Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 04:27 AM EST

PDB ID	:	3NDM
Title	:	Crystal structure of Rho-Associated Protein Kinase (ROCK1) with a potent isoquinolone derivative
Authors	:	Li, X.
Deposited on	:	2010-06-07
Resolution	:	3.30 Å(reported)

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

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

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

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

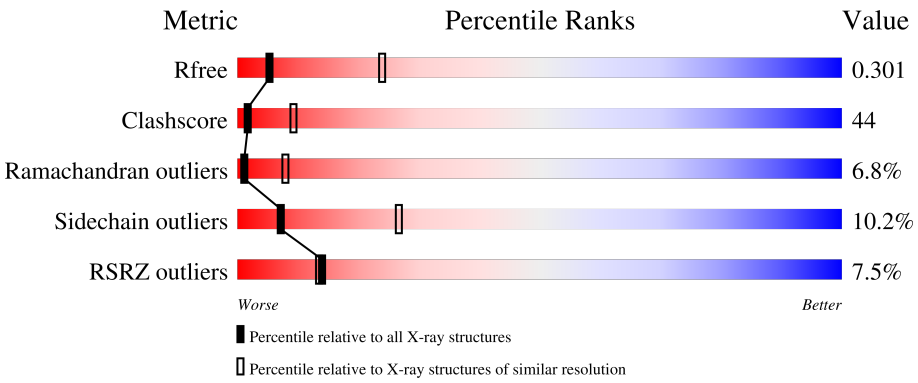
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	415	14% 32% 50% 9% • 8%
1	B	415	3% 32% 52% 11% • 5%
1	C	415	9% 31% 48% 9% • 11%
1	D	415	2% 33% 54% 8% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12746 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.

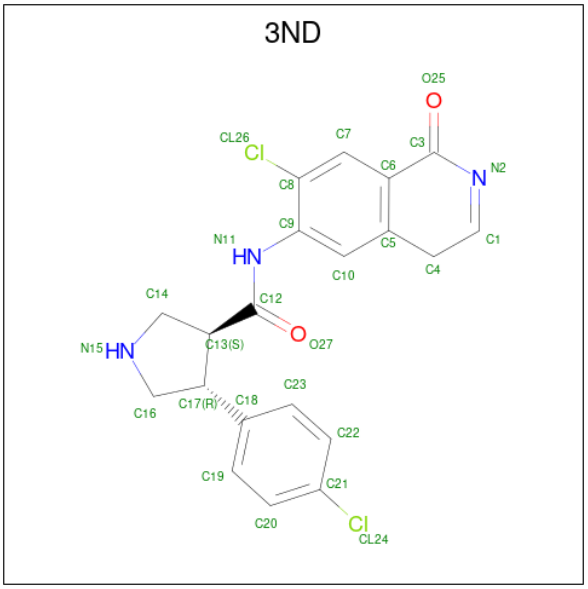
- Molecule 1 is a protein called Rho-Associated Protein Kinase (ROCK1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	383	3128	2005	517	584	22	0	0	0
1	B	396	3222	2059	532	610	21	0	0	0
1	C	371	3028	1944	493	569	22	0	0	0
1	D	396	3222	2059	532	610	21	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q13464
A	2	SER	-	expression tag	UNP Q13464
A	3	LEU	-	expression tag	UNP Q13464
A	4	HIS	-	expression tag	UNP Q13464
A	5	MET	-	expression tag	UNP Q13464
B	1	GLY	-	expression tag	UNP Q13464
B	2	SER	-	expression tag	UNP Q13464
B	3	LEU	-	expression tag	UNP Q13464
B	4	HIS	-	expression tag	UNP Q13464
B	5	MET	-	expression tag	UNP Q13464
C	1	GLY	-	expression tag	UNP Q13464
C	2	SER	-	expression tag	UNP Q13464
C	3	LEU	-	expression tag	UNP Q13464
C	4	HIS	-	expression tag	UNP Q13464
C	5	MET	-	expression tag	UNP Q13464
D	1	GLY	-	expression tag	UNP Q13464
D	2	SER	-	expression tag	UNP Q13464
D	3	LEU	-	expression tag	UNP Q13464
D	4	HIS	-	expression tag	UNP Q13464
D	5	MET	-	expression tag	UNP Q13464

- Molecule 2 is (3S,4R)-N-(7-chloro-1-oxo-1,4-dihydroisoquinolin-6-yl)-4-(4-chlorophenyl)pyrrolidine-3-carboxamide (three-letter code: 3ND) (formula: $C_{20}H_{17}Cl_2N_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		
2	C	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		
2	D	1	Total	C	Cl	N	O	0	0
			27	20	2	3	2		

- Molecule 3 is water.

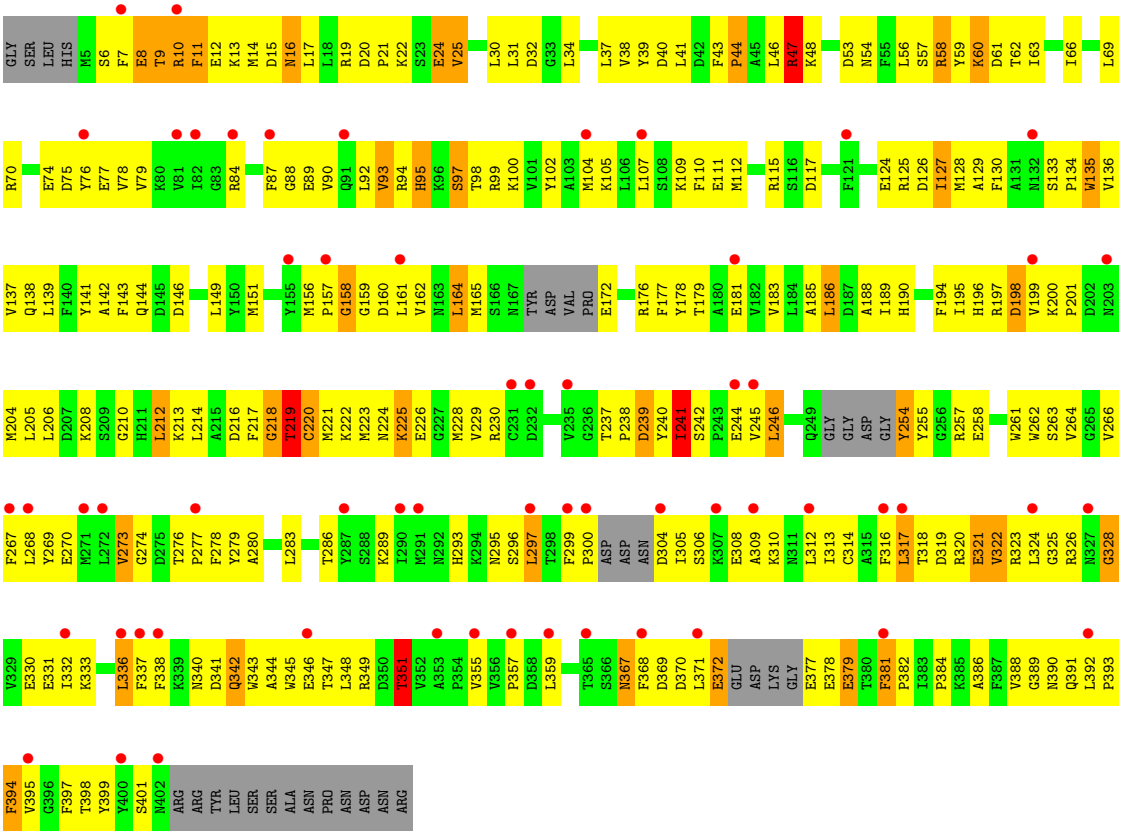
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	16	Total	O	0	0
			16	16		
3	C	15	Total	O	0	0
			15	15		
3	D	14	Total	O	0	0
			14	14		

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.

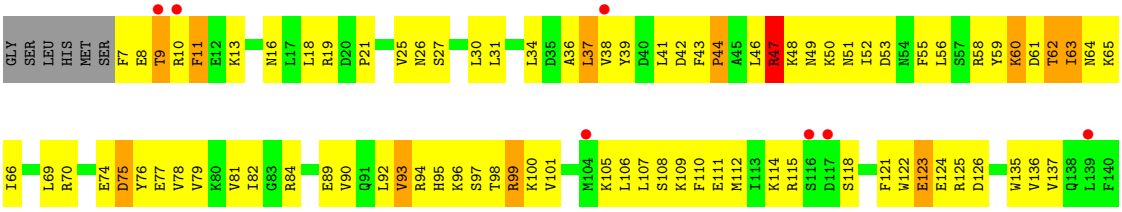
• Molecule 1: Rho-Associated Protein Kinase (ROCK1)

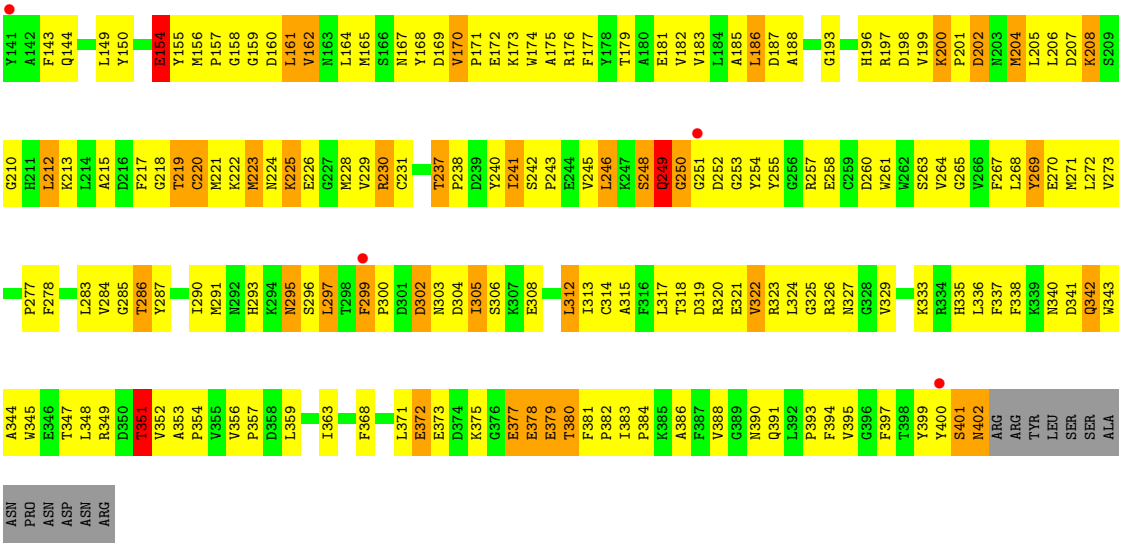
Chain A:



• Molecule 1: Rho-Associated Protein Kinase (ROCK1)

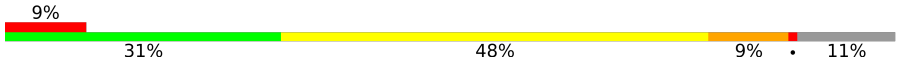
Chain B:

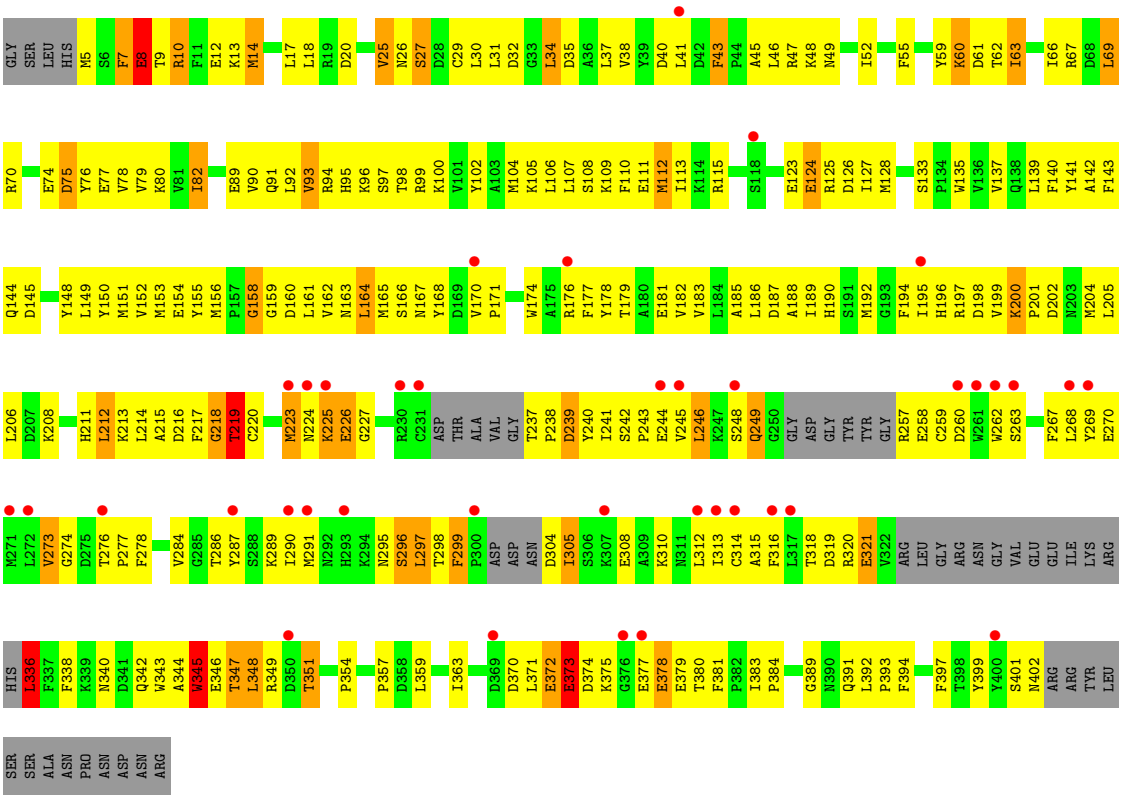




• Molecule 1: Rho-Associated Protein Kinase (ROCK1)

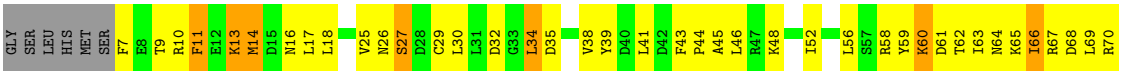
Chain C:

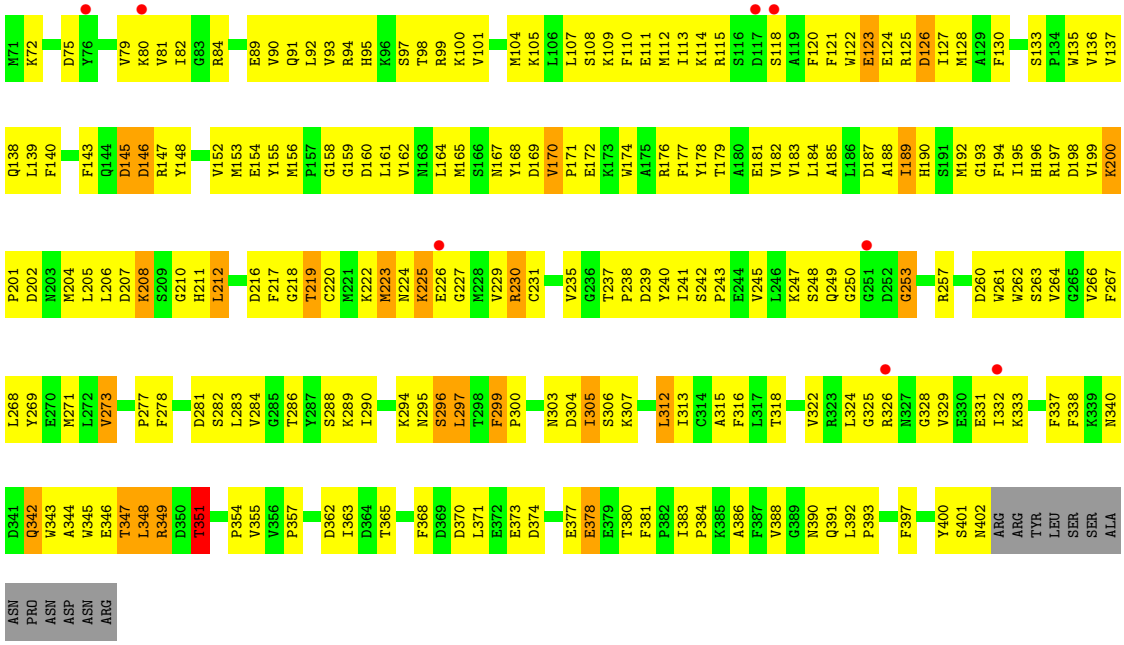




• Molecule 1: Rho-Associated Protein Kinase (ROCK1)

Chain D:




M71 K72 D75 Y76 V79 K80 V81 I82 G83 R84 E89 V90 Q91 L92 V93 R94 H95 K96 S97 T98 R99 K100 V101 M104 K105 L106 L107 S108 K109 F110 E111 M112 I113 K114 R115 S116 D117 S118 A119 F120 F121 W122 E123 E124 R125 D126 I127 M128 A129 F130 S133 P134 W135 V136 V137
Q138 L139 F140 F143 Q144 D145 D146 R147 Y148 V152 M153 E154 Y155 M156 P157 G158 G159 D160 L161 V162 N163 L164 M165 S166 N167 Y168 D169 V170 P171 E172 K173 W174 A175 R176 F177 Y178 T179 A180 E181 V182 V183 L184 A185 L186 D187 A188 I189 H190 S191 M192 G193 F194 I195 H196 R197 D198 V199 K200
P201 D202 N203 M204 L205 L206 D207 K208 S209 G210 H211 L212 D216 F217 G218 T219 C220 M221 K222 M223 N224 K225 E226 G227 M228 V229 R230 C231 V235 G236 T237 P238 D239 Y240 I241 S242 P243 E244 V245 L246 K247 S248 Q249 G250 G251 D252 G253 R257 D260 W261 W262 S263 V264 G265 V266 F267
L268 Y269 E270 M271 L272 V273 P277 F278 D281 S282 L283 V284 G285 T286 Y287 S288 K289 I290 K294 N295 S296 L297 T298 F299 P300 N303 D304 I305 S306 K307 L312 I313 C314 A315 F316 L317 T318 V322 R323 L324 G325 R326 N327 G328 V329 E330 E331 I332 K333 F337 F338 K339 N340
D341 Q342 W343 A344 W345 E346 T347 L348 R349 D350 T351 P354 V355 V356 P357 D362 I363 D364 T365 F368 D369 D370 L371 E372 E373 D374 E377 E378 E379 T380 F381 P382 I383 P384 K385 A386 F387 V388 G389 N390 Q391 L392 P393 F397 Y400 S401 N402 ARG ARG TYR LEU SER SER ALA
ASN PRO ASN ASP ASN ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.78Å 83.55Å 177.96Å 90.00° 119.95° 90.00°	Depositor
Resolution (Å)	42.53 – 3.30 44.72 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.53-3.30) 99.6 (44.72-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 3.32Å)	Xtriage
Refinement program	PHENIX 1.6.1_357	Depositor
R, R_{free}	0.241 , 0.310 0.232 , 0.301	Depositor DCC
R_{free} test set	1402 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å^2)	129.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 160.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12746	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3ND

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.39	0/3199	0.57	0/4314
1	B	0.55	0/3299	0.67	0/4457
1	C	0.49	0/3098	0.62	1/4180 (0.0%)
1	D	0.56	0/3299	0.67	0/4457
All	All	0.50	0/12895	0.63	1/17408 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	336	LEU	CA-CB-CG	-5.52	102.60	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3128	0	3048	269	0
1	B	3222	0	3120	282	0
1	C	3028	0	2943	304	0
1	D	3222	0	3120	292	0
2	B	27	0	17	7	0
2	C	27	0	17	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	27	0	17	5	0
3	A	20	0	0	5	0
3	B	16	0	0	3	0
3	C	15	0	0	5	0
3	D	14	0	0	1	0
All	All	12746	0	12282	1105	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 44.

