0.89
1:D:341:HIS:ND1	1:D:342:PRO:CD	2.32	0.89
1:C:105:ARG:HB3	1:C:106:PRO:HD3	1.54	0.89
1:C:149:PHE:CD2	1:C:153:MET:HE2	2.06	0.89
1:C:353:TRP:O	1:C:356:VAL:HG23	1.72	0.89
1:E:42:VAL:HG12	1:E:69:ILE:HG23	1.54	0.89
1:A:47:VAL:HG12	1:A:76:LEU:CD2	2.02	0.89
1:B:212:LEU:CD2	1:B:238:ILE:HD11	2.02	0.89
1:C:298:LYS:CB	1:C:298:LYS:HZ3	1.85	0.89
1:C:162:ILE:HD12	1:C:163:ASP:N	1.88	0.89
1:D:52:SER:OG	1:D:55:GLU:HB2	1.74	0.88
1:C:434:THR:HG21	1:C:441:SER:HB2	1.55	0.88
1:C:298:LYS:NZ	1:C:298:LYS:CB	2.30	0.88
1:D:391:VAL:CG1	1:D:394:TRP:CD1	2.56	0.88
1:F:278:GLN:HE21	1:F:278:GLN:C	1.75	0.88
1:D:366:VAL:HG12	1:D:388:GLY:HA3	1.55	0.88
1:D:389:LEU:HD21	1:D:420:LEU:HD23	1.53	0.88
1:D:153:MET:HA	1:D:198:ILE:HD11	1.53	0.88
1:C:26:LEU:O	1:C:30:ARG:HG3	1.73	0.88
1:D:341:HIS:CG	1:D:342:PRO:CD	2.56	0.88
1:D:26:LEU:O	1:D:30:ARG:HG3	1.74	0.88
1:D:194:PHE:O	1:D:194:PHE:HD1	1.57	0.88
1:F:112:SER:CB	1:F:113:PRO:HD3	2.04	0.88
1:F:159:LEU:C	1:F:159:LEU:CD1	2.42	0.88
1:C:16:LEU:HD21	1:C:31:LEU:HD23	1.55	0.88
1:D:26:LEU:N	1:D:27:PRO:HD2	1.89	0.87
1:D:38:ARG:HB3	1:D:449:ILE:HD12	1.55	0.87
1:F:149:PHE:HE2	1:F:153:MET:HE2	1.39	0.87
1:F:434:THR:HG22	1:F:441:SER:CB	2.04	0.87
1:D:266:VAL:HB	1:D:295:TRP:CD1	2.09	0.87
1:A:54:ALA:HB2	1:A:304:LYS:CE	2.03	0.87
1:F:434:THR:HG21	1:F:441:SER:OG	1.73	0.87
1:B:218:SER:OG	1:B:430:LYS:HD3	1.73	0.87
1:C:278:GLN:HE21	1:C:369:TRP:HH2	1.16	0.87
1:C:383:GLU:HG2	1:C:384:LYS:NZ	1.88	0.87
1:C:434:THR:CG2	1:C:441:SER:H	1.86	0.87
1:B:16:LEU:HD11	1:B:32:ALA:HB2	1.56	0.86
1:C:278:GLN:NE2	1:C:369:TRP:CZ2	2.43	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:PHE:HB2	1:F:271:ARG:HH12	1.37	0.86
1:B:198:ILE:O	1:B:202:VAL:HG23	1.76	0.86
1:D:394:TRP:CD1	1:D:402:ILE:HD11	2.06	0.86
1:E:65:ILE:HG13	1:E:246:ALA:HB1	1.57	0.86
1:D:394:TRP:CE2	1:D:402:ILE:CD1	2.59	0.86
1:B:34:MET:CE	1:B:241:LEU:HA	2.05	0.86
1:A:34:MET:CE	1:A:241:LEU:CD2	2.51	0.86
1:F:222:GLU:CD	1:F:222:GLU:H	1.78	0.86
1:C:124:LEU:O	1:C:128:VAL:HG23	1.76	0.85
1:F:223:ALA:O	1:F:227:VAL:HG23	1.76	0.85
1:C:183:ILE:HG23	1:C:187:MET:CE	2.05	0.85
1:F:143:MET:HE3	1:F:145:SER:H	1.39	0.85
1:C:300:GLY:H	1:C:307:LYS:HG2	1.29	0.85
1:F:297:LEU:HD13	1:F:297:LEU:N	1.91	0.85
1:D:63:PHE:CZ	1:D:71:ARG:HB2	2.12	0.85
1:D:394:TRP:CG	1:D:402:ILE:CD1	2.60	0.84
1:A:285:ALA:HB1	1:A:407:ILE:HG22	1.56	0.84
1:A:272:THR:CB	1:A:301:LYS:HA	2.08	0.84
1:E:335:GLN:OE1	2:E:500:UDP:C2'	2.24	0.84
1:E:346:GLY:CA	1:E:415:MET:HE3	2.08	0.84
1:F:298:LYS:HB3	1:F:298:LYS:HZ3	1.43	0.84
1:A:43:THR:HA	1:A:70:THR:HG22	1.59	0.84
1:B:203:SER:O	1:B:206:HIS:CG	2.30	0.84
1:C:112:SER:HB2	1:C:113:PRO:HD3	1.57	0.84
1:F:171:GLU:HA	1:F:177:PRO:HA	1.57	0.84
1:C:213:ILE:CG2	1:C:215:THR:CG2	2.57	0.83
1:D:218:SER:OG	1:D:430:LYS:HE2	1.78	0.83
1:F:143:MET:CE	1:F:145:SER:N	2.41	0.83
1:C:84:LEU:HD22	1:C:84:LEU:N	1.94	0.83
1:C:238:ILE:H	1:C:238:ILE:HD13	1.42	0.83
1:A:299:GLY:H	1:A:330:LYS:NZ	1.77	0.83
1:D:211:VAL:O	1:D:212:LEU:HD23	1.78	0.83
1:B:276:LYS:HZ2	1:B:280:ARG:HH21	1.24	0.83
1:C:225:GLU:OE1	1:C:225:GLU:HA	1.77	0.83
1:E:346:GLY:HA3	1:E:415:MET:CE	2.08	0.83
1:C:314:LEU:HD12	1:C:328:ILE:HD12	1.60	0.82
1:B:107:LEU:HD12	1:B:107:LEU:O	1.79	0.82
1:C:401:LEU:HD12	1:C:402:ILE:CA	2.08	0.82
1:F:143:MET:CE	1:F:145:SER:CA	2.56	0.82
1:B:263:VAL:CG2	1:B:344:ILE:HD12	2.09	0.82
1:C:298:LYS:HB2	1:C:298:LYS:HZ2	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LYS:HB2	1:C:298:LYS:HZ3	1.39	0.82
1:C:171:GLU:HA	1:C:177:PRO:HB3	1.62	0.82
1:C:268:PHE:O	1:C:272:THR:CG2	2.27	0.82
1:D:151:CYS:HA	1:D:154:ALA:HB3	1.61	0.82
1:F:90:PHE:HB2	1:F:271:ARG:NH1	1.92	0.82
1:B:34:MET:CE	1:B:242:GLU:H	1.87	0.81
1:B:156:LEU:HD13	1:B:156:LEU:O	1.79	0.81
1:A:272:THR:CB	1:A:301:LYS:HG2	2.10	0.81
1:D:212:LEU:N	1:D:212:LEU:CD2	2.41	0.81
1:E:394:TRP:O	1:E:400:LYS:HD2	1.81	0.81
1:C:295:TRP:CE2	1:C:297:LEU:CD1	2.64	0.81
1:A:173:PRO:CB	1:A:230:ASN:HD21	1.94	0.81
1:F:401:LEU:HD23	1:F:401:LEU:O	1.79	0.81
1:D:273:ALA:HB1	1:D:371:GLN:CG	2.10	0.81
1:B:218:SER:OG	1:B:430:LYS:CD	2.29	0.81
1:B:434:THR:HG22	1:B:441:SER:HB2	1.63	0.81
1:A:278:GLN:HE22	1:A:402:ILE:H	1.26	0.80
1:C:84:LEU:H	1:C:84:LEU:CD2	1.94	0.80
1:C:353:TRP:HA	1:C:356:VAL:HG23	1.61	0.80
1:B:289:SER:CB	1:B:411:MET:HE3	2.11	0.80
1:C:334:LYS:O	1:C:338:ILE:HG13	1.82	0.80
1:C:394:TRP:CE2	1:C:402:ILE:CD1	2.65	0.80
1:F:159:LEU:O	1:F:159:LEU:CD1	2.30	0.80
1:D:350:HIS:HE1	1:D:352:GLY:CA	1.94	0.80
1:B:289:SER:HB3	1:B:411:MET:HE3	1.62	0.80
1:C:105:ARG:HG2	1:C:105:ARG:HH11	1.47	0.80
1:C:175:LEU:CD1	1:C:176:GLY:O	2.30	0.80
1:D:278:GLN:O	1:D:278:GLN:NE2	2.15	0.80
1:D:220:GLU:O	1:D:224:ILE:CG1	2.30	0.80
1:B:34:MET:CE	1:B:241:LEU:HD23	2.11	0.80
1:F:198:ILE:O	1:F:202:VAL:HG23	1.80	0.80
1:A:88:ASP:OD1	1:A:89:PRO:HD2	1.81	0.80
1:B:156:LEU:CD1	1:B:156:LEU:O	2.30	0.80
1:B:85:ARG:CB	1:B:193:PHE:CE1	2.64	0.80
1:C:434:THR:HG21	1:C:441:SER:CB	2.07	0.79
1:F:424:ALA:O	1:F:427:VAL:HG23	1.82	0.79
1:B:271:ARG:HG2	1:B:271:ARG:NH1	1.88	0.79
1:E:38:ARG:CG	1:E:38:ARG:NH1	2.39	0.79
1:F:50:THR:CG2	1:F:52:SER:O	2.30	0.79
1:A:173:PRO:HB2	1:A:230:ASN:ND2	1.97	0.79
1:D:10:VAL:O	1:D:10:VAL:CG1	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:ASN:O	1:E:358:GLU:CG	2.29	0.79
1:F:314:LEU:HD12	1:F:328:ILE:HD13	1.65	0.79
1:C:210:GLY:HA2	1:C:234:HIS:HB2	1.65	0.79
1:F:372:HIS:O	1:F:375:GLN:HG3	1.83	0.79
1:A:282:LEU:HD13	1:A:369:TRP:HZ3	1.48	0.79
1:C:300:GLY:N	1:C:307:LYS:CG	2.41	0.79
1:D:410:LYS:CE	1:D:413:GLU:OE1	2.30	0.79
1:E:168:ASP:O	1:E:180:MET:HB2	1.83	0.79
1:F:286:LEU:CD2	1:F:411:MET:SD	2.70	0.79
1:D:350:HIS:HE1	1:D:352:GLY:HA3	1.46	0.79
1:B:42:VAL:HG13	1:B:69:ILE:HG23	1.65	0.79
1:C:50:THR:CG2	1:C:52:SER:O	2.30	0.79
1:D:391:VAL:O	1:D:391:VAL:HG12	1.83	0.79
1:B:126:SER:O	1:B:129:THR:CG2	2.30	0.78
1:B:223:ALA:O	1:B:227:VAL:CG2	2.30	0.78
1:B:102:HIS:O	1:B:105:ARG:HG3	1.82	0.78
1:D:378:ASN:O	1:D:381:VAL:CG2	2.30	0.78
1:A:407:ILE:HG23	1:A:411:MET:CE	2.14	0.78
1:B:90:PHE:O	1:B:94:MET:CG	2.30	0.78
1:F:143:MET:CE	1:F:145:SER:H	1.94	0.78
1:F:254:TRP:CG	1:F:327:LEU:HD22	2.18	0.78
1:C:183:ILE:HG23	1:C:187:MET:HE1	1.65	0.78
1:B:16:LEU:HD13	1:B:28:PHE:O	1.83	0.78
1:C:149:PHE:CD2	1:C:153:MET:CE	2.66	0.78
1:A:407:ILE:O	1:A:411:MET:HE2	1.84	0.78
1:D:269:GLY:HA2	1:D:350:HIS:CD2	2.19	0.78
1:E:175:LEU:HD12	1:E:175:LEU:N	1.98	0.78
1:D:10:VAL:O	1:D:10:VAL:HG13	1.83	0.78
1:C:278:GLN:NE2	1:C:369:TRP:HH2	1.74	0.77
1:E:166:ASN:OD1	1:E:166:ASN:N	2.18	0.77
1:F:434:THR:HG23	1:F:441:SER:H	1.49	0.77
1:D:47:VAL:HG11	1:D:97:ILE:HD11	1.67	0.77
1:C:387:LEU:O	1:C:387:LEU:CD2	2.31	0.77
1:D:152:LEU:HD21	1:D:183:ILE:HG12	1.66	0.77
1:B:159:LEU:O	1:B:159:LEU:HD12	1.85	0.77
1:C:227:VAL:HG11	1:C:235:ILE:CD1	2.07	0.77
1:D:211:VAL:O	1:D:212:LEU:CD2	2.32	0.77
1:E:14:ILE:HD11	1:E:452:PHE:CD2	2.20	0.77
1:E:434:THR:HG23	1:E:441:SER:HB2	1.65	0.77
1:B:212:LEU:HD23	1:B:238:ILE:CD1	2.11	0.77
1:C:434:THR:HG23	1:C:441:SER:H	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:THR:CG2	1:C:52:SER:H	1.98	0.77
1:E:38:ARG:HG3	1:E:38:ARG:NH1	1.88	0.76
1:C:295:TRP:CZ2	1:C:297:LEU:CD1	2.67	0.76
1:C:435:ARG:NE	1:C:435:ARG:HA	2.00	0.76
1:A:93:GLN:HA	1:A:96:THR:HG22	1.65	0.76
1:B:284:ALA:CB	1:B:404:ARG:NH1	2.49	0.76
1:A:50:THR:HG22	1:A:52:SER:O	1.85	0.76
1:C:53:ALA:CB	1:C:304:LYS:HD3	2.13	0.76
1:A:47:VAL:HG12	1:A:76:LEU:CG	2.16	0.76
1:C:366:VAL:HG13	1:C:388:GLY:HA3	1.66	0.76
1:C:394:TRP:CD2	1:C:402:ILE:HD13	2.21	0.76
1:D:350:HIS:CE1	1:D:352:GLY:CA	2.68	0.76
1:D:354:ASN:CB	2:D:500:UDP:H5'1	2.15	0.76
1:A:19:CYS:HB3	1:A:97:ILE:HD12	1.67	0.76
1:C:27:PRO:HG3	1:C:354:ASN:HD21	0.63	0.76
1:C:389:LEU:HD12	1:C:414:VAL:HG22	1.67	0.76
1:A:255:LEU:HD23	1:A:341:HIS:HD2	1.51	0.75
1:D:266:VAL:HG13	1:D:348:VAL:HB	1.68	0.75
1:B:212:LEU:CB	1:B:238:ILE:CD1	2.44	0.75
1:C:141:THR:CG2	1:C:208:VAL:HG11	2.16	0.75
1:E:424:ALA:O	1:E:427:VAL:CG1	2.35	0.75
1:F:105:ARG:HB2	1:F:105:ARG:HH11	1.50	0.75
1:A:149:PHE:CE2	1:A:374:ASP:HA	2.22	0.75
1:E:84:LEU:HD13	1:E:84:LEU:N	2.00	0.75
1:C:318:PHE:O	1:C:322:THR:HG23	1.87	0.75
1:F:297:LEU:N	1:F:297:LEU:CD1	2.50	0.75
1:A:13:HIS:O	1:A:14:ILE:HD13	1.87	0.75
1:A:407:ILE:HG23	1:A:411:MET:HE1	1.62	0.75
1:D:391:VAL:CG1	1:D:394:TRP:CG	2.69	0.75
1:B:27:PRO:HA	1:B:30:ARG:HG3	1.69	0.75
1:C:295:TRP:CZ2	1:C:297:LEU:HD11	2.23	0.74
1:E:169:ALA:CB	1:E:178:ILE:O	2.32	0.74
1:E:426:GLU:O	1:E:430:LYS:HG3	1.87	0.74
1:F:124:LEU:O	1:F:128:VAL:HG23	1.87	0.74
1:C:105:ARG:HE	1:C:135:LEU:HD11	1.53	0.74
1:C:367:LEU:HB2	1:C:414:VAL:HG21	1.68	0.74
1:D:389:LEU:CD2	1:D:420:LEU:HD22	2.18	0.74
1:C:378:ASN:O	1:C:381:VAL:HG12	1.87	0.74
1:C:149:PHE:HD2	1:C:153:MET:CE	2.01	0.74
1:F:149:PHE:HE2	1:F:153:MET:CE	2.00	0.74
1:B:47:VAL:HG11	1:B:97:ILE:HD12	1.65	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ALA:HB2	1:C:304:LYS:HE3	1.70	0.73
1:A:407:ILE:O	1:A:411:MET:CE	2.36	0.73
1:E:13:HIS:HB3	1:E:115:LEU:HA	1.70	0.73
1:A:47:VAL:HG12	1:A:76:LEU:HG	1.70	0.73
1:B:16:LEU:CD1	1:B:28:PHE:O	2.36	0.73
1:D:350:HIS:CE1	1:D:352:GLY:HA3	2.23	0.73
1:C:353:TRP:C	1:C:356:VAL:HG23	2.09	0.73
1:B:434:THR:CG2	1:B:441:SER:CB	2.65	0.73
1:C:300:GLY:CA	1:C:307:LYS:CG	2.52	0.73
1:D:218:SER:OG	1:D:430:LYS:CE	2.36	0.73
1:E:15:ALA:HB2	1:E:115:LEU:HD22	1.70	0.73
1:F:143:MET:HE1	1:F:145:SER:C	2.09	0.73
1:A:320:GLU:O	1:A:323:LYS:HB3	1.88	0.73
1:B:213:ILE:CG2	1:B:215:THR:HG22	2.17	0.73
1:C:54:ALA:H	1:C:304:LYS:CD	2.00	0.73
1:C:175:LEU:HD13	1:C:176:GLY:O	1.89	0.73
1:D:278:GLN:HE21	1:D:278:GLN:C	1.92	0.73
1:D:448:LEU:C	1:D:448:LEU:CD1	2.51	0.73
1:A:341:HIS:CE1	1:A:342:PRO:HG2	2.24	0.72
1:B:224:ILE:C	1:B:227:VAL:HG23	2.08	0.72
1:C:88:ASP:O	1:C:92:ILE:CG1	2.34	0.72
1:D:16:LEU:HD22	1:D:32:ALA:HB2	1.71	0.72
1:D:274:LEU:HD22	1:D:278:GLN:HG2	1.71	0.72
1:A:105:ARG:HB2	1:A:106:PRO:HD3	1.71	0.72
1:F:298:LYS:HA	1:F:298:LYS:HE2	1.71	0.72
1:A:30:ARG:HG2	1:A:242:GLU:O	1.89	0.72
1:B:47:VAL:CG1	1:B:97:ILE:HD13	2.01	0.72
1:E:19:CYS:HB2	1:E:121:ASP:OD2	1.89	0.72
1:B:146:SER:OG	1:B:149:PHE:CB	2.37	0.72
1:A:34:MET:HE2	1:A:241:LEU:HD23	1.65	0.72
1:B:276:LYS:NZ	1:B:280:ARG:NH2	2.37	0.72
1:D:24:HIS:HA	1:D:144:THR:HG21	1.71	0.72
1:D:153:MET:CA	1:D:198:ILE:HD11	2.19	0.72
1:C:183:ILE:CG2	1:C:187:MET:CE	2.67	0.72
1:C:378:ASN:O	1:C:381:VAL:CG1	2.38	0.72
1:E:42:VAL:HG12	1:E:69:ILE:CG2	2.19	0.72
1:F:50:THR:HG22	1:F:52:SER:H	1.55	0.72
1:A:98:ALA:HB1	1:A:127:GLN:HG3	1.72	0.72
1:A:299:GLY:H	1:A:330:LYS:HZ3	1.36	0.72
1:B:34:MET:HE3	1:B:241:LEU:HD23	1.71	0.72
1:D:215:THR:HG22	1:D:216:PHE:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:MET:CE	1:F:145:SER:CB	2.67	0.72
1:A:212:LEU:N	1:A:212:LEU:HD12	2.05	0.72
1:B:226:ALA:O	1:B:230:ASN:HB2	1.90	0.72
1:C:352:GLY:O	1:C:356:VAL:HG22	1.89	0.72
1:E:18:PRO:HG3	1:E:28:PHE:CB	2.20	0.72
1:C:50:THR:HG23	1:C:52:SER:N	2.05	0.71
1:D:194:PHE:HD1	1:D:194:PHE:C	1.92	0.71
1:A:34:MET:HE3	1:A:241:LEU:HD23	1.68	0.71
1:E:299:GLY:HA3	1:E:313:MET:HE3	1.72	0.71
1:F:50:THR:HG22	1:F:52:SER:O	1.90	0.71
1:A:72:LEU:HG	1:A:107:LEU:HD11	1.72	0.71
1:B:141:THR:CG2	1:B:211:VAL:HG13	2.20	0.71
1:D:15:ALA:HA	1:D:43:THR:O	1.88	0.71
1:D:113:PRO:N	1:D:113:PRO:O	2.23	0.71
1:E:76:LEU:CD2	1:E:76:LEU:H	2.03	0.71
1:F:424:ALA:C	1:F:427:VAL:HG23	2.10	0.71
1:F:238:ILE:O	1:F:238:ILE:CG2	2.36	0.71
1:A:13:HIS:C	1:A:14:ILE:HD13	2.10	0.71
1:E:90:PHE:CE2	1:E:271:ARG:CB	2.74	0.71
1:E:112:SER:HB3	1:E:113:PRO:HD3	1.70	0.71
1:C:232:VAL:HG13	1:C:234:HIS:CE1	2.25	0.71
1:C:353:TRP:CA	1:C:356:VAL:HG23	2.19	0.71
1:F:50:THR:HG21	1:F:55:GLU:HB2	1.71	0.71
1:D:394:TRP:CD2	1:D:402:ILE:HD13	2.25	0.71
1:D:251:ASP:OD1	1:D:251:ASP:N	2.24	0.70
1:F:143:MET:HE1	1:F:145:SER:HB3	1.73	0.70
1:C:300:GLY:HA3	1:C:307:LYS:CB	2.21	0.70
1:D:317:SER:O	1:D:321:ARG:HG3	1.90	0.70
1:D:389:LEU:HD21	1:D:420:LEU:HD22	1.68	0.70
1:F:143:MET:CE	1:F:145:SER:C	2.60	0.70
1:C:383:GLU:CG	1:C:384:LYS:NZ	2.54	0.70
1:F:187:MET:O	1:F:195:SER:HB2	1.91	0.70
1:B:34:MET:HE3	1:B:241:LEU:CD2	2.21	0.70
1:B:266:VAL:HB	1:B:295:TRP:CD1	2.27	0.70
1:D:350:HIS:HE1	1:D:352:GLY:N	1.88	0.70
1:E:243:SER:CB	1:E:336:GLU:OE1	2.40	0.70
1:B:76:LEU:HD13	1:B:96:THR:HG21	1.71	0.70
1:A:285:ALA:HB1	1:A:407:ILE:CG2	2.21	0.70
1:D:339:LEU:CB	1:D:362:LEU:HD12	2.22	0.70
1:B:155:TYR:CD2	1:B:173:PRO:HD3	2.26	0.70
1:D:152:LEU:HD21	1:D:183:ILE:CG1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:PHE:O	1:D:194:PHE:CD1	2.44	0.70
1:C:383:GLU:HG2	1:C:384:LYS:HZ1	1.55	0.70
1:E:175:LEU:HD12	1:E:175:LEU:H	1.56	0.70
1:F:50:THR:HG22	1:F:52:SER:N	2.07	0.70
1:F:412:ILE:HG23	1:F:416:GLN:HG3	1.73	0.70
1:D:354:ASN:HB3	2:D:500:UDP:H5'1	1.74	0.69
1:E:65:ILE:HG13	1:E:246:ALA:CB	2.22	0.69
1:F:50:THR:HG21	1:F:52:SER:O	1.92	0.69
1:C:27:PRO:CG	1:C:354:ASN:ND2	2.28	0.69
1:F:296:VAL:C	1:F:297:LEU:HD13	2.12	0.69
1:C:353:TRP:HA	1:C:356:VAL:HG21	1.72	0.69
1:D:16:LEU:CD2	1:D:28:PHE:O	2.40	0.69
1:C:187:MET:O	1:C:195:SER:HB2	1.92	0.69
1:B:321:ARG:HG2	1:B:321:ARG:HH11	1.56	0.69
1:D:26:LEU:N	1:D:27:PRO:CD	2.55	0.69
1:D:194:PHE:C	1:D:194:PHE:CD1	2.66	0.69
1:D:391:VAL:HG12	1:D:394:TRP:CG	2.25	0.69
1:E:90:PHE:HE2	1:E:271:ARG:HB3	1.56	0.69
1:C:445:LEU:O	1:C:449:ILE:HG12	1.93	0.69
1:E:76:LEU:H	1:E:76:LEU:HD23	1.56	0.69
1:F:424:ALA:HA	1:F:427:VAL:CG2	2.22	0.69
1:B:156:LEU:CD1	1:B:156:LEU:C	2.61	0.69
1:D:153:MET:HB3	1:D:198:ILE:HD11	1.74	0.69
1:D:215:THR:CG2	1:D:216:PHE:N	2.55	0.69
1:F:232:VAL:O	1:F:232:VAL:HG22	1.92	0.69
1:F:286:LEU:HD21	1:F:411:MET:CE	2.22	0.69
1:A:47:VAL:HG12	1:A:76:LEU:HD21	1.61	0.69
1:C:54:ALA:N	1:C:304:LYS:HD2	2.04	0.69
1:E:252:LEU:N	1:E:253:PRO:CD	2.55	0.69
1:E:260:PRO:O	1:E:261:GLU:HB3	1.93	0.69
1:A:227:VAL:HG11	1:A:235:ILE:HD12	1.75	0.69
1:B:192:ASP:OD1	1:B:192:ASP:C	2.31	0.69
1:C:189:ASP:C	1:C:189:ASP:OD1	2.30	0.69
1:C:335:GLN:HB2	2:C:500:UDP:O2	1.93	0.69
1:C:50:THR:CG2	1:C:52:SER:N	2.55	0.68
1:D:410:LYS:HE3	1:D:413:GLU:OE1	1.93	0.68
1:E:152:LEU:HD21	1:E:183:ILE:HG13	1.75	0.68
1:E:183:ILE:HG23	1:E:187:MET:HE2	1.74	0.68
1:E:84:LEU:HD13	1:E:84:LEU:H	1.57	0.68
1:E:188:LEU:N	1:E:188:LEU:HD23	2.07	0.68
1:F:88:ASP:O	1:F:92:ILE:CG1	2.33	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:HIS:ND1	1:D:352:GLY:N	2.36	0.68
1:D:394:TRP:CD2	1:D:402:ILE:CD1	2.76	0.68
1:B:156:LEU:CD1	1:B:160:LEU:CG	2.61	0.68
1:E:307:LYS:CG	1:E:330:LYS:HZ1	2.06	0.68
1:F:143:MET:HE2	1:F:145:SER:N	2.08	0.68
1:A:254:TRP:CE2	1:A:258:GLN:OE1	2.46	0.68
1:D:14:ILE:HG13	1:D:40:CYS:SG	2.33	0.68
1:E:280:ARG:NE	1:E:280:ARG:HA	2.07	0.68
1:D:50:THR:HG21	1:D:55:GLU:HB3	1.75	0.68
1:E:49:PRO:CD	1:E:76:LEU:HD21	2.21	0.68
1:A:258:GLN:HA	1:A:258:GLN:HE21	1.57	0.68
1:B:35:LEU:O	1:B:40:CYS:HB2	1.94	0.68
1:C:64:THR:HG22	1:E:82:SER:CA	2.23	0.68
1:C:141:THR:HG23	1:C:208:VAL:HG11	1.76	0.68
1:D:268:PHE:O	1:D:350:HIS:CD2	2.47	0.67
1:E:72:LEU:HD11	1:E:111:LEU:HD11	1.76	0.67
1:E:215:THR:HG21	1:E:220:GLU:HG3	1.75	0.67
1:D:434:THR:HG22	1:D:441:SER:H	1.60	0.67
1:F:13:HIS:C	1:F:14:ILE:HD13	2.14	0.67
1:E:394:TRP:O	1:E:400:LYS:CD	2.42	0.67
1:F:206:HIS:CD2	1:F:207:LYS:HG2	2.30	0.67
1:B:289:SER:CB	1:B:411:MET:CE	2.69	0.67
1:C:300:GLY:H	1:C:307:LYS:CD	2.08	0.67
1:B:100:SER:O	1:B:103:LEU:HB2	1.94	0.67
1:E:23:GLY:O	1:E:27:PRO:HG2	1.94	0.67
1:F:42:VAL:HB	1:F:69:ILE:HG23	1.75	0.67
1:E:347:PHE:CD1	1:E:348:VAL:N	2.63	0.67
1:C:244:TYR:O	1:C:245:ASP:HB2	1.95	0.67
1:B:141:THR:HG22	1:B:211:VAL:HG13	1.75	0.67
1:D:424:ALA:O	1:D:427:VAL:CG1	2.36	0.67
1:E:26:LEU:HD12	2:E:500:UDP:H4'	1.77	0.67
1:F:101:VAL:HG13	1:F:131:LEU:HD21	1.77	0.67
1:F:271:ARG:HD2	1:F:271:ARG:O	1.95	0.67
1:B:146:SER:OG	1:B:149:PHE:HB3	1.95	0.67
1:B:158:LYS:O	1:B:162:ILE:HG13	1.94	0.67
1:D:153:MET:HB3	1:D:198:ILE:CD1	2.25	0.67
1:C:314:LEU:HD12	1:C:328:ILE:CD1	2.24	0.67
1:B:26:LEU:N	1:B:27:PRO:HD2	2.09	0.66
1:C:46:THR:HG21	1:C:59:LEU:CD2	2.24	0.66
1:C:366:VAL:CG1	1:C:388:GLY:HA3	2.25	0.66
1:B:50:THR:CG2	1:B:52:SER:O	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ASN:HD21	1:C:91:PHE:HB3	1.59	0.66
1:D:350:HIS:ND1	1:D:350:HIS:C	2.48	0.66
1:E:159:LEU:HD23	1:E:159:LEU:C	2.16	0.66
1:E:307:LYS:CG	1:E:330:LYS:NZ	2.58	0.66
1:F:101:VAL:O	1:F:131:LEU:HD21	1.96	0.66
1:D:24:HIS:O	1:D:27:PRO:CG	2.42	0.66
1:B:212:LEU:HB3	1:B:238:ILE:HD12	0.78	0.66
1:C:156:LEU:HB3	1:C:157:PRO:HD3	1.77	0.66
1:F:188:LEU:O	1:F:190:PRO:HD3	1.95	0.66
1:A:273:ALA:O	1:A:301:LYS:HE3	1.96	0.66
1:C:260:PRO:O	1:C:261:GLU:HB2	1.95	0.66
1:C:295:TRP:CE2	1:C:297:LEU:HD13	2.30	0.66
1:C:387:LEU:HD23	1:C:387:LEU:C	2.13	0.66
1:D:317:SER:O	1:D:321:ARG:CG	2.43	0.66
1:B:50:THR:HG21	1:B:55:GLU:HB2	1.78	0.66
1:C:243:SER:CB	1:C:336:GLU:OE2	2.44	0.66
1:F:203:SER:O	1:F:206:HIS:CE1	2.48	0.66
1:F:390:TRP:CH2	1:F:392:ARG:HD3	2.31	0.66
1:B:104:LEU:HD13	1:B:108:LEU:HD11	1.77	0.66
1:C:25:LEU:HD12	1:C:25:LEU:O	1.96	0.66
1:C:407:ILE:O	1:C:411:MET:HG3	1.96	0.66
1:C:60:SER:O	1:C:64:THR:HG23	1.96	0.66
1:C:284:ALA:CB	1:C:404:ARG:HD3	2.26	0.66
1:D:391:VAL:HG11	1:D:394:TRP:CE2	2.30	0.66
1:E:227:VAL:HG13	1:E:232:VAL:HB	1.78	0.66
1:C:366:VAL:HG12	1:C:387:LEU:HD22	1.78	0.66
1:F:434:THR:CG2	1:F:441:SER:N	2.56	0.66
1:A:282:LEU:HD13	1:A:369:TRP:CZ3	2.29	0.66
1:B:101:VAL:O	1:B:104:LEU:HB2	1.96	0.65
1:C:16:LEU:CD2	1:C:31:LEU:HD23	2.26	0.65
1:D:445:LEU:O	1:D:449:ILE:HG13	1.96	0.65
1:B:13:HIS:HD2	1:B:113:PRO:O	1.78	0.65
1:E:397:GLY:O	1:E:398:GLN:CB	2.44	0.65
1:B:212:LEU:CG	1:B:238:ILE:HD11	2.25	0.65
1:C:260:PRO:HA	1:C:343:ALA:HA	1.79	0.65
1:D:149:PHE:HE2	1:D:153:MET:HE2	1.62	0.65
1:B:25:LEU:HD12	1:B:25:LEU:O	1.96	0.65
1:E:254:TRP:O	1:E:258:GLN:NE2	2.30	0.65
1:E:338:ILE:O	1:E:344:ILE:HG13	1.96	0.65
1:A:278:GLN:HE22	1:A:402:ILE:N	1.94	0.65
1:B:263:VAL:HG22	1:B:344:ILE:CD1	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:THR:HA	1:D:70:THR:HG22	1.79	0.65
1:C:222:GLU:CD	1:C:222:GLU:H	2.00	0.65
1:C:286:LEU:HD23	1:C:411:MET:SD	2.36	0.65
1:C:350:HIS:O	1:C:351:CYS:HB2	1.96	0.65
1:D:410:LYS:NZ	1:D:413:GLU:OE1	2.30	0.65
1:F:152:LEU:HD21	1:F:183:ILE:HG12	1.79	0.65
1:A:233:ASP:N	1:A:233:ASP:OD1	2.29	0.65
1:B:276:LYS:HD2	1:B:313:MET:HA	1.78	0.65
1:C:387:LEU:CD2	1:C:387:LEU:C	2.64	0.65
1:D:194:PHE:O	1:D:198:ILE:HG22	1.96	0.65
1:D:339:LEU:HB2	1:D:362:LEU:HD12	1.77	0.65
1:E:16:LEU:CD2	1:E:32:ALA:HB2	2.20	0.65
1:F:146:SER:HB3	1:F:353:TRP:CE3	2.32	0.65
1:C:238:ILE:HD13	1:C:238:ILE:N	2.12	0.65
1:C:434:THR:HG22	1:C:441:SER:H	1.60	0.65
1:D:127:GLN:OE1	1:D:127:GLN:N	2.30	0.65
1:A:285:ALA:CB	1:A:407:ILE:CG2	2.75	0.65
1:B:394:TRP:CD2	1:B:402:ILE:HD12	2.32	0.65
1:D:51:VAL:HG11	1:D:90:PHE:CE1	2.32	0.65
1:D:171:GLU:HB2	1:D:177:PRO:HG3	1.79	0.65
1:D:391:VAL:CG1	1:D:391:VAL:O	2.45	0.65
1:E:350:HIS:HE1	2:E:500:UDP:O1B	1.80	0.65
1:F:408:ALA:O	1:F:412:ILE:HD12	1.97	0.65
1:A:50:THR:CG2	1:A:52:SER:O	2.45	0.65
1:A:407:ILE:HG22	1:A:411:MET:HE3	1.74	0.65
1:B:22:MET:HE1	1:B:25:LEU:HD23	1.77	0.65
1:D:149:PHE:CE2	1:D:153:MET:HE2	2.31	0.65
1:D:269:GLY:O	2:D:500:UDP:H5	1.79	0.65
1:F:254:TRP:O	1:F:258:GLN:NE2	2.29	0.65
1:B:192:ASP:OD1	1:B:194:PHE:N	2.30	0.64
1:C:284:ALA:HB1	1:C:404:ARG:HD3	1.79	0.64
1:F:149:PHE:CE2	1:F:153:MET:HE2	2.27	0.64
1:A:278:GLN:NE2	1:A:402:ILE:H	1.95	0.64
1:B:269:GLY:CA	1:B:350:HIS:CE1	2.81	0.64
1:F:50:THR:CG2	1:F:52:SER:H	2.10	0.64
1:F:143:MET:HE3	1:F:145:SER:CB	2.27	0.64
1:B:284:ALA:HB1	1:B:404:ARG:HH11	1.62	0.64
1:A:402:ILE:HG22	1:A:407:ILE:CD1	2.28	0.64
1:D:197:PHE:O	1:D:201:ASN:ND2	2.30	0.64
1:D:224:ILE:O	1:D:227:VAL:HG23	1.97	0.64
1:C:138:SER:OG	1:C:209:LYS:CG	2.34	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ILE:HD13	1:C:180:MET:CE	2.28	0.64
1:C:215:THR:OG1	1:C:220:GLU:HG3	1.97	0.64
1:F:104:LEU:N	1:F:104:LEU:HD23	2.12	0.64
1:F:303:ASP:OD1	1:F:303:ASP:N	2.28	0.64
1:A:14:ILE:HG21	1:A:35:LEU:CD1	2.26	0.64
1:B:47:VAL:HG13	1:B:97:ILE:HD11	1.77	0.64
1:B:448:LEU:O	1:B:448:LEU:HD12	1.98	0.64
1:C:105:ARG:HG2	1:C:105:ARG:NH1	2.10	0.64
1:C:434:THR:HG21	1:C:441:SER:OG	1.98	0.64
1:D:269:GLY:CA	1:D:350:HIS:CD2	2.80	0.64
1:E:402:ILE:CG2	1:E:406:GLU:HG2	2.27	0.64
1:F:278:GLN:NE2	1:F:278:GLN:O	2.30	0.64
1:B:34:MET:HE1	1:B:241:LEU:HD23	1.78	0.64
1:B:193:PHE:HD1	1:B:193:PHE:H	1.41	0.64
1:C:374:ASP:OD1	1:C:375:GLN:N	2.30	0.64
1:A:164:VAL:HG11	1:A:190:PRO:HD3	1.80	0.64
1:C:383:GLU:OE2	1:C:384:LYS:NZ	2.30	0.64
1:C:434:THR:CG2	1:C:441:SER:N	2.60	0.64
1:F:440:ASP:N	1:F:440:ASP:OD1	2.30	0.64
1:A:76:LEU:HD13	1:A:96:THR:HG23	1.80	0.64
1:D:61:ALA:O	1:D:65:ILE:HD12	1.98	0.64
1:E:48:LYS:O	1:E:76:LEU:CD2	2.46	0.64
1:C:170:ILE:CD1	1:C:180:MET:CE	2.76	0.63
1:F:101:VAL:HG12	1:F:131:LEU:HD11	1.80	0.63
1:D:349:SER:OG	1:D:351:CYS:N	2.30	0.63
1:E:159:LEU:O	1:E:163:ASP:CB	2.46	0.63
1:B:275:SER:O	1:B:279:ILE:HG13	1.98	0.63
1:F:298:LYS:HB3	1:F:298:LYS:NZ	2.13	0.63
1:B:104:LEU:O	1:B:108:LEU:HD12	1.98	0.63
1:D:22:MET:HE1	1:D:26:LEU:HD21	1.81	0.63
1:F:254:TRP:CE3	1:F:327:LEU:HD21	2.31	0.63
1:C:255:LEU:HD21	1:C:344:ILE:HD11	1.79	0.63
1:F:26:LEU:O	1:F:30:ARG:CG	2.46	0.63
1:A:272:THR:CB	1:A:301:LYS:CG	2.77	0.63
1:B:224:ILE:HA	1:B:227:VAL:CG2	2.29	0.63
1:D:184:PRO:HG2	1:D:187:MET:CE	2.27	0.63
1:D:389:LEU:HD23	1:D:420:LEU:CD2	2.27	0.63
1:E:212:LEU:HD12	1:E:212:LEU:N	2.13	0.63
1:C:320:GLU:OE2	1:C:320:GLU:HA	1.99	0.62
1:E:347:PHE:HD1	1:E:348:VAL:N	1.97	0.62
1:D:212:LEU:HA	1:D:236:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:SER:OG	1:B:149:PHE:N	2.30	0.62
1:C:295:TRP:HB3	1:C:328:ILE:HG22	1.80	0.62
1:D:394:TRP:CG	1:D:402:ILE:HD13	2.32	0.62
1:E:286:LEU:CG	1:E:411:MET:HE1	2.28	0.62
1:C:307:LYS:O	1:C:330:LYS:HE3	1.99	0.62
1:D:47:VAL:CG1	1:D:97:ILE:HD11	2.29	0.62
1:A:271:ARG:HB3	1:A:301:LYS:O	2.00	0.62
1:D:153:MET:CB	1:D:198:ILE:HD11	2.29	0.62
1:F:219:PHE:HE1	1:F:385:ALA:CB	2.11	0.62
1:A:217:ASN:OD1	1:A:217:ASN:N	2.33	0.62
1:B:218:SER:CB	1:B:430:LYS:HD2	2.29	0.62
1:E:108:LEU:HD22	1:E:115:LEU:HD11	1.82	0.62
1:A:274:LEU:HD22	1:A:278:GLN:HG2	1.80	0.62
1:D:184:PRO:CG	1:D:187:MET:HE2	2.29	0.62
1:A:129:THR:HG22	1:A:207:LYS:HD2	1.81	0.62
1:C:23:GLY:O	1:C:27:PRO:HG2	2.00	0.62
1:C:30:ARG:O	1:C:34:MET:HG3	1.98	0.62
1:E:159:LEU:HD23	1:E:159:LEU:O	1.99	0.62
1:F:86:ASN:HD21	1:F:92:ILE:N	1.98	0.62
1:B:286:LEU:HD21	1:B:293:PHE:CD2	2.35	0.61
1:D:341:HIS:CE1	1:D:342:PRO:HD2	2.30	0.61
1:F:19:CYS:HB2	1:F:121:ASP:OD2	2.00	0.61
1:F:90:PHE:O	1:F:94:MET:HG3	1.99	0.61
1:F:143:MET:HE1	1:F:145:SER:CB	2.30	0.61
1:D:402:ILE:O	1:D:402:ILE:HG23	2.00	0.61
1:E:235:ILE:HD12	1:E:235:ILE:O	2.00	0.61
