Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 05:51 PM EDT

PDB ID	:	1IXR
Title	:	RuvA-RuvB complex
Authors	:	Yamada, K.; Miyata, T.; Tsuchiya, D.; Oyama, T.; Fujiwara, Y.; Ohnishi, T.; Iwasaki, H.; Shinagawa, H.; Ariyoshi, M.; Mayanagi, K.; Morikawa, K.
Deposited on	:	2002-07-04
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 ⓘ symbol.

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

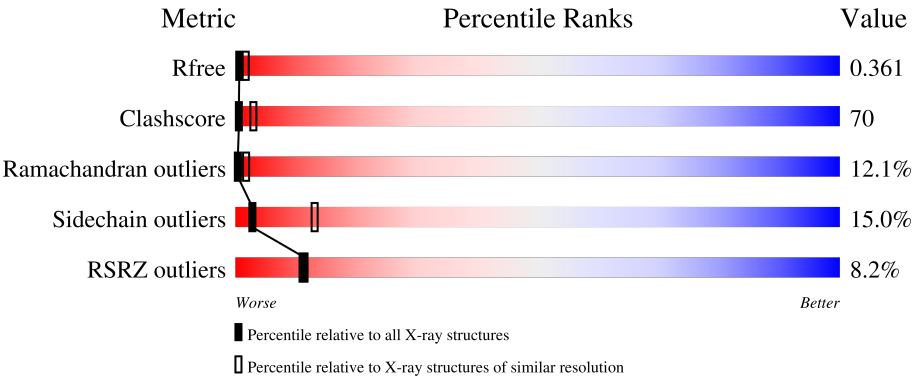
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	191	2% 19% 41% 10% • 29%
1	B	191	2% 29% 50% 19% •
2	C	312	15% 19% 61% 17% ••

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4904 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 Holliday junction DNA helicase ruvA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1018	665	175	177	1			
1	B	191	Total	C	N	O	S	0	0	0
			1440	929	252	257	2			

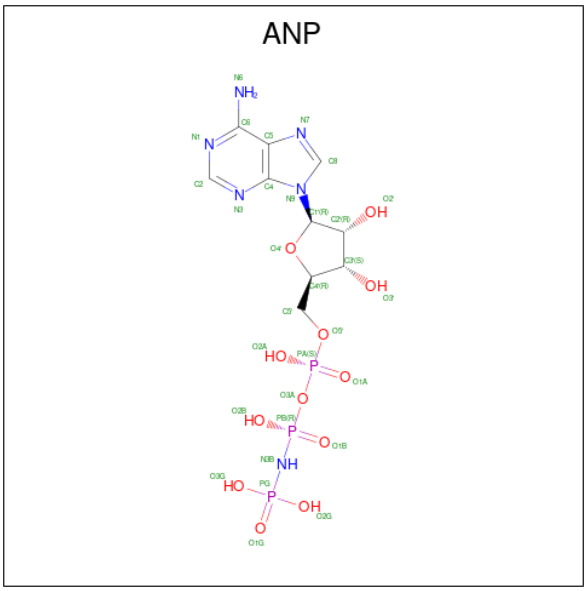
- Molecule 2 is a protein called RuvB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	308	Total	C	N	O	S	0	0	0
			2415	1528	445	438	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	309	ARG	TYR	engineered mutation	UNP Q5SL87

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



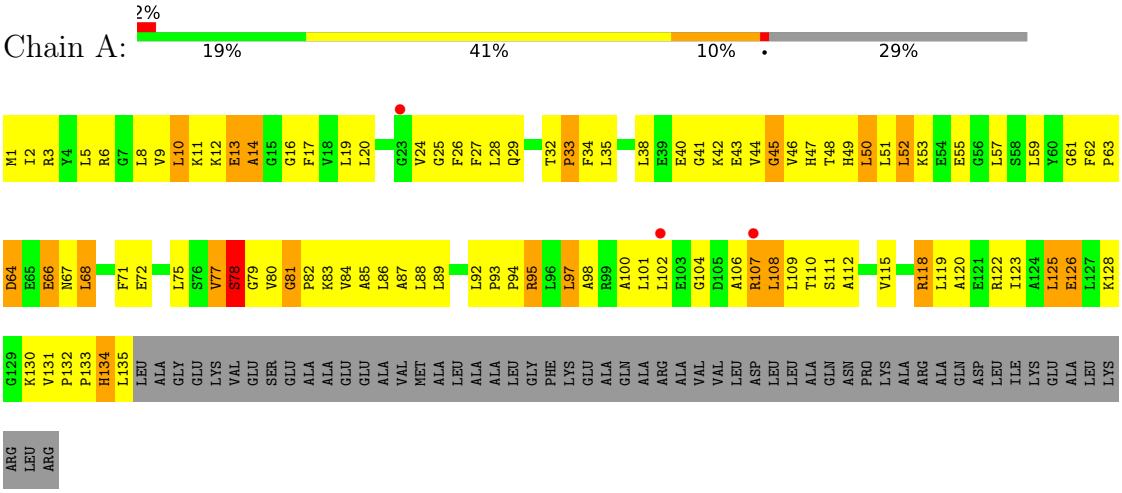
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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.

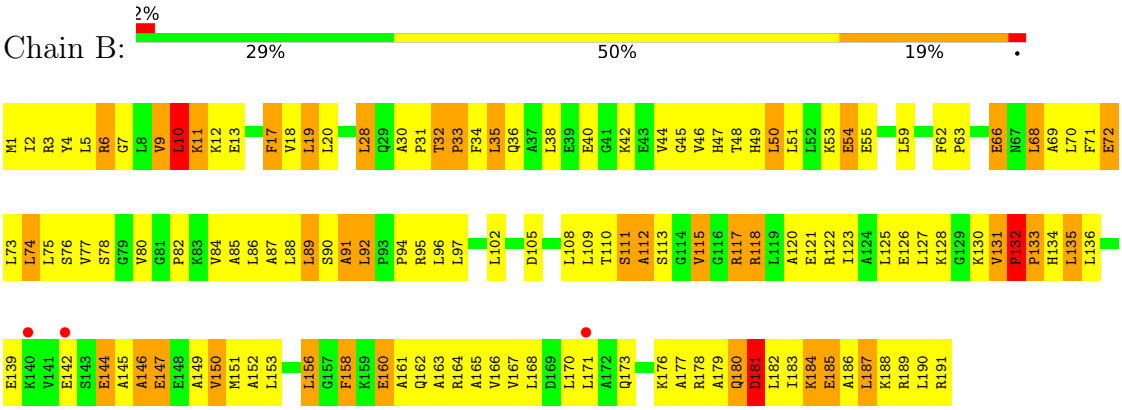
• Molecule 1: Holliday junction DNA helicase ruvA

Chain A:



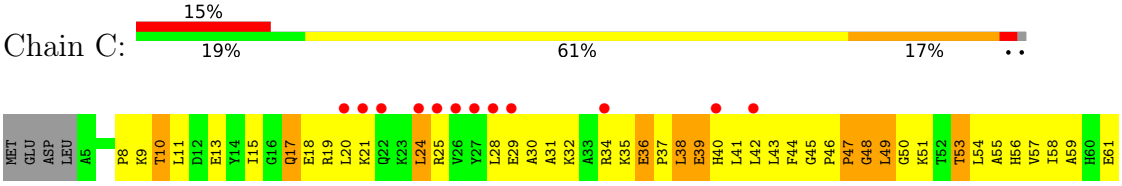
• Molecule 1: Holliday junction DNA helicase ruvA

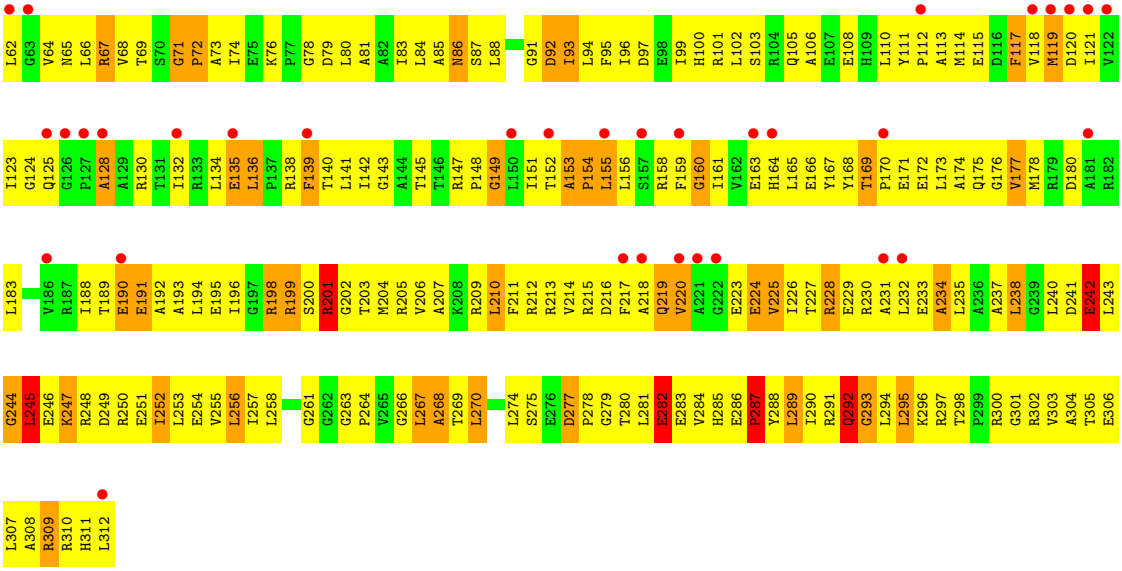
Chain B:



• Molecule 2: RuvB

Chain C:




L62 G63 V64 N65 L66 R67 V68 T69 S70 G71 P72 A73 I74 E75 K76 P77 G78 D79 L80 A81 A82 I83 L84 A85 N86 S87 L88 G91 D92 I93 L94 F95 I96 D97 E98 I99 H100 R101 L102 S103 R104 Q105 A106 E107 E108 H109 L110 Y111 P112 A113 M114 E115 D116 F117 V118 M119 D120 I121 V122
I123 G124 Q125 G126 P127 A128 A129 R130 T131 I132 R133 L134 E135 L136 P137 R138 F139 T140 L141 I142 G143 A144 T145 T146 R147 P148 G149 L150 I151 T152 A153 P154 L155 L156 S157 R158 F159 G160 I161 V162 E163 H164 L165 E166 Y167 Y168 T169 P170 E171 E172 L173 A174 Q175 G176 V177 M178 R179 D180 A181 R182
L183 V186 R187 I188 T189 E190 E191 A192 A193 L194 E195 I196 G197 R198 R199 S200 R201 G202 T203 M204 R205 V206 A207 R208 R209 L210 F211 R212 R213 V214 R215 D216 F217 A218 Q219 V220 A221 G222 E223 E224 V225 I226 T227 R228 E229 R230 A231 L232 E233 A234 L235 A236 A237 L238 G239 L240 D241 E242 L243
G244 L245 E246 K247 R248 D249 R250 E251 T252 L253 E254 V255 L256 I257 L258 G261 G262 G263 P264 V265 G266 L267 A268 T269 L270 L274 S275 E276 D277 P278 G279 T280 L281 E282 E283 V284 H285 E286 P287 Y288 L289 I290 R291 Q292 G293 L294 L295 K296 R297 T298 P299 R300 G301 R302 V303 A304 T305 E306
L307 A308 R309 R310 H311 L312