All (1105) 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:A:66:ILE:HD11	1:B:25:VAL:HG21	1.35	1.08
1:A:399:TYR:CE2	1:A:401:SER:HB2	1.91	1.04
1:A:230:ARG:HH21	1:A:254:TYR:HB2	1.23	1.02
1:C:78:VAL:HA	1:C:93:VAL:HG12	1.42	1.00
1:B:38:VAL:HG21	1:B:63:ILE:HG13	1.41	0.99
1:D:161:LEU:HD23	1:D:267:PHE:HZ	1.27	0.99
1:D:34:LEU:HD12	1:D:63:ILE:HD11	1.48	0.96
1:B:159:GLY:HA2	1:B:368:PHE:HE2	1.31	0.96
1:B:149:LEU:HD22	1:B:397:PHE:CD2	2.01	0.95
1:A:381:PHE:HD2	1:A:382:PRO:HD2	1.27	0.95
1:B:159:GLY:HA2	1:B:368:PHE:CE2	2.03	0.94
1:C:141:TYR:HH	1:D:7:PHE:HZ	0.97	0.92
1:C:90:VAL:HG22	1:C:105:LYS:HB2	1.48	0.91
1:D:105:LYS:HE2	1:D:107:LEU:HD21	1.51	0.90
1:D:289:LYS:HD3	1:D:296:SER:OG	1.72	0.90
1:C:30:LEU:HB3	1:D:30:LEU:HB3	1.52	0.89
1:A:149:LEU:HD22	1:A:397:PHE:CD2	2.07	0.89
1:D:190:HIS:HB3	1:D:257:ARG:HH12	1.35	0.88
1:D:261:TRP:O	1:D:264:VAL:HB	1.73	0.88
1:B:225:LYS:HG3	1:C:379:GLU:HG2	1.56	0.88
1:A:78:VAL:HA	1:A:93:VAL:HG12	1.54	0.87
1:A:324:LEU:HG	1:A:332:ILE:HG12	1.57	0.86
1:C:187:ASP:HA	1:C:190:HIS:HD2	1.40	0.86
1:D:165:MET:HE1	1:D:271:MET:HA	1.58	0.86
1:A:87:PHE:HE1	1:A:115:ARG:HG3	1.40	0.85
1:C:139:LEU:HD11	1:C:141:TYR:O	1.76	0.85
1:B:181:GLU:HG2	1:B:348:LEU:HD21	1.57	0.85
1:D:190:HIS:HB3	1:D:257:ARG:NH1	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:PHE:CD2	1:A:382:PRO:HD2	2.13	0.84
1:D:181:GLU:HB3	1:D:212:LEU:HD22	1.59	0.84
1:B:41:LEU:HD22	1:B:52:ILE:HD13	1.59	0.84
1:B:399:TYR:CZ	1:B:401:SER:HB3	2.14	0.83
1:B:268:LEU:HD23	1:B:313:ILE:HG13	1.61	0.82
1:A:304:ASP:N	1:A:310:LYS:HZ1	1.78	0.82
1:C:38:VAL:HG21	1:C:63:ILE:HG13	1.60	0.82
1:C:225:LYS:H	1:C:225:LYS:HD3	1.43	0.82
1:A:196:HIS:HE1	1:A:216:ASP:O	1.62	0.82
1:C:43:PHE:CD1	1:C:384:PRO:HD2	2.13	0.82
1:D:159:GLY:HA2	1:D:368:PHE:HE2	1.43	0.82
1:B:174:TRP:CD1	1:B:354:PRO:HB3	2.15	0.81
1:A:144:GLN:HB3	1:A:149:LEU:HD23	1.62	0.81
1:C:8:GLU:CD	1:C:8:GLU:H	1.84	0.81
1:C:305:ILE:HD13	1:C:305:ILE:H	1.44	0.81
1:B:215:ALA:HB1	2:B:900:3ND:H4A	1.62	0.81
1:C:25:VAL:HG23	1:C:25:VAL:O	1.81	0.81
1:D:184:LEU:HD21	1:D:333:LYS:NZ	1.96	0.81
1:A:261:TRP:HE3	1:A:264:VAL:HG21	1.46	0.81
1:D:184:LEU:HD21	1:D:333:LYS:HZ1	1.46	0.81
1:C:158:GLY:HA3	1:C:206:LEU:O	1.81	0.80
1:A:241:ILE:HG12	1:A:246:LEU:HD13	1.62	0.80
1:B:258:GLU:HG3	1:B:320:ARG:HG3	1.63	0.80
1:B:399:TYR:OH	1:B:401:SER:HB3	1.81	0.80
1:C:171:PRO:HD2	1:C:174:TRP:CE3	2.17	0.80
1:D:159:GLY:HA2	1:D:368:PHE:CE2	2.16	0.80
1:A:179:THR:O	1:A:183:VAL:HG23	1.82	0.79
1:C:13:LYS:O	1:C:17:LEU:HD13	1.83	0.78
1:D:362:ASP:OD2	1:D:363:ILE:HG23	1.83	0.78
1:A:159:GLY:HA2	1:A:368:PHE:CZ	2.17	0.78
1:A:47:ARG:HH11	1:A:47:ARG:HG2	1.46	0.78
1:B:105:LYS:HE2	1:B:107:LEU:HD21	1.65	0.78
1:B:137:VAL:HG11	2:B:900:3ND:H1	1.64	0.78
1:B:246:LEU:HG	1:B:287:TYR:CE1	2.18	0.78
1:C:393:PRO:HA	1:D:58:ARG:HH22	1.48	0.78
1:C:393:PRO:HA	1:D:58:ARG:NH2	1.99	0.78
1:B:160:ASP:OD2	1:B:162:VAL:HG12	1.84	0.77
1:D:217:PHE:HB3	1:D:220:CYS:SG	2.24	0.77
1:C:200:LYS:HE3	1:C:202:ASP:HB2	1.66	0.77
1:B:177:PHE:CE2	1:B:354:PRO:HD2	2.20	0.76
1:A:392:LEU:HD22	1:B:55:PHE:CD1	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HD12	1:B:63:ILE:HD11	1.67	0.76
1:D:182:VAL:HG21	1:D:267:PHE:HE2	1.50	0.76
1:C:215:ALA:HB1	2:C:900:3ND:H4A	1.67	0.76
1:D:218:GLY:O	1:D:219:THR:HG23	1.86	0.76
1:B:246:LEU:HG	1:B:287:TYR:HE1	1.49	0.76
1:D:286:THR:O	1:D:290:ILE:HG13	1.86	0.76
1:D:200:LYS:HE2	1:D:202:ASP:HB2	1.68	0.76
1:A:25:VAL:HG23	1:A:25:VAL:O	1.84	0.76
1:A:268:LEU:HD22	1:A:312:LEU:HD13	1.66	0.76
1:C:179:THR:O	1:C:183:VAL:HG23	1.86	0.76
1:A:39:TYR:CE1	1:A:146:ASP:HB3	2.21	0.75
1:B:81:VAL:HG21	1:B:373:GLU:HA	1.66	0.75
1:B:181:GLU:HG2	1:B:348:LEU:CD2	2.16	0.75
1:C:170:VAL:HG13	1:C:174:TRP:HB2	1.66	0.75
1:A:136:VAL:HG12	1:A:137:VAL:O	1.87	0.75
1:B:158:GLY:HA3	1:B:206:LEU:HB2	1.66	0.75
1:A:262:TRP:HB2	1:A:323:ARG:NH1	2.01	0.74
1:B:322:VAL:HG22	1:B:322:VAL:O	1.86	0.74
1:C:41:LEU:HD22	1:C:52:ILE:HD13	1.67	0.74
1:D:204:MET:C	1:D:205:LEU:HD23	2.07	0.74
1:A:261:TRP:CE3	1:A:264:VAL:HG21	2.23	0.74
1:C:241:ILE:HD11	1:C:245:VAL:HG11	1.69	0.74
1:C:69:LEU:O	1:D:10:ARG:HD2	1.87	0.74
1:A:31:LEU:HG	1:B:30:LEU:HD13	1.69	0.74
1:B:245:VAL:O	1:B:248:SER:HB2	1.88	0.73
1:C:66:ILE:O	1:C:70:ARG:HG3	1.87	0.73
1:B:400:TYR:O	1:B:401:SER:HB2	1.88	0.73
1:D:212:LEU:O	1:D:212:LEU:HD23	1.87	0.73
1:D:261:TRP:HE3	1:D:264:VAL:HG21	1.54	0.73
1:A:78:VAL:HA	1:A:93:VAL:CG1	2.18	0.73
1:B:161:LEU:HD11	1:B:206:LEU:HD21	1.71	0.73
1:C:69:LEU:HD12	1:D:14:MET:SD	2.28	0.73
1:D:41:LEU:HD22	1:D:52:ILE:HD13	1.69	0.73
1:B:66:ILE:O	1:B:70:ARG:HG3	1.89	0.73
1:C:115:ARG:HG2	1:C:115:ARG:HH21	1.54	0.72
1:A:156:MET:SD	1:A:213:LYS:HD2	2.28	0.72
1:B:202:ASP:O	2:B:900:3ND:H14A	1.89	0.72
1:D:161:LEU:O	1:D:165:MET:HG3	1.88	0.72
1:C:29:CYS:O	1:C:32:ASP:HB2	1.89	0.72
1:C:299:PHE:CZ	1:C:310:LYS:HG2	2.24	0.72
1:C:90:VAL:HA	1:C:105:LYS:HA	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:GLU:OE2	1:C:213:LYS:HE3	1.90	0.72
1:D:161:LEU:HD23	1:D:267:PHE:CZ	2.18	0.71
1:B:92:LEU:HD13	1:B:155:TYR:CD1	2.25	0.71
1:D:177:PHE:CE2	1:D:354:PRO:HD2	2.26	0.71
1:D:392:LEU:N	1:D:393:PRO:HD2	2.05	0.71
1:D:111:GLU:HB3	1:D:115:ARG:NH2	2.05	0.71
1:B:84:ARG:NH2	1:B:372:GLU:HG3	2.05	0.71
1:B:246:LEU:C	1:B:248:SER:H	1.90	0.71
1:A:321:GLU:H	1:A:321:GLU:CD	1.94	0.71
1:B:212:LEU:HG	1:B:213:LYS:N	2.02	0.71
1:B:161:LEU:CD1	1:B:206:LEU:HD21	2.21	0.71
1:C:141:TYR:HB2	1:C:152:VAL:HB	1.73	0.70
1:D:241:ILE:HD11	1:D:245:VAL:HB	1.73	0.70
1:A:66:ILE:O	1:A:70:ARG:HG3	1.92	0.70
1:A:137:VAL:HG23	1:A:214:LEU:O	1.91	0.70
1:B:381:PHE:HD2	1:B:382:PRO:HD2	1.57	0.70
1:C:34:LEU:O	1:C:38:VAL:HG23	1.92	0.70
1:A:158:GLY:HA3	1:A:206:LEU:O	1.91	0.70
1:B:84:ARG:HH22	1:B:372:GLU:HG3	1.56	0.70
1:D:41:LEU:HD13	1:D:52:ILE:HG23	1.72	0.70
1:A:38:VAL:HG21	1:A:63:ILE:HG13	1.72	0.70
1:C:343:TRP:HB3	1:C:351:THR:HG21	1.73	0.70
1:A:69:LEU:HD22	1:B:10:ARG:HB3	1.72	0.70
1:B:149:LEU:HD22	1:B:397:PHE:HD2	1.55	0.70
1:C:199:VAL:O	1:C:200:LYS:HB3	1.91	0.70
1:D:189:ILE:HA	1:D:192:MET:CE	2.22	0.70
1:A:109:LYS:HB3	1:A:394:PHE:HE1	1.57	0.69
1:D:343:TRP:CD2	1:D:348:LEU:HD13	2.26	0.69
1:C:269:TYR:CZ	1:C:273:VAL:HG21	2.27	0.69
1:A:58:ARG:HH22	1:B:393:PRO:HA	1.55	0.69
1:D:333:LYS:HB3	1:D:345:TRP:NE1	2.07	0.69
1:C:18:LEU:HD22	1:D:27:SER:HB3	1.73	0.69
1:A:230:ARG:NH2	1:A:254:TYR:HB2	2.04	0.69
1:D:266:VAL:HG13	1:D:277:PRO:HD2	1.75	0.69
1:B:225:LYS:HG3	1:C:379:GLU:CG	2.23	0.69
1:C:123:GLU:O	1:C:127:ILE:HG13	1.92	0.69
1:D:237:THR:HG22	1:D:238:PRO:HD2	1.75	0.69
1:C:79:VAL:HG11	1:C:92:LEU:HD23	1.74	0.69
1:C:217:PHE:HB3	1:C:220:CYS:SG	2.33	0.69
1:D:104:MET:HG3	1:D:152:VAL:HG22	1.76	0.68
1:C:373:GLU:O	1:C:373:GLU:HG3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:O	1:A:93:VAL:HG13	1.93	0.68
1:D:84:ARG:HD3	1:D:89:GLU:HB3	1.74	0.68
1:A:226:GLU:O	1:A:228:MET:HG2	1.93	0.68
1:C:262:TRP:CZ2	1:C:290:ILE:HG23	2.28	0.68
1:A:14:MET:SD	1:B:69:LEU:HB2	2.34	0.67
1:C:76:TYR:HE2	1:C:152:VAL:HG21	1.59	0.67
1:A:229:VAL:O	1:A:254:TYR:HD1	1.76	0.67
1:B:108:SER:HB3	1:B:111:GLU:HB2	1.76	0.67
1:B:136:VAL:HG12	1:B:137:VAL:O	1.94	0.67
1:D:225:LYS:HD3	1:D:225:LYS:H	1.59	0.67
1:A:8:GLU:CD	1:A:8:GLU:H	1.97	0.67
1:D:109:LYS:NZ	1:D:145:ASP:O	2.23	0.67
1:A:308:GLU:HB3	1:A:337:PHE:HA	1.76	0.67
1:C:189:ILE:HA	1:C:192:MET:HE2	1.77	0.67
1:C:304:ASP:N	3:C:419:HOH:O	2.27	0.67
1:A:330:GLU:OE2	1:A:333:LYS:HD2	1.95	0.67
1:B:59:TYR:O	1:B:60:LYS:C	2.32	0.66
1:D:82:ILE:HB	1:D:368:PHE:HD1	1.60	0.66
1:C:345:TRP:HA	1:C:345:TRP:CE3	2.29	0.66
1:C:345:TRP:HA	1:C:345:TRP:HE3	1.60	0.66
1:D:123:GLU:O	1:D:127:ILE:HG13	1.96	0.66
1:A:115:ARG:HG2	1:A:115:ARG:HH21	1.60	0.66
1:A:176:ARG:HD3	1:A:338:PHE:HA	1.77	0.66
1:A:328:GLY:O	1:A:331:GLU:HG2	1.96	0.66
1:B:225:LYS:CG	1:C:379:GLU:HG2	2.25	0.66
1:D:35:ASP:OD1	1:D:67:ARG:NE	2.28	0.66
1:C:8:GLU:CD	1:C:8:GLU:N	2.49	0.66
1:B:179:THR:O	1:B:183:VAL:HG23	1.96	0.66
1:C:93:VAL:HB	3:C:423:HOH:O	1.95	0.66
1:C:343:TRP:CB	1:C:351:THR:HG21	2.25	0.66
1:C:9:THR:O	1:C:12:GLU:N	2.28	0.66
1:B:38:VAL:HG11	1:B:63:ILE:HG21	1.78	0.66
1:C:142:ALA:HB3	1:C:399:TYR:HB3	1.78	0.66
1:C:140:PHE:O	1:C:141:TYR:CD1	2.49	0.66
1:D:322:VAL:HB	1:D:326:ARG:HH21	1.60	0.66
1:A:6:SER:O	1:A:9:THR:HB	1.94	0.65
1:B:277:PRO:HG2	1:B:278:PHE:CD2	2.31	0.65
1:C:187:ASP:HA	1:C:190:HIS:CD2	2.26	0.65
1:C:199:VAL:HB	1:C:263:SER:HB3	1.78	0.65
1:D:238:PRO:O	1:D:241:ILE:HG22	1.96	0.65
1:D:392:LEU:N	1:D:393:PRO:CD	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:O	1:A:17:LEU:HD13	1.97	0.65
1:B:174:TRP:NE1	1:B:354:PRO:HB3	2.11	0.65
1:C:78:VAL:HA	1:C:93:VAL:CG1	2.21	0.65
1:C:205:LEU:O	1:C:212:LEU:HA	1.96	0.65
1:C:258:GLU:HG3	1:C:320:ARG:HG3	1.79	0.65
1:B:182:VAL:HG21	1:B:204:MET:HE2	1.79	0.65
1:C:204:MET:HB3	1:C:212:LEU:HD12	1.79	0.65
1:D:182:VAL:HG22	1:D:212:LEU:HD11	1.79	0.65
1:D:286:THR:HA	1:D:289:LYS:HB2	1.77	0.65
1:A:127:ILE:HD11	1:A:194:PHE:CD2	2.32	0.65
1:A:225:LYS:H	1:A:225:LYS:HD3	1.62	0.65
1:A:312:LEU:HD12	1:A:337:PHE:CD2	2.32	0.65
1:B:308:GLU:HB3	1:B:337:PHE:HA	1.79	0.65
1:D:158:GLY:HA3	1:D:206:LEU:O	1.97	0.65
1:D:277:PRO:C	1:D:278:PHE:CD2	2.70	0.64
1:A:186:LEU:HD22	1:A:190:HIS:NE2	2.12	0.64
1:B:55:PHE:HD2	1:B:56:LEU:HD23	1.62	0.64
1:C:170:VAL:HG22	1:C:174:TRP:HE3	1.61	0.64
1:D:38:VAL:HG21	1:D:63:ILE:HG13	1.79	0.64
1:D:82:ILE:HB	1:D:368:PHE:CD1	2.33	0.64
1:B:401:SER:HA	1:B:402:ASN:C	2.18	0.64
1:A:43:PHE:CD1	1:A:384:PRO:HD2	2.33	0.64
1:D:391:GLN:C	1:D:393:PRO:HD2	2.18	0.64
1:B:193:GLY:O	1:B:222:LYS:HG3	1.98	0.64
1:D:154:GLU:O	1:D:154:GLU:HG3	1.97	0.64
1:C:45:ALA:O	1:C:48:LYS:HD3	1.98	0.63
1:C:63:ILE:HD13	1:C:66:ILE:HD12	1.80	0.63
1:C:75:ASP:C	1:C:76:TYR:HD1	2.02	0.63
1:D:66:ILE:O	1:D:70:ARG:HG3	1.99	0.63
1:D:189:ILE:HA	1:D:192:MET:HE2	1.78	0.63
1:D:363:ILE:HG13	1:D:363:ILE:O	1.98	0.63
1:A:268:LEU:CD2	1:A:312:LEU:HD13	2.28	0.63
1:A:269:TYR:CE2	1:A:273:VAL:HG21	2.33	0.63
1:A:278:PHE:O	1:A:286:THR:HG23	1.98	0.63
1:A:224:ASN:HB2	1:A:225:LYS:HZ2	1.64	0.63
1:B:196:HIS:O	1:B:197:ARG:HB2	1.96	0.63
1:A:34:LEU:HD12	1:A:63:ILE:HD11	1.81	0.63
1:C:27:SER:HB3	1:D:18:LEU:HD22	1.79	0.63
1:D:262:TRP:HZ2	1:D:290:ILE:CG2	2.10	0.63
1:D:333:LYS:HE2	1:D:345:TRP:CE2	2.34	0.63
1:C:208:LYS:C	1:C:357:PRO:HG2	2.18	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLU:HG2	3:A:424:HOH:O	1.99	0.62
1:C:204:MET:C	1:C:205:LEU:HD23	2.19	0.62
1:D:165:MET:CE	1:D:271:MET:HA	2.28	0.62
1:A:47:ARG:HH11	1:A:47:ARG:CG	2.11	0.62
1:A:32:ASP:OD2	1:A:398:THR:HB	1.99	0.62
1:A:395:VAL:O	1:B:58:ARG:NH1	2.33	0.62
1:B:156:MET:HE1	1:B:207:ASP:HB3	1.81	0.62
1:C:76:TYR:CE2	1:C:152:VAL:HG21	2.33	0.62
1:D:262:TRP:HZ2	1:D:290:ILE:HG23	1.65	0.62
1:D:164:LEU:HD11	1:D:178:TYR:OH	1.98	0.62
1:D:46:LEU:HD21	1:D:386:ALA:HA	1.81	0.62
1:A:77:GLU:O	1:A:93:VAL:HG12	2.00	0.62
1:B:31:LEU:HB3	1:B:70:ARG:NH1	2.13	0.62
1:D:146:ASP:OD1	1:D:146:ASP:N	2.25	0.62
1:A:161:LEU:HD23	1:A:267:PHE:CZ	2.34	0.62
1:A:161:LEU:HD23	1:A:267:PHE:HZ	1.63	0.62
1:A:47:ARG:HG2	1:A:47:ARG:NH1	2.11	0.62
1:D:138:GLN:HG2	1:D:140:PHE:CE2	2.35	0.62
1:D:333:LYS:HE2	1:D:345:TRP:CD2	2.35	0.62
1:C:128:MET:CE	1:C:153:MET:SD	2.88	0.61
1:B:295:ASN:O	1:B:297:LEU:N	2.33	0.61
1:D:269:TYR:CE2	1:D:273:VAL:HG21	2.35	0.61
1:A:226:GLU:HG3	1:A:228:MET:HG3	1.82	0.61
1:B:381:PHE:CD2	1:B:382:PRO:HD2	2.36	0.61
1:C:92:LEU:O	1:C:93:VAL:HG13	2.01	0.61
1:A:224:ASN:HB2	1:A:225:LYS:NZ	2.14	0.61
1:B:167:ASN:O	1:B:168:TYR:CD1	2.53	0.61
1:C:41:LEU:HD22	1:C:52:ILE:CD1	2.29	0.61
1:D:307:LYS:NZ	1:D:307:LYS:HB3	2.15	0.61
1:B:165:MET:CE	1:B:271:MET:HA	2.30	0.61
1:C:224:ASN:OD1	1:C:226:GLU:HG2	2.01	0.61
1:D:59:TYR:O	1:D:60:LYS:C	2.38	0.61
1:D:211:HIS:HB3	1:D:349:ARG:HH21	1.64	0.61
1:B:230:ARG:HB3	1:B:230:ARG:NH1	2.16	0.61
1:C:94:ARG:N	3:C:423:HOH:O	2.33	0.61
1:C:76:TYR:HE2	1:C:152:VAL:CG2	2.14	0.60
1:C:108:SER:O	1:C:112:MET:HB2	2.01	0.60
1:C:111:GLU:OE1	1:C:115:ARG:NH2	2.30	0.60
1:C:297:LEU:HD21	1:C:314:CYS:SG	2.40	0.60
1:A:330:GLU:OE2	1:A:330:GLU:HA	2.01	0.60