1:B:275:SER:O	1:B:279:ILE:CG1	2.48	0.61
1:B:341:HIS:ND1	1:B:342:PRO:HD2	2.15	0.61
1:C:320:GLU:OE2	1:C:323:LYS:CE	2.49	0.61
1:F:129:THR:CG2	1:F:130:ASP:N	2.63	0.61
1:D:47:VAL:HB	1:D:97:ILE:CD1	2.31	0.61
1:D:184:PRO:CG	1:D:187:MET:CE	2.78	0.61
1:F:143:MET:HE3	1:F:145:SER:N	2.06	0.61
1:F:354:ASN:O	1:F:358:GLU:HG3	2.00	0.61
1:B:213:ILE:HG23	1:B:215:THR:CG2	2.28	0.61
1:B:272:THR:CB	1:B:301:LYS:HA	2.31	0.61
1:C:434:THR:HG22	1:C:441:SER:N	2.16	0.61
1:F:369:TRP:O	1:F:371:GLN:NE2	2.30	0.61
1:A:341:HIS:ND1	1:A:342:PRO:N	2.49	0.61
1:B:218:SER:HB3	1:B:430:LYS:HD2	1.83	0.61
1:C:198:ILE:O	1:C:202:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:ARG:HB2	1:F:192:ASP:HA	1.83	0.61
1:C:292:ARG:HA	1:C:325:LYS:O	2.00	0.60
1:F:360:ALA:HB2	1:F:387:LEU:HD11	1.82	0.60
1:A:238:ILE:O	1:A:238:ILE:HG22	2.00	0.60
1:D:411:MET:O	1:D:414:VAL:HG12	2.01	0.60
1:F:389:LEU:HD12	1:F:414:VAL:HB	1.84	0.60
1:C:371:GLN:HE21	1:C:397:GLY:HA3	1.67	0.60
1:C:383:GLU:HG2	1:C:384:LYS:CE	2.31	0.60
1:E:347:PHE:HD1	1:E:348:VAL:H	1.49	0.60
1:F:424:ALA:CA	1:F:427:VAL:HG23	2.32	0.60
1:C:434:THR:HG22	1:C:441:SER:CA	2.31	0.60
1:D:211:VAL:O	1:D:236:LEU:N	2.28	0.60
1:B:321:ARG:HG2	1:B:321:ARG:NH1	2.14	0.60
1:D:35:LEU:O	1:D:40:CYS:HB2	2.02	0.60
1:F:112:SER:CB	1:F:113:PRO:CD	2.78	0.60
1:A:108:LEU:HD13	1:A:137:ILE:HD11	1.83	0.60
1:D:278:GLN:OE1	1:D:402:ILE:HG22	2.02	0.60
1:E:42:VAL:CG1	1:E:69:ILE:HG23	2.28	0.60
1:D:22:MET:CE	1:D:25:LEU:HD23	2.32	0.60
1:A:51:VAL:HG11	1:A:90:PHE:CE1	2.36	0.60
1:A:298:LYS:NZ	2:A:500:UDP:O4	2.29	0.60
1:D:115:LEU:CB	1:D:137:ILE:CD1	2.75	0.60
1:F:131:LEU:N	1:F:131:LEU:HD12	2.17	0.60
1:A:254:TRP:CD2	1:A:258:GLN:OE1	2.55	0.59
1:D:105:ARG:HB2	1:D:106:PRO:HD3	1.84	0.59
1:D:350:HIS:ND1	1:D:351:CYS:N	2.50	0.59
1:E:76:LEU:HD23	1:E:76:LEU:N	2.16	0.59
1:A:36:ASP:OD1	1:A:36:ASP:C	2.41	0.59
1:A:293:PHE:CE1	1:A:326:GLY:HA3	2.38	0.59
1:B:42:VAL:HG12	1:B:69:ILE:HG12	1.81	0.59
1:D:155:TYR:C	1:D:157:PRO:HD2	2.23	0.59
1:D:156:LEU:HD11	1:D:160:LEU:HG	1.83	0.59
1:E:264:LEU:HD12	1:E:346:GLY:HA3	1.82	0.59
1:E:286:LEU:HG	1:E:411:MET:HE1	1.84	0.59
1:F:38:ARG:HG2	1:F:446:GLN:NE2	2.16	0.59
1:C:353:TRP:CA	1:C:356:VAL:CG2	2.74	0.59
1:C:394:TRP:CE2	1:C:402:ILE:HD12	2.36	0.59
1:E:53:ALA:H	1:E:304:LYS:CG	2.15	0.59
1:E:350:HIS:O	1:E:375:GLN:HB3	2.01	0.59
1:F:289:SER:HA	1:F:412:ILE:HD11	1.83	0.59
1:A:22:MET:HG3	1:A:332:TRP:CH2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:O	1:A:63:PHE:CD2	2.54	0.59
1:A:408:ALA:HA	1:A:411:MET:HE3	1.84	0.59
1:B:212:LEU:CG	1:B:238:ILE:CD1	2.79	0.59
1:C:335:GLN:HB2	2:C:500:UDP:C2	2.36	0.59
1:F:23:GLY:O	1:F:27:PRO:HG2	2.03	0.59
1:D:285:ALA:HB1	1:D:407:ILE:HG22	1.83	0.59
1:E:238:ILE:HG22	1:E:238:ILE:O	2.01	0.59
1:B:155:TYR:CG	1:B:155:TYR:O	2.56	0.59
1:C:371:GLN:O	1:C:397:GLY:O	2.21	0.59
1:D:22:MET:HE3	1:D:25:LEU:HD23	1.85	0.59
1:B:26:LEU:O	1:B:30:ARG:HG3	2.02	0.59
1:B:286:LEU:HA	1:B:411:MET:HE1	1.84	0.59
1:C:309:GLU:O	1:C:330:LYS:HD2	2.03	0.59
1:D:342:PRO:HD2	1:D:343:ALA:H	1.68	0.59
1:F:266:VAL:HG13	1:F:348:VAL:HB	1.85	0.59
1:A:26:LEU:HB3	1:A:30:ARG:NH2	2.17	0.58
1:A:50:THR:HG21	1:A:55:GLU:HB2	1.85	0.58
1:B:263:VAL:CG2	1:B:344:ILE:CD1	2.78	0.58
1:D:125:THR:O	1:D:207:LYS:NZ	2.36	0.58
1:E:169:ALA:HB1	1:E:178:ILE:C	2.22	0.58
1:F:311:GLU:HA	1:F:311:GLU:OE1	2.02	0.58
1:A:88:ASP:OD1	1:A:89:PRO:CD	2.50	0.58
1:B:85:ARG:CB	1:B:193:PHE:HE1	2.14	0.58
1:D:296:VAL:HG12	1:D:296:VAL:O	2.01	0.58
1:D:448:LEU:O	1:D:448:LEU:CD1	2.30	0.58
1:C:54:ALA:HB2	1:C:304:LYS:CE	2.33	0.58
1:C:171:GLU:HA	1:C:177:PRO:CB	2.33	0.58
1:F:105:ARG:HB3	1:F:106:PRO:HD3	1.85	0.58
1:A:10:VAL:HG23	1:A:10:VAL:O	2.02	0.58
1:A:350:HIS:CD2	1:A:352:GLY:N	2.67	0.58
1:B:276:LYS:HZ1	1:B:280:ARG:NH2	1.97	0.58
1:C:165:ALA:O	1:C:166:ASN:CB	2.49	0.58
1:C:383:GLU:CG	1:C:384:LYS:HZ3	2.16	0.58
1:F:296:VAL:C	1:F:297:LEU:CD1	2.72	0.58
1:A:147:ALA:HB2	1:A:215:THR:HG21	1.86	0.58
1:C:193:PHE:CD1	1:C:193:PHE:C	2.77	0.58
1:D:126:SER:O	1:D:129:THR:CG2	2.46	0.58
1:D:130:ASP:OD1	1:D:130:ASP:N	2.29	0.58
1:D:192:ASP:OD1	1:D:194:PHE:N	2.30	0.58
1:F:216:PHE:CE2	1:F:219:PHE:HB2	2.39	0.58
1:C:374:ASP:OD1	1:C:374:ASP:C	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:ALA:HB1	1:D:371:GLN:CB	2.33	0.58
1:C:394:TRP:CD2	1:C:402:ILE:CD1	2.85	0.58
1:F:23:GLY:O	1:F:27:PRO:CG	2.51	0.58
1:A:26:LEU:N	1:A:27:PRO:HD2	2.19	0.58
1:E:216:PHE:N	1:E:216:PHE:CD1	2.72	0.58
1:F:105:ARG:HB2	1:F:105:ARG:NH1	2.18	0.58
1:F:269:GLY:O	1:F:298:LYS:HG3	2.04	0.58
1:A:152:LEU:HD21	1:A:187:MET:HE1	1.86	0.57
1:B:156:LEU:O	1:B:156:LEU:HD12	2.03	0.57
1:B:271:ARG:NH1	1:B:302:VAL:HG12	2.19	0.57
1:C:125:THR:OG1	1:C:141:THR:HG21	2.03	0.57
1:E:447:ARG:CG	1:E:447:ARG:NH1	2.35	0.57
1:F:264:LEU:HD13	1:F:415:MET:SD	2.44	0.57
1:F:434:THR:HA	1:F:439:GLY:HA3	1.86	0.57
1:F:445:LEU:O	1:F:449:ILE:HG13	2.04	0.57
1:A:135:LEU:HG	1:C:87:ASP:HB2	1.84	0.57
1:B:22:MET:CE	1:B:22:MET:HA	2.34	0.57
1:B:434:THR:HG21	1:B:441:SER:OG	2.04	0.57
1:C:76:LEU:HD22	1:C:96:THR:HG22	1.87	0.57
1:B:38:ARG:HB2	1:B:449:ILE:HD13	1.86	0.57
1:B:271:ARG:CB	1:B:301:LYS:O	2.42	0.57
1:F:215:THR:O	1:F:237:PRO:HB3	2.05	0.57
1:F:328:ILE:O	1:F:328:ILE:HG13	2.04	0.57
1:A:278:GLN:NE2	1:A:401:LEU:HD12	2.19	0.57
1:B:155:TYR:O	1:B:155:TYR:CD1	2.58	0.57
1:D:273:ALA:CB	1:D:371:GLN:CG	2.80	0.57
1:D:341:HIS:CG	1:D:342:PRO:HD3	2.35	0.57
1:F:50:THR:CG2	1:F:55:GLU:HB2	2.35	0.57
1:F:143:MET:CE	1:F:145:SER:HB3	2.34	0.57
1:F:424:ALA:HA	1:F:427:VAL:HG23	1.87	0.57
1:B:10:VAL:HG11	1:B:68:ARG:NH2	2.19	0.57
1:B:16:LEU:HD21	1:B:32:ALA:HB2	1.85	0.57
1:B:26:LEU:O	1:B:30:ARG:CG	2.53	0.57
1:B:175:LEU:HD22	1:B:176:GLY:H	1.70	0.57
1:B:368:ALA:HB3	1:B:390:TRP:HB2	1.87	0.57
1:C:170:ILE:CD1	1:C:180:MET:HE3	2.35	0.57
1:C:353:TRP:HE3	1:C:378:ASN:ND2	2.03	0.57
1:A:335:GLN:NE2	2:A:500:UDP:H2'	2.20	0.57
1:B:50:THR:HG21	1:B:52:SER:O	2.05	0.57
1:B:105:ARG:NH2	1:B:134:ASP:OD2	2.37	0.57
1:D:47:VAL:HG23	1:D:76:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:GLY:CA	1:E:415:MET:CE	2.78	0.57
1:D:50:THR:CG2	1:D:55:GLU:HB3	2.34	0.56
1:D:334:LYS:HB3	1:D:337:GLN:HB3	1.87	0.56
1:E:16:LEU:HD23	1:E:28:PHE:O	2.05	0.56
1:A:140:TYR:CZ	1:A:448:LEU:HD11	2.40	0.56
1:B:42:VAL:HG13	1:B:69:ILE:HG12	1.81	0.56
1:B:180:MET:HA	1:B:183:ILE:HG13	1.86	0.56
1:F:434:THR:HG21	1:F:441:SER:HB2	1.65	0.56
1:A:435:ARG:NH1	1:A:442:GLU:OE1	2.38	0.56
1:C:89:PRO:HG3	1:C:302:VAL:HG21	1.88	0.56
1:F:143:MET:HE2	1:F:145:SER:O	2.05	0.56
1:F:390:TRP:CZ2	1:F:392:ARG:HD3	2.41	0.56
1:C:135:LEU:HD12	1:C:135:LEU:N	2.19	0.56
1:C:183:ILE:CG2	1:C:187:MET:HE2	2.34	0.56
1:D:211:VAL:HG23	1:D:234:HIS:CD2	2.40	0.56
1:D:274:LEU:HD22	1:D:278:GLN:CG	2.34	0.56
1:A:52:SER:OG	1:A:55:GLU:HG3	2.06	0.56
1:C:371:GLN:NE2	1:C:397:GLY:HA3	2.21	0.56
1:C:435:ARG:HA	1:C:435:ARG:HE	1.69	0.56
1:D:435:ARG:O	1:D:435:ARG:HD3	2.05	0.56
1:F:86:ASN:ND2	1:F:92:ILE:N	2.53	0.56
1:C:170:ILE:CD1	1:C:180:MET:HE1	2.35	0.56
1:D:115:LEU:CB	1:D:137:ILE:HD11	2.09	0.56
1:E:334:LYS:O	1:E:338:ILE:HD12	2.06	0.56
1:E:335:GLN:CD	2:E:500:UDP:H2'	2.24	0.56
1:F:120:SER:OG	1:F:128:VAL:CG1	2.45	0.56
1:F:286:LEU:CD2	1:F:411:MET:CE	2.83	0.56
1:D:124:LEU:O	1:D:128:VAL:HG23	2.06	0.56
1:E:14:ILE:CD1	1:E:452:PHE:CD2	2.88	0.56
1:C:46:THR:HG21	1:C:59:LEU:HD21	1.85	0.56
1:D:16:LEU:HD23	1:D:28:PHE:O	2.05	0.56
1:D:100:SER:O	1:D:103:LEU:HB2	2.06	0.56
1:D:410:LYS:NZ	1:D:410:LYS:HA	2.21	0.56
1:E:168:ASP:O	1:E:180:MET:CB	2.51	0.56
1:F:424:ALA:HA	1:F:427:VAL:HG21	1.88	0.56
1:B:24:HIS:HA	1:B:144:THR:HG21	1.88	0.56
1:B:52:SER:HG	1:B:55:GLU:HG3	1.71	0.56
1:C:50:THR:HG23	1:C:51:VAL:N	2.21	0.56
1:F:143:MET:HE1	1:F:145:SER:CA	2.36	0.56
1:F:434:THR:HG22	1:F:441:SER:H	1.69	0.56
1:C:74:PHE:HZ	1:C:104:LEU:HG	1.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LEU:HD13	1:C:115:LEU:HG	1.86	0.56
1:C:394:TRP:CZ2	1:C:402:ILE:CD1	2.88	0.56
1:A:350:HIS:HE1	2:A:500:UDP:O2B	1.89	0.55
1:B:284:ALA:HB1	1:B:404:ARG:NH1	2.18	0.55
1:D:24:HIS:C	1:D:27:PRO:HD2	2.27	0.55
1:D:268:PHE:O	1:D:350:HIS:HD2	1.86	0.55
1:E:158:LYS:O	1:E:162:ILE:HG22	2.06	0.55
1:F:260:PRO:O	1:F:261:GLU:HB2	2.06	0.55
1:C:170:ILE:HD13	1:C:180:MET:HE3	1.88	0.55
1:C:217:ASN:O	1:C:221:SER:HB2	2.06	0.55
1:B:266:VAL:HG13	1:B:348:VAL:HG22	1.89	0.55
1:C:445:LEU:O	1:C:449:ILE:CG1	2.54	0.55
1:D:47:VAL:CB	1:D:97:ILE:HD11	2.36	0.55
1:E:112:SER:CB	1:E:113:PRO:HD3	2.36	0.55
1:D:268:PHE:O	1:D:350:HIS:HB3	2.06	0.55
1:D:354:ASN:HB2	2:D:500:UDP:H5'1	1.87	0.55
1:E:213:ILE:HG22	1:E:237:PRO:HA	1.89	0.55
1:D:156:LEU:N	1:D:157:PRO:CD	2.70	0.55
1:D:389:LEU:HD13	1:D:413:GLU:HG2	1.88	0.55
1:E:374:ASP:O	1:E:377:VAL:CG1	2.54	0.55
1:A:258:GLN:HA	1:A:258:GLN:NE2	2.20	0.55
1:D:105:ARG:HB2	1:D:106:PRO:CD	2.36	0.55
1:D:424:ALA:C	1:D:427:VAL:HG12	2.23	0.55
1:D:23:GLY:O	1:D:354:ASN:ND2	2.40	0.55
1:D:216:PHE:N	1:D:216:PHE:CD1	2.75	0.55
1:B:107:LEU:HD12	1:B:107:LEU:C	2.26	0.55
1:B:276:LYS:HZ1	1:B:280:ARG:HH21	1.45	0.55
1:B:268:PHE:HZ	1:B:369:TRP:CE3	2.25	0.55
1:B:269:GLY:HA3	1:B:350:HIS:CE1	2.41	0.55
1:F:149:PHE:CE2	1:F:153:MET:CE	2.86	0.55
1:A:34:MET:HE3	1:A:241:LEU:CD2	2.29	0.55
1:B:65:ILE:HG22	1:B:66:HIS:CE1	2.42	0.55
1:B:341:HIS:CG	1:B:342:PRO:HD2	2.42	0.55
1:D:45:ILE:HA	1:D:72:LEU:O	2.07	0.55
1:D:278:GLN:HE21	1:D:278:GLN:CA	2.18	0.55
1:D:303:ASP:HB3	1:D:306:ASP:HB2	1.88	0.55
1:E:434:THR:HG23	1:E:441:SER:CB	2.37	0.55
1:F:101:VAL:CG1	1:F:131:LEU:HD21	2.37	0.55
1:D:156:LEU:N	1:D:157:PRO:HD2	2.21	0.54
1:E:213:ILE:HG23	1:E:215:THR:H	1.71	0.54
1:D:149:PHE:HD2	1:D:153:MET:HE3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:VAL:HB	1:D:235:ILE:HA	1.90	0.54
1:D:269:GLY:CA	1:D:350:HIS:HD2	2.19	0.54
1:D:389:LEU:CD2	1:D:420:LEU:HD21	2.32	0.54
1:F:368:ALA:HB3	1:F:390:TRP:HB2	1.89	0.54
1:A:173:PRO:CB	1:A:230:ASN:ND2	2.62	0.54
1:C:225:GLU:OE1	1:C:225:GLU:CA	2.53	0.54
1:C:286:LEU:CD2	1:C:411:MET:SD	2.96	0.54
1:C:335:GLN:NE2	2:C:500:UDP:H2'	2.22	0.54
1:F:401:LEU:C	1:F:402:ILE:HD12	2.28	0.54
1:C:214:ASN:OD1	1:C:241:LEU:HG	2.08	0.54
1:C:74:PHE:HZ	1:C:104:LEU:HA	1.73	0.54
1:C:216:PHE:N	1:C:216:PHE:CD1	2.76	0.54
1:F:434:THR:HG22	1:F:441:SER:N	2.22	0.54
1:A:372:HIS:N	1:A:375:GLN:OE1	2.30	0.54
1:D:134:ASP:N	1:D:134:ASP:OD1	2.40	0.54
1:D:150:PHE:O	1:D:154:ALA:N	2.38	0.54
1:D:151:CYS:O	1:D:155:TYR:N	2.31	0.54
1:D:440:ASP:O	1:D:444:LEU:HG	2.07	0.54
1:F:101:VAL:HG13	1:F:131:LEU:CD2	2.37	0.54
1:F:298:LYS:HE2	1:F:298:LYS:CA	2.38	0.54
1:B:234:HIS:ND1	1:B:234:HIS:N	2.42	0.54
1:B:242:GLU:OE2	1:B:435:ARG:HD3	2.08	0.54
1:B:335:GLN:HB2	2:B:500:UDP:C2	2.43	0.54
1:C:401:LEU:HD12	1:C:401:LEU:O	2.05	0.54
1:D:156:LEU:O	1:D:156:LEU:HD12	2.08	0.54
1:E:445:LEU:O	1:E:449:ILE:HG13	2.07	0.54
1:B:105:ARG:HB2	1:B:106:PRO:HD3	1.89	0.54
1:B:156:LEU:HD11	1:B:160:LEU:CD1	2.37	0.54
1:D:25:LEU:C	1:D:27:PRO:HD2	2.27	0.54
1:D:60:SER:O	1:D:64:THR:OG1	2.21	0.54
1:C:101:VAL:O	1:C:104:LEU:HB2	2.08	0.54
1:D:339:LEU:HB3	1:D:362:LEU:HD12	1.90	0.54
1:E:18:PRO:HG3	1:E:28:PHE:HB3	1.90	0.54
1:E:227:VAL:HG11	1:E:235:ILE:HG21	1.89	0.54
1:F:295:TRP:CE2	1:F:297:LEU:HD11	2.43	0.54
1:A:59:LEU:HD22	1:A:63:PHE:CE2	2.43	0.54
1:A:97:ILE:HG22	1:A:124:LEU:HD11	1.90	0.54
1:A:341:HIS:ND1	1:A:342:PRO:CG	2.71	0.54
1:C:63:PHE:CE1	1:C:71:ARG:CB	2.80	0.54
1:E:122:PHE:CE2	1:E:153:MET:HE2	2.43	0.54
1:F:38:ARG:NH2	1:F:442:GLU:OE1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:LEU:HB3	1:F:341:HIS:CD2	2.43	0.54
1:F:300:GLY:HA3	1:F:307:LYS:CG	2.38	0.54
1:A:38:ARG:HB3	1:A:449:ILE:HD13	1.88	0.53
1:B:34:MET:CE	1:B:241:LEU:CA	2.83	0.53
1:C:105:ARG:NE	1:C:135:LEU:HD11	2.19	0.53
1:D:149:PHE:CD2	1:D:153:MET:HE3	2.43	0.53
1:D:295:TRP:CE3	1:D:328:ILE:CD1	2.91	0.53
1:C:12:ALA:HB1	1:C:116:SER:OG	2.08	0.53
1:C:351:CYS:SG	1:C:368:ALA:HB1	2.48	0.53
1:D:344:ILE:HD13	1:D:344:ILE:N	2.22	0.53
1:B:155:TYR:CE1	1:B:159:LEU:CB	2.86	0.53
1:D:30:ARG:O	1:D:34:MET:HG3	2.09	0.53
1:E:141:THR:HG23	1:E:211:VAL:HG22	1.89	0.53
1:A:34:MET:O	1:A:38:ARG:HD2	2.08	0.53
1:D:47:VAL:HB	1:D:97:ILE:HD13	1.90	0.53
1:D:342:PRO:CD	1:D:343:ALA:H	2.21	0.53
1:F:112:SER:HB3	1:F:113:PRO:CD	2.26	0.53
1:B:147:ALA:HB2	1:B:215:THR:HG21	1.90	0.53
1:C:170:ILE:HD13	1:C:180:MET:HE1	1.91	0.53
1:C:262:SER:HB2	1:C:292:ARG:HH11	1.71	0.53
1:D:28:PHE:O	1:D:31:LEU:HB3	2.08	0.53
1:F:401:LEU:CD2	1:F:401:LEU:O	2.50	0.53
1:B:273:ALA:HB1	1:B:371:GLN:CG	2.38	0.53
1:C:293:PHE:CD1	1:C:293:PHE:O	2.62	0.53
1:C:319:VAL:HG22	1:C:328:ILE:HD11	1.90	0.53
1:E:26:LEU:HB3	1:E:30:ARG:HH11	1.73	0.53
1:E:255:LEU:HD21	1:E:344:ILE:HD11	1.91	0.53
1:E:280:ARG:HE	1:E:280:ARG:CA	2.20	0.53
1:F:167:ARG:NH2	1:F:170:ILE:HD13	2.23	0.53
1:A:299:GLY:N	1:A:330:LYS:NZ	2.54	0.53
1:E:18:PRO:HG3	1:E:28:PHE:CG	2.42	0.53
1:D:427:VAL:HG13	1:D:428:ARG:N	2.24	0.53
1:B:156:LEU:N	1:B:157:PRO:HD2	2.24	0.53
1:C:98:ALA:O	1:C:101:VAL:HG22	2.09	0.53
1:C:335:GLN:NE2	2:C:500:UDP:O2'	2.42	0.53
1:E:309:GLU:O	1:E:330:LYS:HE2	2.09	0.53
1:F:341:HIS:HD2	1:F:343:ALA:HB3	1.72	0.53
1:B:156:LEU:C	1:B:156:LEU:HD12	2.28	0.52
1:B:274:LEU:HD22	1:B:278:GLN:HG2	1.90	0.52
1:F:22:MET:CE	1:F:58:HIS:CD2	2.92	0.52
1:B:280:ARG:NE	1:B:313:MET:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ARG:HB3	1:C:242:GLU:O	2.09	0.52
1:C:74:PHE:HZ	1:C:104:LEU:CA	2.22	0.52
1:C:227:VAL:CG1	1:C:228:ARG:N	2.72	0.52
1:F:46:THR:O	1:F:73:GLU:HA	2.09	0.52
1:A:309:GLU:O	1:A:330:LYS:HE3	2.09	0.52
1:D:13:HIS:HA	1:D:41:ALA:HB3	1.91	0.52
1:D:101:VAL:O	1:D:104:LEU:HB2	2.10	0.52
1:C:34:MET:O	1:C:38:ARG:HG2	2.09	0.52
1:C:149:PHE:CD2	1:C:153:MET:HE1	2.44	0.52
1:E:220:GLU:HB3	1:E:223:ALA:HB3	1.90	0.52
1:E:332:TRP:CH2	2:E:500:UDP:C2	2.97	0.52
1:A:255:LEU:HD23	1:A:341:HIS:CD2	2.37	0.52
1:D:233:ASP:N	1:D:233:ASP:OD1	2.42	0.52
1:E:26:LEU:HB2	1:E:27:PRO:CD	2.39	0.52
1:F:402:ILE:N	1:F:402:ILE:HD12	2.24	0.52
1:A:269:GLY:O	1:A:298:LYS:HE2	2.10	0.52
1:C:298:LYS:HZ3	1:C:298:LYS:HB3	1.72	0.52
1:E:447:ARG:HH11	1:E:447:ARG:CB	2.22	0.52
1:F:119:VAL:O	1:F:119:VAL:CG2	2.56	0.52
1:B:47:VAL:HG22	1:B:76:LEU:HG	1.91	0.52
1:C:62:PHE:HD1	1:C:244:TYR:CD2	2.28	0.52
1:C:238:ILE:N	1:C:238:ILE:CD1	2.72	0.52
1:C:348:VAL:HG22	1:C:367:LEU:HD23	1.91	0.52
1:D:378:ASN:HA	1:D:381:VAL:CG2	2.39	0.52
1:E:16:LEU:CD2	1:E:28:PHE:O	2.58	0.52
1:C:27:PRO:CD	1:C:354:ASN:ND2	2.73	0.52
1:C:437:VAL:HG12	1:C:438:ASP:N	2.24	0.52
1:E:419:LYS:O	1:E:423:SER:HB3	2.10	0.52
1:B:218:SER:OG	1:B:430:LYS:HD2	2.08	0.52
1:D:402:ILE:HG23	1:D:407:ILE:HD11	1.91	0.52
1:F:101:VAL:O	1:F:104:LEU:HG	2.09	0.52
1:F:236:LEU:HD23	1:F:236:LEU:N	2.23	0.52
1:A:212:LEU:N	1:A:212:LEU:CD1	2.72	0.52
1:E:65:ILE:HG21	1:E:246:ALA:HB2	1.91	0.52
1:E:84:LEU:N	1:E:84:LEU:CD1	2.73	0.52
1:E:156:LEU:N	1:E:157:PRO:HD2	2.25	0.52
1:F:403:GLY:O	1:F:407:ILE:CG1	2.47	0.52
1:A:402:ILE:CG2	1:A:407:ILE:CD1	2.87	0.51
1:B:155:TYR:CE2	1:B:173:PRO:HD3	2.45	0.51
1:D:278:GLN:NE2	1:D:278:GLN:CA	2.73	0.51
1:E:252:LEU:N	1:E:253:PRO:HD2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:ARG:HG3	1:E:292:ARG:HH21	1.75	0.51
1:F:374:ASP:OD1	1:F:375:GLN:N	2.42	0.51
1:B:22:MET:HA	1:B:22:MET:HE2	1.92	0.51
1:F:64:THR:CG2	1:F:65:ILE:N	2.72	0.51
1:F:143:MET:HE3	1:F:145:SER:CA	2.40	0.51
1:B:402:ILE:O	1:B:402:ILE:HG12	2.09	0.51
1:C:286:LEU:HD13	1:C:293:PHE:CD2	2.45	0.51
1:D:143:MET:HG2	1:D:212:LEU:O	2.11	0.51
1:E:175:LEU:N	1:E:175:LEU:CD1	2.72	0.51
1:E:282:LEU:O	1:E:282:LEU:HD12	2.10	0.51
1:A:138:SER:HB3	1:A:209:LYS:HG3	1.91	0.51
1:B:155:TYR:HE1	1:B:159:LEU:HB2	1.71	0.51
1:B:321:ARG:NH1	1:B:321:ARG:CG	2.72	0.51
1:B:334:LYS:HB3	1:B:337:GLN:HB3	1.91	0.51
1:C:62:PHE:HD1	1:C:244:TYR:CE2	2.29	0.51
1:C:147:ALA:HB3	1:C:220:GLU:OE2	2.10	0.51
1:D:340:ALA:HA	1:D:362:LEU:HD13	1.92	0.51
1:C:135:LEU:N	1:C:135:LEU:CD1	2.73	0.51
1:D:349:SER:OG	1:D:351:CYS:HA	2.11	0.51
1:E:234:HIS:ND1	1:E:234:HIS:N	2.59	0.51
1:E:292:ARG:HH21	1:E:292:ARG:CG	2.23	0.51
1:E:374:ASP:O	1:E:377:VAL:HG13	2.10	0.51
1:A:16:LEU:HD13	1:A:28:PHE:O	2.11	0.51
1:B:347:PHE:CZ	1:B:349:SER:HB2	2.46	0.51
1:C:175:LEU:CD1	1:C:176:GLY:N	2.74	0.51
1:C:254:TRP:O	1:C:258:GLN:NE2	2.44	0.51
1:F:380:GLY:HA2	1:F:390:TRP:CE3	2.46	0.51
1:B:264:LEU:O	1:B:293:PHE:HA	2.10	0.51
1:C:394:TRP:HE1	1:C:406:GLU:CD	2.14	0.51
1:F:156:LEU:HB3	1:F:157:PRO:HD3	1.91	0.51
1:B:434:THR:HG23	1:B:441:SER:HB2	1.89	0.51
1:B:50:THR:HG22	1:B:52:SER:O	2.10	0.51
1:C:59:LEU:O	1:C:63:PHE:CD2	2.64	0.51
1:C:293:PHE:CD1	1:C:293:PHE:C	2.84	0.51
1:F:99:THR:O	1:F:102:HIS:CD2	2.64	0.51
1:F:129:THR:HG23	1:F:130:ASP:N	2.26	0.51
1:F:402:ILE:HG22	1:F:407:ILE:HG12	1.92	0.51
1:F:421:ARG:CZ	1:F:421:ARG:HB2	2.40	0.51
1:A:126:SER:OG	1:A:204:SER:OG	2.23	0.51
1:B:16:LEU:CD1	1:B:32:ALA:HB2	2.35	0.51
1:C:378:ASN:O	1:C:381:VAL:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:HIS:CG	1:E:342:PRO:HD2	2.46	0.51
1:F:288:LYS:NZ	1:F:405:GLU:CG	2.74	0.51
1:F:183:ILE:HG23	1:F:187:MET:HE3	1.93	0.50
1:A:372:HIS:O	1:A:375:GLN:OE1	2.30	0.50
1:B:42:VAL:HG11	1:B:69:ILE:HG12	1.87	0.50
1:B:268:PHE:CZ	1:B:369:TRP:CE3	2.99	0.50
1:B:434:THR:HG23	1:B:441:SER:H	1.76	0.50
1:C:74:PHE:CZ	1:C:104:LEU:CG	2.83	0.50
1:C:314:LEU:CD1	1:C:328:ILE:HD12	2.36	0.50
1:A:264:LEU:HD11	1:A:348:VAL:HG23	1.93	0.50
1:C:35:LEU:O	1:C:40:CYS:HB2	2.12	0.50
1:C:261:GLU:N	1:C:343:ALA:O	2.45	0.50
1:C:278:GLN:NE2	1:C:369:TRP:HZ2	2.03	0.50
1:D:13:HIS:HD2	1:D:41:ALA:O	1.95	0.50
1:D:218:SER:OG	1:D:430:LYS:HE3	2.12	0.50
1:D:285:ALA:HB1	1:D:407:ILE:CG2	2.42	0.50
1:E:26:LEU:CB	1:E:27:PRO:CD	2.89	0.50
1:E:212:LEU:N	1:E:212:LEU:CD1	2.74	0.50
1:A:402:ILE:HG21	1:A:407:ILE:HG13	1.92	0.50
1:B:65:ILE:HG22	1:B:66:HIS:ND1	2.27	0.50
1:B:185:PRO:HG2	1:B:186:LYS:N	2.27	0.50
1:B:212:LEU:CD2	1:B:238:ILE:CD1	2.81	0.50
1:F:196:ALA:O	1:F:200:SER:OG	2.30	0.50
1:A:98:ALA:HB2	1:A:124:LEU:HD22	1.93	0.50
1:E:211:VAL:O	1:E:211:VAL:HG12	2.12	0.50
1:A:36:ASP:OD1	1:A:36:ASP:O	2.30	0.50
1:D:50:THR:CG2	1:D:52:SER:O	2.59	0.50
1:D:149:PHE:CE2	1:D:153:MET:CE	2.95	0.50
1:A:14:ILE:HG21	1:A:35:LEU:HD13	1.93	0.50
1:C:47:VAL:HG12	1:C:76:LEU:HG	1.93	0.50
1:C:112:SER:CB	1:C:113:PRO:HD3	2.31	0.50
1:C:125:THR:OG1	1:C:141:THR:CG2	2.59	0.50
1:D:16:LEU:HD21	1:D:31:LEU:HB3	1.92	0.50
1:F:184:PRO:HD2	1:F:187:MET:CE	2.41	0.50
1:C:118:ILE:HG23	1:C:118:ILE:O	2.11	0.50
1:D:372:HIS:O	1:D:375:GLN:OE1	2.30	0.50
1:F:121:ASP:OD1	1:F:122:PHE:N	2.45	0.50
1:A:255:LEU:CD2	1:A:341:HIS:CD2	2.95	0.50
1:A:402:ILE:CG2	1:A:407:ILE:HG13	2.42	0.50
1:B:47:VAL:CG2	1:B:76:LEU:CG	2.90	0.50
1:B:224:ILE:CA	1:B:227:VAL:CG2	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:TRP:CE3	1:D:328:ILE:HD11	2.47	0.50
1:E:146:SER:HB3	1:E:353:TRP:CE3	2.47	0.50
1:E:394:TRP:CG	1:E:402:ILE:HD12	2.47	0.50
1:E:184:PRO:HG3	1:E:373:GLY:O	2.12	0.49
1:E:259:PRO:O	1:E:262:SER:OG	2.30	0.49
1:F:14:ILE:HD12	1:F:117:ALA:HB3	1.94	0.49
1:F:172:ILE:O	1:F:175:LEU:O	2.30	0.49
1:B:293:PHE:C	1:B:293:PHE:CD1	2.85	0.49
1:C:54:ALA:N	1:C:304:LYS:CD	2.69	0.49
1:C:273:ALA:CB	1:C:301:LYS:HA	2.42	0.49
1:D:63:PHE:O	1:D:66:HIS:O	2.30	0.49
1:E:251:ASP:C	1:E:253:PRO:HD2	2.32	0.49
1:F:77:LEU:HB3	1:F:78:PRO:CD	2.42	0.49
1:F:351:CYS:HA	1:F:356:VAL:HG23	1.93	0.49
1:A:285:ALA:CB	1:A:407:ILE:HG21	2.42	0.49
1:A:402:ILE:HG22	1:A:407:ILE:HD11	1.93	0.49
1:B:47:VAL:CG2	1:B:76:LEU:HD23	2.37	0.49
1:B:85:ARG:CB	1:B:193:PHE:CZ	2.94	0.49
1:B:233:ASP:O	1:B:233:ASP:OD1	2.30	0.49
2:C:500:UDP:O2A	2:C:500:UDP:O1B	2.30	0.49
1:D:235:ILE:O	1:D:235:ILE:HG23	2.12	0.49
1:F:156:LEU:HB3	1:F:157:PRO:CD	2.43	0.49
1:A:26:LEU:HD12	2:A:500:UDP:O4'	2.12	0.49
1:B:134:ASP:N	1:B:134:ASP:OD1	2.45	0.49
1:C:300:GLY:N	1:C:307:LYS:CD	2.72	0.49
1:E:38:ARG:NE	1:E:442:GLU:OE1	2.28	0.49
1:A:380:GLY:O	1:A:384:LYS:HG3	2.13	0.49
1:B:141:THR:O	1:B:212:LEU:HD13	2.13	0.49
1:B:448:LEU:HD12	1:B:448:LEU:C	2.32	0.49
1:C:89:PRO:CG	1:C:302:VAL:HG21	2.42	0.49
1:C:446:GLN:HA	1:C:449:ILE:HG13	1.94	0.49
1:B:24:HIS:O	1:B:28:PHE:HD1	1.96	0.49
1:C:259:PRO:O	1:C:262:SER:OG	2.30	0.49
1:C:295:TRP:CE2	1:C:297:LEU:HD12	2.47	0.49
1:F:401:LEU:HD23	1:F:402:ILE:CA	2.43	0.49
1:A:427:VAL:HG13	1:A:428:ARG:N	2.27	0.49
1:D:391:VAL:CG1	1:D:394:TRP:CD2	2.96	0.49
1:E:280:ARG:NE	1:E:280:ARG:CA	2.72	0.49
1:E:394:TRP:CD2	1:E:402:ILE:HD12	2.48	0.49
1:F:91:PHE:CG	1:F:193:PHE:CE2	3.00	0.49
1:F:255:LEU:HB3	1:F:341:HIS:NE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:ARG:HB3	1:E:106:PRO:HD3	1.93	0.49
1:E:425:GLY:O	1:E:428:ARG:HB3	2.12	0.49
1:E:445:LEU:O	1:E:449:ILE:CG1	2.61	0.49
1:F:254:TRP:CE3	1:F:327:LEU:HD23	2.44	0.49
1:B:13:HIS:CD2	1:B:113:PRO:O	2.63	0.49
1:C:208:VAL:O	1:C:234:HIS:HD2	1.95	0.49
1:D:317:SER:O	1:D:321:ARG:HG2	2.13	0.49
1:D:402:ILE:CG2	1:D:407:ILE:HD11	2.43	0.49
1:F:434:THR:HG22	1:F:441:SER:CA	2.43	0.49
1:A:40:CYS:SG	1:A:449:ILE:HG12	2.53	0.49
1:A:88:ASP:HB3	1:A:91:PHE:HB2	1.94	0.49
1:A:258:GLN:NE2	1:A:258:GLN:CA	2.73	0.49
1:A:407:ILE:O	1:A:411:MET:HE3	2.13	0.49
1:B:63:PHE:CE2	1:B:71:ARG:HB2	2.47	0.49
1:B:269:GLY:HA2	1:B:350:HIS:CE1	2.48	0.49
1:C:234:HIS:ND1	1:C:234:HIS:N	2.59	0.49
1:C:383:GLU:HG2	1:C:384:LYS:HE2	1.94	0.49
1:D:14:ILE:HG22	1:D:15:ALA:N	2.27	0.49
1:D:442:GLU:OE1	1:D:442:GLU:O	2.30	0.49
1:E:15:ALA:HB3	1:E:118:ILE:HD13	1.95	0.49
1:E:22:MET:HE2	1:E:58:HIS:CD2	2.47	0.49
1:B:192:ASP:OD1	1:B:193:PHE:N	2.46	0.48
1:E:20:ALA:HB2	1:E:93:GLN:HG2	1.93	0.48
1:F:91:PHE:HB3	1:F:193:PHE:CE2	2.48	0.48
1:C:383:GLU:HA	1:C:388:GLY:O	2.12	0.48
1:D:340:ALA:CA	1:D:362:LEU:HD13	2.43	0.48
1:A:255:LEU:CD2	1:A:341:HIS:HD2	2.24	0.48
1:A:414:VAL:HG13	1:A:415:MET:N	2.29	0.48
1:B:40:CYS:SG	1:B:449:ILE:HG12	2.53	0.48
1:C:62:PHE:CD1	1:C:244:TYR:CD2	3.00	0.48
1:C:263:VAL:HG11	1:C:344:ILE:HD13	1.95	0.48
1:D:182:SER:O	1:D:396:TRP:CH2	2.66	0.48
1:D:297:LEU:HD22	1:D:314:LEU:HD11	1.95	0.48
1:E:274:LEU:N	1:E:274:LEU:HD23	2.28	0.48
1:F:105:ARG:HB3	1:F:106:PRO:CD	2.42	0.48
1:F:131:LEU:N	1:F:131:LEU:CD1	2.76	0.48
1:F:170:ILE:HG13	1:F:171:GLU:N	2.28	0.48
1:A:407:ILE:HG23	1:A:411:MET:HE2	1.94	0.48
1:C:120:SER:O	1:C:141:THR:HA	2.13	0.48
1:D:127:GLN:O	1:D:130:ASP:OD1	2.30	0.48
1:D:449:ILE:O	1:D:452:PHE:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:GLU:HG3	1:E:318:PHE:CE1	2.48	0.48
1:E:350:HIS:H	1:E:350:HIS:CD2	2.32	0.48
1:E:409:GLU:HG3	1:E:410:LYS:N	2.25	0.48
1:F:298:LYS:HA	1:F:298:LYS:CE	2.37	0.48
1:A:51:VAL:CG1	1:A:90:PHE:CE1	2.96	0.48
1:B:271:ARG:HH12	1:B:302:VAL:HG12	1.76	0.48
1:D:238:ILE:O	1:D:238:ILE:HG22	2.12	0.48
1:E:228:ARG:CG	1:E:235:ILE:HD11	2.44	0.48