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	61.58Å 195.11Å 246.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.30 42.03 – 3.19	Depositor EDS
% Data completeness (in resolution range)	89.4 (12.00-3.30) 97.4 (42.03-3.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.268 , 0.335 0.281 , 0.361	Depositor DCC
R_{free} test set	1195 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	92.1	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 118.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	4904	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: ANP

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	0.56	0/1036	0.89	3/1400 (0.2%)
1	B	0.50	0/1460	0.86	2/1968 (0.1%)
2	C	0.39	0/2452	0.71	0/3311
All	All	0.47	0/4948	0.80	5/6679 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	131	VAL	C-N-CD	-14.28	89.18	120.60
1	A	79	GLY	N-CA-C	-7.51	94.32	113.10
1	B	131	VAL	C-N-CA	6.63	149.84	122.00
1	A	45	GLY	N-CA-C	-5.42	99.55	113.10
1	A	29	GLN	N-CA-C	-5.20	96.96	111.00

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	1018	0	1090	119	0
1	B	1440	0	1539	193	0
2	C	2415	0	2515	401	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	31	0	13	1	0
All	All	4904	0	5157	701	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 70.

All (701) 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)
2:C:264:PRO:HA	2:C:302:ARG:O	1.46	1.14
1:B:73:LEU:O	1:B:76:SER:HB3	1.54	1.08
1:A:78:SER:HB2	1:A:122:ARG:HH22	1.16	1.07
2:C:119:MET:HB2	2:C:136:LEU:HD11	1.36	1.04
2:C:306:GLU:HA	2:C:309:ARG:HD3	1.34	1.04
2:C:136:LEU:HD12	2:C:136:LEU:H	1.19	1.03
2:C:298:THR:HG22	2:C:300:ARG:H	1.23	1.02
2:C:189:THR:HG22	2:C:227:THR:HA	1.40	1.02
1:B:153:LEU:HD23	1:B:163:ALA:HB1	1.39	1.02
1:A:118:ARG:HD3	1:A:118:ARG:H	1.20	1.01
1:B:96:LEU:HD21	1:B:108:LEU:HD11	1.39	1.01
2:C:58:ILE:HG22	2:C:62:LEU:HD11	1.37	1.00
1:B:10:LEU:HB3	1:B:18:VAL:HG23	1.44	0.98
2:C:68:VAL:HG12	2:C:95:PHE:HB3	1.46	0.98
1:B:110:THR:O	1:B:115:VAL:HG12	1.62	0.97
2:C:195:GLU:OE2	2:C:232:LEU:HD12	1.66	0.95
2:C:238:LEU:C	2:C:240:LEU:H	1.73	0.93
2:C:66:LEU:HD13	2:C:93:ILE:HB	1.53	0.89
1:B:151:MET:HB3	2:C:123:ILE:HD11	1.53	0.88
2:C:295:LEU:HD12	2:C:296:LYS:N	1.88	0.88
2:C:79:ASP:O	2:C:83:ILE:HG13	1.74	0.88
2:C:286:GLU:CD	2:C:302:ARG:HE	1.78	0.87
2:C:42:LEU:HD12	2:C:143:GLY:O	1.72	0.87
2:C:58:ILE:O	2:C:62:LEU:HG	1.75	0.87
2:C:253:LEU:O	2:C:257:ILE:HG22	1.76	0.86
2:C:195:GLU:OE2	2:C:232:LEU:HB2	1.75	0.86
2:C:295:LEU:HD12	2:C:296:LYS:H	1.41	0.85
1:A:78:SER:HB2	1:A:122:ARG:NH2	1.88	0.85
2:C:25:ARG:HA	2:C:28:LEU:HD12	1.58	0.85
1:A:50:LEU:HD12	1:A:51:LEU:N	1.92	0.85
1:A:9:VAL:HG21	1:A:38:LEU:HD11	1.60	0.84
2:C:64:VAL:HG11	2:C:91:GLY:HA3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:232:LEU:O	2:C:232:LEU:HD23	1.77	0.83
2:C:203:THR:HB	2:C:206:VAL:HG22	1.61	0.83
2:C:189:THR:CG2	2:C:227:THR:HA	2.08	0.83
1:A:81:GLY:HA3	1:A:84:VAL:HG23	1.61	0.82
1:B:163:ALA:O	1:B:167:VAL:HG23	1.78	0.82
2:C:311:HIS:O	2:C:312:LEU:HB2	1.79	0.82
2:C:250:ARG:HD2	2:C:254:GLU:OE2	1.78	0.82
2:C:95:PHE:HE1	2:C:97:ASP:HB2	1.44	0.81
2:C:210:LEU:O	2:C:214:VAL:HG23	1.81	0.81
2:C:117:PHE:HB2	2:C:136:LEU:O	1.80	0.81
1:A:32:THR:HB	1:A:33:PRO:HD3	1.63	0.81
2:C:191:GLU:HB2	2:C:228:ARG:HH11	1.43	0.81
2:C:56:HIS:HA	2:C:66:LEU:HD23	1.62	0.80
2:C:17:GLN:HG2	2:C:19:ARG:H	1.46	0.80
1:B:12:LYS:O	1:B:13:GLU:HG3	1.81	0.80
2:C:201:ARG:H	2:C:201:ARG:HD3	1.47	0.80
2:C:136:LEU:H	2:C:136:LEU:CD1	1.96	0.79
2:C:168:TYR:O	2:C:173:LEU:HG	1.83	0.79
2:C:270:LEU:HD11	2:C:274:LEU:HD12	1.62	0.78
1:A:75:LEU:O	1:A:80:VAL:HG13	1.84	0.78
2:C:248:ARG:O	2:C:252:ILE:HG13	1.84	0.78
1:B:153:LEU:CD2	1:B:163:ALA:HB1	2.14	0.78
1:A:95:ARG:HD3	1:A:95:ARG:H	1.48	0.77
1:B:153:LEU:HD23	1:B:163:ALA:CB	2.14	0.77
2:C:136:LEU:HD12	2:C:136:LEU:N	1.99	0.77
1:B:28:LEU:N	1:B:28:LEU:HD23	1.99	0.77
2:C:99:ILE:O	2:C:102:LEU:HG	1.85	0.77
1:B:150:VAL:HG22	1:B:167:VAL:HG21	1.66	0.77
1:A:130:LYS:O	1:A:132:PRO:HD3	1.84	0.76
1:B:92:LEU:HD23	1:B:92:LEU:H	1.50	0.76
2:C:80:LEU:HD23	2:C:80:LEU:H	1.46	0.76
1:A:68:LEU:O	1:A:68:LEU:HD12	1.86	0.76
1:A:68:LEU:HD12	1:A:68:LEU:C	2.06	0.76
2:C:201:ARG:C	2:C:291:ARG:HH22	1.89	0.76
1:B:53:LYS:HG2	1:B:54:GLU:H	1.49	0.75
1:A:102:LEU:N	1:A:131:VAL:HG21	2.02	0.75
2:C:191:GLU:O	2:C:194:LEU:HB2	1.86	0.75
1:B:10:LEU:HB3	1:B:18:VAL:CG2	2.16	0.75
2:C:191:GLU:HB2	2:C:228:ARG:NH1	2.00	0.75
2:C:238:LEU:C	2:C:240:LEU:N	2.38	0.75
2:C:284:VAL:HG12	2:C:284:VAL:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:LEU:H	1:B:70:LEU:HD22	1.52	0.75
2:C:195:GLU:OE2	2:C:232:LEU:CD1	2.35	0.75
2:C:267:LEU:HD11	2:C:282:GLU:HB3	1.70	0.74
2:C:282:GLU:HA	2:C:286:GLU:HB2	1.70	0.74
2:C:9:LYS:HB3	2:C:57:VAL:HG13	1.68	0.74
1:A:118:ARG:H	1:A:118:ARG:CD	1.97	0.74
2:C:173:LEU:HD11	2:C:203:THR:N	2.02	0.74
2:C:30:ALA:O	2:C:34:ARG:HG2	1.88	0.73
2:C:173:LEU:O	2:C:177:VAL:HG23	1.88	0.73
2:C:9:LYS:HG2	2:C:57:VAL:HG22	1.70	0.73
1:B:131:VAL:HG12	1:B:132:PRO:CG	2.18	0.73
2:C:288:TYR:CZ	2:C:292:GLN:HG3	2.23	0.73
2:C:238:LEU:O	2:C:240:LEU:HG	1.88	0.73
1:A:59:LEU:HD13	1:B:1:MET:HG3	1.70	0.73
2:C:25:ARG:O	2:C:29:GLU:HG3	1.89	0.73
1:B:66:GLU:O	1:B:69:ALA:HB3	1.90	0.72
2:C:55:ALA:HA	2:C:58:ILE:CG1	2.17	0.72
2:C:306:GLU:HA	2:C:309:ARG:CD	2.17	0.72
2:C:167:TYR:HB3	2:C:202:GLY:HA3	1.71	0.72
1:B:158:PHE:CD1	1:B:190:LEU:HD13	2.25	0.72
2:C:200:SER:OG	2:C:207:ALA:HA	1.90	0.72
1:B:34:PHE:HB2	1:B:63:PRO:HG3	1.71	0.72
2:C:100:HIS:CE1	2:C:101:ARG:HG3	2.26	0.71
2:C:55:ALA:HA	2:C:58:ILE:HB	1.72	0.71
1:B:144:GLU:HG2	1:B:147:GLU:H	1.55	0.71
1:B:50:LEU:HD23	1:B:51:LEU:H	1.55	0.70
2:C:42:LEU:O	2:C:43:LEU:HD23	1.91	0.70
1:A:78:SER:CB	1:A:122:ARG:HH22	1.99	0.70
1:B:173:GLN:HE22	1:B:189:ARG:HH22	1.39	0.70
1:B:50:LEU:CD2	1:B:51:LEU:H	2.04	0.70
2:C:201:ARG:NH1	2:C:288:TYR:CD2	2.59	0.70
2:C:209:ARG:N	2:C:212:ARG:HH21	1.90	0.70
2:C:198:ARG:HD2	2:C:243:LEU:HD11	1.74	0.69
1:B:108:LEU:HD23	1:B:108:LEU:O	1.93	0.69
2:C:245:LEU:HD11	2:C:294:LEU:CD1	2.22	0.69
2:C:55:ALA:HA	2:C:58:ILE:CB	2.23	0.69
2:C:242:GLU:OE1	2:C:245:LEU:HB2	1.92	0.69
2:C:55:ALA:HA	2:C:58:ILE:HG13	1.75	0.69
1:A:133:PRO:O	1:A:135:LEU:N	2.26	0.68
2:C:199:ARG:HG2	2:C:199:ARG:HH11	1.57	0.68
2:C:153:ALA:HB1	2:C:154:PRO:HD2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:225:VAL:O	2:C:230:ARG:HD3	1.93	0.68
2:C:46:PRO:HG2	2:C:49:LEU:HD11	1.76	0.68
2:C:46:PRO:HG3	2:C:167:TYR:CZ	2.29	0.68
2:C:201:ARG:H	2:C:201:ARG:CD	2.06	0.68
1:B:151:MET:HB3	2:C:123:ILE:CD1	2.24	0.67
2:C:192:ALA:HB1	2:C:231:ALA:HB2	1.74	0.67
1:B:73:LEU:HD11	1:B:127:LEU:HD13	1.76	0.67
1:A:25:GLY:HA3	1:B:4:TYR:HB3	1.76	0.67
1:B:28:LEU:HD23	1:B:28:LEU:H	1.59	0.67
2:C:306:GLU:O	2:C:309:ARG:HG2	1.95	0.67
1:A:119:LEU:O	1:A:123:ILE:HG13	1.94	0.67
2:C:81:ALA:HA	2:C:84:LEU:HD12	1.76	0.67
2:C:298:THR:HG22	2:C:300:ARG:N	2.04	0.67
1:A:88:LEU:HD23	1:A:112:ALA:HB2	1.77	0.67
2:C:245:LEU:HD11	2:C:294:LEU:HD13	1.76	0.67
2:C:48:GLY:HA3	2:C:203:THR:CG2	2.25	0.67
2:C:61:GLU:O	2:C:62:LEU:HD23	1.95	0.66
2:C:40:HIS:HB2	2:C:160:GLY:H	1.59	0.66
2:C:64:VAL:HG11	2:C:91:GLY:CA	2.25	0.66
2:C:11:LEU:HD11	2:C:21:LYS:HE2	1.76	0.66
2:C:59:ALA:HB1	2:C:64:VAL:O	1.95	0.66
2:C:93:ILE:HG23	2:C:140:THR:OG1	1.94	0.66
2:C:119:MET:HB2	2:C:136:LEU:CD1	2.21	0.66
1:A:63:PRO:HG2	1:A:67:ASN:HD22	1.61	0.66
2:C:252:ILE:HG23	2:C:274:LEU:HD11	1.78	0.66
2:C:125:GLN:HE21	2:C:125:GLN:HA	1.61	0.66
1:B:28:LEU:HB3	1:B:59:LEU:HB3	1.77	0.65
1:B:131:VAL:HG12	1:B:132:PRO:HG3	1.78	0.65
2:C:191:GLU:OE1	2:C:228:ARG:HB2	1.96	0.65
1:B:112:ALA:H	1:B:115:VAL:HG12	1.61	0.65
2:C:247:LYS:O	2:C:251:GLU:HG3	1.97	0.65
1:B:183:ILE:HG22	1:B:184:LYS:N	2.11	0.65
1:B:70:LEU:HD22	1:B:70:LEU:N	2.12	0.65
2:C:48:GLY:HA3	2:C:203:THR:HG23	1.78	0.65
2:C:65:ASN:O	2:C:93:ILE:HD12	1.96	0.65
1:A:102:LEU:HB2	1:A:131:VAL:HB	1.79	0.64
1:A:43:GLU:HG2	1:A:44:VAL:H	1.61	0.64