1:C:244:GLU:CD	1:C:320:ARG:HB2	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLU:OE1	1:B:308:GLU:HA	2.01	0.60
1:B:144:GLN:NE2	1:B:394:PHE:O	2.31	0.60
1:B:321:GLU:O	1:B:326:ARG:CZ	2.50	0.60
1:D:174:TRP:CD1	1:D:354:PRO:HB3	2.37	0.60
1:C:113:ILE:HG13	1:C:381:PHE:HZ	1.65	0.60
1:C:278:PHE:O	1:C:286:THR:HG23	2.01	0.60
1:D:81:VAL:HG21	1:D:373:GLU:HA	1.83	0.60
1:D:108:SER:O	1:D:112:MET:HE2	2.01	0.60
1:A:196:HIS:CE1	1:A:216:ASP:O	2.51	0.60
1:B:165:MET:HE2	1:B:271:MET:HA	1.84	0.60
1:A:135:TRP:HA	1:A:135:TRP:CE3	2.37	0.60
1:A:237:THR:HG23	1:A:238:PRO:HD2	1.83	0.60
1:B:109:LYS:HE2	1:B:394:PHE:CD1	2.37	0.60
1:B:110:PHE:CG	1:B:379:GLU:HB3	2.37	0.60
1:C:156:MET:HG3	1:C:205:LEU:HD12	1.84	0.60
1:A:135:TRP:CH2	1:A:181:GLU:HG2	2.36	0.59
1:B:265:GLY:HA3	1:B:317:LEU:CD1	2.32	0.59
1:D:181:GLU:HB3	1:D:212:LEU:CD2	2.31	0.59
1:B:164:LEU:HD23	1:B:164:LEU:O	2.01	0.59
1:C:40:ASP:OD2	1:C:391:GLN:HB2	2.02	0.59
1:C:135:TRP:CH2	1:C:181:GLU:HG2	2.37	0.59
1:B:225:LYS:H	1:B:225:LYS:HD3	1.67	0.59
1:C:223:MET:HE3	1:C:227:GLY:HA2	1.83	0.59
1:D:243:PRO:HD3	1:D:262:TRP:CE2	2.37	0.59
1:B:7:PHE:C	1:B:9:THR:H	2.06	0.59
1:B:224:ASN:HD21	1:B:228:MET:HB2	1.68	0.59
1:C:299:PHE:CE2	1:C:305:ILE:HD11	2.37	0.59
1:C:66:ILE:HD11	1:D:25:VAL:HG11	1.84	0.59
1:B:114:LYS:HE2	1:B:115:ARG:NH1	2.18	0.59
1:A:14:MET:HE1	1:B:69:LEU:HD12	1.84	0.59
1:B:230:ARG:HD2	1:C:380:THR:HG21	1.85	0.59
1:C:262:TRP:HZ2	1:C:290:ILE:HG23	1.68	0.59
1:D:160:ASP:OD2	1:D:162:VAL:HG12	2.02	0.59
1:A:11:PHE:O	1:A:15:ASP:OD2	2.21	0.59
1:A:208:LYS:C	1:A:357:PRO:HG2	2.23	0.59
1:B:204:MET:HB3	1:B:212:LEU:HD12	1.85	0.58
1:C:139:LEU:HD12	1:C:152:VAL:O	2.03	0.58
1:C:392:LEU:N	1:C:393:PRO:CD	2.66	0.58
1:D:44:PRO:HD3	3:D:417:HOH:O	2.03	0.58
1:A:308:GLU:OE1	1:A:336:LEU:HB3	2.02	0.58
1:C:249:GLN:CD	1:C:249:GLN:H	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:MET:HE1	1:C:270:GLU:HG2	1.85	0.58
1:C:176:ARG:HD3	1:C:340:ASN:HD22	1.69	0.58
1:D:277:PRO:O	1:D:278:PHE:CD2	2.56	0.58
1:A:321:GLU:CD	1:A:321:GLU:N	2.56	0.58
1:A:14:MET:CE	1:B:69:LEU:HD12	2.33	0.58
1:D:179:THR:O	1:D:183:VAL:HG23	2.03	0.58
1:B:379:GLU:OE1	1:B:379:GLU:HA	2.04	0.58
1:C:161:LEU:HD11	1:C:206:LEU:HD21	1.86	0.58
1:B:42:ASP:OD1	1:B:42:ASP:O	2.22	0.58
1:D:136:VAL:HG12	1:D:137:VAL:O	2.04	0.58
1:D:324:LEU:HG	1:D:332:ILE:HG12	1.86	0.57
1:B:41:LEU:HD22	1:B:52:ILE:CD1	2.33	0.57
1:A:190:HIS:CE1	1:A:257:ARG:HB2	2.39	0.57
1:B:175:ALA:CB	1:B:272:LEU:HD21	2.34	0.57
1:C:164:LEU:O	1:C:168:TYR:HB2	2.04	0.57
1:B:246:LEU:C	1:B:248:SER:N	2.58	0.57
1:C:242:SER:HB3	1:C:262:TRP:CG	2.40	0.57
1:D:110:PHE:C	1:D:110:PHE:CD2	2.77	0.57
1:D:195:ILE:HD12	1:D:229:VAL:CG1	2.34	0.57
1:B:241:ILE:HG13	1:B:242:SER:N	2.18	0.57
1:D:211:HIS:HB3	1:D:349:ARG:NH2	2.19	0.57
1:A:95:HIS:CE1	1:A:97:SER:HB3	2.40	0.57
1:A:149:LEU:HB3	1:A:397:PHE:CE2	2.40	0.57
1:C:59:TYR:O	1:C:60:LYS:C	2.43	0.57
1:D:238:PRO:HG3	1:D:283:LEU:HD13	1.86	0.57
1:B:84:ARG:HA	1:B:89:GLU:HA	1.86	0.57
1:B:223:MET:HA	1:B:229:VAL:HG12	1.86	0.57
1:C:344:ALA:O	1:C:345:TRP:C	2.43	0.57
1:D:137:VAL:HG11	2:D:900:3ND:H1	1.86	0.57
1:A:59:TYR:O	1:A:60:LYS:C	2.43	0.57
1:C:174:TRP:O	1:C:177:PHE:HB3	2.05	0.57
1:D:225:LYS:H	1:D:225:LYS:CD	2.15	0.56
1:D:295:ASN:O	1:D:297:LEU:N	2.38	0.56
1:A:196:HIS:HD2	1:A:198:ASP:N	2.04	0.56
1:A:269:TYR:CZ	1:A:273:VAL:HG21	2.41	0.56
1:B:43:PHE:CD1	1:B:384:PRO:HD2	2.40	0.56
1:C:156:MET:HE1	1:C:213:LYS:HE3	1.88	0.56
1:A:205:LEU:O	1:A:212:LEU:HA	2.05	0.56
1:A:399:TYR:CE2	1:A:401:SER:CB	2.79	0.56
1:B:59:TYR:O	1:B:61:ASP:N	2.38	0.56
1:B:77:GLU:HB2	1:B:96:LYS:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LEU:HD13	1:D:155:TYR:CD1	2.40	0.56
1:C:375:LYS:HB3	1:C:377:GLU:HG3	1.87	0.56
1:C:59:TYR:O	1:C:61:ASP:N	2.39	0.56
1:C:242:SER:HB2	1:C:243:PRO:CD	2.36	0.56
1:B:186:LEU:HD21	1:B:260:ASP:HB3	1.86	0.56
1:A:58:ARG:NH2	1:B:393:PRO:HA	2.21	0.56
1:C:25:VAL:O	1:C:25:VAL:CG2	2.53	0.56
1:D:242:SER:HB2	1:D:243:PRO:HD2	1.86	0.56
1:A:78:VAL:CA	1:A:93:VAL:HG12	2.32	0.56
1:D:289:LYS:HD3	1:D:296:SER:HG	1.70	0.56
1:A:229:VAL:O	1:A:254:TYR:HA	2.06	0.56
1:C:9:THR:O	1:C:10:ARG:C	2.45	0.55
1:D:114:LYS:HG2	1:D:115:ARG:HD3	1.87	0.55
1:D:199:VAL:O	1:D:200:LYS:HB3	2.06	0.55
1:D:125:ARG:NE	1:D:397:PHE:O	2.40	0.55
1:A:133:SER:OG	1:A:135:TRP:HB2	2.06	0.55
1:A:37:LEU:HD21	1:B:37:LEU:HD21	1.88	0.55
1:B:357:PRO:HB3	1:B:359:LEU:HD21	1.87	0.55
1:C:43:PHE:HE1	1:C:384:PRO:HG2	1.70	0.55
1:C:108:SER:O	1:C:112:MET:HE2	2.06	0.55
1:A:6:SER:HB3	1:A:9:THR:OG1	2.06	0.55
1:A:381:PHE:HD2	1:A:382:PRO:CD	2.10	0.55
1:B:55:PHE:CD2	1:B:56:LEU:HD23	2.42	0.55
1:D:257:ARG:CZ	1:D:257:ARG:HB3	2.36	0.55
1:D:305:ILE:N	1:D:305:ILE:HD13	2.21	0.55
1:B:261:TRP:O	1:B:264:VAL:HB	2.06	0.55
1:B:313:ILE:HG22	1:B:314:CYS:N	2.21	0.55
1:D:268:LEU:HD23	1:D:313:ILE:HG12	1.89	0.55
1:D:333:LYS:HB3	1:D:345:TRP:CE2	2.41	0.55
1:D:127:ILE:HD11	1:D:194:PHE:CD2	2.42	0.55
1:A:181:GLU:HB3	1:A:212:LEU:HD22	1.88	0.55
1:A:135:TRP:HH2	1:A:181:GLU:HG2	1.71	0.55
1:B:13:LYS:HA	1:B:16:ASN:ND2	2.22	0.55
1:D:237:THR:CG2	1:D:238:PRO:HD2	2.36	0.55
1:A:162:VAL:HB	1:A:201:PRO:HB2	1.89	0.54
1:D:224:ASN:HB2	1:D:225:LYS:NZ	2.22	0.54
1:B:124:GLU:HG3	1:B:217:PHE:HB2	1.89	0.54
1:C:239:ASP:HB3	1:C:276:THR:HG21	1.88	0.54
1:D:184:LEU:CD2	1:D:333:LYS:NZ	2.68	0.54
1:A:157:PRO:HB2	1:A:359:LEU:HD21	1.88	0.54
1:D:299:PHE:HD2	1:D:300:PRO:CD	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ASN:HA	1:C:166:SER:OG	2.07	0.54
1:C:208:LYS:O	1:C:357:PRO:HG2	2.06	0.54
1:C:346:GLU:CD	1:C:346:GLU:H	2.10	0.54
1:A:61:ASP:CG	1:C:372:GLU:HG2	2.28	0.54
1:C:98:THR:O	1:C:100:LYS:N	2.40	0.54
1:C:389:GLY:HA3	1:C:392:LEU:HD12	1.88	0.54
1:D:98:THR:O	1:D:100:LYS:N	2.40	0.54
1:A:210:GLY:HA3	1:A:355:VAL:O	2.07	0.54
1:A:229:VAL:N	1:A:255:TYR:O	2.38	0.54
1:C:242:SER:HB3	1:C:262:TRP:CD1	2.42	0.54
1:D:56:LEU:O	1:D:60:LYS:HB2	2.07	0.54
1:A:70:ARG:NH1	3:A:416:HOH:O	2.26	0.54
1:A:381:PHE:CZ	1:A:390:ASN:HB3	2.42	0.54
1:B:377:GLU:HG3	1:B:378:GLU:N	2.23	0.54
1:C:107:LEU:HB2	1:C:149:LEU:HB2	1.88	0.54
1:C:399:TYR:CZ	1:C:401:SER:HB3	2.43	0.54
1:A:217:PHE:HB3	1:A:220:CYS:SG	2.48	0.54
1:A:242:SER:OG	1:A:245:VAL:HG23	2.07	0.54
1:A:262:TRP:O	1:A:266:VAL:HG23	2.06	0.54
1:D:225:LYS:HD3	1:D:225:LYS:N	2.22	0.54
1:A:46:LEU:O	1:A:48:LYS:N	2.40	0.54
1:A:186:LEU:CD2	1:A:190:HIS:NE2	2.71	0.54
1:A:306:SER:O	1:A:310:LYS:HG3	2.08	0.54
1:C:161:LEU:HD23	1:C:267:PHE:HZ	1.73	0.54
1:A:204:MET:HB3	1:A:212:LEU:HD12	1.90	0.54
1:D:182:VAL:CG2	1:D:212:LEU:HD11	2.37	0.54
1:D:218:GLY:O	1:D:219:THR:CG2	2.56	0.54
1:B:286:THR:O	1:B:290:ILE:HG13	2.08	0.53
1:D:59:TYR:O	1:D:61:ASP:N	2.41	0.53
1:A:110:PHE:CZ	1:A:379:GLU:HB3	2.42	0.53
1:A:377:GLU:N	1:A:378:GLU:HA	2.21	0.53
1:C:176:ARG:CD	1:C:340:ASN:HD22	2.21	0.53
1:D:65:LYS:O	1:D:68:ASP:HB2	2.08	0.53
1:A:160:ASP:HA	1:A:204:MET:O	2.07	0.53
1:D:135:TRP:HZ3	1:D:181:GLU:OE2	1.92	0.53
1:D:346:GLU:CD	1:D:346:GLU:H	2.11	0.53
1:A:54:ASN:HA	3:A:422:HOH:O	2.07	0.53
1:B:187:ASP:OD1	1:B:329:VAL:HG11	2.09	0.53
1:B:314:CYS:O	1:B:318:THR:CG2	2.57	0.53
1:C:212:LEU:HD23	1:C:212:LEU:O	2.08	0.53
1:D:196:HIS:O	1:D:197:ARG:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:VAL:HB	1:A:92:LEU:O	2.09	0.53
1:B:106:LEU:HG	1:B:150:TYR:CD2	2.44	0.53
1:B:161:LEU:HD23	1:B:267:PHE:HZ	1.72	0.53
1:C:150:TYR:CD1	1:C:150:TYR:N	2.77	0.53
1:C:295:ASN:O	1:C:297:LEU:N	2.42	0.53
1:D:147:ARG:HB2	1:D:148:TYR:CD1	2.44	0.53
1:D:230:ARG:NH2	1:D:253:GLY:O	2.42	0.53
1:A:59:TYR:O	1:A:61:ASP:N	2.42	0.53
1:A:244:GLU:CG	1:A:320:ARG:HD3	2.38	0.53
1:C:109:LYS:HE2	1:C:394:PHE:CD1	2.43	0.53
1:A:367:ASN:OD1	1:A:367:ASN:N	2.41	0.53
1:C:30:LEU:HB3	1:D:30:LEU:CB	2.33	0.53
1:C:43:PHE:CE1	1:C:384:PRO:HD2	2.44	0.53
1:D:400:TYR:O	1:D:401:SER:HB2	2.08	0.53
1:A:61:ASP:OD2	1:C:372:GLU:HG2	2.08	0.53
1:B:173:LYS:HG2	1:B:176:ARG:HH12	1.74	0.53
1:C:5:MET:O	1:C:5:MET:CG	2.57	0.53
1:C:128:MET:HE1	1:C:153:MET:SD	2.49	0.53
1:C:160:ASP:OD2	1:C:162:VAL:HG12	2.08	0.53
1:C:161:LEU:CD1	1:C:206:LEU:HD21	2.38	0.53
1:A:135:TRP:HA	1:A:135:TRP:HE3	1.73	0.52
1:B:186:LEU:CD2	1:B:260:ASP:HB3	2.40	0.52
1:C:269:TYR:CE1	1:C:273:VAL:HG21	2.43	0.52
1:D:182:VAL:HG21	1:D:267:PHE:CE2	2.37	0.52
1:D:231:CYS:O	1:D:253:GLY:HA3	2.09	0.52
1:D:46:LEU:HD21	1:D:386:ALA:CA	2.38	0.52
1:A:46:LEU:C	1:A:48:LYS:H	2.12	0.52
1:B:46:LEU:CD2	1:B:386:ALA:HA	2.39	0.52
1:B:382:PRO:O	1:B:384:PRO:HD3	2.09	0.52
1:D:177:PHE:CD2	1:D:354:PRO:HG2	2.44	0.52
1:D:189:ILE:HA	1:D:192:MET:HE3	1.92	0.52
1:A:177:PHE:CD1	1:A:348:LEU:HD11	2.45	0.52
1:C:189:ILE:HG23	1:C:194:PHE:HB2	1.91	0.52
1:D:69:LEU:HD23	1:D:69:LEU:N	2.23	0.52
1:D:89:GLU:HA	2:D:900:3ND:H22	1.91	0.52
1:B:225:LYS:H	1:B:225:LYS:CD	2.16	0.52
1:B:340:ASN:HB2	1:B:342:GLN:OE1	2.10	0.52
1:C:289:LYS:HD3	1:C:296:SER:OG	2.10	0.52
1:C:299:PHE:HE2	1:C:305:ILE:HD11	1.74	0.52
1:D:177:PHE:CE2	1:D:354:PRO:CD	2.92	0.52
1:A:344:ALA:O	1:A:345:TRP:C	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLU:HA	2:C:900:3ND:H22	1.92	0.52
1:C:94:ARG:C	3:C:423:HOH:O	2.47	0.52
1:A:110:PHE:C	1:A:110:PHE:CD2	2.83	0.52
1:A:262:TRP:CD1	1:A:262:TRP:C	2.82	0.52
1:A:343:TRP:HB3	1:A:351:THR:HG21	1.92	0.52
1:C:338:PHE:CD1	1:C:345:TRP:CH2	2.98	0.52
1:B:308:GLU:OE1	1:B:336:LEU:HB2	2.10	0.52
1:D:195:ILE:HD12	1:D:229:VAL:HG11	1.92	0.52
1:B:155:TYR:CD2	1:B:157:PRO:HD3	2.45	0.51
1:C:79:VAL:HG23	1:C:93:VAL:HA	1.91	0.51
1:C:199:VAL:HB	1:C:263:SER:CB	2.40	0.51
1:D:299:PHE:HD2	1:D:300:PRO:HD2	1.75	0.51
1:B:82:ILE:HG21	1:B:92:LEU:HB2	1.91	0.51
1:B:277:PRO:HG2	1:B:278:PHE:CE2	2.45	0.51
1:B:308:GLU:HG3	1:B:336:LEU:HB3	1.91	0.51
1:D:94:ARG:HA	1:D:100:LYS:O	2.10	0.51
1:D:230:ARG:NH1	1:D:230:ARG:HB3	2.25	0.51
1:A:286:THR:HA	1:A:289:LYS:HG3	1.92	0.51
1:A:388:VAL:HG23	1:A:389:GLY:N	2.26	0.51
1:D:46:LEU:C	1:D:48:LYS:H	2.14	0.51
1:A:10:ARG:NH1	1:B:75:ASP:OD1	2.44	0.51
1:A:92:LEU:HD12	1:A:102:TYR:O	2.10	0.51
1:B:172:GLU:OE2	1:B:306:SER:HB2	2.10	0.51
1:C:14:MET:HE1	1:D:69:LEU:HB2	1.93	0.51
1:C:74:GLU:C	1:C:76:TYR:H	2.13	0.51
1:D:211:HIS:CB	1:D:349:ARG:NH2	2.73	0.51
1:D:261:TRP:CE3	1:D:264:VAL:HG21	2.41	0.51
1:D:344:ALA:O	1:D:345:TRP:C	2.49	0.51
1:A:90:VAL:HA	1:A:105:LYS:HA	1.93	0.51
1:B:156:MET:HE1	1:B:213:LYS:HE3	1.92	0.51
1:B:225:LYS:HD3	1:B:225:LYS:N	2.26	0.51
1:C:241:ILE:HD11	1:C:245:VAL:CG1	2.40	0.51
1:B:60:LYS:HE3	1:B:64:ASN:HD21	1.74	0.51
1:C:49:ASN:C	1:C:49:ASN:OD1	2.49	0.51
1:C:168:TYR:HE2	1:C:174:TRP:HH2	1.58	0.51
1:A:13:LYS:HA	1:A:16:ASN:HD21	1.75	0.51
1:C:177:PHE:CD1	1:C:348:LEU:HD11	2.46	0.51
1:D:109:LYS:O	1:D:113:ILE:HG12	2.10	0.51
1:D:262:TRP:CZ2	1:D:290:ILE:CG2	2.91	0.51
1:A:117:ASP:HB3	3:A:419:HOH:O	2.11	0.51
1:A:295:ASN:O	1:A:297:LEU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:VAL:C	1:B:248:SER:HB2	2.30	0.51
1:D:105:LYS:HE3	2:D:900:3ND:CL24	2.47	0.51
1:B:223:MET:HE1	1:B:257:ARG:HH22	1.76	0.50
1:C:375:LYS:HD2	1:C:377:GLU:OE1	2.09	0.50
1:A:230:ARG:HG2	1:A:254:TYR:CE1	2.47	0.50
1:B:98:THR:O	1:B:100:LYS:N	2.44	0.50
1:C:74:GLU:O	1:C:76:TYR:N	2.44	0.50
1:C:305:ILE:HD13	1:C:305:ILE:N	2.22	0.50
1:D:184:LEU:CD2	1:D:333:LYS:HZ2	2.24	0.50
1:D:212:LEU:HD23	1:D:212:LEU:C	2.31	0.50
1:A:164:LEU:CD2	1:A:178:TYR:HE1	2.25	0.50
1:A:199:VAL:HB	1:A:263:SER:HB3	1.93	0.50
1:D:223:MET:SD	1:D:257:ARG:NH2	2.84	0.50
1:B:156:MET:CE	1:B:207:ASP:HB3	2.40	0.50
1:C:110:PHE:C	1:C:110:PHE:CD2	2.85	0.50
1:C:135:TRP:CE3	1:C:135:TRP:HA	2.47	0.50
1:D:120:PHE:O	1:D:123:GLU:HG2	2.11	0.50
1:D:242:SER:HA	1:D:262:TRP:NE1	2.26	0.50
1:A:316:PHE:C	1:A:318:THR:H	2.14	0.50
1:A:321:GLU:O	1:A:326:ARG:HD3	2.11	0.50
1:B:199:VAL:O	1:B:200:LYS:HB3	2.12	0.50
1:D:205:LEU:HD23	1:D:205:LEU:N	2.27	0.50
1:A:200:LYS:HB2	1:A:201:PRO:HD2	1.93	0.50
1:B:74:GLU:C	1:B:76:TYR:H	2.15	0.50
1:C:195:ILE:HG23	1:C:260:ASP:OD2	2.12	0.50
1:A:225:LYS:H	1:A:225:LYS:CD	2.24	0.50
1:C:392:LEU:N	1:C:393:PRO:HD2	2.26	0.50
1:D:240:TYR:O	1:D:241:ILE:C	2.50	0.50
1:A:125:ARG:HH21	1:A:399:TYR:HB2	1.77	0.50
1:A:333:LYS:HD3	1:A:345:TRP:CD1	2.47	0.50
1:D:205:LEU:O	1:D:212:LEU:HA	2.11	0.50
1:B:63:ILE:HG22	1:B:64:ASN:N	2.25	0.50