1:F:175:LEU:HG	1:F:176:GLY:N	2.29	0.48
1:F:205:LEU:HD22	1:F:211:VAL:CG2	2.44	0.48
1:F:259:PRO:O	1:F:262:SER:OG	2.30	0.48
1:A:13:HIS:HE1	1:A:43:THR:OG1	1.97	0.48
1:A:254:TRP:O	1:A:258:GLN:CG	2.51	0.48
1:B:22:MET:HE3	1:B:55:GLU:HA	1.95	0.48
1:B:185:PRO:CG	1:B:186:LYS:N	2.76	0.48
1:C:89:PRO:HG3	1:C:302:VAL:CG2	2.43	0.48
1:C:270:SER:OG	2:C:500:UDP:O3B	2.29	0.48
1:D:146:SER:OG	1:D:378:ASN:OD1	2.29	0.48
1:D:402:ILE:O	1:D:402:ILE:CG2	2.61	0.48
1:E:26:LEU:CD1	2:E:500:UDP:H4'	2.42	0.48
1:E:169:ALA:CB	1:E:179:SER:HA	2.28	0.48
1:E:300:GLY:HA3	1:E:307:LYS:CG	2.44	0.48
1:E:23:GLY:O	1:E:27:PRO:CG	2.61	0.48
1:A:15:ALA:HA	1:A:43:THR:O	2.13	0.48
1:A:45:ILE:HA	1:A:72:LEU:O	2.14	0.48
1:C:213:ILE:HG21	1:C:215:THR:CG2	2.41	0.48
1:C:278:GLN:HE22	1:C:369:TRP:HZ2	1.60	0.48
1:D:185:PRO:O	1:D:188:LEU:HB2	2.13	0.48
1:E:299:GLY:HA3	1:E:313:MET:CE	2.42	0.48
1:F:180:MET:HA	1:F:183:ILE:HD12	1.95	0.48
1:F:238:ILE:O	1:F:435:ARG:NH1	2.46	0.48
1:A:149:PHE:CD2	1:A:374:ASP:HA	2.48	0.48
1:A:341:HIS:ND1	1:A:342:PRO:HG2	2.27	0.48
1:C:46:THR:HG21	1:C:59:LEU:HD22	1.93	0.48
1:C:233:ASP:CG	1:C:233:ASP:O	2.52	0.48
1:C:366:VAL:HG13	1:C:366:VAL:O	2.14	0.48
1:E:346:GLY:N	1:E:415:MET:HE3	2.28	0.48
1:E:409:GLU:CG	1:E:410:LYS:N	2.77	0.48
1:F:143:MET:CE	1:F:145:SER:O	2.62	0.48
1:F:376:SER:HB2	1:F:396:TRP:CH2	2.48	0.48
1:B:145:SER:OG	1:B:149:PHE:HD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ILE:CG2	1:B:215:THR:CG2	2.89	0.48
1:D:183:ILE:HG23	1:D:184:PRO:HD2	1.96	0.48
1:E:412:ILE:O	1:E:416:GLN:HG3	2.14	0.48
1:F:13:HIS:O	1:F:14:ILE:HD13	2.14	0.48
1:F:387:LEU:HG	1:F:427:VAL:HG11	1.95	0.48
1:A:274:LEU:CD2	1:A:278:GLN:HG2	2.44	0.47
1:B:47:VAL:HG22	1:B:76:LEU:CG	2.44	0.47
1:B:47:VAL:HG23	1:B:76:LEU:CD2	2.38	0.47
1:D:26:LEU:O	1:D:30:ARG:CG	2.53	0.47
1:E:347:PHE:CE1	1:E:348:VAL:O	2.67	0.47
1:F:86:ASN:HD21	1:F:91:PHE:HB2	1.79	0.47
1:A:34:MET:HE2	1:A:241:LEU:CD2	2.34	0.47
1:A:414:VAL:CG1	1:A:415:MET:N	2.77	0.47
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.69	0.47
1:B:224:ILE:HA	1:B:227:VAL:HG21	1.94	0.47
1:C:108:LEU:HD23	1:C:111:LEU:HD11	1.95	0.47
1:C:335:GLN:NE2	2:C:500:UDP:C2'	2.76	0.47
1:E:30:ARG:O	1:E:34:MET:HG3	2.13	0.47
1:F:150:PHE:O	1:F:150:PHE:CD1	2.67	0.47
1:B:50:THR:CG2	1:B:55:GLU:HB2	2.43	0.47
1:C:76:LEU:CD1	1:C:93:GLN:NE2	2.77	0.47
1:C:353:TRP:CZ3	1:C:381:VAL:HG11	2.49	0.47
1:D:51:VAL:HG11	1:D:90:PHE:CD1	2.49	0.47
1:D:152:LEU:O	1:D:156:LEU:HB2	2.15	0.47
1:E:280:ARG:HA	1:E:280:ARG:HE	1.77	0.47
1:F:119:VAL:O	1:F:119:VAL:HG22	2.13	0.47
1:C:90:PHE:O	1:C:94:MET:HG3	2.14	0.47
1:D:71:ARG:O	1:D:71:ARG:CG	2.59	0.47
1:D:254:TRP:O	1:D:254:TRP:CE3	2.67	0.47
1:F:59:LEU:O	1:F:63:PHE:HD2	1.98	0.47
1:D:63:PHE:CE2	1:D:71:ARG:HB2	2.50	0.47
1:F:254:TRP:CE2	1:F:327:LEU:HD22	2.44	0.47
1:B:98:ALA:HB1	1:B:127:GLN:HG3	1.95	0.47
1:B:251:ASP:OD1	1:B:251:ASP:N	2.45	0.47
1:C:38:ARG:NH2	1:C:442:GLU:OE2	2.47	0.47
1:D:198:ILE:HG23	1:D:199:SER:N	2.29	0.47
1:D:389:LEU:HD23	1:D:420:LEU:HD22	1.93	0.47
1:E:108:LEU:HD22	1:E:115:LEU:CD1	2.44	0.47
1:E:292:ARG:CG	1:E:292:ARG:NH2	2.76	0.47
1:F:263:VAL:CG1	1:F:344:ILE:HD13	2.44	0.47
1:C:76:LEU:HD11	1:C:93:GLN:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LEU:HD13	1:C:293:PHE:CG	2.49	0.47
1:D:38:ARG:HB3	1:D:449:ILE:CD1	2.37	0.47
1:F:146:SER:HB3	1:F:353:TRP:CZ3	2.50	0.47
1:A:14:ILE:O	1:A:42:VAL:HA	2.15	0.47
1:C:193:PHE:CD1	1:C:194:PHE:N	2.82	0.47
1:C:213:ILE:CG2	1:C:215:THR:HG23	2.44	0.47
1:C:288:LYS:HD2	1:C:288:LYS:HA	1.64	0.47
1:D:24:HIS:O	1:D:27:PRO:HD2	2.15	0.47
1:F:167:ARG:HH22	1:F:170:ILE:HD13	1.80	0.47
1:F:236:LEU:HD13	1:F:448:LEU:HD13	1.97	0.47
1:C:47:VAL:HG13	1:C:74:PHE:HB3	1.96	0.47
1:C:50:THR:CG2	1:C:51:VAL:N	2.77	0.47
1:C:394:TRP:CZ2	1:C:402:ILE:HD11	2.50	0.47
1:D:47:VAL:CB	1:D:97:ILE:CD1	2.93	0.47
1:D:51:VAL:CG1	1:D:90:PHE:HE1	2.28	0.47
1:E:372:HIS:CD2	1:E:372:HIS:O	2.68	0.47
1:F:120:SER:HG	1:F:128:VAL:HG11	1.74	0.47
1:C:347:PHE:HD1	1:C:348:VAL:N	2.14	0.46
1:E:48:LYS:O	1:E:76:LEU:HD22	2.15	0.46
1:E:105:ARG:N	1:E:106:PRO:CD	2.78	0.46
1:F:425:GLY:HA2	1:F:428:ARG:NH2	2.30	0.46
1:A:353:TRP:CZ3	1:A:356:VAL:HG11	2.50	0.46
1:F:401:LEU:CD2	1:F:402:ILE:N	2.66	0.46
1:A:70:THR:HG23	1:A:72:LEU:HD13	1.97	0.46
1:A:118:ILE:HG22	1:A:139:THR:HG22	1.97	0.46
1:C:353:TRP:CE3	1:C:378:ASN:ND2	2.82	0.46
1:D:198:ILE:HG23	1:D:199:SER:H	1.80	0.46
1:F:184:PRO:HD2	1:F:187:MET:HE3	1.97	0.46
1:A:420:LEU:HD23	1:A:420:LEU:O	2.16	0.46
1:B:212:LEU:N	1:B:212:LEU:HD13	2.25	0.46
1:B:213:ILE:HB	1:B:235:ILE:HD11	1.97	0.46
1:B:289:SER:HB3	1:B:411:MET:HE2	1.87	0.46
1:D:142:LEU:HA	1:D:212:LEU:O	2.16	0.46
1:A:129:THR:CG2	1:A:207:LYS:HD2	2.45	0.46
1:A:156:LEU:N	1:A:157:PRO:HD2	2.30	0.46
1:B:348:VAL:HG22	1:B:348:VAL:O	2.15	0.46
1:C:233:ASP:O	1:C:233:ASP:OD1	2.33	0.46
1:D:76:LEU:HD13	1:D:96:THR:HG22	1.93	0.46
1:D:150:PHE:HA	1:D:153:MET:HG3	1.98	0.46
1:F:274:LEU:HG	1:F:278:GLN:HB3	1.96	0.46
1:A:164:VAL:HG11	1:A:190:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:C	1:A:175:LEU:CD1	2.84	0.46
1:B:285:ALA:HB2	1:B:404:ARG:HA	1.98	0.46
1:D:14:ILE:N	1:D:41:ALA:O	2.30	0.46
1:D:48:LYS:HA	1:D:49:PRO:C	2.36	0.46
1:D:254:TRP:CH2	1:D:326:GLY:HA2	2.50	0.46
1:F:27:PRO:HG3	1:F:354:ASN:OD1	2.15	0.46
1:F:131:LEU:CD1	1:F:131:LEU:H	2.28	0.46
1:B:34:MET:HE3	1:B:241:LEU:HD22	1.97	0.46
1:B:193:PHE:N	1:B:193:PHE:CD1	2.69	0.46
1:D:211:VAL:O	1:D:212:LEU:HD22	2.12	0.46
1:D:254:TRP:O	1:D:258:GLN:NE2	2.49	0.46
1:E:129:THR:HG21	1:E:207:LYS:HD3	1.97	0.46
1:A:307:LYS:CG	1:A:330:LYS:HZ1	2.28	0.46
1:B:149:PHE:CD2	1:B:153:MET:HE3	2.51	0.46
1:D:268:PHE:O	1:D:350:HIS:CB	2.64	0.46
1:B:30:ARG:O	1:B:34:MET:HG3	2.15	0.46
1:C:59:LEU:O	1:C:63:PHE:HD2	1.99	0.46
1:C:356:VAL:CG1	1:C:382:VAL:CG2	2.94	0.46
1:D:278:GLN:NE2	1:D:278:GLN:HA	2.31	0.46
1:D:367:LEU:CD1	1:D:389:LEU:O	2.53	0.46
1:A:338:ILE:O	1:A:344:ILE:HG13	2.16	0.46
1:C:293:PHE:CE1	1:C:326:GLY:HA3	2.50	0.46
1:F:93:GLN:O	1:F:97:ILE:HG13	2.16	0.46
1:A:286:LEU:O	1:A:289:SER:OG	2.30	0.45
1:B:26:LEU:N	1:B:27:PRO:CD	2.78	0.45
1:B:276:LYS:O	1:B:280:ARG:HG3	2.16	0.45
1:D:51:VAL:CG1	1:D:90:PHE:CE1	2.99	0.45
1:F:129:THR:CG2	1:F:130:ASP:OD1	2.64	0.45
1:F:380:GLY:HA2	1:F:390:TRP:CZ3	2.51	0.45
1:B:128:VAL:O	1:B:131:LEU:HB2	2.17	0.45
1:C:366:VAL:O	1:C:388:GLY:HA3	2.16	0.45
1:C:394:TRP:CH2	1:C:402:ILE:HD11	2.52	0.45
1:E:332:TRP:CZ2	2:E:500:UDP:O2	2.69	0.45
1:F:310:VAL:O	1:F:313:MET:HG2	2.15	0.45
1:A:149:PHE:CD1	1:A:149:PHE:O	2.69	0.45
1:A:350:HIS:HB2	1:A:371:GLN:CG	2.46	0.45
1:B:146:SER:HG	1:B:149:PHE:H	1.58	0.45
1:B:218:SER:HG	1:B:430:LYS:HD3	1.76	0.45
1:C:433:GLU:O	1:C:439:GLY:HA3	2.16	0.45
1:A:350:HIS:CD2	1:A:350:HIS:C	2.89	0.45
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ALA:HA	1:D:179:SER:HA	1.98	0.45
1:A:116:SER:OG	1:A:453:ASN:O	2.29	0.45
1:B:50:THR:CG2	1:B:52:SER:H	2.30	0.45
1:B:275:SER:O	1:B:279:ILE:HG12	2.16	0.45
1:C:352:GLY:O	1:C:356:VAL:CG2	2.63	0.45
1:D:45:ILE:HG12	1:D:72:LEU:HD12	1.99	0.45
1:D:50:THR:HG22	1:D:52:SER:O	2.15	0.45
1:F:203:SER:O	1:F:206:HIS:ND1	2.50	0.45
1:F:412:ILE:O	1:F:416:GLN:HG2	2.17	0.45
1:F:445:LEU:O	1:F:449:ILE:CG1	2.64	0.45
1:D:14:ILE:O	1:D:42:VAL:HA	2.16	0.45
1:D:105:ARG:CB	1:D:106:PRO:CD	2.95	0.45
1:E:26:LEU:HB2	1:E:27:PRO:HD2	1.98	0.45
1:E:350:HIS:CE1	2:E:500:UDP:O3A	2.70	0.45
1:F:194:PHE:O	1:F:198:ILE:HG13	2.16	0.45
1:F:205:LEU:HD22	1:F:211:VAL:HG21	1.98	0.45
1:A:282:LEU:O	1:A:286:LEU:N	2.45	0.45
1:B:149:PHE:CD2	1:B:374:ASP:HB2	2.51	0.45
1:C:104:LEU:HB3	1:C:131:LEU:HD11	1.98	0.45
1:C:278:GLN:OE1	1:C:401:LEU:HA	2.17	0.45
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.80	0.45
1:F:298:LYS:CA	1:F:298:LYS:CE	2.94	0.45
1:B:14:ILE:O	1:B:42:VAL:HA	2.16	0.45
1:C:17:PHE:CD1	1:C:17:PHE:C	2.91	0.45
1:C:172:ILE:O	1:C:175:LEU:O	2.34	0.45
1:D:47:VAL:O	1:D:48:LYS:HD2	2.16	0.45
1:D:244:TYR:O	1:D:244:TYR:CG	2.70	0.45
1:E:354:ASN:HB2	2:E:500:UDP:H5'1	1.99	0.45
1:F:124:LEU:O	1:F:128:VAL:CG2	2.62	0.45
1:F:150:PHE:O	1:F:150:PHE:HD1	2.00	0.45
1:B:226:ALA:O	1:B:230:ASN:CB	2.62	0.45
1:C:263:VAL:HG11	1:C:344:ILE:CD1	2.47	0.45
1:D:252:LEU:C	1:D:254:TRP:N	2.69	0.45
1:F:58:HIS:O	1:F:62:PHE:N	2.39	0.45
1:F:313:MET:HG2	1:F:313:MET:H	1.62	0.45
1:B:434:THR:CG2	1:B:441:SER:OG	2.63	0.45
1:C:26:LEU:HB2	1:C:27:PRO:HD3	1.98	0.45
1:F:98:ALA:O	1:F:127:GLN:HG2	2.18	0.45
1:F:288:LYS:HZ1	1:F:405:GLU:CG	2.30	0.45
1:B:125:THR:O	1:B:207:LYS:NZ	2.50	0.44
1:B:135:LEU:HG	1:F:87:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:PRO:HB3	1:B:420:LEU:CD2	2.47	0.44
1:D:391:VAL:CG1	1:D:394:TRP:CE2	3.00	0.44
1:E:295:TRP:CE3	1:E:328:ILE:HD13	2.52	0.44
1:F:86:ASN:HD21	1:F:91:PHE:CB	2.29	0.44
1:F:163:ASP:O	1:F:164:VAL:C	2.52	0.44
1:F:394:TRP:N	1:F:394:TRP:CD1	2.84	0.44
1:B:155:TYR:CD2	1:B:173:PRO:CD	2.98	0.44
1:B:185:PRO:CD	1:B:186:LYS:H	2.31	0.44
1:C:304:LYS:HB3	1:C:304:LYS:HE2	1.68	0.44
1:C:338:ILE:O	1:C:344:ILE:HG13	2.16	0.44
1:D:52:SER:OG	1:D:55:GLU:OE2	2.30	0.44
1:D:152:LEU:HD11	1:D:183:ILE:HD11	1.98	0.44
1:D:287:GLU:H	1:D:287:GLU:HG3	1.53	0.44
1:E:159:LEU:C	1:E:159:LEU:CD2	2.84	0.44
1:E:433:GLU:O	1:E:439:GLY:HA3	2.16	0.44
1:F:280:ARG:HG2	1:F:281:GLU:N	2.31	0.44
1:A:299:GLY:N	1:A:330:LYS:HZ3	2.07	0.44
1:B:16:LEU:HD11	1:B:32:ALA:CB	2.38	0.44
1:B:52:SER:HB2	1:B:304:LYS:CG	2.47	0.44
1:D:27:PRO:HG3	1:D:144:THR:CG2	2.47	0.44
1:B:211:VAL:O	1:B:235:ILE:HA	2.17	0.44
1:B:265:PHE:HE2	1:B:335:GLN:HG2	1.80	0.44
1:C:27:PRO:HD3	1:C:354:ASN:ND2	2.32	0.44
1:C:307:LYS:CD	1:C:307:LYS:C	2.86	0.44
1:D:378:ASN:HA	1:D:381:VAL:HG22	1.99	0.44
1:F:314:LEU:HD13	1:F:318:PHE:CE2	2.52	0.44
1:A:152:LEU:CD2	1:A:187:MET:HE1	2.46	0.44
1:E:26:LEU:HD12	2:E:500:UDP:C4'	2.46	0.44
1:B:105:ARG:HB2	1:B:106:PRO:CD	2.48	0.44
1:E:215:THR:HG23	1:E:353:TRP:HZ2	1.81	0.44
1:E:350:HIS:HE1	2:E:500:UDP:PB	2.41	0.44
1:F:314:LEU:HD12	1:F:328:ILE:CD1	2.43	0.44
1:D:272:THR:CB	1:D:301:LYS:HA	2.47	0.44
1:D:389:LEU:HD11	1:D:414:VAL:HA	2.00	0.44
1:D:410:LYS:HA	1:D:410:LYS:HZ2	1.83	0.44
1:E:372:HIS:O	1:E:372:HIS:CG	2.70	0.44
1:E:374:ASP:O	1:E:377:VAL:HG12	2.17	0.44
1:F:143:MET:HE3	1:F:145:SER:HB2	1.99	0.44
1:A:105:ARG:HB2	1:A:106:PRO:CD	2.43	0.44
1:A:402:ILE:HG22	1:A:402:ILE:O	2.17	0.44
1:B:24:HIS:O	1:B:28:PHE:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLN:O	1:B:281:GLU:HB2	2.18	0.44
1:D:235:ILE:O	1:D:236:LEU:HD12	2.17	0.44
1:D:328:ILE:O	1:D:328:ILE:HG23	2.18	0.44
1:A:402:ILE:CG2	1:A:407:ILE:HD11	2.47	0.44
1:B:185:PRO:HG2	1:B:186:LYS:H	1.83	0.44
1:B:276:LYS:CG	1:B:313:MET:HB3	2.47	0.44
1:C:96:THR:O	1:C:100:SER:OG	2.34	0.44
1:C:376:SER:HB2	1:C:396:TRP:CH2	2.52	0.44
1:B:132:VAL:CB	1:B:139:THR:HG21	2.48	0.43
1:C:22:MET:HE3	1:C:332:TRP:CH2	2.53	0.43
1:D:274:LEU:CD2	1:D:278:GLN:HG2	2.44	0.43
1:D:300:GLY:H	1:D:307:LYS:HB2	1.83	0.43
1:A:122:PHE:O	1:A:122:PHE:CG	2.70	0.43
1:B:16:LEU:HD21	1:B:32:ALA:CB	2.49	0.43
1:B:101:VAL:HG11	1:B:127:GLN:HB3	2.00	0.43
1:C:263:VAL:CG1	1:C:344:ILE:HD13	2.48	0.43
1:C:295:TRP:NE1	1:C:297:LEU:HD12	2.33	0.43
1:C:394:TRP:HE1	1:C:406:GLU:CG	2.31	0.43
1:D:391:VAL:HG11	1:D:394:TRP:CG	2.30	0.43
1:E:28:PHE:CZ	1:E:142:LEU:HB3	2.53	0.43
1:E:169:ALA:HB2	1:E:179:SER:CA	2.30	0.43
1:A:59:LEU:HD22	1:A:63:PHE:CZ	2.53	0.43
1:A:227:VAL:HG13	1:A:232:VAL:HB	2.00	0.43
2:A:500:UDP:O1A	2:A:500:UDP:O1B	2.36	0.43
1:B:310:VAL:N	1:B:310:VAL:C	2.72	0.43
1:C:146:SER:HB3	1:C:353:TRP:CE3	2.53	0.43
1:E:101:VAL:HG22	1:E:127:GLN:HB3	1.99	0.43
1:E:272:THR:HG23	1:E:372:HIS:CE1	2.53	0.43
1:E:447:ARG:NH1	1:E:447:ARG:CB	2.81	0.43
1:F:140:TYR:CE1	1:F:452:PHE:HE1	2.36	0.43
1:A:38:ARG:HH21	1:A:442:GLU:CD	2.22	0.43
1:B:50:THR:HG23	1:B:52:SER:H	1.83	0.43
1:B:193:PHE:O	1:B:196:ALA:N	2.51	0.43
1:B:276:LYS:HE3	1:B:276:LYS:HB3	1.53	0.43
1:B:321:ARG:HH11	1:B:321:ARG:CG	2.24	0.43
1:C:273:ALA:HB3	1:C:301:LYS:HA	2.00	0.43
1:D:113:PRO:N	1:D:113:PRO:C	2.71	0.43
1:F:59:LEU:O	1:F:63:PHE:CD2	2.71	0.43
1:F:143:MET:HE2	1:F:145:SER:C	2.38	0.43
1:F:254:TRP:CZ3	1:F:327:LEU:HD23	2.53	0.43
1:A:10:VAL:HG12	1:A:39:GLY:HA2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD12	1:A:212:LEU:H	1.82	0.43
1:A:273:ALA:O	1:A:301:LYS:CE	2.65	0.43
1:B:110:SER:HB3	1:F:303:ASP:OD2	2.18	0.43
1:E:358:GLU:OE1	2:E:500:UDP:O3'	2.35	0.43
1:F:341:HIS:HD2	1:F:343:ALA:CB	2.32	0.43
1:A:299:GLY:H	1:A:330:LYS:HZ1	1.64	0.43
1:A:427:VAL:CG1	1:A:428:ARG:N	2.81	0.43
1:B:90:PHE:CE2	1:B:271:ARG:NH1	2.87	0.43
1:C:366:VAL:O	1:C:388:GLY:CA	2.67	0.43
1:A:347:PHE:N	1:A:365:PRO:O	2.50	0.43
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.87	0.43
1:B:149:PHE:CE2	1:B:374:ASP:HB3	2.53	0.43
1:C:75:GLN:HA	1:C:75:GLN:OE1	2.18	0.43
1:C:353:TRP:HB2	1:C:378:ASN:HD21	1.82	0.43
1:D:66:HIS:CB	1:D:69:ILE:HG13	2.49	0.43
1:D:341:HIS:CE1	1:D:342:PRO:CD	2.97	0.43
1:D:392:ARG:HE	1:D:392:ARG:HB2	1.46	0.43
1:C:16:LEU:HG	1:C:119:VAL:HB	2.00	0.43
1:C:156:LEU:HB3	1:C:157:PRO:CD	2.48	0.43
1:C:160:LEU:HD23	1:C:160:LEU:HA	1.68	0.43
1:C:423:SER:O	1:C:427:VAL:HG23	2.19	0.43
1:D:184:PRO:HA	1:D:185:PRO:HD3	1.87	0.43
1:D:340:ALA:N	1:D:362:LEU:HD13	2.34	0.43
1:F:212:LEU:HD12	1:F:212:LEU:N	2.34	0.43
1:B:408:ALA:HA	1:B:411:MET:HE2	2.00	0.43
1:E:38:ARG:HH11	1:E:38:ARG:HG2	1.74	0.43
1:B:366:VAL:HG23	1:B:387:LEU:HG	2.01	0.43
1:C:105:ARG:HB3	1:C:106:PRO:CD	2.36	0.43
1:C:150:PHE:O	1:C:150:PHE:CD1	2.72	0.43
1:D:119:VAL:HG13	1:D:140:TYR:HB2	2.00	0.43
1:F:86:ASN:HD22	1:F:92:ILE:HG12	1.77	0.43
1:F:350:HIS:HE1	2:F:500:UDP:O2B	2.02	0.43
1:B:229:ARG:O	1:B:229:ARG:CG	2.38	0.42
1:B:370:PRO:HG3	1:B:379:ALA:HB2	2.00	0.42
1:D:47:VAL:HG23	1:D:76:LEU:CD2	2.47	0.42
1:D:349:SER:OG	1:D:351:CYS:CA	2.67	0.42
1:E:107:LEU:HA	1:F:190:PRO:HB2	2.01	0.42
1:E:255:LEU:HB3	1:E:341:HIS:CE1	2.53	0.42
1:E:382:VAL:HG13	1:E:387:LEU:HB3	2.00	0.42
1:A:43:THR:CB	1:A:72:LEU:HD22	2.49	0.42
1:B:26:LEU:O	1:B:30:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ARG:HH11	1:B:271:ARG:CG	2.04	0.42
1:C:149:PHE:HD2	1:C:153:MET:HE1	1.76	0.42
1:C:224:ILE:O	1:C:227:VAL:HG12	2.19	0.42
1:E:410:LYS:HD2	1:E:410:LYS:HA	1.62	0.42
1:A:18:PRO:HD2	1:A:18:PRO:O	2.18	0.42
1:A:350:HIS:HE1	2:A:500:UDP:PB	2.43	0.42
1:B:27:PRO:CA	1:B:30:ARG:HG3	2.43	0.42
1:B:434:THR:HG23	1:B:441:SER:CB	2.48	0.42
1:D:255:LEU:HD12	1:D:255:LEU:HA	1.67	0.42
1:E:286:LEU:HD23	1:E:411:MET:HE1	1.75	0.42
1:F:118:ILE:HG13	1:F:119:VAL:N	2.34	0.42
1:A:14:ILE:HG12	1:A:40:CYS:HB3	2.01	0.42
1:B:210:GLY:HA2	1:B:234:HIS:HB2	2.01	0.42
1:C:271:ARG:O	1:C:302:VAL:HG12	2.18	0.42
1:B:211:VAL:C	1:B:212:LEU:CD1	2.59	0.42
1:B:216:PHE:N	1:B:216:PHE:CD1	2.88	0.42
1:C:378:ASN:C	1:C:381:VAL:HG12	2.39	0.42
1:C:380:GLY:HA2	1:C:390:TRP:CE3	2.54	0.42
1:D:24:HIS:O	1:D:27:PRO:CD	2.67	0.42
1:E:162:ILE:HG13	1:E:162:ILE:O	2.19	0.42
1:E:313:MET:HE2	1:E:313:MET:HB3	1.76	0.42
1:B:149:PHE:CE2	1:B:153:MET:HE2	2.55	0.42
1:B:185:PRO:CG	1:B:186:LYS:H	2.32	0.42
1:C:376:SER:HB2	1:C:396:TRP:CZ3	2.54	0.42
1:D:156:LEU:CD1	1:D:160:LEU:HG	2.49	0.42
1:E:22:MET:CE	1:E:58:HIS:CD2	3.01	0.42
1:E:141:THR:HG22	1:E:208:VAL:HG11	2.01	0.42
1:E:265:PHE:CD2	1:E:339:LEU:HD21	2.54	0.42
1:A:164:VAL:HG11	1:A:190:PRO:CG	2.49	0.42
1:B:27:PRO:O	1:B:30:ARG:HB2	2.20	0.42
1:D:149:PHE:CD2	1:D:153:MET:CE	3.01	0.42
1:D:234:HIS:ND1	1:D:234:HIS:N	2.62	0.42
1:E:105:ARG:HH12	1:E:134:ASP:HB2	1.85	0.42
1:E:376:SER:O	1:E:379:ALA:HB3	2.20	0.42
1:F:76:LEU:HD22	1:F:96:THR:HG22	2.01	0.42
1:A:47:VAL:CG1	1:A:76:LEU:HD23	2.40	0.42
1:A:207:LYS:O	1:A:207:LYS:HG2	2.17	0.42
1:A:428:ARG:O	1:A:428:ARG:HG2	2.17	0.42
1:B:35:LEU:HD23	1:B:449:ILE:HD11	2.01	0.42
1:B:72:LEU:HD22	1:B:107:LEU:HD11	2.02	0.42
1:B:273:ALA:HB1	1:B:371:GLN:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:CD1	1:C:135:LEU:H	2.32	0.42
1:C:383:GLU:CD	1:C:384:LYS:NZ	2.73	0.42
1:D:105:ARG:HG2	1:D:131:LEU:CD1	2.34	0.42
1:F:14:ILE:HD13	1:F:14:ILE:N	2.35	0.42
1:F:318:PHE:O	1:F:322:THR:CG2	2.44	0.42
1:B:121:ASP:OD1	1:B:122:PHE:N	2.53	0.42
1:E:47:VAL:HA	1:E:74:PHE:O	2.20	0.42
1:E:63:PHE:CE1	1:E:71:ARG:HB2	2.54	0.42
1:E:72:LEU:HD23	1:E:72:LEU:HA	1.83	0.42
1:F:183:ILE:HG23	1:F:184:PRO:HD2	2.01	0.42
1:F:286:LEU:HD21	1:F:411:MET:HE1	2.02	0.42
1:B:276:LYS:HG2	1:B:313:MET:CB	2.49	0.42
1:B:394:TRP:CE3	1:B:402:ILE:HD12	2.55	0.42
1:C:79:TYR:CD1	1:C:79:TYR:C	2.92	0.42
1:C:380:GLY:O	1:C:384:LYS:HE2	2.20	0.42
1:D:149:PHE:CE1	1:D:374:ASP:HA	2.55	0.42
1:F:88:ASP:HB3	1:F:91:PHE:HB2	2.02	0.42
1:A:32:ALA:HB1	1:A:42:VAL:HG11	2.03	0.41
1:A:194:PHE:CE1	1:A:198:ILE:HD11	2.55	0.41
1:E:307:LYS:CG	1:E:330:LYS:HZ2	2.33	0.41
1:F:84:LEU:HG	1:F:193:PHE:HA	2.02	0.41
1:F:350:HIS:CD2	1:F:352:GLY:H	2.38	0.41
1:A:42:VAL:HB	1:A:69:ILE:HG12	2.02	0.41
1:B:10:VAL:HA	1:B:39:GLY:C	2.40	0.41
1:B:30:ARG:NH2	2:B:500:UDP:O3'	2.51	0.41
1:B:268:PHE:CE2	1:B:274:LEU:CD1	3.03	0.41
1:C:171:GLU:CA	1:C:177:PRO:HB3	2.41	0.41
1:D:47:VAL:O	1:D:47:VAL:HG13	2.20	0.41
1:D:220:GLU:HB3	1:D:223:ALA:HB3	2.01	0.41
1:E:255:LEU:HD12	1:E:255:LEU:HA	1.81	0.41
1:E:297:LEU:HD12	1:E:297:LEU:HA	1.85	0.41
1:F:111:LEU:HD23	1:F:111:LEU:HA	1.83	0.41
1:A:408:ALA:O	1:A:412:ILE:HG13	2.20	0.41
1:C:162:ILE:CD1	1:C:163:ASP:N	2.71	0.41
1:C:172:ILE:HA	1:C:173:PRO:HD3	1.74	0.41
1:C:281:GLU:OE1	1:C:404:ARG:HG2	2.19	0.41
1:C:321:ARG:CG	1:C:321:ARG:HH21	2.34	0.41
1:D:38:ARG:CB	1:D:449:ILE:HD12	2.39	0.41
1:D:105:ARG:CB	1:D:106:PRO:HD3	2.48	0.41
1:E:30:ARG:NH2	1:E:358:GLU:OE2	2.54	0.41
1:E:243:SER:CB	1:E:336:GLU:CD	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:PHE:C	1:E:293:PHE:CD1	2.94	0.41
1:E:376:SER:HB2	1:E:396:TRP:CH2	2.55	0.41
1:F:295:TRP:CZ3	1:F:314:LEU:HD11	2.55	0.41
1:B:276:LYS:HD2	1:B:313:MET:CA	2.48	0.41
1:C:46:THR:HB	1:C:59:LEU:HD11	2.03	0.41
1:C:105:ARG:NH1	1:C:105:ARG:CG	2.72	0.41
1:D:192:ASP:OD1	1:D:194:PHE:CB	2.68	0.41
1:D:402:ILE:HG23	1:D:407:ILE:CD1	2.50	0.41
1:F:26:LEU:N	1:F:27:PRO:HD2	2.36	0.41
1:B:271:ARG:NH1	1:B:271:ARG:CG	2.65	0.41
1:D:118:ILE:HG22	1:D:139:THR:HB	2.02	0.41
1:D:389:LEU:CD1	1:D:413:GLU:HG2	2.50	0.41
1:E:447:ARG:NH1	1:E:447:ARG:HB3	2.35	0.41
1:F:174:ASP:HB2	1:F:226:ALA:HA	2.01	0.41
1:A:105:ARG:CB	1:A:106:PRO:HD3	2.47	0.41
1:A:248:LYS:HB3	1:A:249:ALA:H	1.46	0.41
1:C:183:ILE:HG23	1:C:187:MET:HE2	1.91	0.41
1:C:282:LEU:HD12	1:C:282:LEU:O	2.20	0.41
1:D:143:MET:N	1:D:212:LEU:O	2.40	0.41
1:D:223:ALA:O	1:D:227:VAL:CG2	2.68	0.41
1:D:266:VAL:O	1:D:295:TRP:HD1	2.04	0.41
1:D:303:ASP:CB	1:D:306:ASP:HB2	2.49	0.41
1:E:289:SER:O	1:E:412:ILE:HD11	2.20	0.41
1:B:104:LEU:O	1:B:108:LEU:CD1	2.68	0.41
1:B:215:THR:OG1	1:B:220:GLU:HG3	2.21	0.41
1:C:156:LEU:N	1:C:157:PRO:HD2	2.36	0.41
1:C:175:LEU:HD13	1:C:176:GLY:N	2.35	0.41
1:C:368:ALA:HB3	1:C:390:TRP:HB2	2.01	0.41
1:C:391:VAL:O	1:C:391:VAL:HG22	2.20	0.41
1:D:107:LEU:HD13	1:D:107:LEU:HA	1.87	0.41
1:D:391:VAL:HG11	1:D:394:TRP:CD2	2.56	0.41
1:E:240:PRO:HG2	1:E:431:ALA:HB1	2.02	0.41
1:F:38:ARG:HG2	1:F:446:GLN:HE22	1.85	0.41
1:F:45:ILE:HA	1:F:72:LEU:O	2.20	0.41
1:F:252:LEU:HA	1:F:253:PRO:HD3	1.87	0.41
1:A:318:PHE:HE2	1:A:328:ILE:HD11	1.85	0.41
1:A:420:LEU:C	1:A:420:LEU:CD2	2.89	0.41
1:B:178:ILE:HD12	1:B:178:ILE:HA	1.82	0.41
1:C:65:ILE:C	1:C:67:PRO:HD3	2.41	0.41
1:D:217:ASN:CG	1:D:218:SER:N	2.73	0.41
1:D:247:LYS:HA	1:D:248:LYS:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:427:VAL:CG1	1:D:428:ARG:N	2.84	0.41
1:E:354:ASN:O	1:E:358:GLU:HG2	2.18	0.41
1:F:294:LEU:HD13	1:F:327:LEU:HD21	2.02	0.41
1:A:402:ILE:HG22	1:A:407:ILE:HD12	2.00	0.41
1:A:413:GLU:O	1:A:417:ASP:HB2	2.19	0.41
1:B:15:ALA:HA	1:B:43:THR:O	2.19	0.41
1:B:411:MET:HE3	1:B:411:MET:HB3	1.90	0.41
1:C:87:ASP:OD1	1:C:87:ASP:C	2.59	0.41
1:C:152:LEU:HD21	1:C:187:MET:HE1	2.03	0.41
1:C:255:LEU:HA	1:C:255:LEU:HD12	1.78	0.41
1:C:383:GLU:CD	1:C:384:LYS:HZ3	2.24	0.41
1:C:435:ARG:NE	1:C:435:ARG:CA	2.67	0.41
1:D:195:SER:HA	1:D:198:ILE:CG2	2.51	0.41
1:E:13:HIS:ND1	1:E:113:PRO:O	2.53	0.41
1:E:149:PHE:HD1	1:E:377:VAL:HG11	1.86	0.41
1:E:350:HIS:CE1	2:E:500:UDP:O1B	2.68	0.41
1:E:394:TRP:O	1:E:400:LYS:HD3	2.21	0.41
1:F:216:PHE:CZ	1:F:219:PHE:HB2	2.56	0.41
1:F:235:ILE:O	1:F:235:ILE:HG23	2.19	0.41
1:F:286:LEU:HD21	1:F:411:MET:HE2	2.02	0.41
1:F:440:ASP:O	1:F:444:LEU:HB2	2.21	0.41
1:A:16:LEU:H	1:A:16:LEU:HG	1.72	0.41
1:B:20:ALA:O	1:B:24:HIS:HB2	2.21	0.41
1:D:27:PRO:HG3	1:D:144:THR:HG21	2.03	0.41
1:D:375:GLN:O	1:D:378:ASN:HB2	2.20	0.41
1:E:84:LEU:HA	1:E:191:SER:O	2.21	0.41
1:E:212:LEU:HG	1:E:238:ILE:HD11	2.03	0.41
1:F:101:VAL:CG1	1:F:131:LEU:HD11	2.50	0.41
1:A:254:TRP:CG	1:A:258:GLN:OE1	2.74	0.40
1:A:307:LYS:CG	1:A:330:LYS:NZ	2.84	0.40
1:B:42:VAL:HG13	1:B:69:ILE:CG2	2.44	0.40
1:B:447:ARG:HD3	1:B:447:ARG:HA	1.82	0.40
1:C:26:LEU:CB	1:C:27:PRO:HD3	2.50	0.40
1:C:384:LYS:HD3	1:C:384:LYS:HA	1.69	0.40
1:D:47:VAL:CG2	1:D:76:LEU:HD21	2.50	0.40
1:D:88:ASP:HB3	1:D:91:PHE:HB2	2.03	0.40
1:D:137:ILE:O	1:D:137:ILE:HG22	2.21	0.40
1:D:288:LYS:HB3	1:D:288:LYS:HE3	1.76	0.40
1:E:213:ILE:HD13	1:E:213:ILE:HA	1.77	0.40
1:F:65:ILE:C	1:F:67:PRO:HD3	2.41	0.40
1:D:192:ASP:OD1	1:D:194:PHE:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:ASP:OD1	1:E:193:PHE:N	2.55	0.40
1:F:234:HIS:O	1:F:234:HIS:ND1	2.48	0.40
1:A:183:ILE:HG23	1:A:187:MET:HE2	2.02	0.40
1:A:341:HIS:CG	1:A:342:PRO:HD2	2.51	0.40
1:B:29:LEU:N	1:B:29:LEU:HD23	2.35	0.40
1:B:218:SER:CB	1:B:430:LYS:CD	2.94	0.40
1:B:299:GLY:H	1:B:330:LYS:HZ1	1.68	0.40
1:D:90:PHE:O	1:D:94:MET:HG3	2.22	0.40
1:E:334:LYS:HB3	1:E:337:GLN:HG3	2.03	0.40
1:E:370:PRO:HG2	1:E:376:SER:HA	2.03	0.40
1:B:285:ALA:HB2	1:B:404:ARG:O	2.21	0.40
1:D:43:THR:CA	1:D:70:THR:HG22	2.49	0.40
1:F:145:SER:O	1:F:213:ILE:HD11	2.22	0.40
1:A:282:LEU:HA	1:A:285:ALA:HB3	2.02	0.40
1:B:25:LEU:O	1:B:29:LEU:HG	2.21	0.40
1:B:211:VAL:CA	1:B:212:LEU:HD12	2.47	0.40
1:C:118:ILE:O	1:C:118:ILE:CG2	2.70	0.40
1:C:264:LEU:HB2	1:C:415:MET:CE	2.52	0.40
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.77	0.40
1:D:227:VAL:O	1:D:232:VAL:HB	2.22	0.40
1:E:332:TRP:CZ2	2:E:500:UDP:C2	3.10	0.40
1:E:351:CYS:HA	1:E:356:VAL:HG23	2.03	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	439/460 (95%)	417 (95%)	15 (3%)	7 (2%)	9 40
1	B	442/460 (96%)	429 (97%)	13 (3%)	0	100 100
1	C	435/460 (95%)	423 (97%)	11 (2%)	1 (0%)	47 82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	432/460 (94%)	417 (96%)	12 (3%)	3 (1%)	22 60
1	E	441/460 (96%)	423 (96%)	16 (4%)	2 (0%)	29 68
1	F	440/460 (96%)	430 (98%)	9 (2%)	1 (0%)	47 82
All	All	2629/2760 (95%)	2539 (97%)	76 (3%)	14 (0%)	29 68