1:A:52:LEU:HD12	1:A:52:LEU:C	2.17	0.64
2:C:48:GLY:O	2:C:50:GLY:N	2.29	0.64
2:C:145:THR:HB	2:C:148:PRO:HG3	1.80	0.64
2:C:93:ILE:HD12	2:C:93:ILE:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLU:O	1:B:130:LYS:HE2	1.98	0.64
2:C:24:LEU:O	2:C:28:LEU:HG	1.98	0.64
2:C:103:SER:HB2	2:C:106:ALA:CB	2.27	0.64
2:C:188:ILE:HB	2:C:226:ILE:CD1	2.27	0.64
2:C:233:GLU:C	2:C:235:LEU:H	2.00	0.64
2:C:111:TYR:O	2:C:114:MET:HB3	1.98	0.64
2:C:101:ARG:O	2:C:102:LEU:HD23	1.97	0.64
2:C:93:ILE:HD12	2:C:93:ILE:H	1.63	0.64
2:C:68:VAL:CG1	2:C:95:PHE:HB3	2.26	0.63
2:C:64:VAL:HB	2:C:92:ASP:HA	1.78	0.63
2:C:201:ARG:HB3	2:C:291:ARG:NH1	2.14	0.63
2:C:270:LEU:CD1	2:C:274:LEU:HD12	2.28	0.63
1:B:12:LYS:HD2	1:B:38:LEU:O	1.97	0.63
2:C:46:PRO:HG2	2:C:49:LEU:CD1	2.29	0.63
2:C:277:ASP:O	2:C:280:THR:N	2.32	0.63
1:A:19:LEU:C	1:A:19:LEU:HD23	2.19	0.63
1:A:28:LEU:N	1:A:28:LEU:HD12	2.14	0.63
2:C:285:HIS:C	2:C:287:PRO:HD2	2.19	0.63
2:C:69:THR:O	2:C:96:ILE:HA	1.98	0.63
2:C:223:GLU:O	2:C:224:GLU:C	2.37	0.63
2:C:294:LEU:O	2:C:305:THR:HG22	1.98	0.63
2:C:288:TYR:HA	2:C:291:ARG:CG	2.27	0.63
1:A:106:ALA:C	1:A:108:LEU:H	2.02	0.63
1:A:125:LEU:C	1:A:125:LEU:HD23	2.19	0.62
2:C:192:ALA:HB2	2:C:228:ARG:N	2.13	0.62
1:A:47:HIS:CE1	1:A:64:ASP:HA	2.34	0.62
1:B:6:ARG:HH11	1:B:6:ARG:HB3	1.63	0.62
2:C:51:LYS:HE2	2:C:165:LEU:HD12	1.80	0.62
1:B:72:GLU:O	1:B:75:LEU:N	2.33	0.62
2:C:192:ALA:O	2:C:195:GLU:N	2.32	0.62
2:C:241:ASP:HB3	2:C:246:GLU:HB2	1.82	0.62
1:B:134:HIS:NE2	1:B:139:GLU:HB2	2.15	0.62
2:C:56:HIS:HA	2:C:66:LEU:CD2	2.28	0.62
1:B:109:LEU:HB2	1:B:120:ALA:HB1	1.81	0.61
2:C:20:LEU:HD22	2:C:163:GLU:OE1	2.01	0.61
1:B:74:LEU:HD12	1:B:80:VAL:HG11	1.80	0.61
2:C:288:TYR:OH	2:C:292:GLN:HG3	2.01	0.61
1:A:95:ARG:H	1:A:95:ARG:CD	2.10	0.61
1:B:70:LEU:H	1:B:70:LEU:CD2	2.13	0.61
2:C:101:ARG:C	2:C:102:LEU:HD23	2.20	0.61
2:C:30:ALA:C	2:C:32:LYS:H	2.02	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:LEU:HD12	2:C:93:ILE:O	2.01	0.61
2:C:68:VAL:HG12	2:C:95:PHE:CB	2.28	0.61
1:B:9:VAL:O	1:B:11:LYS:N	2.34	0.61
1:A:50:LEU:HD12	1:A:50:LEU:C	2.19	0.61
1:B:92:LEU:HD13	1:B:108:LEU:HD21	1.81	0.61
2:C:188:ILE:HA	2:C:226:ILE:HG13	1.82	0.61
2:C:210:LEU:HD12	2:C:210:LEU:H	1.64	0.61
2:C:201:ARG:HG2	2:C:288:TYR:CG	2.36	0.60
2:C:229:GLU:O	2:C:233:GLU:HB2	2.00	0.60
2:C:21:LYS:O	2:C:25:ARG:HG2	2.00	0.60
2:C:24:LEU:HD23	2:C:28:LEU:HD11	1.83	0.60
2:C:41:LEU:HB3	2:C:142:ILE:HD13	1.83	0.60
2:C:103:SER:HB2	2:C:106:ALA:HB2	1.83	0.60
2:C:189:THR:HG23	2:C:192:ALA:CB	2.31	0.60
2:C:200:SER:O	2:C:202:GLY:N	2.34	0.60
1:B:36:GLN:C	1:B:38:LEU:H	2.05	0.60
1:A:47:HIS:ND1	1:A:64:ASP:HA	2.17	0.60
1:B:180:GLN:NE2	2:C:135:GLU:HB2	2.17	0.60
2:C:34:ARG:HG3	2:C:35:LYS:H	1.67	0.60
1:A:28:LEU:HG	1:A:59:LEU:HB3	1.84	0.60
1:A:133:PRO:O	1:A:135:LEU:HG	2.01	0.60
1:B:32:THR:O	1:B:33:PRO:C	2.40	0.60
1:B:184:LYS:O	1:B:186:ALA:N	2.34	0.60
1:B:136:LEU:HD22	1:B:136:LEU:N	2.16	0.60
2:C:230:ARG:HA	2:C:233:GLU:HB3	1.82	0.60
2:C:267:LEU:HD11	2:C:282:GLU:CB	2.31	0.60
2:C:35:LYS:NZ	2:C:138:ARG:HH21	2.01	0.59
2:C:58:ILE:CG2	2:C:62:LEU:HD11	2.24	0.59
2:C:153:ALA:HB1	2:C:154:PRO:CD	2.32	0.59
2:C:198:ARG:O	2:C:198:ARG:HD3	2.00	0.59
1:A:10:LEU:HD13	1:A:20:LEU:HD13	1.85	0.59
2:C:49:LEU:HG	2:C:166:GLU:O	2.02	0.59
2:C:204:MET:O	2:C:207:ALA:HB3	2.03	0.59
1:A:46:VAL:HG21	1:A:61:GLY:HA3	1.84	0.59
2:C:198:ARG:CD	2:C:243:LEU:HD11	2.32	0.59
2:C:210:LEU:HD13	2:C:211:PHE:CE2	2.38	0.59
1:B:72:GLU:O	1:B:73:LEU:C	2.41	0.58
2:C:191:GLU:HA	2:C:194:LEU:HD23	1.84	0.58
1:A:77:VAL:HG13	1:A:126:GLU:HG2	1.86	0.58
1:B:164:ARG:O	1:B:168:LEU:HD23	2.03	0.58
2:C:35:LYS:HZ3	2:C:138:ARG:HH21	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:119:MET:CB	2:C:136:LEU:HD11	2.22	0.58
2:C:83:ILE:CG2	2:C:94:LEU:HD21	2.33	0.58
1:B:17:PHE:CZ	1:B:19:LEU:HD12	2.38	0.58
1:B:156:LEU:HD21	2:C:121:ILE:HG21	1.85	0.58
2:C:199:ARG:HG3	2:C:244:GLY:H	1.68	0.58
1:A:43:GLU:HG2	1:A:44:VAL:N	2.19	0.58
1:B:132:PRO:HB2	1:B:135:LEU:HB3	1.86	0.58
1:A:125:LEU:HD23	1:A:125:LEU:O	2.03	0.58
2:C:9:LYS:HD3	2:C:57:VAL:HA	1.86	0.58
1:B:132:PRO:O	1:B:132:PRO:CD	2.51	0.57
1:A:97:LEU:HD22	1:A:101:LEU:HG	1.87	0.57
2:C:188:ILE:HA	2:C:226:ILE:O	2.05	0.57
2:C:245:LEU:H	2:C:245:LEU:HD23	1.69	0.57
2:C:199:ARG:NH1	2:C:235:LEU:HD21	2.20	0.57
2:C:290:ILE:HD11	2:C:297:ARG:HG3	1.85	0.57
1:A:32:THR:HB	1:A:33:PRO:CD	2.33	0.57
2:C:41:LEU:HB3	2:C:142:ILE:CD1	2.35	0.57
2:C:204:MET:HA	2:C:207:ALA:HB3	1.86	0.57
2:C:298:THR:CG2	2:C:300:ARG:H	2.09	0.57
1:A:118:ARG:HD3	1:A:118:ARG:N	2.05	0.57
2:C:279:GLY:O	2:C:283:GLU:HB2	2.05	0.57
2:C:288:TYR:HA	2:C:291:ARG:HG3	1.87	0.57
1:B:173:GLN:HE22	1:B:189:ARG:NH2	2.03	0.56
1:B:108:LEU:HD23	1:B:108:LEU:C	2.24	0.56
1:B:144:GLU:OE1	1:B:147:GLU:HB2	2.05	0.56
2:C:95:PHE:CE1	2:C:97:ASP:HB2	2.33	0.56
2:C:141:LEU:HD23	2:C:142:ILE:N	2.19	0.56
2:C:200:SER:HA	2:C:206:VAL:HG23	1.87	0.56
2:C:282:GLU:HA	2:C:286:GLU:CB	2.35	0.56
1:B:28:LEU:N	1:B:28:LEU:CD2	2.69	0.56
2:C:118:VAL:C	2:C:136:LEU:HD13	2.25	0.56
1:B:156:LEU:HD21	2:C:121:ILE:CG2	2.35	0.56
1:A:8:LEU:HD12	1:A:42:LYS:O	2.05	0.56
1:B:9:VAL:HB	1:B:40:GLU:HA	1.87	0.56
1:B:185:GLU:OE2	1:B:188:LYS:HD3	2.06	0.56
1:A:68:LEU:C	1:A:68:LEU:CD1	2.74	0.56
1:A:119:LEU:HG	1:A:123:ILE:HD11	1.87	0.56
2:C:242:GLU:OE2	2:C:243:LEU:N	2.38	0.56
2:C:264:PRO:CA	2:C:303:VAL:HG12	2.35	0.56
1:B:131:VAL:CG1	1:B:132:PRO:HB3	2.36	0.56
2:C:145:THR:HG22	2:C:147:ARG:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HG22	1:A:46:VAL:HG12	1.89	0.55
2:C:58:ILE:HG22	2:C:62:LEU:CD1	2.23	0.55
2:C:173:LEU:HD22	2:C:204:MET:SD	2.46	0.55
2:C:267:LEU:HD21	2:C:282:GLU:HB3	1.87	0.55
2:C:121:ILE:N	2:C:132:ILE:O	2.37	0.55
2:C:153:ALA:O	2:C:155:LEU:N	2.39	0.55
1:B:62:PHE:CZ	1:B:71:PHE:CG	2.94	0.55
1:B:110:THR:O	1:B:115:VAL:CG1	2.46	0.55
2:C:229:GLU:HG3	2:C:230:ARG:N	2.20	0.55
1:B:3:ARG:NH1	1:B:68:LEU:HD13	2.21	0.55
1:A:97:LEU:HD22	1:A:101:LEU:CG	2.36	0.55
2:C:256:LEU:CD1	2:C:304:ALA:HB2	2.36	0.55
1:B:66:GLU:HG3	1:B:135:LEU:HD13	1.89	0.55
1:B:96:LEU:CD2	1:B:108:LEU:HD11	2.26	0.55
2:C:71:GLY:O	2:C:73:ALA:N	2.40	0.55
2:C:180:ASP:O	2:C:183:LEU:HG	2.06	0.55
1:B:149:ALA:HA	1:B:183:ILE:HG13	1.89	0.55
2:C:36:GLU:O	2:C:38:LEU:HD23	2.07	0.55
2:C:45:GLY:HA3	2:C:165:LEU:O	2.07	0.55
1:A:94:PRO:HG2	1:A:95:ARG:HD3	1.89	0.54
2:C:257:ILE:HG23	2:C:258:LEU:N	2.22	0.54
1:A:5:LEU:HD21	1:A:26:PHE:CD2	2.42	0.54
2:C:36:GLU:N	2:C:37:PRO:CD	2.70	0.54
1:A:33:PRO:O	1:A:34:PHE:C	2.43	0.54
1:B:17:PHE:CE1	1:B:19:LEU:HD12	2.42	0.54
1:B:66:GLU:O	1:B:70:LEU:CD2	2.55	0.54
1:B:84:VAL:HG12	1:B:88:LEU:HD12	1.88	0.54
2:C:282:GLU:HA	2:C:286:GLU:CG	2.37	0.54
1:B:178:ARG:HD2	1:B:181:ASP:OD1	2.07	0.54
1:B:49:HIS:ND1	1:B:72:GLU:OE1	2.41	0.54
2:C:39:GLU:HB3	2:C:160:GLY:HA3	1.87	0.54
2:C:211:PHE:HA	2:C:214:VAL:CG2	2.38	0.54
2:C:249:ASP:OD1	2:C:289:LEU:HD21	2.06	0.54
1:B:96:LEU:HD21	1:B:108:LEU:CD1	2.25	0.54
2:C:125:GLN:HA	2:C:125:GLN:NE2	2.22	0.54
1:B:2:ILE:N	1:B:2:ILE:HD13	2.23	0.54
2:C:64:VAL:HG21	2:C:91:GLY:O	2.07	0.54
1:A:53:LYS:HB3	1:A:55:GLU:OE1	2.08	0.54
1:B:183:ILE:O	1:B:186:ALA:HB3	2.08	0.54
2:C:42:LEU:CD2	2:C:44:PHE:HE1	2.21	0.54
2:C:67:ARG:O	2:C:94:LEU:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HD23	1:B:97:LEU:HD23	1.90	0.54
1:A:84:VAL:O	1:A:87:ALA:HB3	2.08	0.54
2:C:306:GLU:O	2:C:308:ALA:N	2.41	0.54
1:B:95:ARG:HG3	1:B:136:LEU:O	2.08	0.53
2:C:80:LEU:HA	2:C:83:ILE:HD12	1.89	0.53
2:C:141:LEU:HD23	2:C:141:LEU:C	2.29	0.53
1:B:89:LEU:HD23	1:B:97:LEU:CD2	2.38	0.53
2:C:201:ARG:HB3	2:C:291:ARG:CZ	2.38	0.53
2:C:111:TYR:N	2:C:112:PRO:CD	2.72	0.53
2:C:286:GLU:OE2	2:C:302:ARG:NE	2.38	0.53
1:A:102:LEU:C	1:A:104:GLY:H	2.11	0.53
1:B:118:ARG:HH11	1:B:118:ARG:HB3	1.74	0.53
2:C:190:GLU:O	2:C:193:ALA:N	2.41	0.53
2:C:288:TYR:O	2:C:289:LEU:C	2.44	0.53
1:B:6:ARG:HH11	1:B:6:ARG:CG	2.22	0.53
1:B:73:LEU:HD21	1:B:131:VAL:HG22	1.88	0.53