1:B:199:VAL:HB	1:B:263:SER:CB	2.41	0.50
1:C:43:PHE:CE1	1:C:384:PRO:HG2	2.47	0.50
1:D:61:ASP:O	1:D:64:ASN:HB2	2.12	0.50
1:D:224:ASN:OD1	1:D:226:GLU:HG2	2.10	0.50
1:B:135:TRP:CH2	1:B:349:ARG:HD2	2.47	0.49
1:B:229:VAL:HG22	1:B:255:TYR:O	2.12	0.49
1:C:174:TRP:CG	1:C:354:PRO:HB3	2.47	0.49
1:C:286:THR:O	1:C:289:LYS:HB2	2.12	0.49
1:C:26:ASN:O	1:C:27:SER:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:VAL:HA	1:D:105:LYS:HA	1.93	0.49
1:D:328:GLY:O	1:D:331:GLU:HG2	2.12	0.49
1:B:34:LEU:O	1:B:38:VAL:HG23	2.13	0.49
1:B:46:LEU:HD21	1:B:386:ALA:HA	1.93	0.49
1:C:137:VAL:HG11	2:C:900:3ND:H1	1.93	0.49
1:C:156:MET:HE1	1:C:213:LYS:CE	2.42	0.49
1:A:333:LYS:HA	1:A:345:TRP:CZ2	2.47	0.49
1:B:174:TRP:CE2	1:B:354:PRO:HB3	2.47	0.49
1:C:63:ILE:HA	1:C:66:ILE:HD12	1.93	0.49
1:A:238:PRO:O	1:A:241:ILE:HG22	2.12	0.49
1:D:46:LEU:C	1:D:48:LYS:N	2.65	0.49
1:B:135:TRP:HA	1:B:135:TRP:CE3	2.48	0.49
1:B:228:MET:HB3	1:B:254:TYR:CE1	2.48	0.49
1:B:323:ARG:O	1:B:324:LEU:C	2.51	0.49
1:C:46:LEU:C	1:C:48:LYS:H	2.15	0.49
1:C:177:PHE:CE2	1:C:354:PRO:HD2	2.46	0.49
1:A:46:LEU:C	1:A:48:LYS:N	2.65	0.49
1:A:109:LYS:CB	1:A:394:PHE:HE1	2.24	0.49
1:A:165:MET:HE1	1:A:270:GLU:O	2.13	0.49
1:A:217:PHE:O	1:A:219:THR:N	2.43	0.49
1:B:185:ALA:O	1:B:188:ALA:HB3	2.12	0.49
1:C:242:SER:HB2	1:C:243:PRO:HD2	1.94	0.49
1:C:244:GLU:OE2	1:C:320:ARG:HB2	2.11	0.49
1:D:17:LEU:N	1:D:17:LEU:HD12	2.28	0.49
1:A:295:ASN:N	1:A:295:ASN:HD22	2.10	0.49
1:A:297:LEU:HD13	1:A:317:LEU:HD23	1.95	0.49
1:B:193:GLY:HA2	1:B:223:MET:CE	2.43	0.49
1:C:26:ASN:ND2	1:C:29:CYS:SG	2.86	0.49
1:C:246:LEU:C	1:C:248:SER:H	2.17	0.49
1:C:319:ASP:OD1	1:C:321:GLU:HG2	2.13	0.49
1:A:279:TYR:CD2	1:A:280:ALA:N	2.81	0.49
1:B:46:LEU:C	1:B:48:LYS:N	2.65	0.49
1:B:110:PHE:CD1	1:B:379:GLU:HB3	2.48	0.49
1:B:240:TYR:O	1:B:241:ILE:C	2.51	0.49
1:C:225:LYS:H	1:C:225:LYS:CD	2.11	0.49
1:C:277:PRO:O	1:C:278:PHE:CG	2.66	0.49
1:D:105:LYS:CE	1:D:107:LEU:HD21	2.35	0.49
1:B:312:LEU:O	1:B:315:ALA:HB3	2.13	0.48
1:B:343:TRP:CD2	1:B:348:LEU:HD13	2.48	0.48
1:B:351:THR:OG1	1:B:352:VAL:N	2.43	0.48
1:C:371:LEU:HG	1:C:372:GLU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:GLU:HB3	1:D:115:ARG:HH22	1.77	0.48
1:D:217:PHE:HB3	1:D:220:CYS:HG	1.78	0.48
1:D:304:ASP:N	1:D:305:ILE:HD13	2.27	0.48
1:A:61:ASP:OD1	1:C:372:GLU:HG2	2.13	0.48
1:D:219:THR:O	1:D:220:CYS:C	2.51	0.48
1:A:278:PHE:HD1	1:A:289:LYS:HB3	1.78	0.48
1:A:343:TRP:CD2	1:A:348:LEU:HD13	2.48	0.48
1:B:49:ASN:OD1	1:B:51:ASN:HB2	2.13	0.48
1:B:78:VAL:HG21	1:B:375:LYS:NZ	2.28	0.48
1:B:171:PRO:HD2	1:B:174:TRP:CE3	2.49	0.48
1:C:158:GLY:CA	1:C:206:LEU:O	2.57	0.48
1:C:164:LEU:CD2	1:C:178:TYR:HE1	2.26	0.48
1:C:316:PHE:C	1:C:318:THR:H	2.17	0.48
1:D:217:PHE:C	1:D:220:CYS:HG	2.16	0.48
1:A:47:ARG:NH1	1:A:53:ASP:OD1	2.46	0.48
1:C:115:ARG:HG2	1:C:115:ARG:NH2	2.26	0.48
1:C:170:VAL:HG13	1:C:174:TRP:CB	2.39	0.48
1:B:135:TRP:HB3	1:B:185:ALA:HA	1.93	0.48
1:B:94:ARG:HD2	1:B:99:ARG:CZ	2.42	0.48
1:C:62:THR:HG22	1:C:63:ILE:N	2.28	0.48
1:C:182:VAL:HG21	1:C:267:PHE:CE2	2.48	0.48
1:C:259:CYS:SG	1:C:260:ASP:N	2.87	0.48
1:D:307:LYS:HB3	1:D:307:LYS:HZ3	1.79	0.48
1:A:199:VAL:O	1:A:200:LYS:HB3	2.14	0.48
1:A:393:PRO:HG2	1:A:394:PHE:CE2	2.48	0.48
1:B:177:PHE:CE2	1:B:354:PRO:CD	2.95	0.48
1:B:265:GLY:HA3	1:B:317:LEU:HD13	1.95	0.48
1:C:154:GLU:O	1:C:154:GLU:HG3	2.13	0.48
1:A:34:LEU:O	1:A:38:VAL:HG23	2.14	0.48
1:A:399:TYR:CZ	1:A:401:SER:HB2	2.46	0.48
1:C:35:ASP:OD1	1:C:67:ARG:NE	2.46	0.48
1:C:109:LYS:NZ	1:C:145:ASP:O	2.43	0.48
1:C:181:GLU:HG3	1:C:348:LEU:HD21	1.95	0.48
1:C:269:TYR:CD2	1:C:277:PRO:HD3	2.49	0.48
1:A:322:VAL:HG22	1:A:322:VAL:O	2.14	0.48
1:B:109:LYS:NZ	1:B:144:GLN:OE1	2.44	0.48
1:B:226:GLU:OE1	1:C:380:THR:O	2.32	0.48
1:B:248:SER:O	1:B:249:GLN:C	2.52	0.48
1:C:128:MET:HE2	1:C:153:MET:SD	2.52	0.48
1:C:143:PHE:CE1	1:C:150:TYR:CG	3.01	0.48
1:C:174:TRP:CD1	1:C:354:PRO:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:PHE:CD1	1:C:345:TRP:HH2	2.32	0.48
1:D:70:ARG:HB3	1:D:400:TYR:OH	2.14	0.48
1:D:322:VAL:CB	1:D:326:ARG:HH21	2.27	0.48
1:B:11:PHE:CG	3:B:419:HOH:O	2.66	0.48
1:B:322:VAL:O	1:B:322:VAL:CG2	2.58	0.48
1:C:7:PHE:HA	1:C:10:ARG:HD2	1.95	0.48
1:C:77:GLU:O	1:C:93:VAL:HG12	2.14	0.48
1:C:211:HIS:CE1	1:C:349:ARG:O	2.66	0.48
1:D:80:LYS:HE3	1:D:370:ASP:OD2	2.14	0.48
1:B:250:GLY:HA2	1:B:251:GLY:HA2	1.67	0.47
1:C:217:PHE:O	1:C:219:THR:N	2.46	0.47
1:C:273:VAL:HG12	1:C:274:GLY:N	2.28	0.47
1:C:393:PRO:CA	1:D:58:ARG:HH22	2.24	0.47
1:D:17:LEU:HD12	1:D:17:LEU:H	1.77	0.47
1:D:164:LEU:HD21	1:D:178:TYR:HE1	1.78	0.47
1:A:115:ARG:HG2	1:A:115:ARG:NH2	2.26	0.47
1:A:240:TYR:O	1:A:241:ILE:C	2.52	0.47
1:A:308:GLU:HB3	1:A:337:PHE:CA	2.43	0.47
1:B:46:LEU:C	1:B:48:LYS:H	2.16	0.47
1:B:93:VAL:O	1:B:101:VAL:HA	2.15	0.47
1:A:297:LEU:HD21	1:A:314:CYS:SG	2.54	0.47
1:B:49:ASN:O	1:B:50:LYS:C	2.52	0.47
1:B:78:VAL:HG21	1:B:375:LYS:HZ1	1.79	0.47
1:C:344:ALA:HB3	1:C:347:THR:HG22	1.94	0.47
1:A:277:PRO:O	1:A:278:PHE:CG	2.68	0.47
1:A:340:ASN:HB2	1:A:342:GLN:OE1	2.13	0.47
1:B:112:MET:O	1:B:118:SER:HB3	2.14	0.47
1:B:181:GLU:HB3	1:B:212:LEU:HD22	1.96	0.47
1:C:76:TYR:N	1:C:76:TYR:CD1	2.81	0.47
1:D:210:GLY:HA3	1:D:355:VAL:O	2.13	0.47
1:A:98:THR:O	1:A:100:LYS:N	2.47	0.47
1:A:333:LYS:HA	1:A:345:TRP:HZ2	1.79	0.47
1:D:128:MET:HB3	1:D:139:LEU:HB2	1.96	0.47
1:B:74:GLU:O	1:B:76:TYR:N	2.47	0.47
1:B:144:GLN:HB3	1:B:149:LEU:HD23	1.97	0.47
1:B:205:LEU:HD11	2:B:900:3ND:C7	2.44	0.47
1:C:8:GLU:N	1:C:8:GLU:OE1	2.47	0.47
1:C:17:LEU:HD12	1:C:17:LEU:N	2.28	0.47
1:D:176:ARG:HD3	1:D:338:PHE:HA	1.95	0.47
1:A:110:PHE:CE1	1:A:379:GLU:HB3	2.50	0.47
1:A:224:ASN:OD1	1:A:226:GLU:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:HD11	1:A:245:VAL:CG1	2.45	0.47
1:B:156:MET:CE	1:B:213:LYS:HD2	2.45	0.47
1:C:338:PHE:CG	1:C:345:TRP:CH2	3.03	0.47
1:D:230:ARG:HB3	1:D:230:ARG:HH11	1.80	0.47
1:D:268:LEU:HG	1:D:313:ILE:HD11	1.96	0.47
1:D:325:GLY:O	1:D:326:ARG:C	2.53	0.47
1:D:343:TRP:CB	1:D:351:THR:HG21	2.45	0.47
1:A:394:PHE:N	1:A:394:PHE:CD2	2.83	0.47
1:B:13:LYS:HA	1:B:16:ASN:HD21	1.79	0.47
1:C:102:TYR:HB3	1:C:153:MET:O	2.15	0.47
1:D:169:ASP:O	1:D:170:VAL:C	2.53	0.47
1:A:7:PHE:HB2	1:B:97:SER:CB	2.45	0.47
1:B:62:THR:O	1:B:65:LYS:N	2.46	0.47
1:B:343:TRP:CE3	1:B:348:LEU:HD13	2.49	0.47
1:B:348:LEU:O	1:B:351:THR:HG23	2.14	0.47
1:C:160:ASP:HA	1:C:204:MET:O	2.15	0.47
1:C:269:TYR:CE2	1:C:273:VAL:HG21	2.50	0.47
1:C:296:SER:O	1:C:298:THR:HG23	2.14	0.47
1:D:158:GLY:HA3	1:D:206:LEU:HB2	1.96	0.47
1:D:257:ARG:NH1	1:D:257:ARG:HB3	2.30	0.47
1:A:8:GLU:O	1:A:12:GLU:HG3	2.15	0.47
1:D:14:MET:HA	1:D:14:MET:CE	2.45	0.47
1:D:45:ALA:O	1:D:48:LYS:HD3	2.15	0.47
1:D:316:PHE:C	1:D:318:THR:H	2.18	0.47
1:A:196:HIS:O	1:A:197:ARG:HB2	2.15	0.46
1:A:238:PRO:C	1:A:240:TYR:H	2.18	0.46
1:B:143:PHE:CE1	1:B:150:TYR:HB2	2.50	0.46
1:C:80:LYS:HD2	1:C:370:ASP:HB3	1.97	0.46
1:C:224:ASN:HB2	1:C:225:LYS:NZ	2.30	0.46
1:C:338:PHE:CG	1:C:345:TRP:HH2	2.32	0.46
1:D:13:LYS:HA	1:D:16:ASN:ND2	2.30	0.46
1:D:46:LEU:CD2	1:D:386:ALA:HA	2.43	0.46
1:D:378:GLU:HA	1:D:378:GLU:OE2	2.15	0.46
1:A:222:LYS:HB2	1:A:222:LYS:HE3	1.33	0.46
1:C:79:VAL:HG12	1:C:80:LYS:N	2.30	0.46
1:B:36:ALA:O	1:B:39:TYR:HB2	2.15	0.46
1:C:104:MET:CE	1:C:106:LEU:HD11	2.46	0.46
1:C:168:TYR:HD2	1:C:174:TRP:HZ3	1.64	0.46
1:D:238:PRO:HG3	1:D:283:LEU:CD1	2.45	0.46
1:A:306:SER:HB2	1:A:309:ALA:CB	2.45	0.46
1:A:316:PHE:CE2	1:A:324:LEU:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:PHE:HZ	1:C:310:LYS:HG2	1.75	0.46
1:C:371:LEU:CG	1:C:372:GLU:H	2.28	0.46
1:D:48:LYS:NZ	1:D:48:LYS:HB3	2.31	0.46
2:D:900:3ND:H19	2:D:900:3ND:H13	1.58	0.46
1:A:195:ILE:O	1:A:197:ARG:HG3	2.15	0.46
1:A:304:ASP:N	1:A:310:LYS:NZ	2.58	0.46
1:C:30:LEU:HD13	1:D:30:LEU:HB2	1.97	0.46
1:D:283:LEU:O	1:D:284:VAL:C	2.54	0.46
1:B:79:VAL:HB	1:B:92:LEU:O	2.15	0.46
1:C:200:LYS:HE3	1:C:202:ASP:CB	2.43	0.46
1:D:401:SER:HA	1:D:402:ASN:HA	1.69	0.46
1:A:212:LEU:HG	1:A:213:LYS:N	2.30	0.46
1:B:197:ARG:NH2	1:B:221:MET:HE3	2.30	0.46
1:B:395:VAL:O	1:B:395:VAL:HG12	2.15	0.46
1:C:217:PHE:HB3	1:C:220:CYS:HG	1.80	0.46
1:C:357:PRO:HB3	1:C:359:LEU:HD21	1.98	0.46
1:D:223:MET:CE	1:D:227:GLY:HA2	2.46	0.46
1:A:199:VAL:HB	1:A:263:SER:CB	2.46	0.46
1:A:218:GLY:O	1:A:219:THR:HG23	2.16	0.46
1:B:176:ARG:HD3	1:B:338:PHE:HA	1.97	0.46
1:B:208:LYS:C	1:B:357:PRO:HG2	2.36	0.46
1:B:329:VAL:O	1:B:333:LYS:HG3	2.16	0.46
1:A:25:VAL:HG11	1:B:66:ILE:HD11	1.97	0.46
1:A:139:LEU:HD11	1:A:141:TYR:O	2.15	0.46
1:B:156:MET:HB3	1:B:206:LEU:O	2.16	0.46
1:D:90:VAL:HG12	1:D:91:GLN:N	2.31	0.46
1:D:177:PHE:CZ	1:D:181:GLU:OE1	2.68	0.46
1:B:325:GLY:O	1:B:326:ARG:C	2.54	0.45
1:C:125:ARG:HD2	1:C:397:PHE:CD1	2.52	0.45
1:D:135:TRP:HB3	1:D:185:ALA:HA	1.99	0.45
1:D:187:ASP:O	1:D:187:ASP:OD2	2.34	0.45
1:D:383:ILE:HG23	1:D:384:PRO:HD2	1.98	0.45
1:A:10:ARG:NH2	1:B:75:ASP:OD2	2.49	0.45
2:B:900:3ND:H19	2:B:900:3ND:H13	1.65	0.45
1:C:162:VAL:HB	1:C:201:PRO:HB2	1.97	0.45
1:D:80:LYS:HZ3	1:D:80:LYS:HB3	1.80	0.45
1:A:306:SER:HB2	1:A:309:ALA:HB2	1.98	0.45
1:A:392:LEU:N	1:A:393:PRO:CD	2.79	0.45
1:C:149:LEU:HD22	1:C:397:PHE:CD2	2.51	0.45
1:C:156:MET:SD	1:C:213:LYS:HD2	2.56	0.45
1:D:267:PHE:O	1:D:271:MET:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:TRP:HA	1:A:345:TRP:CE3	2.50	0.45
1:B:7:PHE:O	1:B:9:THR:N	2.45	0.45
1:B:193:GLY:HA2	1:B:223:MET:HE2	1.98	0.45
1:B:258:GLU:HG3	1:B:320:ARG:CG	2.42	0.45
1:D:34:LEU:O	1:D:38:VAL:HG23	2.16	0.45
1:A:295:ASN:N	1:A:295:ASN:ND2	2.64	0.45
1:B:245:VAL:O	1:B:245:VAL:HG12	2.15	0.45
1:C:159:GLY:O	1:C:205:LEU:HA	2.16	0.45
1:D:208:LYS:C	1:D:357:PRO:HG2	2.37	0.45
1:D:224:ASN:HB2	1:D:225:LYS:HZ3	1.79	0.45
1:A:135:TRP:HB3	1:A:185:ALA:HA	1.99	0.45
1:B:43:PHE:HA	1:B:44:PRO:HD2	1.67	0.45
1:C:168:TYR:CE2	1:C:174:TRP:HH2	2.34	0.45
1:D:10:ARG:O	1:D:13:LYS:N	2.50	0.45
1:D:267:PHE:CZ	1:D:271:MET:HE1	2.52	0.45
1:D:282:SER:O	1:D:283:LEU:C	2.55	0.45
1:D:338:PHE:CD1	1:D:345:TRP:HZ2	2.34	0.45
1:A:308:GLU:CD	1:A:336:LEU:HB3	2.37	0.45
1:C:115:ARG:HH21	1:C:115:ARG:CG	2.25	0.45
1:C:135:TRP:HB3	1:C:185:ALA:HA	1.98	0.45
1:D:34:LEU:HD22	1:D:34:LEU:HA	1.51	0.45
1:B:344:ALA:O	1:B:345:TRP:C	2.54	0.45
1:C:149:LEU:HB3	1:C:397:PHE:CE2	2.52	0.45
1:D:294:LYS:HE2	1:D:294:LYS:HB2	1.74	0.45
1:D:388:VAL:HG21	1:D:390:ASN:ND2	2.32	0.45
1:A:277:PRO:O	1:A:278:PHE:CD2	2.69	0.45
1:C:240:TYR:O	1:C:241:ILE:C	2.53	0.45
1:D:25:VAL:O	1:D:30:LEU:HD11	2.16	0.45
1:D:199:VAL:HB	1:D:263:SER:CB	2.46	0.45
1:A:19:ARG:O	1:A:21:PRO:HD3	2.16	0.45
1:A:31:LEU:HD22	1:A:66:ILE:HG21	1.99	0.45
1:A:34:LEU:HD22	1:A:34:LEU:HA	1.62	0.45
1:A:125:ARG:NE	1:A:397:PHE:O	2.50	0.45
1:B:246:LEU:HD12	1:B:246:LEU:HA	1.66	0.45
1:C:75:ASP:OD2	1:D:10:ARG:NH2	2.49	0.45
1:C:195:ILE:O	1:C:197:ARG:HG3	2.17	0.45
1:C:200:LYS:HG3	1:C:202:ASP:H	1.82	0.45
1:C:204:MET:O	1:C:205:LEU:HD23	2.17	0.45
1:D:26:ASN:O	1:D:27:SER:C	2.54	0.45
1:D:200:LYS:HE2	1:D:202:ASP:CB	2.43	0.45
1:D:383:ILE:HA	1:D:384:PRO:HD3	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:HG12	1:A:246:LEU:CD1	2.38	0.44
1:B:65:LYS:NZ	1:B:65:LYS:HB3	2.31	0.44
1:B:90:VAL:HA	1:B:105:LYS:HA	1.98	0.44
1:B:231:CYS:HB3	1:B:255:TYR:OH	2.17	0.44
1:B:321:GLU:O	1:B:326:ARG:NE	2.50	0.44
1:C:177:PHE:HD2	1:C:178:TYR:CD2	2.34	0.44
1:C:258:GLU:CG	1:C:320:ARG:HG3	2.45	0.44
1:D:110:PHE:CE1	1:D:380:THR:C	2.90	0.44
1:A:56:LEU:O	1:A:60:LYS:HB3	2.17	0.44
1:A:111:GLU:OE1	1:A:115:ARG:NH2	2.38	0.44
1:B:229:VAL:HG21	1:B:255:TYR:CE2	2.53	0.44
1:B:388:VAL:HG21	1:B:390:ASN:ND2	2.31	0.44
1:C:17:LEU:N	1:C:17:LEU:CD1	2.80	0.44
1:C:215:ALA:CB	2:C:900:3ND:H4A	2.43	0.44
1:D:322:VAL:HB	1:D:326:ARG:NH2	2.28	0.44
1:A:176:ARG:NE	1:A:337:PHE:O	2.48	0.44
1:A:185:ALA:O	1:A:188:ALA:HB3	2.17	0.44
1:A:330:GLU:O	1:A:333:LYS:HB2	2.17	0.44
1:B:65:LYS:O	1:B:69:LEU:HG	2.17	0.44
1:B:154:GLU:O	1:B:154:GLU:HG2	2.16	0.44
1:B:377:GLU:HG3	1:B:378:GLU:H	1.82	0.44
1:C:82:ILE:HG21	1:C:92:LEU:HB2	1.99	0.44
1:D:197:ARG:CZ	1:D:235:VAL:HG21	2.47	0.44
1:A:37:LEU:HD22	1:A:41:LEU:HD11	1.98	0.44
1:A:262:TRP:HH2	1:A:293:HIS:HB3	1.82	0.44
1:A:348:LEU:O	1:A:351:THR:HG23	2.18	0.44