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	A	173	PRO
1	A	249	ALA
1	E	301	LYS
1	A	248	LYS
1	D	173	PRO
1	A	247	LYS
1	A	310	VAL
1	F	310	VAL
1	C	113	PRO
1	D	18	PRO
1	A	136	PRO
1	D	237	PRO
1	E	113	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	310/390 (80%)	247 (80%)	63 (20%)	1 6
1	B	301/390 (77%)	230 (76%)	71 (24%)	1 3
1	C	328/390 (84%)	253 (77%)	75 (23%)	1 4
1	D	297/390 (76%)	211 (71%)	86 (29%)	0 2
1	E	322/390 (83%)	264 (82%)	58 (18%)	1 9
1	F	335/390 (86%)	275 (82%)	60 (18%)	2 9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1893/2340 (81%)	1480 (78%)	413 (22%)	1 5

All (413) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	38	ARG
1	A	46	THR
1	A	48	LYS
1	A	50	THR
1	A	56	SER
1	A	64	THR
1	A	72	LEU
1	A	99	THR
1	A	100	SER
1	A	101	VAL
1	A	118	ILE
1	A	124	LEU
1	A	125	THR
1	A	129	THR
1	A	131	LEU
1	A	135	LEU
1	A	155	TYR
1	A	159	LEU
1	A	162	ILE
1	A	173	PRO
1	A	175	LEU
1	A	187	MET
1	A	194	PHE
1	A	198	ILE
1	A	204	SER
1	A	207	LYS
1	A	217	ASN
1	A	220	GLU
1	A	227	VAL
1	A	233	ASP
1	A	234	HIS
1	A	235	ILE
1	A	248	LYS
1	A	258	GLN
1	A	266	VAL
1	A	270	SER