2:C:244:GLY:O	2:C:245:LEU:C	2.46	0.53
1:B:160:GLU:CD	1:B:164:ARG:HH21	2.11	0.53
2:C:15:ILE:HD12	2:C:15:ILE:H	1.72	0.53
2:C:47:PRO:O	2:C:49:LEU:N	2.36	0.53
1:A:88:LEU:HD23	1:A:112:ALA:CB	2.37	0.53
1:A:92:LEU:HD11	1:A:108:LEU:HD22	1.90	0.53
2:C:172:GLU:O	2:C:175:GLN:HB3	2.09	0.53
1:B:96:LEU:HD23	1:B:96:LEU:O	2.09	0.53
1:B:132:PRO:O	1:B:132:PRO:HD2	2.07	0.53
2:C:46:PRO:O	2:C:49:LEU:HD13	2.08	0.53
2:C:51:LYS:HB2	3:C:313:ANP:O2G	2.09	0.53
1:A:101:LEU:O	1:A:104:GLY:N	2.41	0.53
1:B:115:VAL:O	1:B:115:VAL:HG23	2.08	0.53
1:B:131:VAL:HG12	1:B:132:PRO:CB	2.39	0.53
2:C:59:ALA:HB2	2:C:93:ILE:HD13	1.91	0.53
2:C:117:PHE:O	2:C:136:LEU:HB2	2.09	0.52
1:A:98:ALA:HA	1:A:101:LEU:HD12	1.91	0.52
2:C:20:LEU:HD12	2:C:21:LYS:N	2.23	0.52
2:C:286:GLU:OE1	2:C:302:ARG:NE	2.42	0.52
2:C:10:THR:O	2:C:57:VAL:HG11	2.09	0.52
2:C:294:LEU:HA	2:C:305:THR:HG22	1.91	0.52
2:C:306:GLU:C	2:C:308:ALA:H	2.13	0.52
1:A:68:LEU:HD11	1:A:72:GLU:CD	2.30	0.52
1:B:161:ALA:O	1:B:162:GLN:C	2.47	0.52
2:C:36:GLU:H	2:C:37:PRO:HD3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PHE:CZ	1:A:71:PHE:CG	2.97	0.52
2:C:20:LEU:HD12	2:C:20:LEU:C	2.30	0.52
2:C:196:ILE:CG2	2:C:211:PHE:HZ	2.23	0.52
1:A:80:VAL:O	1:A:82:PRO:HD3	2.10	0.52
1:B:146:ALA:O	1:B:149:ALA:HB3	2.10	0.52
2:C:189:THR:HG23	2:C:192:ALA:HB2	1.91	0.52
2:C:270:LEU:HD12	2:C:270:LEU:O	2.10	0.52
2:C:289:LEU:HD12	2:C:295:LEU:HD23	1.92	0.52
1:A:17:PHE:HE1	1:A:19:LEU:HB2	1.75	0.52
1:A:52:LEU:HD12	1:A:53:LYS:N	2.25	0.52
1:B:161:ALA:HA	1:B:164:ARG:HG2	1.91	0.51
1:A:125:LEU:C	1:A:125:LEU:CD2	2.79	0.51
2:C:100:HIS:CD2	2:C:145:THR:HG23	2.45	0.51
1:A:13:GLU:O	1:A:14:ALA:HB2	2.09	0.51
1:B:91:ALA:CB	1:B:112:ALA:HB1	2.40	0.51
1:B:152:ALA:HB2	2:C:132:ILE:CD1	2.40	0.51
2:C:24:LEU:HD11	2:C:41:LEU:HD22	1.91	0.51
2:C:38:LEU:CD2	2:C:140:THR:HG21	2.41	0.51
2:C:241:ASP:HB3	2:C:246:GLU:CB	2.41	0.51
1:A:12:LYS:HG3	1:A:40:GLU:HB3	1.93	0.51
1:A:81:GLY:C	1:A:83:LYS:N	2.56	0.51
1:B:112:ALA:O	1:B:115:VAL:CG1	2.59	0.51
1:B:150:VAL:CG2	1:B:167:VAL:HG21	2.39	0.51
2:C:266:GLY:O	2:C:268:ALA:N	2.43	0.51
2:C:248:ARG:NH2	2:C:274:LEU:O	2.44	0.51
2:C:292:GLN:O	2:C:293:GLY:C	2.49	0.51
2:C:124:GLY:HA3	2:C:128:ALA:HA	1.92	0.51
2:C:198:ARG:HG3	2:C:198:ARG:HH11	1.76	0.51
1:B:6:ARG:HH11	1:B:6:ARG:CB	2.23	0.51
1:B:118:ARG:HH11	1:B:118:ARG:CB	2.24	0.51
1:B:82:PRO:O	1:B:86:LEU:HB2	2.10	0.51
2:C:17:GLN:HG2	2:C:18:GLU:N	2.26	0.50
2:C:105:GLN:HA	2:C:108:GLU:HG3	1.91	0.50
2:C:191:GLU:CA	2:C:194:LEU:HD23	2.41	0.50
2:C:9:LYS:CB	2:C:57:VAL:HG13	2.36	0.50
2:C:200:SER:CA	2:C:206:VAL:HG23	2.40	0.50
2:C:125:GLN:HE21	2:C:125:GLN:CA	2.23	0.50
2:C:211:PHE:O	2:C:214:VAL:HB	2.11	0.50
2:C:264:PRO:N	2:C:303:VAL:HG12	2.26	0.50
1:B:92:LEU:HD11	1:B:97:LEU:HD13	1.94	0.50
2:C:270:LEU:HD12	2:C:270:LEU:C	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ALA:HB1	1:B:34:PHE:HD1	1.77	0.50
1:B:34:PHE:CB	1:B:63:PRO:HG3	2.41	0.50
1:B:66:GLU:HG3	1:B:135:LEU:CD1	2.42	0.50
2:C:110:LEU:O	2:C:110:LEU:HD23	2.12	0.50
2:C:134:LEU:O	2:C:135:GLU:HB2	2.12	0.50
2:C:285:HIS:N	2:C:287:PRO:HD2	2.27	0.50
2:C:266:GLY:O	2:C:267:LEU:C	2.50	0.50
2:C:292:GLN:O	2:C:294:LEU:HG	2.12	0.50
1:B:80:VAL:HG21	1:B:123:ILE:HG12	1.93	0.49
1:B:131:VAL:HG12	1:B:132:PRO:HB3	1.93	0.49
1:A:93:PRO:HB3	1:A:95:ARG:HE	1.77	0.49
1:A:102:LEU:HB2	1:A:131:VAL:CB	2.41	0.49
1:B:7:GLY:HA3	1:B:19:LEU:HD23	1.94	0.49
2:C:189:THR:HG23	2:C:192:ALA:HB3	1.94	0.49
1:A:97:LEU:O	1:A:100:ALA:N	2.46	0.49
2:C:40:HIS:HB3	2:C:159:PHE:CD2	2.47	0.49
2:C:152:THR:O	2:C:153:ALA:O	2.30	0.49
2:C:54:LEU:O	2:C:58:ILE:HG13	2.12	0.49
2:C:112:PRO:HB3	2:C:118:VAL:HG23	1.94	0.49
2:C:195:GLU:O	2:C:199:ARG:HD3	2.11	0.49
2:C:227:THR:O	2:C:229:GLU:N	2.46	0.49
2:C:286:GLU:N	2:C:287:PRO:CD	2.75	0.49
1:A:12:LYS:HD3	1:A:38:LEU:O	2.12	0.49
2:C:148:PRO:O	2:C:149:GLY:C	2.51	0.49
2:C:8:PRO:O	2:C:13:GLU:OE1	2.30	0.49
2:C:35:LYS:HZ3	2:C:35:LYS:HB3	1.77	0.49
2:C:64:VAL:HB	2:C:92:ASP:CA	2.43	0.49
2:C:264:PRO:HB3	2:C:303:VAL:CG1	2.42	0.49
1:A:3:ARG:NH1	1:A:72:GLU:OE1	2.46	0.49
1:A:32:THR:O	1:A:33:PRO:C	2.51	0.49
1:A:95:ARG:HD3	1:A:95:ARG:N	2.22	0.49
2:C:35:LYS:HZ3	2:C:138:ARG:NH2	2.10	0.49
2:C:55:ALA:C	2:C:57:VAL:N	2.63	0.49
2:C:205:ARG:O	2:C:209:ARG:HG2	2.13	0.49
1:A:82:PRO:O	1:A:86:LEU:HG	2.12	0.49
1:B:47:HIS:HB3	1:B:68:LEU:HD12	1.94	0.49
2:C:51:LYS:O	2:C:54:LEU:HB3	2.13	0.49
2:C:196:ILE:HG12	2:C:211:PHE:HZ	1.77	0.49
1:A:100:ALA:O	1:A:101:LEU:C	2.50	0.48
1:B:94:PRO:HG2	1:B:95:ARG:H	1.77	0.48
2:C:105:GLN:O	2:C:108:GLU:N	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:PHE:CD1	2:C:139:PHE:N	2.81	0.48
1:B:9:VAL:O	1:B:9:VAL:HG12	2.12	0.48
1:B:44:VAL:HG22	1:B:45:GLY:N	2.28	0.48
2:C:46:PRO:O	2:C:49:LEU:HD22	2.12	0.48
1:A:63:PRO:CG	1:A:67:ASN:HD22	2.26	0.48
1:B:92:LEU:HD13	1:B:108:LEU:CD2	2.44	0.48
2:C:190:GLU:O	2:C:191:GLU:C	2.52	0.48
2:C:245:LEU:HD11	2:C:294:LEU:HD11	1.95	0.48
2:C:298:THR:O	2:C:301:GLY:N	2.41	0.48
1:B:160:GLU:O	1:B:163:ALA:N	2.47	0.48
2:C:201:ARG:NH1	2:C:288:TYR:HD2	2.10	0.48
1:B:167:VAL:CG1	1:B:182:LEU:HD21	2.43	0.48
1:B:176:LYS:HG3	1:B:176:LYS:O	2.12	0.48
1:B:184:LYS:O	1:B:187:LEU:N	2.46	0.48
2:C:311:HIS:ND1	2:C:311:HIS:C	2.66	0.48
1:B:3:ARG:O	1:B:48:THR:N	2.43	0.48
2:C:9:LYS:CA	2:C:57:VAL:HG13	2.44	0.48
2:C:100:HIS:ND1	2:C:151:ILE:HG21	2.28	0.48
2:C:153:ALA:C	2:C:155:LEU:H	2.16	0.48
2:C:211:PHE:C	2:C:215:ARG:HH11	2.17	0.48
1:B:164:ARG:HG3	1:B:165:ALA:N	2.28	0.47
2:C:154:PRO:O	2:C:156:LEU:HD23	2.14	0.47
1:A:64:ASP:C	1:A:66:GLU:N	2.64	0.47
1:B:150:VAL:O	1:B:153:LEU:N	2.47	0.47
1:B:94:PRO:O	1:B:95:ARG:C	2.52	0.47
1:A:88:LEU:HA	1:A:112:ALA:HB2	1.96	0.47
1:B:105:ASP:HB3	1:B:108:LEU:HB3	1.95	0.47
1:B:112:ALA:O	1:B:115:VAL:HG13	2.14	0.47
2:C:191:GLU:O	2:C:228:ARG:NH1	2.47	0.47
2:C:288:TYR:O	2:C:289:LEU:O	2.33	0.47
1:A:62:PHE:CE2	1:A:71:PHE:CD2	3.03	0.47
2:C:196:ILE:HG12	2:C:211:PHE:CZ	2.49	0.47
1:B:6:ARG:HD3	1:B:45:GLY:CA	2.44	0.47
2:C:168:TYR:O	2:C:169:THR:O	2.32	0.47
2:C:188:ILE:HG12	2:C:189:THR:N	2.29	0.47
1:A:46:VAL:O	1:A:48:THR:HG23	2.15	0.47
1:A:59:LEU:HD13	1:B:1:MET:CG	2.40	0.47
1:B:10:LEU:HD13	1:B:20:LEU:CD1	2.45	0.47
1:B:144:GLU:O	1:B:145:ALA:C	2.53	0.47
2:C:199:ARG:HG2	2:C:199:ARG:NH1	2.27	0.47
2:C:238:LEU:O	2:C:238:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:40:HIS:HB2	2:C:160:GLY:N	2.28	0.47
1:A:6:ARG:HA	1:A:45:GLY:HA2	1.97	0.47
1:A:27:PHE:C	1:A:28:LEU:HD12	2.35	0.47
1:A:106:ALA:C	1:A:108:LEU:N	2.69	0.46
1:B:80:VAL:CG2	1:B:123:ILE:HG12	2.46	0.46
1:B:118:ARG:O	1:B:121:GLU:HB2	2.15	0.46
1:B:158:PHE:CE1	2:C:76:LYS:HD3	2.50	0.46
2:C:95:PHE:HA	2:C:142:ILE:O	2.15	0.46
2:C:166:GLU:HG3	2:C:167:TYR:H	1.81	0.46
2:C:17:GLN:HB2	2:C:168:TYR:HE1	1.80	0.46
2:C:76:LYS:C	2:C:78:GLY:H	2.18	0.46
2:C:254:GLU:O	2:C:258:LEU:HB2	2.16	0.46
2:C:284:VAL:O	2:C:284:VAL:CG1	2.59	0.46
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.71	0.46
2:C:66:LEU:HD12	2:C:67:ARG:N	2.29	0.46
2:C:205:ARG:C	2:C:207:ALA:H	2.17	0.46
2:C:212:ARG:N	2:C:215:ARG:HH11	2.13	0.46
1:B:34:PHE:CG	1:B:63:PRO:HG3	2.50	0.46
1:B:84:VAL:HG12	1:B:88:LEU:CD1	2.45	0.46
1:B:7:GLY:N	1:B:19:LEU:HD21	2.30	0.46
2:C:47:PRO:O	2:C:49:LEU:HD13	2.15	0.46
2:C:309:ARG:HG2	2:C:310:ARG:H	1.81	0.46
1:B:171:LEU:HD21	1:B:177:ALA:HB3	1.98	0.46
2:C:113:ALA:HB1	2:C:139:PHE:CZ	2.50	0.46
1:A:82:PRO:HA	1:A:85:ALA:HB3	1.98	0.46
1:B:108:LEU:O	1:B:111:SER:HB2	2.16	0.46
2:C:188:ILE:CA	2:C:226:ILE:HG13	2.46	0.46
2:C:245:LEU:HD21	2:C:294:LEU:CD1	2.46	0.46
1:A:24:VAL:HG22	1:B:5:LEU:CD2	2.46	0.46
2:C:170:PRO:O	2:C:174:ALA:HB2	2.15	0.46
2:C:192:ALA:HB1	2:C:231:ALA:CB	2.43	0.46
2:C:277:ASP:O	2:C:278:PRO:C	2.52	0.46
2:C:21:LYS:O	2:C:25:ARG:N	2.44	0.46
2:C:31:ALA:HA	2:C:35:LYS:O	2.16	0.46
2:C:36:GLU:N	2:C:37:PRO:HD3	2.29	0.46
2:C:38:LEU:HD21	2:C:140:THR:HG21	1.98	0.46
2:C:42:LEU:HD23	2:C:44:PHE:HE1	1.81	0.46