1:B:210:GLY:O	1:B:353:ALA:CB	2.65	0.44
1:B:242:SER:HB2	1:B:243:PRO:HD2	1.99	0.44
1:B:322:VAL:HA	1:B:326:ARG:HH21	1.82	0.44
1:C:74:GLU:C	1:C:76:TYR:N	2.71	0.44
1:C:135:TRP:HH2	1:C:181:GLU:HG2	1.80	0.44
1:C:141:TYR:OH	1:D:7:PHE:HZ	1.78	0.44
1:D:162:VAL:HB	1:D:201:PRO:HB2	1.99	0.44
1:A:24:GLU:OE2	1:B:58:ARG:HG3	2.17	0.44
1:A:208:LYS:O	1:A:357:PRO:HG2	2.17	0.44
1:B:69:LEU:N	1:B:69:LEU:HD23	2.33	0.44
1:B:302:ASP:O	1:B:304:ASP:N	2.50	0.44
1:C:43:PHE:CD2	1:C:43:PHE:N	2.82	0.44
1:C:186:LEU:O	1:C:190:HIS:CD2	2.70	0.44
1:C:402:ASN:C	1:D:11:PHE:CE2	2.91	0.44
1:D:93:VAL:O	1:D:101:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ARG:NH2	1:B:56:LEU:HB2	2.31	0.44
1:B:399:TYR:CZ	1:B:401:SER:CB	2.94	0.44
1:C:34:LEU:HD12	1:C:63:ILE:HD11	2.00	0.44
1:D:241:ILE:HD11	1:D:245:VAL:CB	2.45	0.44
1:A:6:SER:N	1:A:9:THR:HB	2.33	0.44
1:A:239:ASP:HB3	1:A:276:THR:HG21	1.98	0.44
1:C:37:LEU:HD22	1:C:41:LEU:HD11	2.00	0.44
1:C:196:HIS:HD2	1:C:198:ASP:H	1.66	0.44
1:C:401:SER:HA	1:C:402:ASN:HA	1.60	0.44
1:D:110:PHE:CE1	1:D:381:PHE:HA	2.53	0.44
1:A:346:GLU:H	1:A:346:GLU:CD	2.20	0.44
1:A:349:ARG:HG2	1:A:349:ARG:HH11	1.82	0.44
1:C:171:PRO:HD2	1:C:174:TRP:CD2	2.51	0.44
1:D:82:ILE:HD11	1:D:90:VAL:HG12	1.98	0.44
1:D:176:ARG:HD3	1:D:337:PHE:O	2.17	0.44
1:D:383:ILE:HG23	1:D:384:PRO:CD	2.48	0.44
1:A:69:LEU:HD22	1:B:10:ARG:CB	2.43	0.44
1:B:200:LYS:HD3	1:B:237:THR:OG1	2.18	0.44
1:C:137:VAL:HG23	1:C:214:LEU:O	2.18	0.44
1:D:79:VAL:HG23	1:D:93:VAL:HA	2.00	0.44
1:B:169:ASP:O	1:B:170:VAL:C	2.55	0.43
1:B:287:TYR:O	1:B:291:MET:HG2	2.18	0.43
1:D:307:LYS:NZ	1:D:307:LYS:CB	2.80	0.43
1:A:88:GLY:O	1:A:89:GLU:HB3	2.18	0.43
1:A:158:GLY:HA3	1:A:206:LEU:HB2	1.99	0.43
1:A:238:PRO:O	1:A:240:TYR:N	2.51	0.43
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.57	0.43
1:B:74:GLU:C	1:B:76:TYR:N	2.71	0.43
1:B:154:GLU:O	1:B:154:GLU:CG	2.66	0.43
1:B:356:VAL:HG13	1:B:357:PRO:HD2	1.98	0.43
1:D:171:PRO:HD2	1:D:174:TRP:CE3	2.53	0.43
1:D:202:ASP:O	2:D:900:3ND:H14A	2.18	0.43
1:D:312:LEU:HD12	1:D:337:PHE:CD2	2.53	0.43
1:D:342:GLN:HE21	1:D:342:GLN:HB3	1.58	0.43
1:A:57:SER:N	3:A:427:HOH:O	2.51	0.43
1:A:312:LEU:HD21	1:A:316:PHE:CE1	2.53	0.43
1:D:167:ASN:O	1:D:168:TYR:CG	2.71	0.43
1:B:205:LEU:CD1	2:B:900:3ND:C6	2.97	0.43
1:B:269:TYR:O	1:B:270:GLU:C	2.57	0.43
1:A:63:ILE:HD13	1:A:63:ILE:HA	1.86	0.43
1:A:104:MET:HA	1:A:151:MET:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:CB	1:A:276:THR:HG21	2.48	0.43
1:B:135:TRP:O	1:B:213:LYS:HA	2.19	0.43
1:B:353:ALA:N	3:B:427:HOH:O	2.40	0.43
1:C:115:ARG:NH2	1:C:115:ARG:CG	2.81	0.43
1:C:315:ALA:HA	1:C:318:THR:CG2	2.48	0.43
1:D:164:LEU:CD1	1:D:178:TYR:OH	2.67	0.43
1:A:129:ALA:HB2	1:A:139:LEU:HD23	2.00	0.43
1:B:110:PHE:C	1:B:110:PHE:CD2	2.92	0.43
1:C:155:TYR:CD1	1:C:156:MET:N	2.86	0.43
1:C:158:GLY:HA3	1:C:206:LEU:HB2	1.99	0.43
1:C:170:VAL:HG22	1:C:174:TRP:CE3	2.47	0.43
1:D:283:LEU:O	1:D:286:THR:N	2.52	0.43
1:A:54:ASN:O	1:A:57:SER:HB2	2.19	0.43
1:B:109:LYS:NZ	1:B:391:GLN:OE1	2.49	0.43
1:B:165:MET:HE3	1:B:271:MET:HA	2.00	0.43
1:C:113:ILE:HG13	1:C:381:PHE:CZ	2.51	0.43
1:C:124:GLU:HG2	1:C:151:MET:CE	2.48	0.43
1:C:223:MET:HE3	1:C:257:ARG:NH2	2.34	0.43
1:D:277:PRO:O	1:D:278:PHE:CG	2.72	0.43
1:A:161:LEU:HB2	1:A:204:MET:HB2	2.01	0.43
1:A:172:GLU:CD	1:A:337:PHE:HE1	2.21	0.43
1:B:43:PHE:CD2	1:B:43:PHE:N	2.85	0.43
1:B:125:ARG:O	1:B:126:ASP:C	2.56	0.43
1:B:162:VAL:HB	1:B:201:PRO:HB2	2.01	0.43
1:B:228:MET:HB3	1:B:254:TYR:HE1	1.84	0.43
1:B:304:ASP:N	1:B:305:ILE:HD13	2.33	0.43
1:B:325:GLY:C	1:B:327:ASN:N	2.71	0.43
1:C:76:TYR:HD1	1:C:76:TYR:N	2.15	0.43
1:C:78:VAL:HG23	1:C:91:GLN:HE21	1.84	0.43
1:C:137:VAL:HG13	1:C:154:GLU:HG2	2.00	0.43
1:C:305:ILE:HD13	3:C:419:HOH:O	2.17	0.43
1:D:110:PHE:CD1	1:D:381:PHE:N	2.86	0.43
1:D:126:ASP:O	1:D:130:PHE:CD1	2.72	0.43
1:D:138:GLN:H	1:D:154:GLU:HG2	1.84	0.43
1:D:185:ALA:O	1:D:188:ALA:HB3	2.19	0.43
1:D:347:THR:O	1:D:349:ARG:N	2.52	0.43
1:A:189:ILE:HG22	1:A:194:PHE:O	2.19	0.43
1:A:324:LEU:O	1:A:332:ILE:HD11	2.18	0.43
1:B:121:PHE:CD1	1:B:122:TRP:N	2.87	0.43
1:B:252:ASP:O	1:B:253:GLY:C	2.58	0.43
1:C:241:ILE:O	1:C:290:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:VAL:O	1:D:371:LEU:HD22	2.19	0.43
1:A:94:ARG:HA	1:A:100:LYS:O	2.19	0.42
1:B:19:ARG:O	1:B:21:PRO:HD3	2.19	0.42
1:D:7:PHE:N	1:D:9:THR:HG1	2.17	0.42
1:D:59:TYR:O	1:D:62:THR:N	2.52	0.42
1:D:80:LYS:HZ3	1:D:80:LYS:CB	2.32	0.42
1:D:347:THR:O	1:D:348:LEU:C	2.57	0.42
1:B:135:TRP:CZ3	1:B:349:ARG:HD2	2.54	0.42
1:B:175:ALA:HB1	1:B:272:LEU:HD21	1.98	0.42
1:B:314:CYS:O	1:B:318:THR:HG22	2.19	0.42
1:B:320:ARG:C	1:B:322:VAL:H	2.22	0.42
1:C:164:LEU:HD21	1:C:178:TYR:HE1	1.82	0.42
1:C:278:PHE:HB3	1:C:289:LYS:HB3	2.01	0.42
1:D:110:PHE:C	1:D:110:PHE:HD2	2.22	0.42
1:B:135:TRP:HA	1:B:135:TRP:HE3	1.84	0.42
1:A:244:GLU:HG3	1:A:320:ARG:HD3	2.01	0.42
1:A:333:LYS:HG2	1:A:345:TRP:CZ2	2.54	0.42
1:B:181:GLU:HG2	1:B:348:LEU:HD23	2.00	0.42
1:C:223:MET:CE	1:C:227:GLY:HA2	2.46	0.42
1:D:29:CYS:O	1:D:32:ASP:HB2	2.18	0.42
1:D:305:ILE:HD13	1:D:305:ILE:H	1.84	0.42
1:A:40:ASP:OD2	1:A:391:GLN:HB2	2.20	0.42
1:A:46:LEU:HD21	1:A:386:ALA:HA	2.02	0.42
1:A:143:PHE:CD2	1:A:143:PHE:N	2.87	0.42
1:C:109:LYS:NZ	1:C:144:GLN:HB2	2.34	0.42
1:C:148:TYR:HB2	1:C:150:TYR:CZ	2.54	0.42
1:C:371:LEU:HG	1:C:372:GLU:HG3	2.00	0.42
1:B:94:ARG:HD2	1:B:99:ARG:NH2	2.34	0.42
1:C:20:ASP:OD1	1:C:20:ASP:C	2.57	0.42
1:C:59:TYR:O	1:C:62:THR:N	2.52	0.42
1:D:112:MET:O	1:D:118:SER:HB3	2.19	0.42
1:A:59:TYR:O	1:A:62:THR:N	2.52	0.42
1:A:79:VAL:HG23	1:A:93:VAL:HA	2.00	0.42
1:A:261:TRP:CE3	1:A:261:TRP:HA	2.54	0.42
1:A:299:PHE:HA	1:A:300:PRO:HD3	1.93	0.42
1:B:237:THR:O	1:B:238:PRO:C	2.56	0.42
1:C:107:LEU:HD23	1:C:107:LEU:HA	1.85	0.42
1:C:167:ASN:O	1:C:168:TYR:CD1	2.73	0.42
1:C:170:VAL:HA	1:C:171:PRO:HD2	1.78	0.42
1:D:165:MET:HE1	1:D:271:MET:CA	2.39	0.42
1:A:34:LEU:O	1:A:34:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:O	1:B:48:LYS:N	2.52	0.42
1:B:81:VAL:HG21	1:B:373:GLU:CA	2.44	0.42
1:B:217:PHE:O	1:B:219:THR:N	2.44	0.42
1:C:109:LYS:HD2	1:C:145:ASP:O	2.19	0.42
1:D:156:MET:HE1	1:D:207:ASP:HB3	2.00	0.42
1:A:159:GLY:O	1:A:205:LEU:HA	2.19	0.42
1:A:241:ILE:HD11	1:A:245:VAL:HG12	2.02	0.42
1:B:335:HIS:CD2	1:B:337:PHE:H	2.37	0.42
1:B:383:ILE:HA	1:B:384:PRO:HD3	1.85	0.42
1:C:345:TRP:CE3	1:C:345:TRP:CA	3.00	0.42
1:B:242:SER:HB2	1:B:243:PRO:CD	2.49	0.42
1:C:286:THR:HA	1:C:289:LYS:HB2	2.02	0.42
1:D:242:SER:OG	1:D:245:VAL:HG23	2.20	0.42
1:A:107:LEU:HB3	1:A:112:MET:CE	2.50	0.41
1:A:269:TYR:CD1	1:A:277:PRO:HB3	2.54	0.41
1:A:279:TYR:CD2	1:A:279:TYR:C	2.92	0.41
1:B:11:PHE:CD2	3:B:419:HOH:O	2.57	0.41
1:B:210:GLY:O	1:B:353:ALA:HB1	2.20	0.41
1:C:46:LEU:C	1:C:48:LYS:N	2.73	0.41
1:C:204:MET:HG2	1:C:212:LEU:HD11	2.02	0.41
1:D:39:TYR:O	1:D:43:PHE:CZ	2.73	0.41
1:A:133:SER:OG	1:A:134:PRO:HD2	2.20	0.41
1:B:237:THR:O	1:B:241:ILE:HG22	2.19	0.41
1:C:241:ILE:HG21	1:C:246:LEU:HD11	2.01	0.41
1:C:268:LEU:HD23	1:C:313:ILE:CG1	2.51	0.41
1:C:372:GLU:H	1:C:372:GLU:HG3	1.52	0.41
1:A:9:THR:HG22	1:A:10:ARG:N	2.35	0.41
1:A:189:ILE:HG23	1:A:194:PHE:HB2	2.03	0.41
1:A:343:TRP:CB	1:A:351:THR:HG21	2.51	0.41
1:B:219:THR:O	1:B:220:CYS:C	2.58	0.41
1:C:200:LYS:CE	1:C:202:ASP:HB2	2.42	0.41
1:D:161:LEU:HD12	1:D:161:LEU:HA	1.69	0.41
1:D:193:GLY:O	1:D:222:LYS:HA	2.20	0.41
1:D:194:PHE:CE1	1:D:222:LYS:HE3	2.55	0.41
1:A:6:SER:O	1:A:9:THR:N	2.53	0.41
1:A:283:LEU:O	1:A:286:THR:N	2.54	0.41
1:B:26:ASN:O	1:B:27:SER:C	2.59	0.41
1:B:43:PHE:CE1	1:B:384:PRO:HD2	2.55	0.41
1:B:285:GLY:C	1:B:287:TYR:N	2.74	0.41
1:C:14:MET:O	1:C:17:LEU:HB2	2.19	0.41
1:C:75:ASP:O	1:C:96:LYS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:THR:O	1:D:100:LYS:HG2	2.21	0.41
1:D:135:TRP:HA	1:D:135:TRP:CE3	2.56	0.41
1:D:160:ASP:HA	1:D:204:MET:O	2.20	0.41
1:A:212:LEU:HD23	1:A:212:LEU:O	2.21	0.41
1:A:293:HIS:O	1:A:297:LEU:HB2	2.21	0.41
1:B:77:GLU:O	1:B:93:VAL:HG12	2.20	0.41
1:B:305:ILE:HD13	1:B:305:ILE:N	2.35	0.41
1:C:182:VAL:HG21	1:C:204:MET:HE1	2.02	0.41
1:C:268:LEU:HD23	1:C:313:ILE:HG13	2.02	0.41
1:C:343:TRP:HZ3	1:C:345:TRP:CE3	2.39	0.41
1:D:13:LYS:O	1:D:17:LEU:HD13	2.20	0.41
1:D:199:VAL:HB	1:D:263:SER:HB2	2.01	0.41
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.84	0.41
1:A:138:GLN:HG2	1:A:139:LEU:N	2.35	0.41
1:B:62:THR:O	1:B:63:ILE:C	2.59	0.41
1:B:106:LEU:HD21	1:B:150:TYR:HE2	1.84	0.41
1:C:287:TYR:O	1:C:291:MET:HG2	2.20	0.41
1:C:343:TRP:CZ3	1:C:345:TRP:CZ3	3.08	0.41
1:D:44:PRO:O	1:D:48:LYS:HG3	2.20	0.41
1:D:343:TRP:HB3	1:D:351:THR:HG21	2.02	0.41
1:A:221:MET:HE3	1:A:221:MET:HB2	1.87	0.41
1:B:199:VAL:HB	1:B:263:SER:HB2	2.03	0.41
1:B:230:ARG:HB3	1:B:230:ARG:CZ	2.50	0.41
1:B:293:HIS:O	1:B:297:LEU:HB2	2.21	0.41
1:B:299:PHE:HD2	1:B:300:PRO:HD2	1.85	0.41
1:B:308:GLU:CD	1:B:336:LEU:HB3	2.40	0.41
1:C:185:ALA:O	1:C:188:ALA:HB3	2.21	0.41
1:C:245:VAL:O	1:C:248:SER:HB2	2.20	0.41
1:D:111:GLU:OE1	1:D:115:ARG:NH2	2.49	0.41
1:D:242:SER:HB2	1:D:243:PRO:CD	2.49	0.41
1:D:378:GLU:OE2	1:D:378:GLU:CA	2.67	0.41
1:A:43:PHE:HA	1:A:44:PRO:HD2	1.58	0.41
1:A:261:TRP:O	1:A:264:VAL:N	2.54	0.41
1:B:92:LEU:HD11	1:B:101:VAL:CG1	2.50	0.41
1:B:196:HIS:N	1:B:260:ASP:OD2	2.46	0.41
1:C:69:LEU:HB3	1:D:14:MET:SD	2.61	0.41
1:C:237:THR:HG23	1:C:238:PRO:HD2	2.03	0.41
1:C:383:ILE:HA	1:C:384:PRO:HD3	1.73	0.41
1:D:340:ASN:HB2	1:D:342:GLN:OE1	2.20	0.41
1:A:74:GLU:O	1:A:76:TYR:N	2.54	0.41
1:B:110:PHE:HE1	1:B:380:THR:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:PRO:HD2	1:B:174:TRP:HB2	2.02	0.41
1:D:139:LEU:HD12	1:D:152:VAL:O	2.21	0.41
1:D:170:VAL:HA	1:D:171:PRO:HD2	1.99	0.41
1:D:172:GLU:OE2	1:D:306:SER:HB2	2.21	0.41
1:A:142:ALA:HB3	1:A:399:TYR:HB3	2.03	0.40
1:A:161:LEU:HD12	1:A:161:LEU:HA	1.84	0.40
1:B:114:LYS:HE2	1:B:115:ARG:CZ	2.51	0.40
1:B:240:TYR:N	1:B:240:TYR:CD2	2.89	0.40
1:C:109:LYS:HA	1:C:112:MET:HE3	2.04	0.40
1:C:308:GLU:OE1	1:C:336:LEU:HB3	2.21	0.40
1:D:143:PHE:CD2	1:D:143:PHE:N	2.88	0.40
1:A:325:GLY:O	1:A:326:ARG:C	2.59	0.40
1:B:78:VAL:O	1:B:78:VAL:HG13	2.21	0.40
1:C:43:PHE:CE1	1:C:384:PRO:CD	3.04	0.40
1:C:75:ASP:O	1:C:76:TYR:HD1	2.03	0.40
1:D:98:THR:OG1	1:D:100:LYS:HG2	2.21	0.40
1:D:159:GLY:O	1:D:205:LEU:HA	2.21	0.40
1:D:196:HIS:CD2	1:D:196:HIS:C	2.94	0.40
1:D:313:ILE:C	1:D:315:ALA:H	2.24	0.40
1:A:22:LYS:HG2	1:A:130:PHE:CE1	2.57	0.40
1:A:84:ARG:HH22	1:A:372:GLU:C	2.23	0.40
1:A:128:MET:HE3	1:A:137:VAL:HB	2.03	0.40
1:B:38:VAL:CG2	1:B:63:ILE:HG13	2.31	0.40
1:B:94:ARG:HA	1:B:100:LYS:O	2.22	0.40
1:B:283:LEU:O	1:B:286:THR:N	2.55	0.40
1:C:55:PHE:HB2	1:D:392:LEU:HB3	2.02	0.40
1:C:196:HIS:HD2	1:C:198:ASP:N	2.19	0.40
1:C:363:ILE:HD13	1:C:363:ILE:HG21	1.81	0.40
1:D:127:ILE:HG22	1:D:128:MET:N	2.36	0.40
1:D:158:GLY:HA3	1:D:206:LEU:C	2.41	0.40
1:D:268:LEU:CD2	1:D:313:ILE:HG12	2.51	0.40
1:A:261:TRP:O	1:A:264:VAL:HB	2.21	0.40
1:A:305:ILE:HG22	1:A:306:SER:N	2.36	0.40
1:B:61:ASP:O	1:B:62:THR:C	2.57	0.40
1:B:77:GLU:HB2	1:B:96:LYS:CG	2.51	0.40
1:B:123:GLU:H	1:B:123:GLU:HG2	1.45	0.40
1:B:161:LEU:HD23	1:B:267:PHE:CZ	2.55	0.40
1:B:205:LEU:HD11	2:B:900:3ND:C6	2.52	0.40
1:C:189:ILE:HG22	1:C:194:PHE:O	2.22	0.40
1:C:218:GLY:O	1:C:219:THR:HG23	2.21	0.40
1:D:16:ASN:HB2	1:D:17:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:PHE:HA	1:D:44:PRO:HD2	1.73	0.40
1:D:121:PHE:HE1	1:D:122:TRP:CE2	2.40	0.40
1:D:177:PHE:CD2	1:D:354:PRO:CD	3.05	0.40
1:A:62:THR:HG21	1:B:25:VAL:HG13	2.03	0.40
1:A:258:GLU:HG3	1:A:320:ARG:HG3	2.03	0.40
1:C:168:TYR:CE2	1:C:174:TRP:CH2	3.09	0.40
1:C:378:GLU:O	1:C:379:GLU:C	2.60	0.40
1:D:48:LYS:NZ	1:D:48:LYS:CB	2.85	0.40
1:D:196:HIS:N	1:D:260:ASP:OD2	2.52	0.40
1:D:247:LYS:HB3	1:D:247:LYS:HE2	1.79	0.40
1:D:299:PHE:HD2	1:D:300:PRO:HD3	1.86	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	373/415 (90%)	282 (76%)	65 (17%)	26 (7%)	1 7
1	B	394/415 (95%)	294 (75%)	70 (18%)	30 (8%)	1 6
1	C	361/415 (87%)	268 (74%)	67 (19%)	26 (7%)	1 7
1	D	394/415 (95%)	286 (73%)	86 (22%)	22 (6%)	2 11
All	All	1522/1660 (92%)	1130 (74%)	288 (19%)	104 (7%)	1 8