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Mol	Chain	Res	Type
1	A	275	SER
1	A	282	LEU
1	A	286	LEU
1	A	288	LYS
1	A	291	CYS
1	A	292	ARG
1	A	302	VAL
1	A	303	ASP
1	A	304	LYS
1	A	310	VAL
1	A	319	VAL
1	A	320	GLU
1	A	337	GLN
1	A	350	HIS
1	A	376	SER
1	A	391	VAL
1	A	399	THR
1	A	402	ILE
1	A	405	GLU
1	A	409	GLU
1	A	416	GLN
1	A	420	LEU
1	A	423	SER
1	A	433	GLU
1	A	434	THR
1	A	451	SER
1	B	16	LEU
1	B	38	ARG
1	B	46	THR
1	B	48	LYS
1	B	50	THR
1	B	51	VAL
1	B	56	SER
1	B	57	ASP
1	B	60	SER
1	B	68	ARG
1	B	101	VAL
1	B	104	LEU
1	B	107	LEU
1	B	110	SER
1	B	118	ILE
1	B	123	THR

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Mol	Chain	Res	Type
1	B	125	THR
1	B	126	SER
1	B	129	THR
1	B	131	LEU
1	B	134	ASP
1	B	137	ILE
1	B	139	THR
1	B	141	THR
1	B	143	MET
1	B	151	CYS
1	B	156	LEU
1	B	159	LEU
1	B	175	LEU
1	B	178	ILE
1	B	183	ILE
1	B	187	MET
1	B	192	ASP
1	B	193	PHE
1	B	195	SER
1	B	199	SER
1	B	207	LYS
1	B	212	LEU
1	B	216	PHE
1	B	221	SER
1	B	227	VAL
1	B	229	ARG
1	B	234	HIS
1	B	235	ILE
1	B	270	SER
1	B	271	ARG
1	B	275	SER
1	B	276	LYS
1	B	277	GLU
1	B	278	GLN
1	B	279	ILE
1	B	282	LEU
1	B	294	LEU
1	B	302	VAL
1	B	308	GLU
1	B	319	VAL
1	B	321	ARG
1	B	328	ILE