1:B:118:ARG:HH11	1:B:118:ARG:CG	2.29	0.45
2:C:35:LYS:CE	2:C:138:ARG:HH21	2.29	0.45
1:A:2:ILE:N	1:A:2:ILE:HD12	2.32	0.45
1:A:106:ALA:O	1:A:108:LEU:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:O	1:B:170:LEU:HB2	2.16	0.45
2:C:114:MET:HG3	2:C:158:ARG:CB	2.47	0.45
2:C:38:LEU:HD23	2:C:38:LEU:H	1.81	0.45
2:C:180:ASP:OD2	2:C:180:ASP:N	2.49	0.45
2:C:224:GLU:O	2:C:226:ILE:HG23	2.16	0.45
2:C:108:GLU:C	2:C:110:LEU:H	2.19	0.45
1:A:46:VAL:O	1:A:46:VAL:HG22	2.15	0.45
2:C:251:GLU:O	2:C:252:ILE:C	2.54	0.45
1:B:9:VAL:HG23	1:B:42:LYS:O	2.16	0.45
1:B:105:ASP:O	1:B:109:LEU:HG	2.17	0.45
1:B:126:GLU:OE1	1:B:126:GLU:HA	2.16	0.45
2:C:34:ARG:O	2:C:35:LYS:HG3	2.16	0.45
2:C:114:MET:SD	2:C:115:GLU:N	2.90	0.45
2:C:170:PRO:O	2:C:174:ALA:CB	2.65	0.45
1:B:178:ARG:HG3	1:B:181:ASP:H	1.81	0.45
2:C:153:ALA:C	2:C:155:LEU:N	2.70	0.45
1:B:152:ALA:HB2	2:C:132:ILE:HD13	1.99	0.45
1:B:150:VAL:HG22	1:B:164:ARG:HA	2.00	0.44
1:B:171:LEU:CD2	1:B:177:ALA:HB3	2.47	0.44
1:A:49:HIS:ND1	1:A:49:HIS:C	2.70	0.44
1:B:178:ARG:O	1:B:179:ALA:C	2.55	0.44
2:C:8:PRO:O	2:C:10:THR:HG23	2.17	0.44
2:C:10:THR:HG23	2:C:13:GLU:OE1	2.17	0.44
2:C:59:ALA:O	2:C:62:LEU:HB2	2.17	0.44
2:C:193:ALA:HA	2:C:196:ILE:HD12	1.99	0.44
1:B:94:PRO:O	1:B:97:LEU:N	2.50	0.44
1:B:178:ARG:HG2	1:B:181:ASP:HB2	2.00	0.44
2:C:199:ARG:HD2	2:C:199:ARG:N	2.33	0.44
1:B:87:ALA:O	1:B:90:SER:N	2.51	0.44
2:C:267:LEU:CD1	2:C:302:ARG:NH2	2.81	0.44
1:B:84:VAL:O	1:B:85:ALA:C	2.55	0.44
2:C:81:ALA:HB2	2:C:119:MET:HE1	1.99	0.44
2:C:74:ILE:O	2:C:74:ILE:HG22	2.17	0.44
2:C:306:GLU:C	2:C:308:ALA:N	2.71	0.44
1:A:102:LEU:CA	1:A:131:VAL:HG21	2.47	0.44
1:B:70:LEU:N	1:B:70:LEU:CD2	2.78	0.44
1:B:77:VAL:HG12	1:B:78:SER:N	2.32	0.44
1:B:89:LEU:CD2	1:B:97:LEU:HD23	2.47	0.44
2:C:30:ALA:C	2:C:32:LYS:N	2.68	0.43
1:A:46:VAL:CG2	1:A:61:GLY:HA3	2.47	0.43
1:A:115:VAL:HG12	1:A:120:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:113:ALA:HB1	2:C:139:PHE:HZ	1.82	0.43
2:C:223:GLU:O	2:C:225:VAL:N	2.50	0.43
1:A:3:ARG:NH2	1:A:72:GLU:OE2	2.46	0.43
1:A:46:VAL:O	1:A:46:VAL:CG2	2.66	0.43
1:B:144:GLU:HG2	1:B:146:ALA:HB3	2.00	0.43
2:C:176:GLY:O	2:C:177:VAL:C	2.56	0.43
2:C:228:ARG:HA	2:C:231:ALA:HB3	2.00	0.43
1:A:16:GLY:HA3	1:A:27:PHE:CE1	2.54	0.43
1:A:19:LEU:HD23	1:A:20:LEU:N	2.34	0.43
1:B:36:GLN:C	1:B:38:LEU:N	2.72	0.43
1:B:73:LEU:CD1	1:B:127:LEU:HD13	2.43	0.43
1:B:152:ALA:CB	1:B:183:ILE:HD11	2.48	0.43
1:B:180:GLN:O	1:B:182:LEU:N	2.52	0.43
1:B:111:SER:O	1:B:112:ALA:HB2	2.19	0.43
2:C:80:LEU:H	2:C:80:LEU:CD2	2.23	0.43
2:C:118:VAL:CA	2:C:136:LEU:HD13	2.48	0.43
2:C:154:PRO:HA	2:C:156:LEU:CD2	2.48	0.43
2:C:251:GLU:O	2:C:255:VAL:HG23	2.19	0.43
2:C:308:ALA:O	2:C:311:HIS:HB3	2.18	0.43
1:A:83:LYS:O	1:A:87:ALA:N	2.36	0.43
1:B:77:VAL:CG1	1:B:78:SER:N	2.81	0.43
2:C:64:VAL:HG21	2:C:91:GLY:C	2.38	0.43
2:C:80:LEU:O	2:C:84:LEU:HG	2.19	0.43
2:C:294:LEU:HA	2:C:305:THR:CG2	2.48	0.43
1:B:160:GLU:O	1:B:161:ALA:C	2.57	0.43
2:C:173:LEU:CD1	2:C:203:THR:N	2.76	0.43
2:C:267:LEU:HD21	2:C:282:GLU:H	1.84	0.43
1:A:28:LEU:N	1:A:28:LEU:CD1	2.80	0.43
1:B:6:ARG:CG	1:B:6:ARG:NH1	2.82	0.43
1:B:10:LEU:CB	1:B:18:VAL:HG23	2.32	0.43
1:B:102:LEU:O	1:B:128:LYS:HA	2.19	0.43
2:C:40:HIS:CD2	2:C:141:LEU:HD13	2.54	0.43
1:B:6:ARG:HD2	1:B:44:VAL:O	2.18	0.43
1:B:87:ALA:O	1:B:88:LEU:C	2.58	0.43
1:B:184:LYS:C	1:B:186:ALA:H	2.22	0.43
2:C:17:GLN:CG	2:C:18:GLU:N	2.81	0.43
2:C:71:GLY:N	2:C:97:ASP:O	2.42	0.43
2:C:120:ASP:HA	2:C:132:ILE:O	2.18	0.43
2:C:266:GLY:C	2:C:268:ALA:N	2.70	0.43
1:A:125:LEU:HA	1:A:128:LYS:HG3	2.00	0.43
1:B:32:THR:OG1	1:B:90:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD23	1:B:92:LEU:N	2.27	0.43
1:A:35:LEU:O	1:A:38:LEU:HB3	2.19	0.42
1:B:168:LEU:N	1:B:168:LEU:HD22	2.33	0.42
1:B:121:GLU:O	1:B:122:ARG:C	2.56	0.42
2:C:35:LYS:HE2	2:C:138:ARG:HH21	1.83	0.42
2:C:76:LYS:C	2:C:78:GLY:N	2.72	0.42
2:C:93:ILE:HG23	2:C:140:THR:O	2.19	0.42
2:C:177:VAL:O	2:C:180:ASP:HB2	2.19	0.42
2:C:229:GLU:CG	2:C:230:ARG:N	2.82	0.42
2:C:261:GLY:C	2:C:263:GLY:H	2.20	0.42
1:A:94:PRO:HD2	1:A:95:ARG:CZ	2.49	0.42
1:B:105:ASP:HB3	1:B:108:LEU:CB	2.49	0.42
2:C:139:PHE:N	2:C:139:PHE:HD1	2.17	0.42
2:C:228:ARG:HG2	2:C:228:ARG:O	2.19	0.42
2:C:300:ARG:HG3	2:C:300:ARG:HH11	1.83	0.42
1:B:31:PRO:HG3	1:B:86:LEU:HD23	2.00	0.42
1:B:158:PHE:CE1	1:B:190:LEU:HB3	2.55	0.42
1:B:6:ARG:HD3	1:B:45:GLY:HA2	2.00	0.42
1:B:152:ALA:HB3	1:B:183:ILE:HD11	2.01	0.42
1:B:184:LYS:C	1:B:186:ALA:N	2.71	0.42
1:A:35:LEU:HD23	1:A:35:LEU:HA	1.60	0.42
1:A:101:LEU:O	1:A:104:GLY:HA2	2.19	0.42
1:B:131:VAL:HG12	1:B:132:PRO:CD	2.48	0.42
2:C:71:GLY:HA3	2:C:102:LEU:HD21	2.02	0.42
1:A:97:LEU:O	1:A:101:LEU:N	2.43	0.42
1:B:62:PHE:CZ	1:B:71:PHE:CD1	3.08	0.42
2:C:38:LEU:HD23	2:C:38:LEU:N	2.35	0.42
2:C:80:LEU:O	2:C:83:ILE:N	2.53	0.42
2:C:231:ALA:O	2:C:235:LEU:HB2	2.20	0.42
1:A:97:LEU:HD22	1:A:101:LEU:HD11	2.01	0.42
2:C:44:PHE:HB2	2:C:164:HIS:HA	2.02	0.42
2:C:88:LEU:HD22	2:C:92:ASP:HB2	2.02	0.42
1:B:133:PRO:HB2	1:B:134:HIS:H	1.58	0.42
2:C:161:ILE:H	2:C:161:ILE:HG12	1.60	0.42
2:C:191:GLU:C	2:C:228:ARG:NH1	2.73	0.42
2:C:227:THR:C	2:C:229:GLU:H	2.23	0.42
2:C:290:ILE:HA	2:C:295:LEU:O	2.20	0.42
1:A:10:LEU:O	1:A:11:LYS:HB2	2.20	0.41
1:A:64:ASP:OD1	1:A:66:GLU:HB3	2.20	0.41
1:B:125:LEU:HD12	1:B:125:LEU:O	2.20	0.41
1:B:150:VAL:O	1:B:151:MET:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:294:LEU:CA	2:C:305:THR:HG22	2.50	0.41
1:B:35:LEU:O	1:B:38:LEU:HB2	2.20	0.41
2:C:53:THR:O	2:C:57:VAL:HG23	2.20	0.41
1:B:42:LYS:HD2	1:B:42:LYS:N	2.34	0.41
1:B:66:GLU:O	1:B:70:LEU:HD23	2.20	0.41
2:C:9:LYS:HD3	2:C:56:HIS:O	2.21	0.41
2:C:175:GLN:O	2:C:176:GLY:C	2.59	0.41
1:A:102:LEU:C	1:A:104:GLY:N	2.73	0.41
2:C:176:GLY:O	2:C:178:MET:N	2.53	0.41
1:B:166:VAL:O	1:B:170:LEU:HG	2.20	0.41
2:C:256:LEU:HD12	2:C:304:ALA:HB2	2.02	0.41
1:A:93:PRO:CB	1:A:95:ARG:HE	2.34	0.41
1:B:19:LEU:CD1	1:B:46:VAL:HG21	2.50	0.41
2:C:8:PRO:HG2	2:C:13:GLU:OE1	2.20	0.41
2:C:76:LYS:O	2:C:78:GLY:N	2.54	0.41
2:C:105:GLN:OE1	2:C:105:GLN:N	2.54	0.41
2:C:145:THR:HG22	2:C:147:ARG:N	2.35	0.41
2:C:188:ILE:HB	2:C:226:ILE:HD11	2.00	0.41
2:C:204:MET:HE3	2:C:204:MET:HB3	1.85	0.41
1:A:112:ALA:HB3	1:A:115:VAL:HG21	2.02	0.41
2:C:64:VAL:HG11	2:C:91:GLY:C	2.41	0.41
2:C:103:SER:HB2	2:C:106:ALA:HB3	2.01	0.41
2:C:83:ILE:HG21	2:C:94:LEU:HD21	2.02	0.41
1:A:81:GLY:O	1:A:82:PRO:C	2.58	0.41
1:A:97:LEU:HD22	1:A:101:LEU:CD1	2.51	0.41
1:B:55:GLU:OE2	1:B:55:GLU:HA	2.20	0.41
1:B:136:LEU:N	1:B:136:LEU:CD2	2.82	0.41
2:C:204:MET:CA	2:C:207:ALA:HB3	2.51	0.41
1:B:150:VAL:HG22	1:B:167:VAL:CG2	2.46	0.41
1:B:183:ILE:O	1:B:184:LYS:C	2.59	0.41
2:C:112:PRO:C	2:C:114:MET:H	2.23	0.41
2:C:232:LEU:HA	2:C:235:LEU:HD23	2.03	0.41
2:C:40:HIS:HD2	2:C:141:LEU:HD13	1.86	0.40
2:C:192:ALA:O	2:C:195:GLU:HB2	2.21	0.40
2:C:267:LEU:HD11	2:C:282:GLU:HG2	2.03	0.40
1:A:2:ILE:HG21	1:A:5:LEU:HD13	2.02	0.40
1:A:107:ARG:HG3	1:A:107:ARG:HH11	1.86	0.40
1:A:119:LEU:HG	1:A:123:ILE:CD1	2.51	0.40
1:B:188:LYS:O	1:B:191:ARG:HD2	2.21	0.40
2:C:81:ALA:O	2:C:85:ALA:N	2.38	0.40
2:C:196:ILE:CG2	2:C:211:PHE:CZ	3.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:224:GLU:O	2:C:225:VAL:C	2.60	0.40
2:C:234:ALA:HA	2:C:237:ALA:HB3	2.01	0.40
1:A:100:ALA:O	1:A:104:GLY:N	2.54	0.40
1:A:134:HIS:O	1:A:134:HIS:ND1	2.54	0.40
1:B:35:LEU:O	1:B:38:LEU:CB	2.70	0.40
2:C:72:PRO:C	2:C:74:ILE:H	2.25	0.40
2:C:242:GLU:HB2	2:C:243:LEU:H	1.71	0.40
1:B:131:VAL:HG13	1:B:132:PRO:HB3	2.02	0.40
2:C:38:LEU:O	2:C:39:GLU:O	2.40	0.40
2:C:240:LEU:O	2:C:241:ASP:HB3	2.21	0.40
2:C:252:ILE:HA	2:C:274:LEU:HD21	2.03	0.40
1:A:8:LEU:HD11	1:A:41:GLY:O	2.22	0.40
2:C:233:GLU:C	2:C:235:LEU:N	2.68	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	133/191 (70%)	95 (71%)	28 (21%)	10 (8%)	1 7
1	B	189/191 (99%)	123 (65%)	45 (24%)	21 (11%)	0 2
2	C	306/312 (98%)	185 (60%)	76 (25%)	45 (15%)	0 1
All	All	628/694 (90%)	403 (64%)	149 (24%)	76 (12%)	0 2