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	99	ARG
1	A	273	VAL
1	A	351	THR

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Mol	Chain	Res	Type
1	B	60	LYS
1	B	99	ARG
1	B	296	SER
1	B	347	THR
1	B	378	GLU
1	C	7	PHE
1	C	60	LYS
1	C	99	ARG
1	C	273	VAL
1	D	60	LYS
1	D	99	ARG
1	D	296	SER
1	D	297	LEU
1	D	347	THR
1	D	378	GLU
1	A	296	SER
1	A	297	LEU
1	A	347	THR
1	A	379	GLU
1	B	8	GLU
1	B	218	GLY
1	B	249	GLN
1	B	250	GLY
1	B	273	VAL
1	B	284	VAL
1	B	297	LEU
1	B	303	ASN
1	B	322	VAL
1	B	401	SER
1	C	47	ARG
1	C	75	ASP
1	C	95	HIS
1	C	296	SER
1	C	297	LEU
1	C	347	THR
1	C	351	THR
1	C	373	GLU
1	C	378	GLU
1	D	75	ASP
1	D	250	GLY
1	D	273	VAL
1	D	351	THR

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Mol	Chain	Res	Type
1	A	9	THR
1	A	47	ARG
1	A	198	ASP
1	A	219	THR
1	B	75	ASP
1	B	220	CYS
1	B	269	TYR
1	B	351	THR
1	C	124	GLU
1	C	219	THR
1	D	198	ASP
1	D	249	GLN
1	A	97	SER
1	A	124	GLU
1	A	220	CYS
1	B	44	PRO
1	B	47	ARG
1	B	198	ASP
1	B	200	LYS
1	B	202	ASP
1	B	208	LYS
1	B	295	ASN
1	C	8	GLU
1	C	345	TRP
1	C	348	LEU
1	D	124	GLU
1	D	170	VAL
1	D	200	LYS
1	D	219	THR
1	D	303	ASN
1	D	348	LEU
1	A	44	PRO
1	A	75	ASP
1	A	317	LEU
1	B	154	GLU
1	B	286	THR
1	C	97	SER
1	C	321	GLU
1	D	11	PHE
1	C	27	SER
1	C	200	LYS
1	C	239	ASP