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Mol	Chain	Res	Type
1	B	329	VAL
1	B	335	GLN
1	B	376	SER
1	B	391	VAL
1	B	392	ARG
1	B	399	THR
1	B	402	ILE
1	B	404	ARG
1	B	435	ARG
1	B	437	VAL
1	B	447	ARG
1	B	448	LEU
1	B	449	ILE
1	C	14	ILE
1	C	17	PHE
1	C	19	CYS
1	C	43	THR
1	C	50	THR
1	C	68	ARG
1	C	71	ARG
1	C	74	PHE
1	C	84	LEU
1	C	87	ASP
1	C	97	ILE
1	C	99	THR
1	C	100	SER
1	C	125	THR
1	C	131	LEU
1	C	139	THR
1	C	143	MET
1	C	145	SER
1	C	170	ILE
1	C	175	LEU
1	C	179	SER
1	C	180	MET
1	C	181	SER
1	C	189	ASP
1	C	193	PHE
1	C	207	LYS
1	C	213	ILE
1	C	215	THR
1	C	216	PHE

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Mol	Chain	Res	Type
1	C	219	PHE
1	C	222	GLU
1	C	225	GLU
1	C	227	VAL
1	C	234	HIS
1	C	238	ILE
1	C	251	ASP
1	C	255	LEU
1	C	258	GLN
1	C	271	ARG
1	C	272	THR
1	C	275	SER
1	C	276	LYS
1	C	279	ILE
1	C	288	LYS
1	C	298	LYS
1	C	303	ASP
1	C	304	LYS
1	C	306	ASP
1	C	320	GLU
1	C	321	ARG
1	C	322	THR
1	C	323	LYS
1	C	329	VAL
1	C	330	LYS
1	C	335	GLN
1	C	338	ILE
1	C	347	PHE
1	C	349	SER
1	C	356	VAL
1	C	362	LEU
1	C	376	SER
1	C	383	GLU
1	C	384	LYS
1	C	387	LEU
1	C	389	LEU
1	C	391	VAL
1	C	399	THR
1	C	400	LYS
1	C	401	LEU
1	C	404	ARG
1	C	406	GLU

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Mol	Chain	Res	Type
1	C	435	ARG
1	C	437	VAL
1	C	449	ILE
1	C	451	SER
1	D	19	CYS
1	D	22	MET
1	D	36	ASP
1	D	40	CYS
1	D	46	THR
1	D	48	LYS
1	D	50	THR
1	D	51	VAL
1	D	57	ASP
1	D	60	SER
1	D	69	ILE
1	D	70	THR
1	D	72	LEU
1	D	73	GLU
1	D	91	PHE
1	D	92	ILE
1	D	93	GLN
1	D	95	GLU
1	D	96	THR
1	D	97	ILE
1	D	99	THR
1	D	118	ILE
1	D	119	VAL
1	D	123	THR
1	D	129	THR
1	D	130	ASP
1	D	131	LEU
1	D	134	ASP
1	D	135	LEU
1	D	137	ILE
1	D	138	SER
1	D	139	THR
1	D	142	LEU
1	D	143	MET
1	D	153	MET
1	D	163	ASP
1	D	173	PRO
1	D	181	SER

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Mol	Chain	Res	Type
1	D	194	PHE
1	D	207	LYS
1	D	208	VAL
1	D	212	LEU
1	D	216	PHE
1	D	221	SER
1	D	227	VAL
1	D	229	ARG
1	D	233	ASP
1	D	251	ASP
1	D	256	ASP
1	D	258	GLN
1	D	274	LEU
1	D	278	GLN
1	D	279	ILE
1	D	282	LEU
1	D	286	LEU
1	D	287	GLU
1	D	303	ASP
1	D	308	GLU
1	D	335	GLN
1	D	350	HIS
1	D	351	CYS
1	D	355	SER
1	D	364	VAL
1	D	366	VAL
1	D	376	SER
1	D	381	VAL
1	D	389	LEU
1	D	391	VAL
1	D	392	ARG
1	D	399	THR
1	D	401	LEU
1	D	406	GLU
1	D	407	ILE
1	D	410	LYS
1	D	411	MET
1	D	414	VAL
1	D	415	MET
1	D	420	LEU
1	D	423	SER
1	D	430	LYS

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Mol	Chain	Res	Type
1	D	434	THR
1	D	435	ARG
1	D	436	GLU
1	D	442	GLU
1	D	447	ARG
1	D	448	LEU
1	E	17	PHE
1	E	19	CYS
1	E	30	ARG
1	E	38	ARG
1	E	40	CYS
1	E	46	THR
1	E	52	SER
1	E	56	SER
1	E	75	GLN
1	E	76	LEU
1	E	84	LEU
1	E	87	ASP
1	E	104	LEU
1	E	105	ARG
1	E	129	THR
1	E	134	ASP
1	E	141	THR
1	E	166	ASN
1	E	171	GLU
1	E	175	LEU
1	E	188	LEU
1	E	204	SER
1	E	213	ILE
1	E	215	THR
1	E	216	PHE
1	E	218	SER
1	E	219	PHE
1	E	227	VAL
1	E	234	HIS
1	E	255	LEU
1	E	258	GLN
1	E	262	SER
1	E	270	SER
1	E	271	ARG
1	E	280	ARG
1	E	292	ARG

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Mol	Chain	Res	Type
1	E	298	LYS
1	E	306	ASP
1	E	323	LYS
1	E	339	LEU
1	E	349	SER
1	E	362	LEU
1	E	371	GLN
1	E	376	SER
1	E	377	VAL
1	E	387	LEU
1	E	391	VAL
1	E	400	LYS
1	E	402	ILE
1	E	410	LYS
1	E	411	MET
1	E	416	GLN
1	E	423	SER
1	E	434	THR
1	E	435	ARG
1	E	444	LEU
1	E	447	ARG
1	E	449	ILE
1	F	17	PHE
1	F	19	CYS
1	F	22	MET
1	F	56	SER
1	F	60	SER
1	F	64	THR
1	F	68	ARG
1	F	76	LEU
1	F	82	SER
1	F	84	LEU
1	F	105	ARG
1	F	115	LEU
1	F	119	VAL
1	F	126	SER
1	F	145	SER
1	F	159	LEU
1	F	163	ASP
1	F	167	ARG
1	F	181	SER
1	F	193	PHE