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	B	10	LEU
1	B	132	PRO
1	B	180	GLN

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Mol	Chain	Res	Type
1	B	185	GLU
2	C	17	GLN
2	C	39	GLU
2	C	49	LEU
2	C	87	SER
2	C	117	PHE
2	C	135	GLU
2	C	153	ALA
2	C	169	THR
2	C	201	ARG
2	C	218	ALA
2	C	247	LYS
2	C	268	ALA
2	C	287	PRO
1	A	14	ALA
1	A	78	SER
1	A	81	GLY
1	A	107	ARG
1	B	115	VAL
1	B	133	PRO
1	B	142	GLU
1	B	158	PHE
1	B	160	GLU
2	C	47	PRO
2	C	92	ASP
2	C	149	GLY
2	C	190	GLU
2	C	219	GLN
2	C	224	GLU
2	C	228	ARG
2	C	293	GLY
2	C	307	LEU
1	B	113	SER
1	B	117	ARG
1	B	144	GLU
1	B	146	ALA
1	B	150	VAL
1	B	181	ASP
2	C	53	THR
2	C	86	ASN
2	C	234	ALA
2	C	267	LEU

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Mol	Chain	Res	Type
2	C	282	GLU
2	C	289	LEU
2	C	292	GLN
1	A	57	LEU
1	A	109	LEU
1	B	91	ALA
1	B	184	LYS
2	C	48	GLY
2	C	72	PRO
2	C	128	ALA
2	C	130	ARG
2	C	154	PRO
2	C	242	GLU
2	C	281	LEU
1	A	33	PRO
1	B	112	ALA
2	C	177	VAL
2	C	245	LEU
2	C	252	ILE
2	C	269	THR
1	A	66	GLU
1	B	111	SER
2	C	71	GLY
1	B	33	PRO
2	C	160	GLY
2	C	244	GLY
1	A	77	VAL
2	C	225	VAL
1	B	9	VAL
2	C	220	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	105/145 (72%)	88 (84%)	17 (16%)	2 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	145/145 (100%)	121 (83%)	24 (17%)	2 10
2	C	249/253 (98%)	215 (86%)	34 (14%)	3 16
All	All	499/543 (92%)	424 (85%)	75 (15%)	3 13