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Mol	Chain	Res	Type
1	D	97	SER
1	D	208	LYS
1	A	218	GLY
1	A	313	ILE
1	A	328	GLY
1	C	158	GLY
1	A	127	ILE
1	B	63	ILE
1	C	218	GLY
1	C	284	VAL
1	A	241	ILE
1	A	274	GLY
1	A	322	VAL
1	B	170	VAL
1	A	158	GLY
1	D	253	GLY

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	343/369 (93%)	307 (90%)	36 (10%)	7 25
1	B	352/369 (95%)	312 (89%)	40 (11%)	5 22
1	C	334/369 (90%)	302 (90%)	32 (10%)	8 29
1	D	352/369 (95%)	319 (91%)	33 (9%)	8 30
All	All	1381/1476 (94%)	1240 (90%)	141 (10%)	7 27

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	10	ARG
1	A	11	PHE
1	A	16	ASN
1	A	20	ASP

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Mol	Chain	Res	Type
1	A	24	GLU
1	A	25	VAL
1	A	47	ARG
1	A	58	ARG
1	A	93	VAL
1	A	95	HIS
1	A	126	ASP
1	A	135	TRP
1	A	164	LEU
1	A	186	LEU
1	A	212	LEU
1	A	219	THR
1	A	223	MET
1	A	225	LYS
1	A	239	ASP
1	A	241	ILE
1	A	246	LEU
1	A	254	TYR
1	A	319	ASP
1	A	321	GLU
1	A	336	LEU
1	A	341	ASP
1	A	342	GLN
1	A	351	THR
1	A	367	ASN
1	A	369	ASP
1	A	370	ASP
1	A	371	LEU
1	A	372	GLU
1	A	381	PHE
1	A	394	PHE
1	B	9	THR
1	B	11	PHE
1	B	18	LEU
1	B	37	LEU
1	B	47	ARG
1	B	53	ASP
1	B	62	THR
1	B	93	VAL
1	B	95	HIS
1	B	123	GLU
1	B	154	GLU

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Mol	Chain	Res	Type
1	B	161	LEU
1	B	162	VAL
1	B	186	LEU
1	B	204	MET
1	B	212	LEU
1	B	219	THR
1	B	223	MET
1	B	225	LYS
1	B	230	ARG
1	B	237	THR
1	B	241	ILE
1	B	246	LEU
1	B	248	SER
1	B	249	GLN
1	B	299	PHE
1	B	302	ASP
1	B	305	ILE
1	B	312	LEU
1	B	319	ASP
1	B	341	ASP
1	B	342	GLN
1	B	351	THR
1	B	363	ILE
1	B	371	LEU
1	B	372	GLU
1	B	377	GLU
1	B	379	GLU
1	B	380	THR
1	B	402	ASN
1	C	8	GLU
1	C	10	ARG
1	C	14	MET
1	C	25	VAL
1	C	31	LEU
1	C	34	LEU
1	C	43	PHE
1	C	63	ILE
1	C	69	LEU
1	C	82	ILE
1	C	93	VAL
1	C	112	MET
1	C	126	ASP

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Mol	Chain	Res	Type
1	C	133	SER
1	C	164	LEU
1	C	212	LEU
1	C	216	ASP
1	C	219	THR
1	C	223	MET
1	C	225	LYS
1	C	226	GLU
1	C	246	LEU
1	C	249	GLN
1	C	299	PHE
1	C	305	ILE
1	C	312	LEU
1	C	336	LEU
1	C	342	GLN
1	C	345	TRP
1	C	372	GLU
1	C	373	GLU
1	C	374	ASP
1	D	13	LYS
1	D	14	MET
1	D	27	SER
1	D	34	LEU
1	D	66	ILE
1	D	72	LYS
1	D	95	HIS
1	D	123	GLU
1	D	126	ASP
1	D	133	SER
1	D	145	ASP
1	D	146	ASP
1	D	153	MET
1	D	189	ILE
1	D	212	LEU
1	D	216	ASP
1	D	223	MET
1	D	225	LYS
1	D	230	ARG
1	D	239	ASP
1	D	248	SER
1	D	281	ASP
1	D	288	SER

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Mol	Chain	Res	Type
1	D	299	PHE
1	D	305	ILE
1	D	312	LEU
1	D	329	VAL
1	D	342	GLN
1	D	349	ARG
1	D	351	THR
1	D	365	THR
1	D	374	ASP
1	D	377	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	196	HIS
1	A	293	HIS
1	A	295	ASN
1	A	311	ASN
1	A	390	ASN
1	B	16	ASN
1	B	51	ASN
1	B	64	ASN
1	B	138	GLN
1	B	190	HIS
1	B	211	HIS
1	B	292	ASN
1	B	295	ASN
1	B	335	HIS
1	B	390	ASN
1	C	26	ASN
1	C	138	GLN
1	C	190	HIS
1	C	196	HIS
1	C	211	HIS
1	C	292	ASN
1	C	295	ASN
1	C	311	ASN
1	C	340	ASN
1	C	342	GLN
1	D	16	ASN
1	D	91	GLN

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Mol	Chain	Res	Type
1	D	138	GLN
1	D	196	HIS
1	D	292	ASN
1	D	295	ASN
1	D	311	ASN
1	D	327	ASN
1	D	342	GLN
1	D	390	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	3ND	D	900	-	28,30,30	1.09	2 (7%)	38,43,43	1.92	8 (21%)
2	3ND	C	900	-	28,30,30	1.10	2 (7%)	38,43,43	1.88	8 (21%)
2	3ND	B	900	-	28,30,30	1.16	3 (10%)	38,43,43	1.95	8 (21%)

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	3ND	D	900	-	-	2/12/32/32	0/3/4/4
2	3ND	C	900	-	-	3/12/32/32	0/3/4/4
2	3ND	B	900	-	-	2/12/32/32	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	900	3ND	C1-N2	3.36	1.36	1.28
2	B	900	3ND	C1-N2	3.36	1.36	1.28
2	C	900	3ND	C1-N2	3.02	1.35	1.28
2	C	900	3ND	C3-N2	-2.65	1.33	1.38
2	B	900	3ND	C18-C17	-2.48	1.48	1.51
2	D	900	3ND	C3-N2	-2.33	1.34	1.38
2	B	900	3ND	C3-N2	-2.27	1.34	1.38

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	900	3ND	C18-C17-C13	-6.49	100.92	114.64
2	D	900	3ND	C18-C17-C13	-6.18	101.57	114.64
2	C	900	3ND	C18-C17-C13	-5.67	102.64	114.64
2	D	900	3ND	C13-C12-N11	5.43	121.18	114.50
2	C	900	3ND	C13-C12-N11	5.13	120.82	114.50
2	B	900	3ND	C13-C12-N11	5.10	120.77	114.50
2	C	900	3ND	C5-C6-C3	-3.66	118.25	120.91
2	D	900	3ND	C5-C6-C3	-3.58	118.31	120.91
2	B	900	3ND	C5-C6-C3	-3.39	118.45	120.91
2	B	900	3ND	C22-C23-C18	-3.26	117.92	121.20
2	D	900	3ND	O27-C12-C13	-3.18	117.89	121.73
2	B	900	3ND	C23-C18-C19	3.09	122.15	118.29
2	D	900	3ND	C22-C23-C18	-3.03	118.14	121.20
2	C	900	3ND	C9-C8-CL26	-3.00	116.13	119.54
2	B	900	3ND	O27-C12-C13	-2.95	118.18	121.73
2	C	900	3ND	C23-C18-C19	2.52	121.44	118.29
2	D	900	3ND	C23-C18-C19	2.47	121.38	118.29
2	D	900	3ND	C9-C8-CL26	-2.47	116.73	119.54
2	C	900	3ND	O27-C12-C13	-2.38	118.86	121.73
2	B	900	3ND	C16-C17-C18	-2.31	111.97	115.03
2	C	900	3ND	O25-C3-N2	-2.13	117.78	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	900	3ND	C6-C3-N2	2.11	120.82	117.88
2	D	900	3ND	C9-N11-C12	-2.07	121.24	126.92
2	B	900	3ND	C7-C8-C9	2.03	123.38	121.72

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	3ND	O27-C12-C13-C17
2	C	900	3ND	O27-C12-C13-C17
2	D	900	3ND	O27-C12-C13-C17
2	B	900	3ND	N11-C12-C13-C17
2	C	900	3ND	N11-C12-C13-C17
2	D	900	3ND	N11-C12-C13-C17
2	C	900	3ND	C8-C9-N11-C12

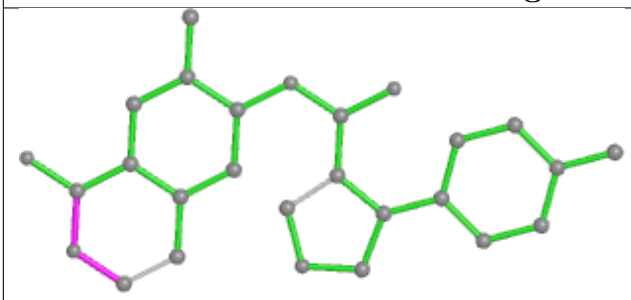
There are no ring outliers.

3 monomers are involved in 16 short contacts:

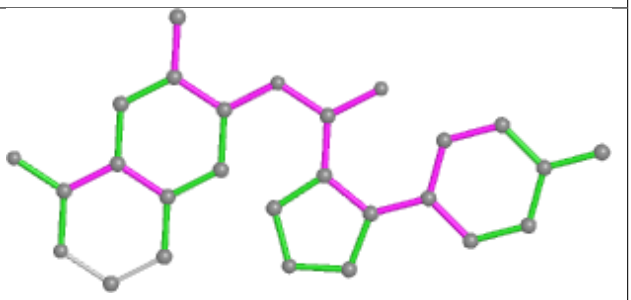
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	3ND	5	0
2	C	900	3ND	4	0
2	B	900	3ND	7	0

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.