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Mol	Chain	Res	Type
1	F	200	SER
1	F	204	SER
1	F	207	LYS
1	F	209	LYS
1	F	218	SER
1	F	219	PHE
1	F	222	GLU
1	F	232	VAL
1	F	235	ILE
1	F	252	LEU
1	F	258	GLN
1	F	266	VAL
1	F	267	SER
1	F	275	SER
1	F	278	GLN
1	F	279	ILE
1	F	291	CYS
1	F	297	LEU
1	F	298	LYS
1	F	303	ASP
1	F	323	LYS
1	F	327	LEU
1	F	335	GLN
1	F	350	HIS
1	F	376	SER
1	F	381	VAL
1	F	387	LEU
1	F	401	LEU
1	F	407	ILE
1	F	409	GLU
1	F	410	LYS
1	F	412	ILE
1	F	414	VAL
1	F	423	SER
1	F	427	VAL
1	F	434	THR
1	F	435	ARG
1	F	440	ASP
1	F	444	LEU
1	F	449	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	127	GLN
1	A	230	ASN
1	A	258	GLN
1	A	278	GLN
1	A	335	GLN
1	A	350	HIS
1	B	13	HIS
1	B	335	GLN
1	C	66	HIS
1	C	93	GLN
1	C	258	GLN
1	C	335	GLN
1	C	354	ASN
1	C	371	GLN
1	D	258	GLN
1	E	350	HIS
1	E	371	GLN
1	E	372	HIS
1	F	24	HIS
1	F	58	HIS
1	F	86	ASN
1	F	206	HIS
1	F	258	GLN
1	F	278	GLN
1	F	341	HIS
1	F	350	HIS
1	F	446	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	UDP	E	500	-	24,26,26	1.25	4 (16%)	37,40,40	1.68	6 (16%)
2	UDP	B	500	-	24,26,26	0.69	0	37,40,40	0.79	1 (2%)
2	UDP	A	500	-	24,26,26	1.27	4 (16%)	37,40,40	1.73	8 (21%)
2	UDP	F	500	-	24,26,26	1.39	5 (20%)	37,40,40	1.61	6 (16%)
2	UDP	C	500	-	24,26,26	1.37	5 (20%)	37,40,40	1.82	8 (21%)
2	UDP	D	500	-	24,26,26	0.70	0	37,40,40	0.86	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	E	500	-	-	2/16/32/32	0/2/2/2
2	UDP	B	500	-	-	4/16/32/32	0/2/2/2
2	UDP	A	500	-	-	6/16/32/32	0/2/2/2
2	UDP	F	500	-	-	3/16/32/32	0/2/2/2
2	UDP	C	500	-	-	5/16/32/32	0/2/2/2
2	UDP	D	500	-	-	4/16/32/32	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	500	UDP	C4-N3	-2.94	1.33	1.38
2	A	500	UDP	C4-N3	-2.92	1.33	1.38
2	F	500	UDP	PB-O1B	2.90	1.59	1.50
2	F	500	UDP	C4-N3	-2.80	1.33	1.38
2	C	500	UDP	C4-N3	-2.75	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	UDP	C2-N3	-2.72	1.33	1.38
2	C	500	UDP	PB-O1B	2.65	1.59	1.50
2	E	500	UDP	C2-N3	-2.49	1.33	1.38
2	F	500	UDP	C2-N3	-2.49	1.33	1.38
2	E	500	UDP	C5-C4	-2.47	1.38	1.43
2	C	500	UDP	C5-C4	-2.46	1.38	1.43
2	C	500	UDP	C2-N3	-2.36	1.33	1.38
2	F	500	UDP	C5-C4	-2.31	1.38	1.43
2	C	500	UDP	C6-N1	-2.20	1.32	1.38
2	A	500	UDP	C6-N1	-2.18	1.32	1.38
2	A	500	UDP	C5-C4	-2.15	1.38	1.43
2	E	500	UDP	C6-N1	-2.02	1.33	1.38
2	F	500	UDP	C6-N1	-2.01	1.33	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	500	UDP	C4-N3-C2	-4.59	120.52	126.58
2	A	500	UDP	C4-N3-C2	-4.56	120.56	126.58
2	A	500	UDP	N3-C2-N1	4.55	120.93	114.89
2	C	500	UDP	C4-N3-C2	-4.43	120.74	126.58
2	F	500	UDP	C4-N3-C2	-4.34	120.86	126.58
2	C	500	UDP	PA-O3A-PB	-4.29	118.11	132.83
2	F	500	UDP	N3-C2-N1	3.93	120.11	114.89
2	E	500	UDP	C5-C4-N3	3.89	120.67	114.84
2	C	500	UDP	N3-C2-N1	3.88	120.04	114.89
2	E	500	UDP	N3-C2-N1	3.77	119.90	114.89
2	A	500	UDP	PA-O3A-PB	-3.72	120.06	132.83
2	F	500	UDP	C5-C4-N3	3.46	120.02	114.84
2	C	500	UDP	C5-C4-N3	3.43	119.98	114.84
2	C	500	UDP	O4-C4-C5	-3.36	119.25	125.16
2	C	500	UDP	O3B-PB-O2B	3.33	120.37	107.64
2	E	500	UDP	O4-C4-C5	-3.19	119.55	125.16
2	A	500	UDP	C5-C4-N3	3.14	119.54	114.84
2	F	500	UDP	O4-C4-C5	-2.83	120.18	125.16
2	F	500	UDP	O2-C2-N1	-2.80	119.06	122.79
2	A	500	UDP	O2-C2-N1	-2.79	119.08	122.79
2	D	500	UDP	C4'-O4'-C1'	-2.76	103.39	109.47
2	F	500	UDP	O3B-PB-O2B	2.61	117.59	107.64
2	A	500	UDP	O4-C4-C5	-2.60	120.59	125.16
2	E	500	UDP	O2-C2-N1	-2.58	119.35	122.79
2	A	500	UDP	O2B-PB-O1B	2.50	120.48	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	UDP	O2-C2-N1	-2.27	119.77	122.79
2	E	500	UDP	PA-O3A-PB	-2.21	125.25	132.83
2	B	500	UDP	O4'-C1'-C2'	-2.15	101.95	106.64
2	C	500	UDP	O3'-C3'-C2'	-2.06	105.15	111.82
2	A	500	UDP	C2'-C3'-C4'	2.01	106.56	102.64

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	UDP	C5'-O5'-PA-O1A
2	B	500	UDP	C5'-O5'-PA-O1A
2	C	500	UDP	C5'-O5'-PA-O1A
2	C	500	UDP	C5'-O5'-PA-O2A
2	D	500	UDP	C5'-O5'-PA-O3A
2	E	500	UDP	C5'-O5'-PA-O2A
2	E	500	UDP	C5'-O5'-PA-O3A
2	F	500	UDP	C5'-O5'-PA-O1A
2	F	500	UDP	C5'-O5'-PA-O2A
2	A	500	UDP	C3'-C4'-C5'-O5'
2	A	500	UDP	O4'-C4'-C5'-O5'
2	D	500	UDP	O4'-C4'-C5'-O5'
2	D	500	UDP	C3'-C4'-C5'-O5'
2	B	500	UDP	PB-O3A-PA-O5'
2	A	500	UDP	C5'-O5'-PA-O3A
2	B	500	UDP	C5'-O5'-PA-O3A
2	C	500	UDP	O4'-C4'-C5'-O5'
2	A	500	UDP	C5'-O5'-PA-O2A
2	B	500	UDP	C5'-O5'-PA-O2A
2	D	500	UDP	C5'-O5'-PA-O1A
2	A	500	UDP	C4'-C5'-O5'-PA
2	C	500	UDP	C3'-C4'-C5'-O5'
2	C	500	UDP	C5'-O5'-PA-O3A
2	F	500	UDP	C5'-O5'-PA-O3A

There are no ring outliers.

6 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	500	UDP	15	0
2	B	500	UDP	2	0

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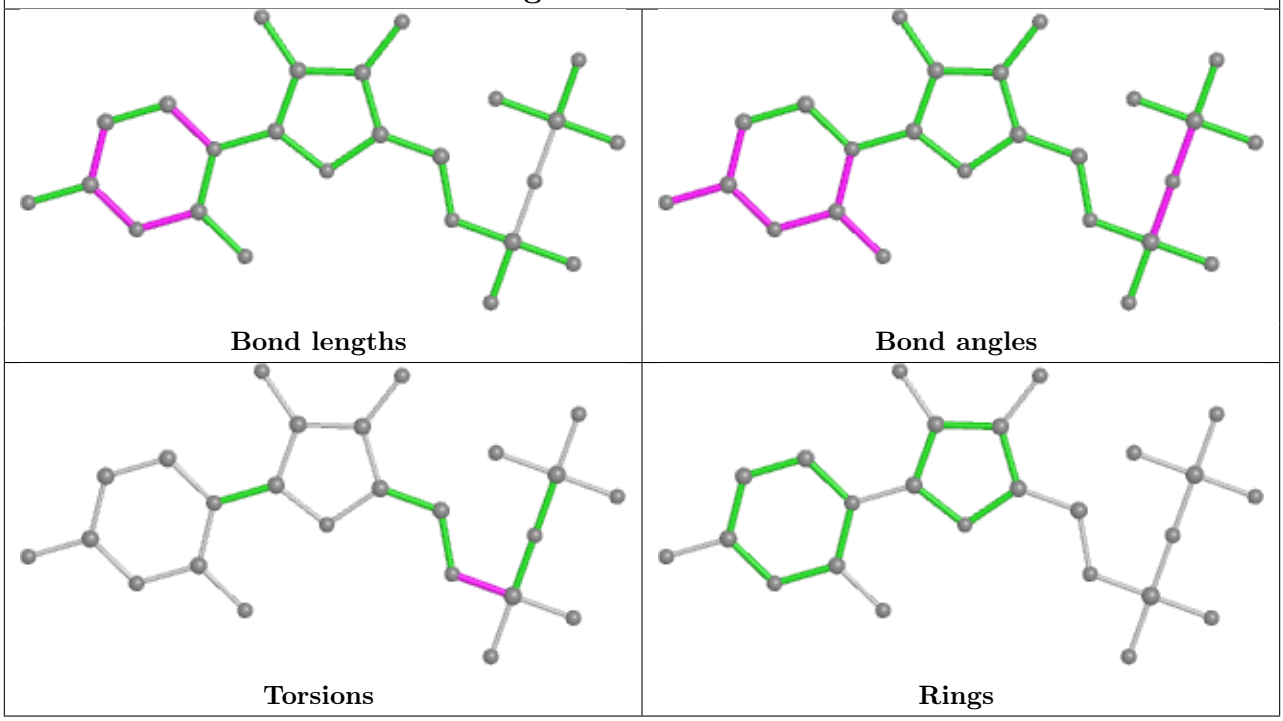
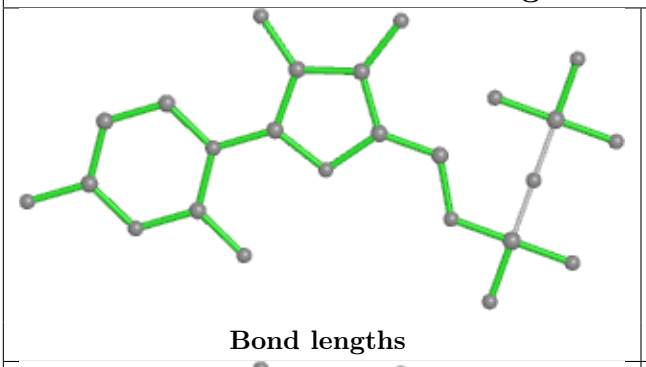
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	UDP	6	0
2	F	500	UDP	1	0
2	C	500	UDP	7	0
2	D	500	UDP	4	0

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.