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	LEU
1	A	13	GLU
1	A	50	LEU
1	A	52	LEU
1	A	64	ASP
1	A	68	LEU
1	A	78	SER
1	A	89	LEU
1	A	95	ARG
1	A	97	LEU
1	A	108	LEU
1	A	110	THR
1	A	111	SER
1	A	118	ARG
1	A	125	LEU
1	A	126	GLU
1	B	6	ARG
1	B	10	LEU
1	B	11	LYS
1	B	17	PHE
1	B	19	LEU
1	B	28	LEU
1	B	32	THR
1	B	35	LEU
1	B	50	LEU
1	B	54	GLU
1	B	66	GLU
1	B	68	LEU
1	B	72	GLU
1	B	74	LEU
1	B	89	LEU
1	B	92	LEU
1	B	117	ARG

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Mol	Chain	Res	Type
1	B	118	ARG
1	B	132	PRO
1	B	135	LEU
1	B	147	GLU
1	B	156	LEU
1	B	181	ASP
1	B	187	LEU
2	C	10	THR
2	C	24	LEU
2	C	36	GLU
2	C	38	LEU
2	C	67	ARG
2	C	86	ASN
2	C	93	ILE
2	C	119	MET
2	C	136	LEU
2	C	139	PHE
2	C	155	LEU
2	C	171	GLU
2	C	191	GLU
2	C	198	ARG
2	C	199	ARG
2	C	201	ARG
2	C	210	LEU
2	C	213	ARG
2	C	216	ASP
2	C	217	PHE
2	C	219	GLN
2	C	220	VAL
2	C	238	LEU
2	C	242	GLU
2	C	245	LEU
2	C	256	LEU
2	C	270	LEU
2	C	275	SER
2	C	277	ASP
2	C	282	GLU
2	C	287	PRO
2	C	292	GLN
2	C	295	LEU
2	C	309	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	49	HIS
1	A	67	ASN
1	B	67	ASN
1	B	173	GLN
2	C	40	HIS
2	C	60	HIS
2	C	86	ASN
2	C	125	GLN
2	C	219	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
3	ANP	C	313	-	29,33,33	2.26	9 (31%)	31,52,52	1.34	4 (12%)