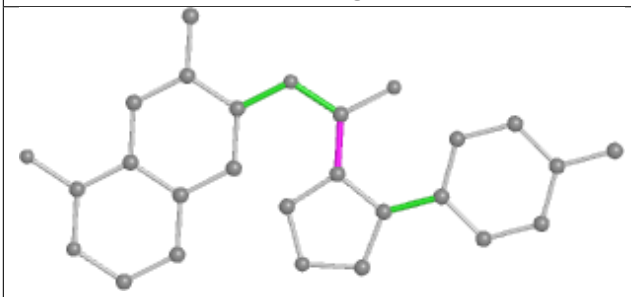
Ligand 3ND D 900



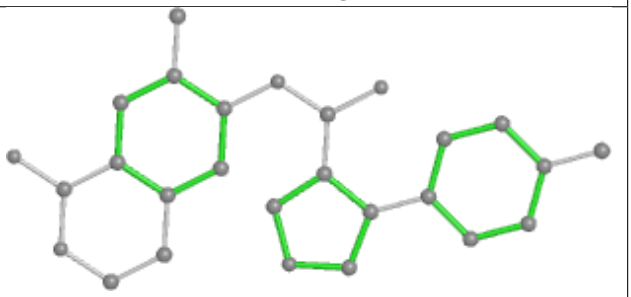
Bond lengths



Bond angles

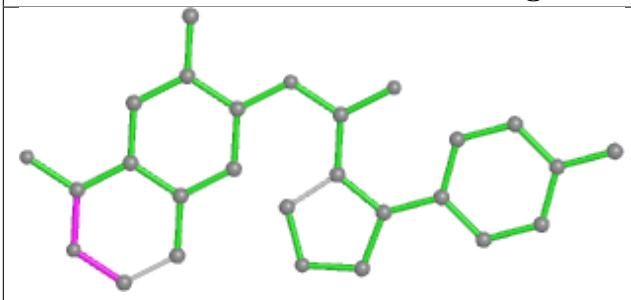


Torsions

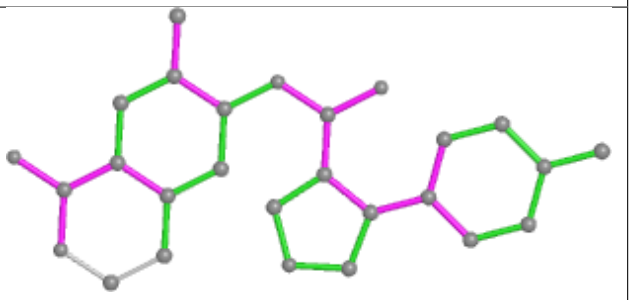


Rings

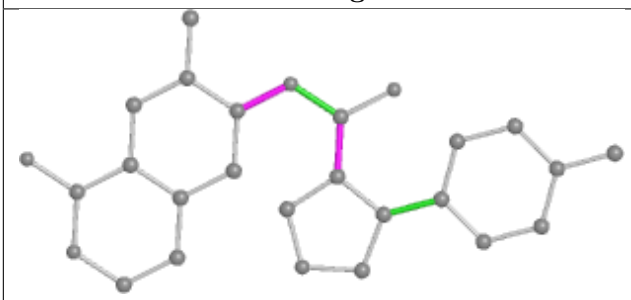
Ligand 3ND C 900



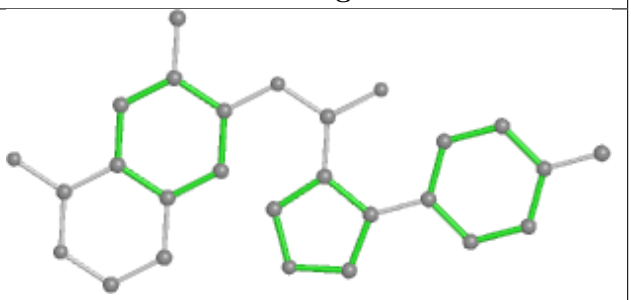
Bond lengths



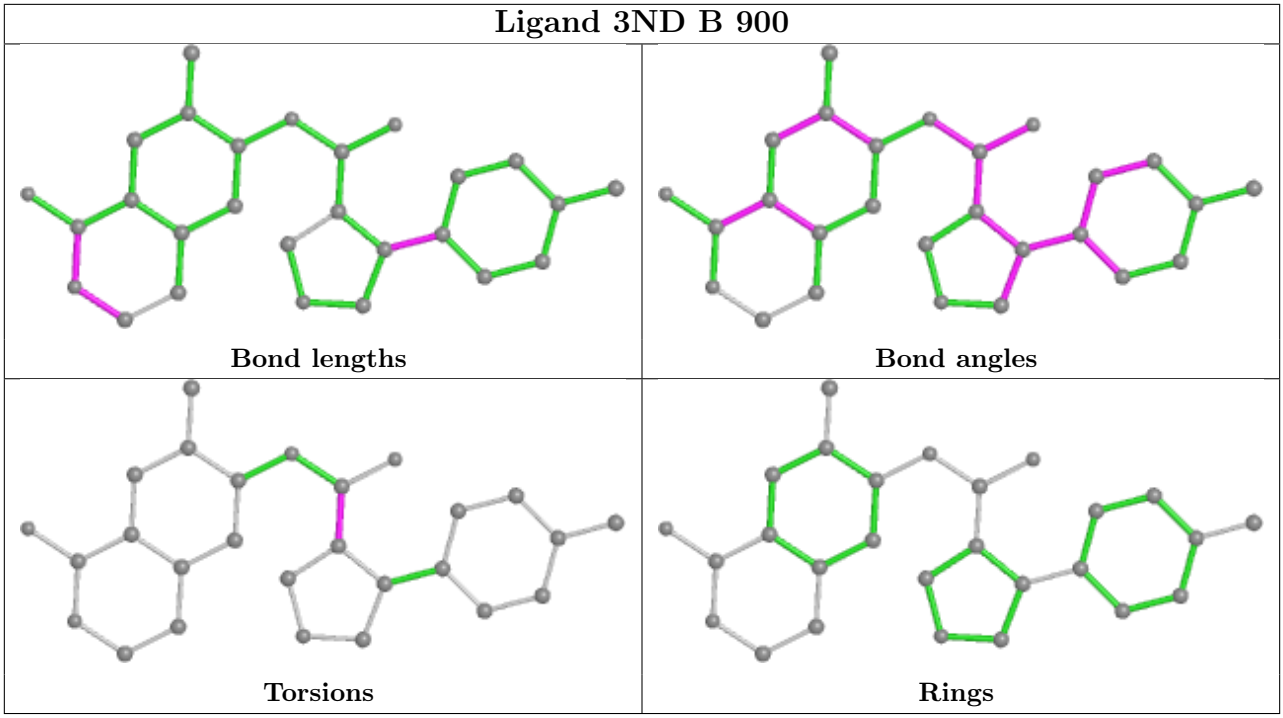
Bond angles



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	383/415 (92%)	0.74	59 (15%)	2	2	102, 200, 300, 366	0
1	B	396/415 (95%)	0.16	11 (2%)	53	51	83, 143, 237, 329	0
1	C	371/415 (89%)	0.44	38 (10%)	6	6	88, 168, 274, 403	0
1	D	396/415 (95%)	0.18	8 (2%)	65	64	82, 153, 232, 336	0
All	All	1546/1660 (93%)	0.38	116 (7%)	14	13	82, 164, 271, 403	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	TYR	6.8
1	A	245	VAL	5.0
1	C	260	ASP	4.9
1	A	336	LEU	4.7
1	A	353	ALA	4.7
1	A	203	ASN	4.5
1	C	245	VAL	4.3
1	C	377	GLU	4.2
1	A	231	CYS	4.1
1	A	268	LEU	4.1
1	C	291	MET	4.1
1	A	76	TYR	4.0
1	A	104	MET	4.0
1	A	327	ASN	4.0
1	A	272	LEU	4.0
1	A	299	PHE	4.0
1	C	317	LEU	4.0
1	A	107	LEU	3.9
1	A	244	GLU	3.8
1	A	338	PHE	3.8
1	C	293	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	7	PHE	3.7
1	D	80	LYS	3.7
1	C	290	ILE	3.6
1	A	359	LEU	3.6
1	A	290	ILE	3.5
1	D	251	GLY	3.4
1	C	313	ILE	3.4
1	C	276	THR	3.3
1	C	248	SER	3.3
1	A	84	ARG	3.3
1	C	262	TRP	3.3
1	C	268	LEU	3.2
1	B	38	VAL	3.2
1	D	226	GLU	3.2
1	C	230	ARG	3.1
1	A	317	LEU	3.1
1	A	402	ASN	3.0
1	A	371	LEU	3.0
1	A	297	LEU	3.0
1	C	376	GLY	2.9
1	B	9	THR	2.9
1	D	326	ARG	2.9
1	C	312	LEU	2.8
1	B	116	SER	2.8
1	A	365	THR	2.8
1	A	199	VAL	2.7
1	A	324	LEU	2.7
1	A	346	GLU	2.7
1	A	87	PHE	2.6
1	A	277	PRO	2.6
1	C	314	CYS	2.6
1	A	357	PRO	2.6
1	C	41	LEU	2.6
1	C	170	VAL	2.6
1	A	132	ASN	2.6
1	A	157	PRO	2.6
1	C	307	LYS	2.5
1	C	176	ARG	2.5
1	A	312	LEU	2.5
1	C	287	TYR	2.5
1	A	316	PHE	2.4
1	C	300	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	118	SER	2.4
1	A	304	ASP	2.4
1	C	231	CYS	2.4
1	C	195	ILE	2.4
1	A	400	TYR	2.4
1	C	225	LYS	2.4
1	A	300	PRO	2.4
1	A	287	TYR	2.4
1	C	263	SER	2.4
1	D	332	ILE	2.4
1	A	337	PHE	2.3
1	C	223	MET	2.3
1	A	235	VAL	2.3
1	A	82	ILE	2.3
1	A	332	ILE	2.3
1	B	139	LEU	2.3
1	A	395	VAL	2.3
1	A	161	LEU	2.3
1	A	81	VAL	2.3
1	A	267	PHE	2.3
1	A	91	GLN	2.3
1	C	244	GLU	2.3
1	A	307	LYS	2.3
1	C	224	ASN	2.2
1	A	155	TYR	2.2
1	A	291	MET	2.2
1	C	271	MET	2.2
1	A	181	GLU	2.2
1	B	251	GLY	2.2
1	A	121	PHE	2.2
1	D	117	ASP	2.2
1	A	355	VAL	2.1
1	A	271	MET	2.1
1	C	272	LEU	2.1
1	C	400	TYR	2.1
1	B	104	MET	2.1
1	A	392	LEU	2.1
1	A	10	ARG	2.1
1	B	117	ASP	2.1
1	C	269	TYR	2.1
1	A	381	PHE	2.1
1	B	10	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	368	PHE	2.1
1	C	350	ASP	2.1
1	D	118	SER	2.0
1	B	299	PHE	2.0
1	C	316	PHE	2.0
1	C	261	TRP	2.0
1	C	369	ASP	2.0
1	A	232	ASP	2.0
1	A	309	ALA	2.0
1	B	141	TYR	2.0
1	D	76	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

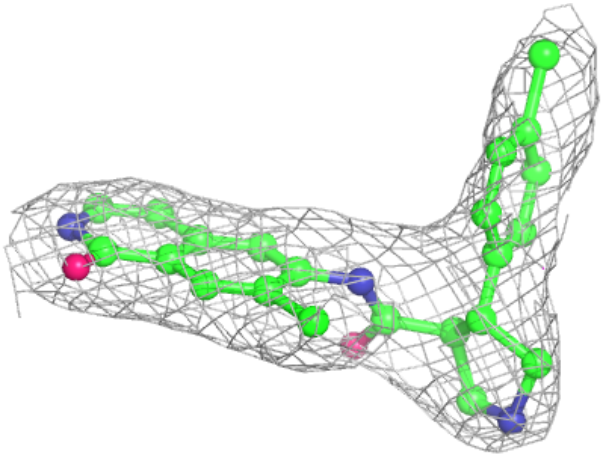
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

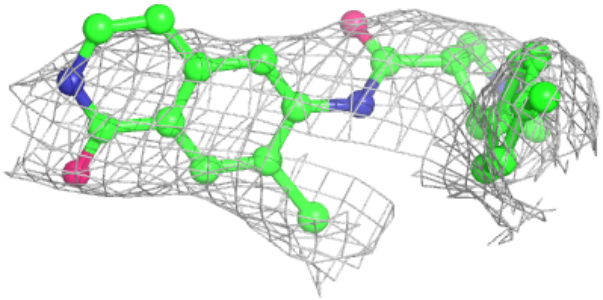
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	3ND	D	900	27/27	0.88	0.33	150,150,150,150	0
2	3ND	B	900	27/27	0.90	0.28	142,142,142,142	0
2	3ND	C	900	27/27	0.92	0.25	138,138,138,138	0

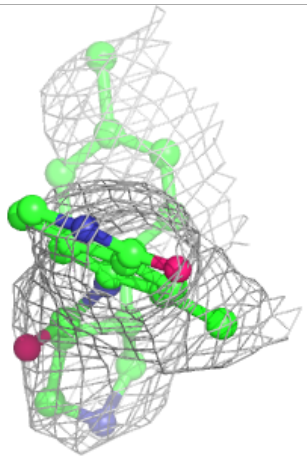
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3ND D 900:

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

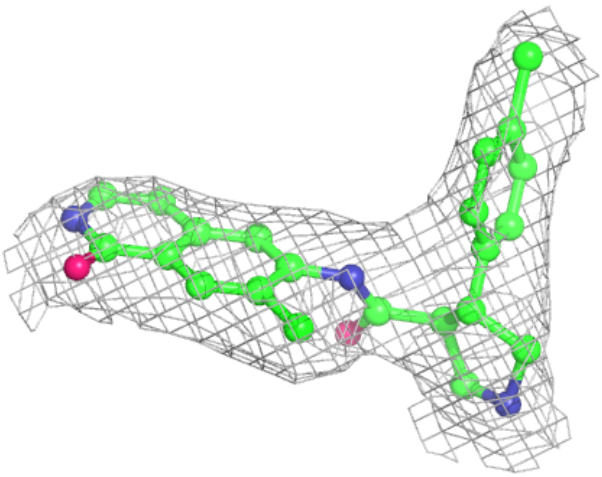


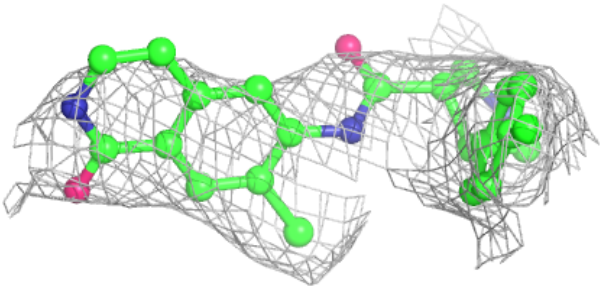


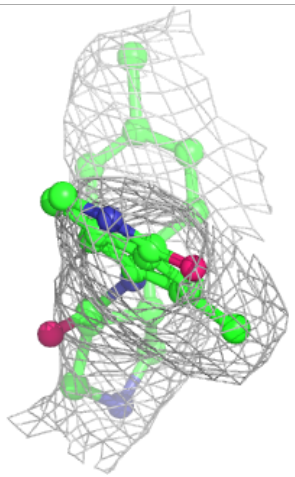


Electron density around 3ND B 900:

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

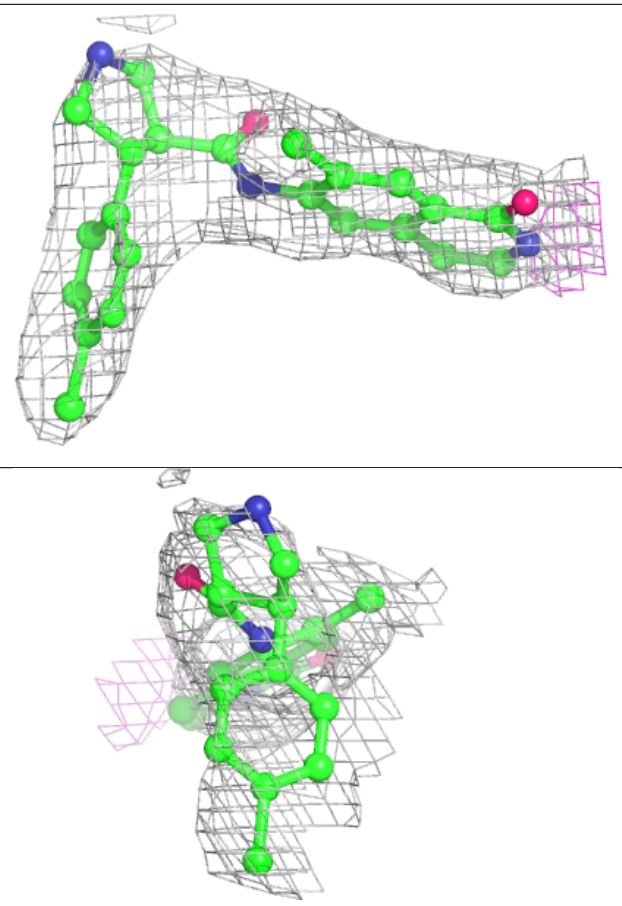






Electron density around 3ND C 900:

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



6.5 Other polymers (i)

There are no such residues in this entry.