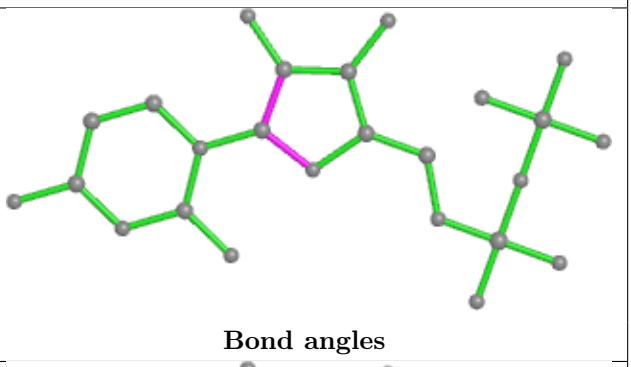
Ligand UDP E 500



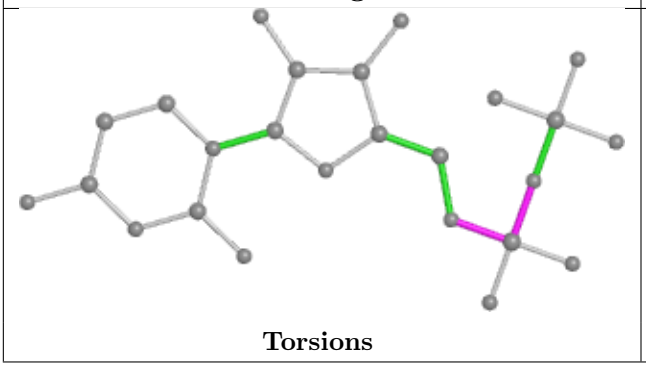
Ligand UDP B 500



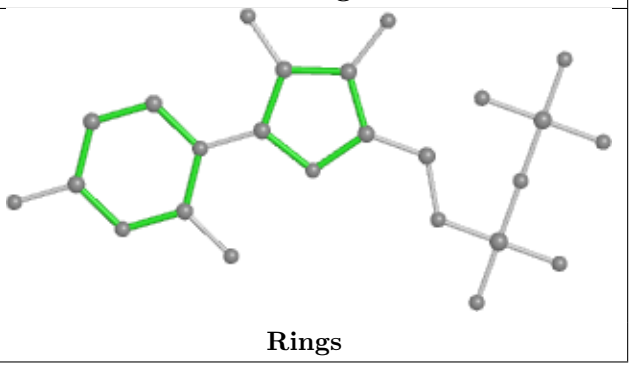
Bond lengths



Bond angles

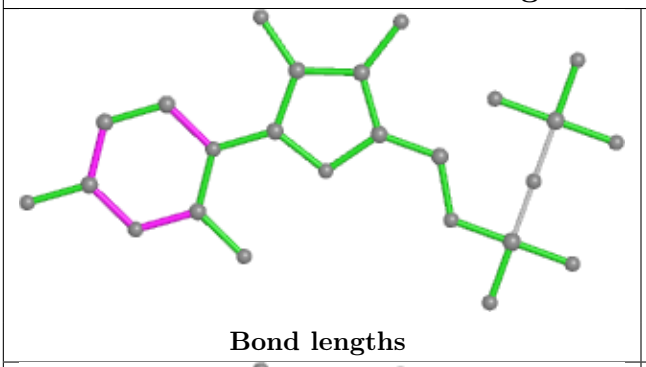


Torsions

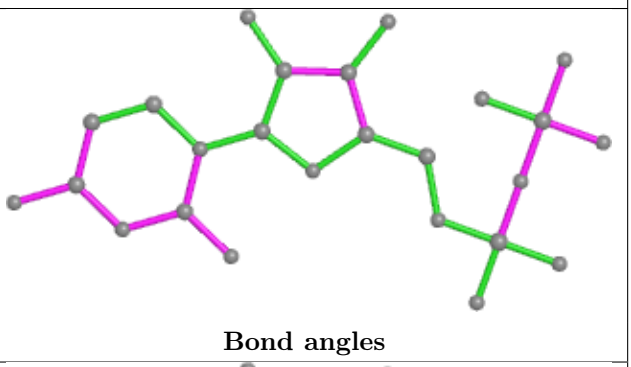


Rings

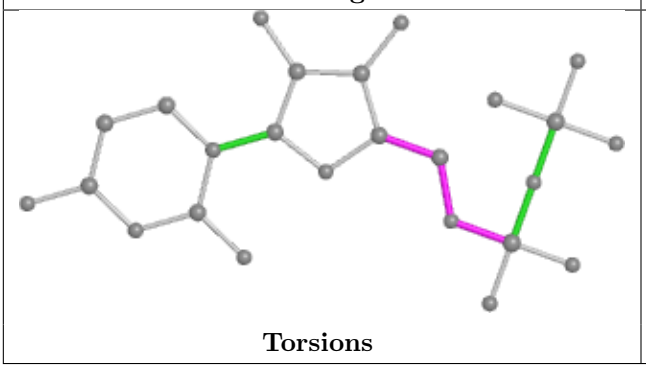
Ligand UDP A 500



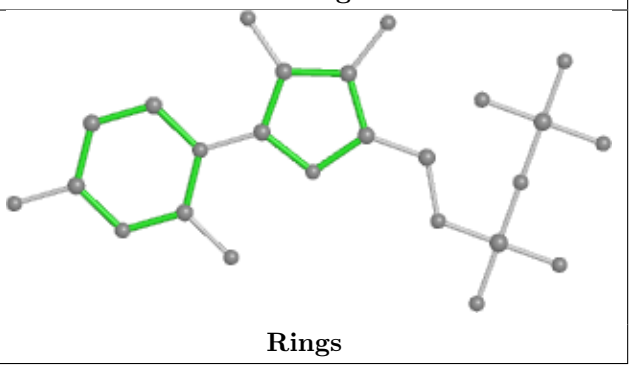
Bond lengths



Bond angles

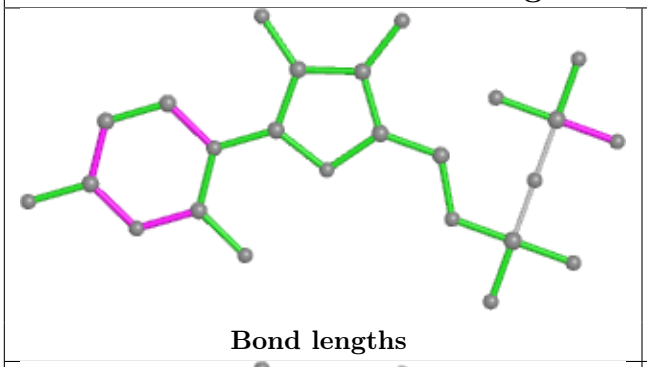


Torsions

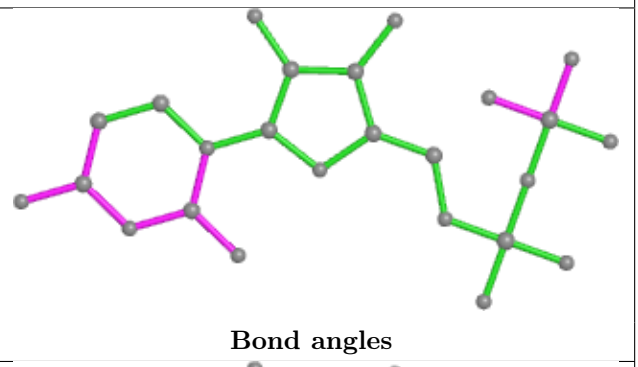


Rings

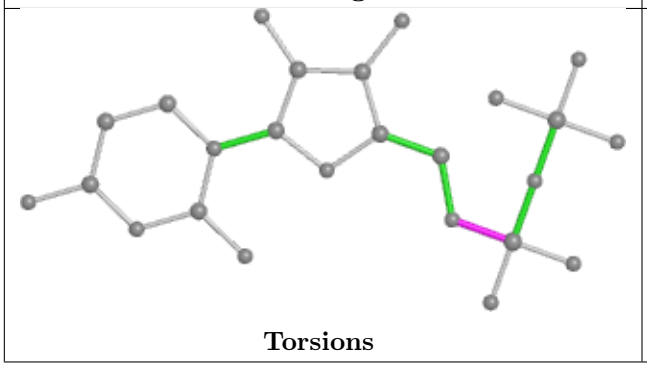
Ligand UDP F 500



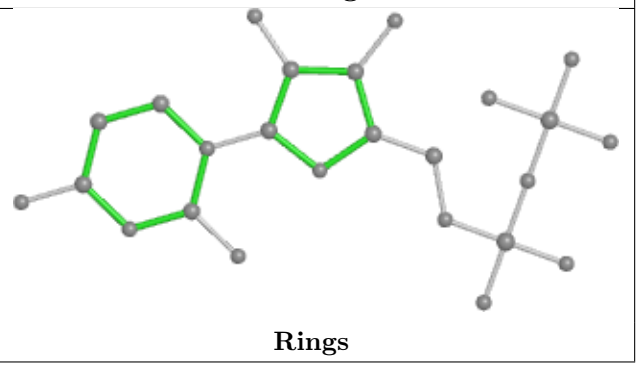
Bond lengths



Bond angles

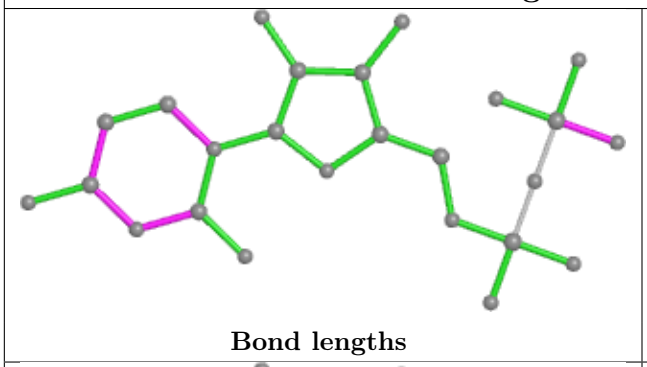


Torsions

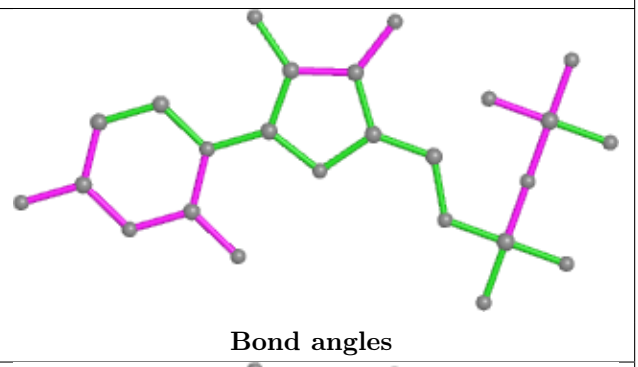


Rings

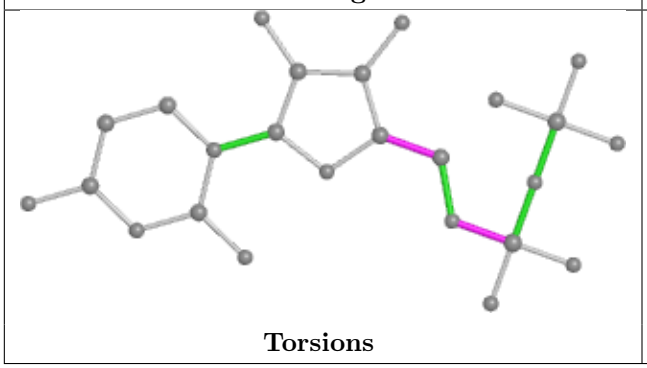
Ligand UDP C 500



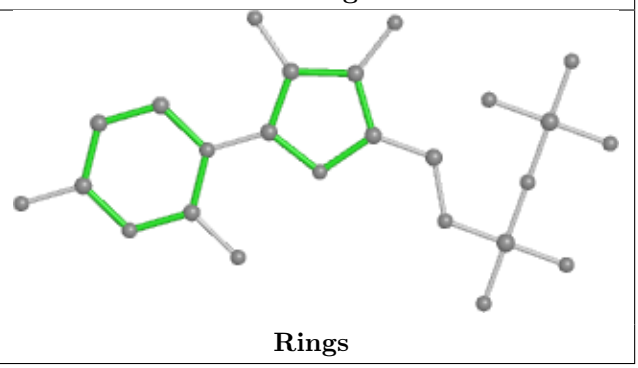
Bond lengths



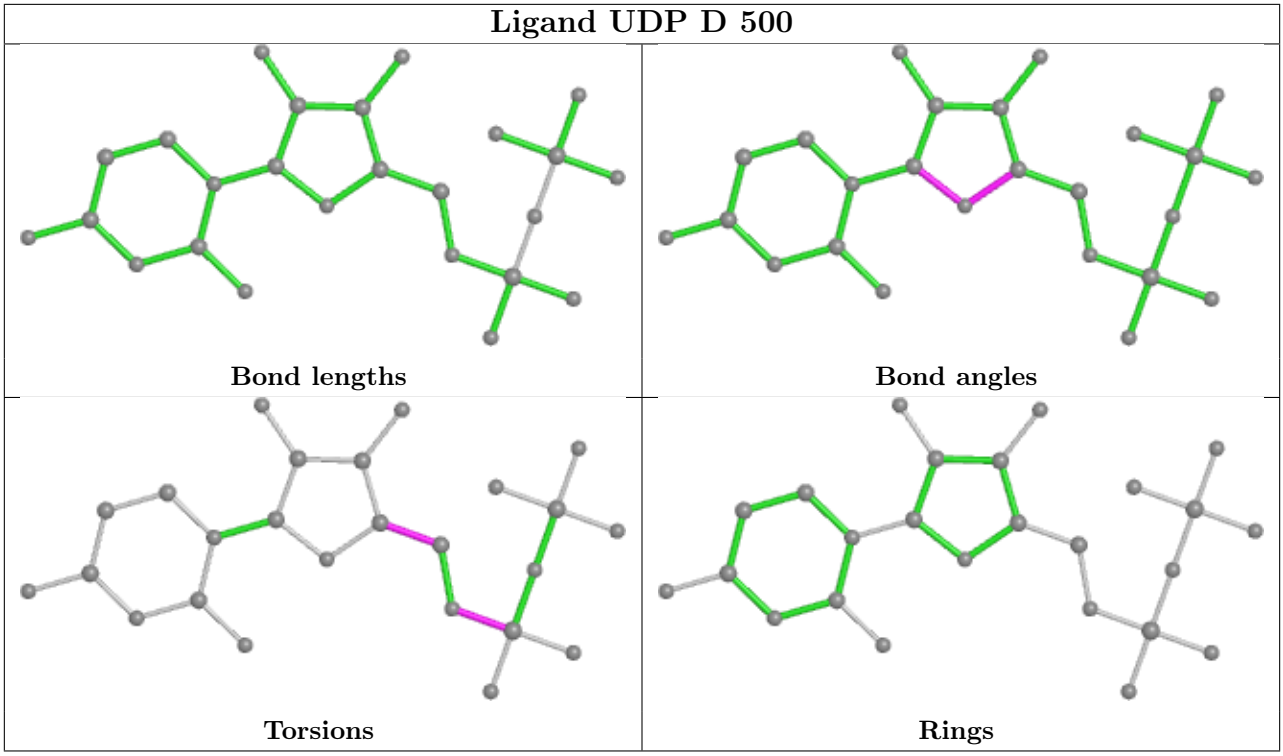
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	443/460 (96%)	-0.02	9 (2%) 65 36	25, 39, 64, 102	0
1	B	445/460 (96%)	0.22	21 (4%) 31 11	28, 48, 75, 116	0
1	C	439/460 (95%)	0.02	5 (1%) 80 56	28, 46, 66, 90	0
1	D	437/460 (95%)	0.30	23 (5%) 26 10	36, 56, 80, 110	0
1	E	443/460 (96%)	0.12	17 (3%) 40 16	30, 45, 68, 108	0
1	F	444/460 (96%)	0.09	14 (3%) 47 20	25, 42, 70, 126	0
All	All	2651/2760 (96%)	0.12	89 (3%) 45 19	25, 46, 73, 126	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	248	LYS	8.7
1	F	249	ALA	8.3
1	D	10	VAL	8.2
1	A	251	ASP	4.9
1	D	177	PRO	4.8
1	D	194	PHE	4.4
1	B	85	ARG	4.4
1	B	86	ASN	4.3
1	B	188	LEU	4.3
1	D	250	HIS	4.1
1	A	250	HIS	4.1
1	B	246	ALA	4.1
1	F	188	LEU	3.8
1	F	250	HIS	3.8
1	B	273	ALA	3.7
1	E	136	PRO	3.6
1	D	187	MET	3.6
1	E	247	LYS	3.5
1	E	250	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	162	ILE	3.5
1	E	246	ALA	3.4
1	A	245	ASP	3.4
1	A	248	LYS	3.3
1	A	175	LEU	3.2
1	A	249	ALA	3.2
1	C	251	ASP	3.1
1	F	252	LEU	3.1
1	E	316	ALA	3.1
1	E	164	VAL	3.1
1	D	175	LEU	3.1
1	D	170	ILE	3.0
1	F	162	ILE	3.0
1	B	10	VAL	3.0
1	E	450	HIS	3.0
1	B	289	SER	2.9
1	F	310	VAL	2.9
1	F	230	ASN	2.9
1	B	332	TRP	2.9
1	B	411	MET	2.9
1	D	168	ASP	2.8
1	E	252	LEU	2.8
1	E	249	ALA	2.8
1	E	248	LYS	2.7
1	B	414	VAL	2.6
1	E	313	MET	2.6
1	E	163	ASP	2.6
1	B	183	ILE	2.6
1	B	250	HIS	2.6
1	D	183	ILE	2.5
1	A	113	PRO	2.5
1	B	398	GLN	2.4
1	F	317	SER	2.4
1	C	450	HIS	2.4
1	D	64	THR	2.4
1	B	170	ILE	2.4
1	E	312	ASP	2.4
1	F	312	ASP	2.4
1	B	301	LYS	2.4
1	D	162	ILE	2.3
1	D	247	LYS	2.3
1	D	167	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	398	GLN	2.3
1	E	165	ALA	2.2
1	D	238	ILE	2.2
1	A	412	ILE	2.2
1	D	198	ILE	2.2
1	E	315	GLY	2.2
1	D	163	ASP	2.2
1	A	79	TYR	2.2
1	D	286	LEU	2.1
1	D	289	SER	2.1
1	B	437	VAL	2.1
1	F	231	GLY	2.1
1	B	319	VAL	2.1
1	B	66	HIS	2.1
1	B	418	GLU	2.1
1	D	159	LEU	2.1
1	D	251	ASP	2.1
1	F	168	ASP	2.1
1	C	313	MET	2.1
1	F	227	VAL	2.1
1	E	135	LEU	2.1
1	B	155	TYR	2.1
1	D	399	THR	2.1
1	B	187	MET	2.1
1	C	11	GLY	2.0
1	C	83	GLY	2.0
1	F	319	VAL	2.0
1	D	454	ASN	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,

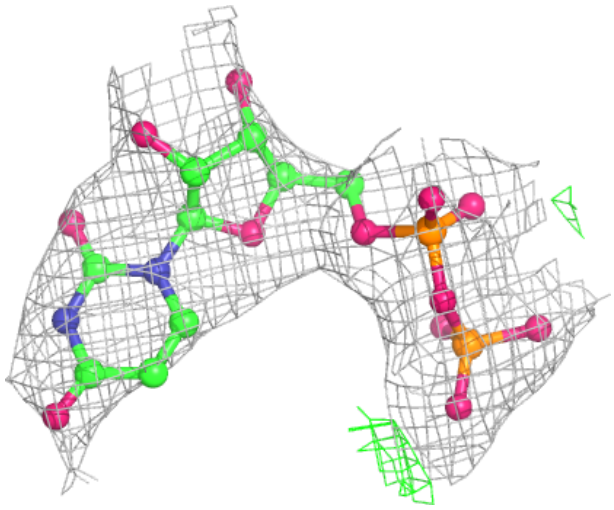
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

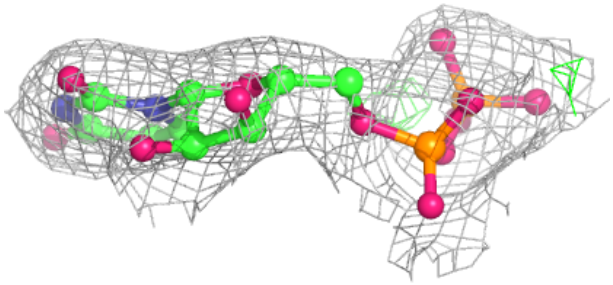
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	UDP	D	500	25/25	0.92	0.21	44,58,68,76	0
2	UDP	C	500	25/25	0.93	0.21	40,46,65,73	0
2	UDP	B	500	25/25	0.93	0.21	43,51,57,70	0
2	UDP	F	500	25/25	0.93	0.21	28,43,56,70	0
2	UDP	E	500	25/25	0.94	0.17	36,47,53,70	0
2	UDP	A	500	25/25	0.94	0.19	33,41,53,70	0

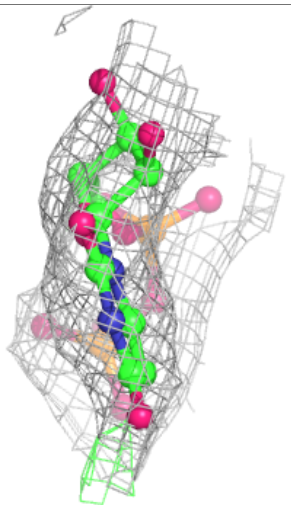
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UDP D 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

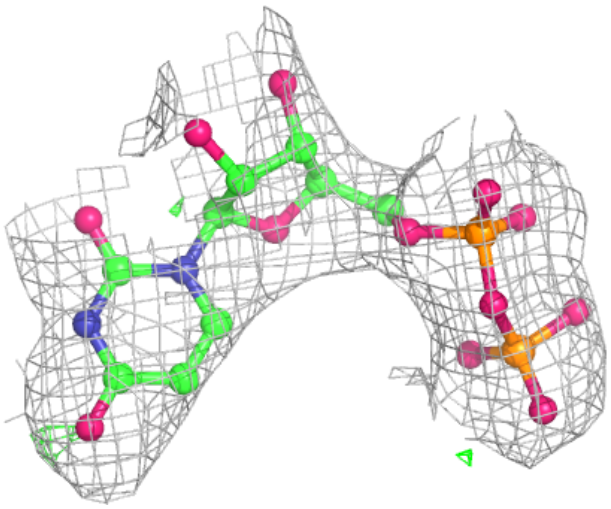


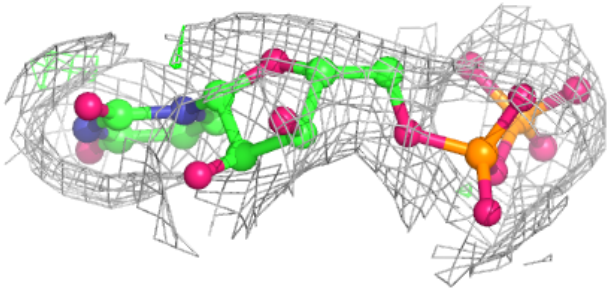


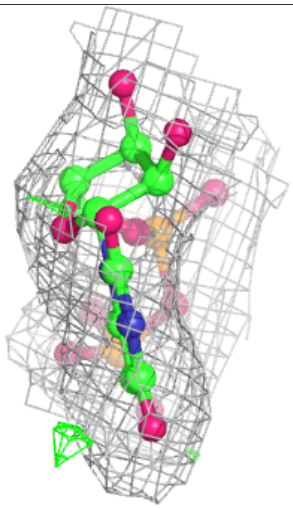


Electron density around UDP C 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

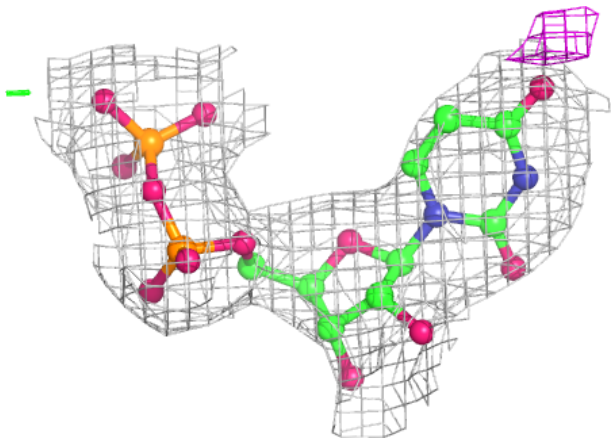


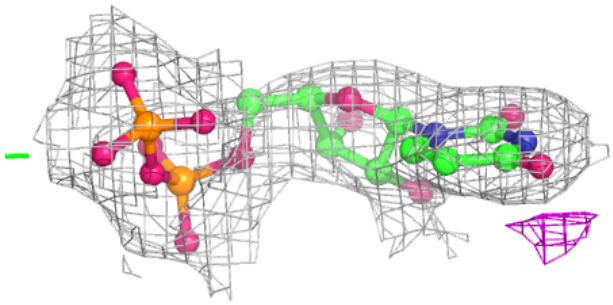


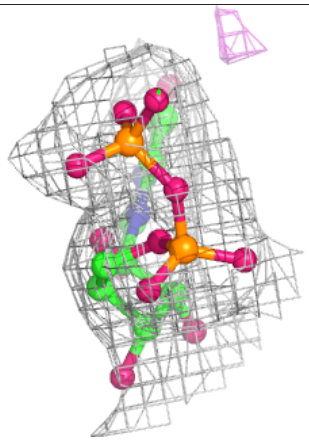


Electron density around UDP B 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

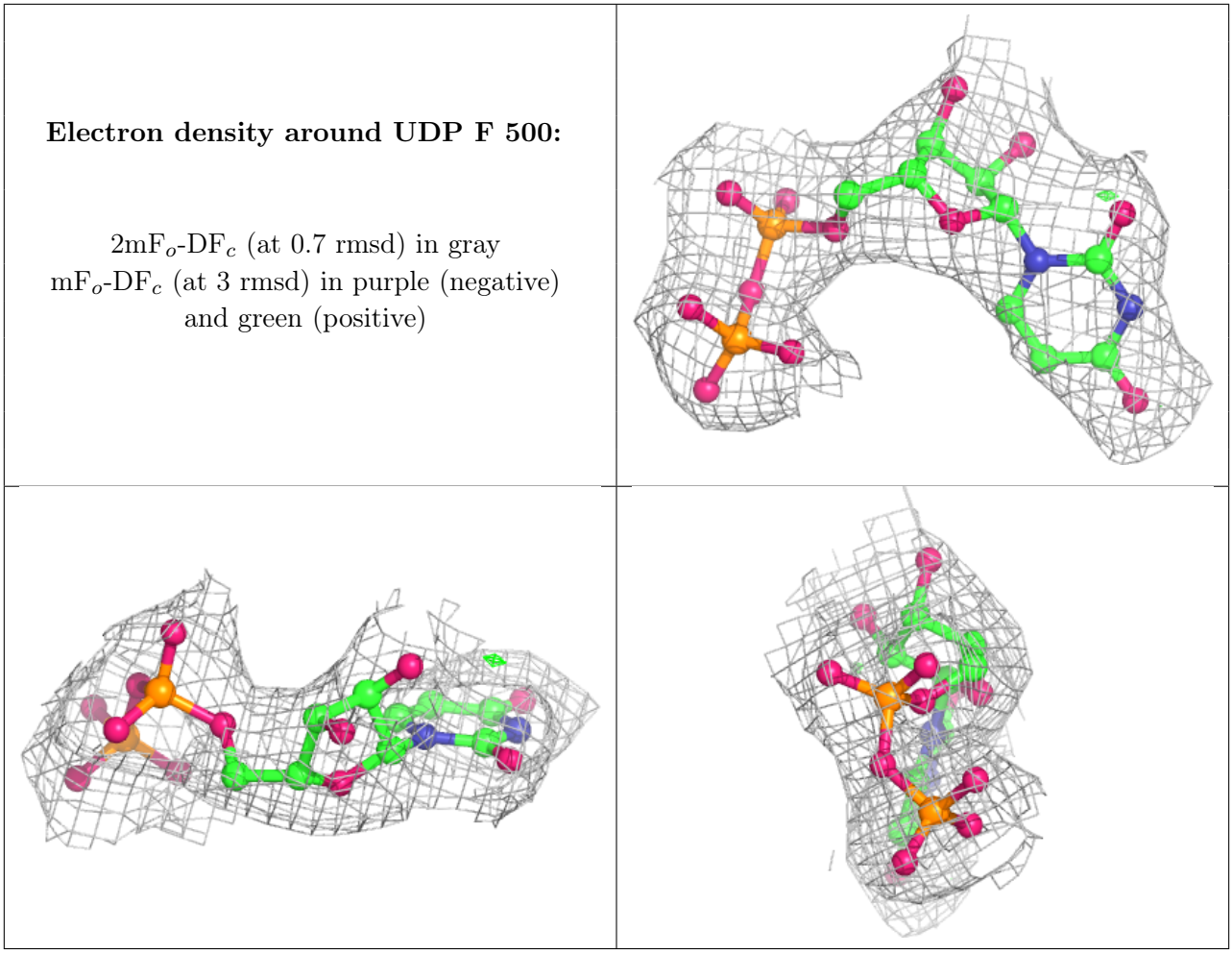






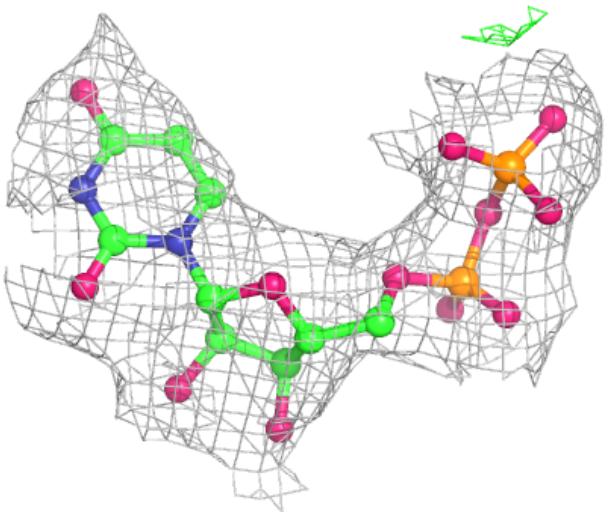
Electron density around UDP F 500:

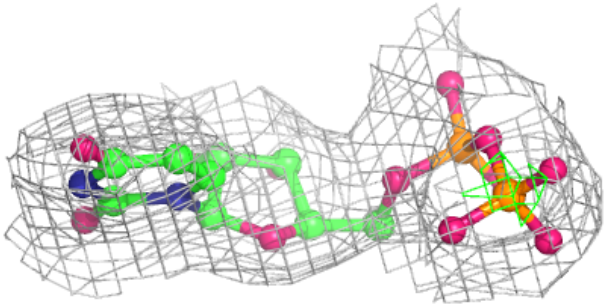
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

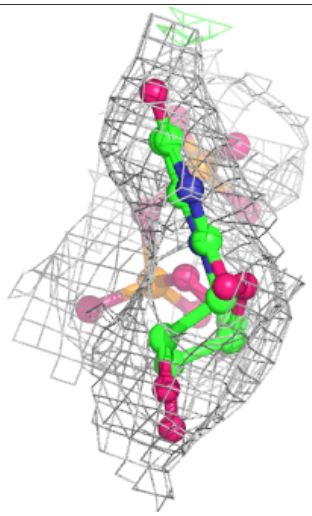


Electron density around UDP E 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

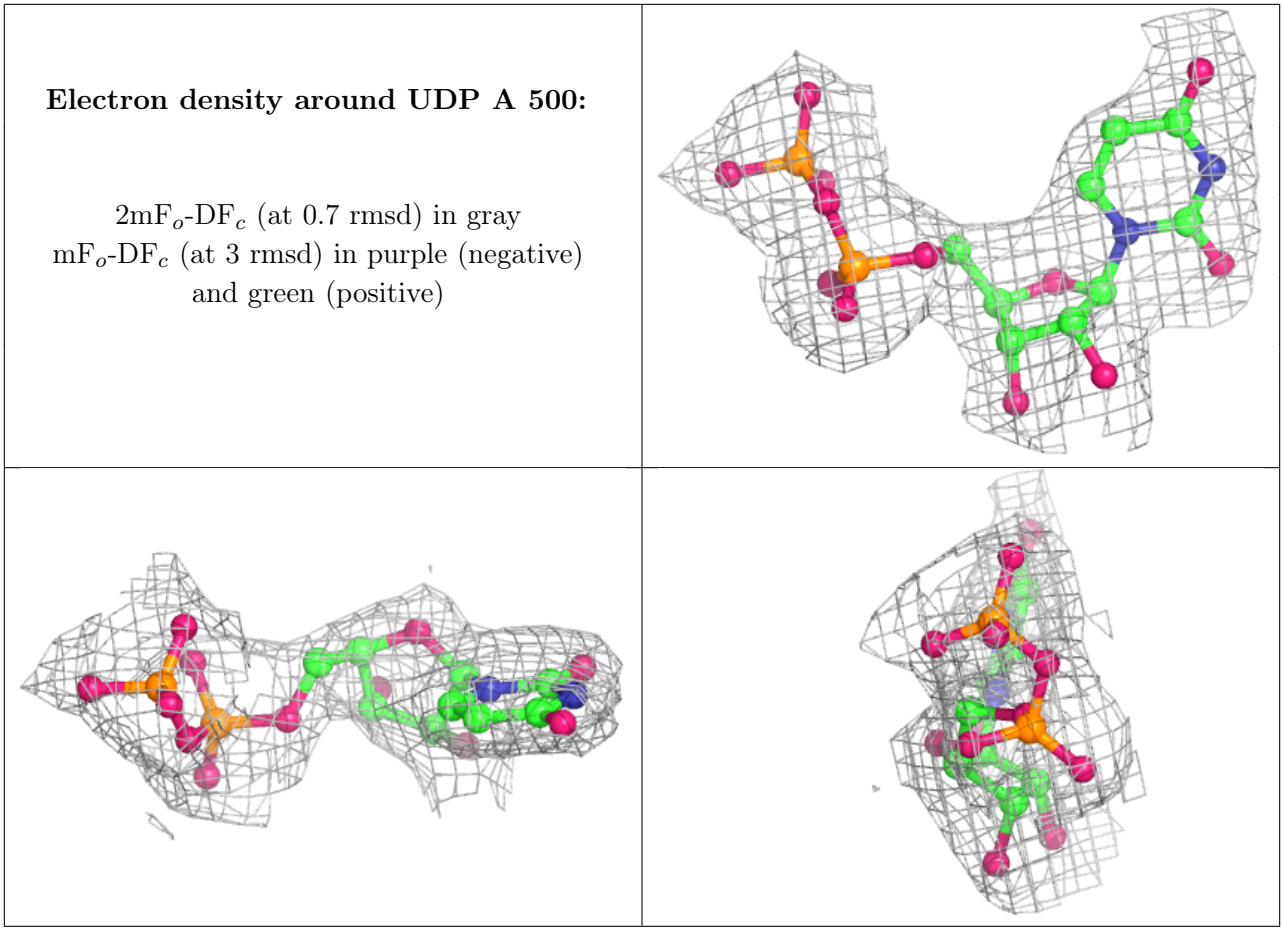






Electron density around UDP A 500:

$2mF_o$-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

There are no such residues in this entry.