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
3	ANP	C	313	-	-	6/14/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	313	ANP	PG-O1G	5.59	1.55	1.46
3	C	313	ANP	C4-N3	5.22	1.42	1.35
3	C	313	ANP	C2-N1	3.93	1.41	1.33
3	C	313	ANP	PB-O2B	-2.89	1.49	1.56
3	C	313	ANP	PB-O1B	2.88	1.50	1.46
3	C	313	ANP	O4'-C1'	2.83	1.45	1.41
3	C	313	ANP	C2-N3	2.59	1.36	1.32
3	C	313	ANP	PB-O3A	2.52	1.62	1.59
3	C	313	ANP	PG-O2G	-2.10	1.51	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	313	ANP	O1G-PG-N3B	-3.42	106.73	111.77
3	C	313	ANP	C4-C5-N7	3.09	112.62	109.40
3	C	313	ANP	O2B-PB-O1B	2.89	115.98	109.92
3	C	313	ANP	O4'-C1'-C2'	2.19	110.13	106.93

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	313	ANP	PB-N3B-PG-O1G
3	C	313	ANP	C5'-O5'-PA-O3A
3	C	313	ANP	C5'-O5'-PA-O1A
3	C	313	ANP	C5'-O5'-PA-O2A
3	C	313	ANP	O4'-C4'-C5'-O5'
3	C	313	ANP	C3'-C4'-C5'-O5'

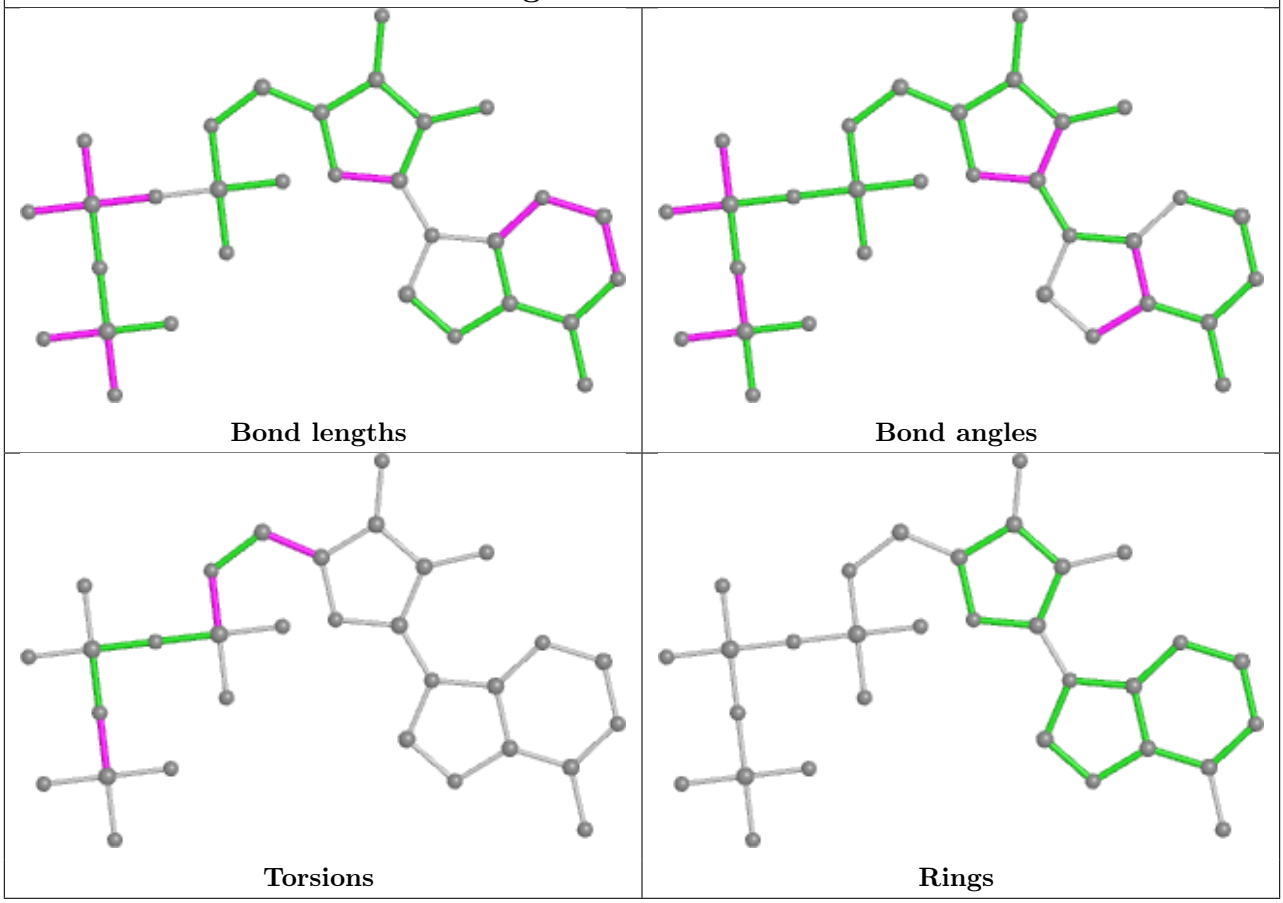
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	313	ANP	1	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 ANP C 313



5.7 Other polymers

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	135/191 (70%)	-0.25	3 (2%) 62 60	10, 38, 96, 200	0
1	B	191/191 (100%)	-0.06	3 (1%) 72 70	4, 55, 151, 200	0
2	C	308/312 (98%)	0.72	46 (14%) 2 2	19, 117, 196, 200	0
All	All	634/694 (91%)	0.28	52 (8%) 11 11	4, 78, 183, 200	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	126	GLY	10.1
2	C	221	ALA	7.9
2	C	127	PRO	5.9
2	C	28	LEU	5.8
2	C	125	GLN	5.8
2	C	20	LEU	5.8
2	C	42	LEU	5.7
2	C	120	ASP	5.7
2	C	232	LEU	5.6
2	C	29	GLU	5.5
2	C	40	HIS	5.5
2	C	231	ALA	5.2
2	C	24	LEU	5.1
2	C	152	THR	4.8
2	C	218	ALA	4.8
2	C	119	MET	4.8
2	C	222	GLY	4.6
2	C	27	TYR	4.2
2	C	26	VAL	3.9
2	C	63	GLY	3.4
2	C	150	LEU	3.3
2	C	155	LEU	3.3
2	C	159	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	217	PHE	2.9
1	B	142	GLU	2.8
2	C	121	ILE	2.8
2	C	186	VAL	2.8
1	A	107	ARG	2.8
2	C	22	GLN	2.7
2	C	25	ARG	2.7
2	C	164	HIS	2.6
2	C	122	VAL	2.6
2	C	118	VAL	2.5
2	C	112	PRO	2.5
2	C	62	LEU	2.4
2	C	157	SER	2.4
2	C	128	ALA	2.3
2	C	139	PHE	2.3
2	C	220	VAL	2.3
2	C	34	ARG	2.3
2	C	132	ILE	2.3
2	C	190	GLU	2.3
2	C	21	LYS	2.2
2	C	170	PRO	2.2
1	A	23	GLY	2.2
1	B	171	LEU	2.2
1	B	140	LYS	2.2
1	A	102	LEU	2.1
2	C	181	ALA	2.1
2	C	135	GLU	2.1
2	C	312	LEU	2.1
2	C	163	GLU	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

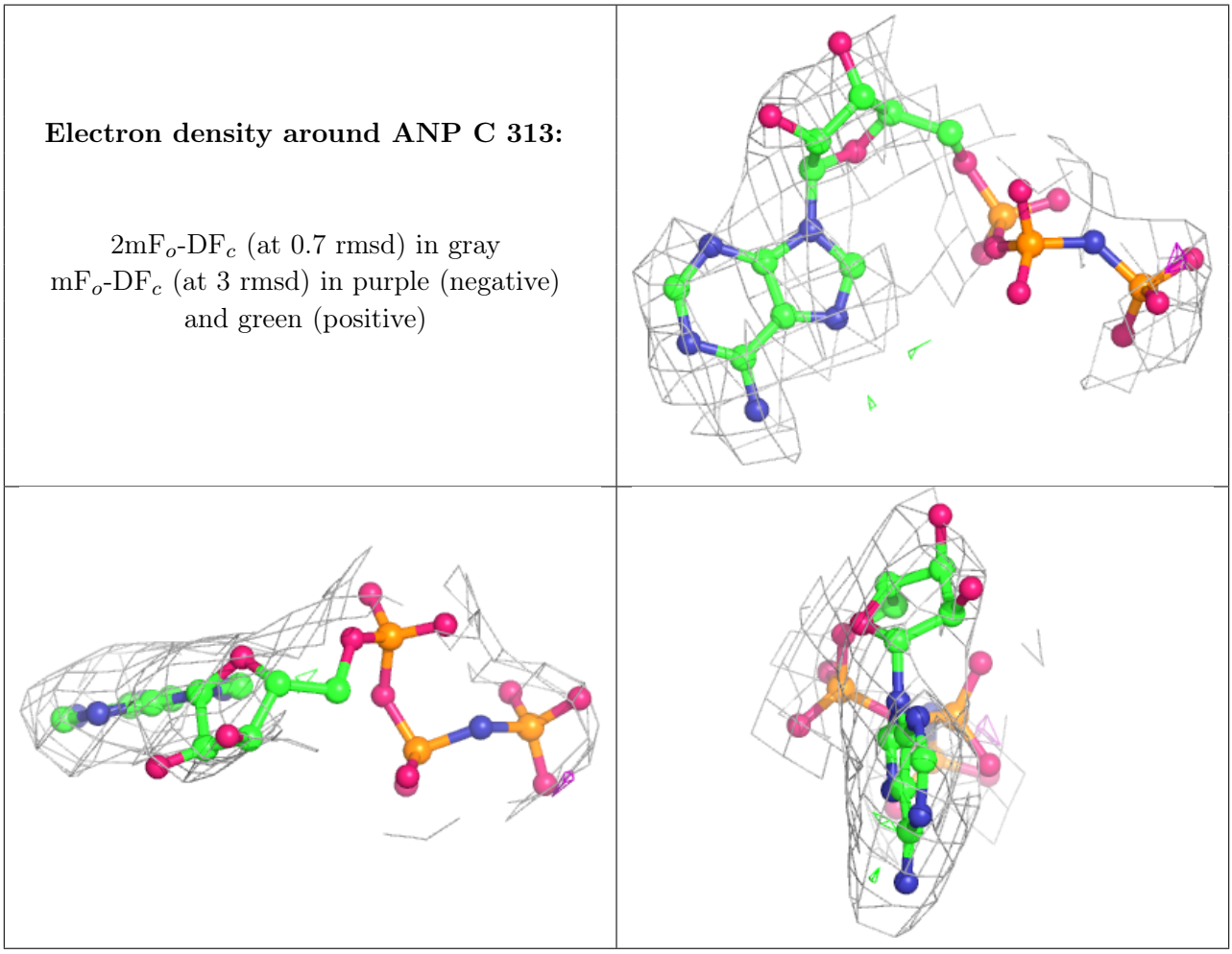
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	ANP	C	313	31/31	0.83	0.23	70,114,114,114	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 ANP C 313:

$2mF_o$-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.