Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2021 – 05:59 AM EDT

PDB ID	:	1S1U
Title	:	Crystal structure of L100I mutant HIV-1 reverse transcriptase in complex with nevirapine
Authors	:	Ren, J.; Nichols, C.E.; Chamberlain, P.P.; Stammers, D.K.
Deposited on	:	2004-01-07
Resolution	:	3.00 Å(reported)

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

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

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

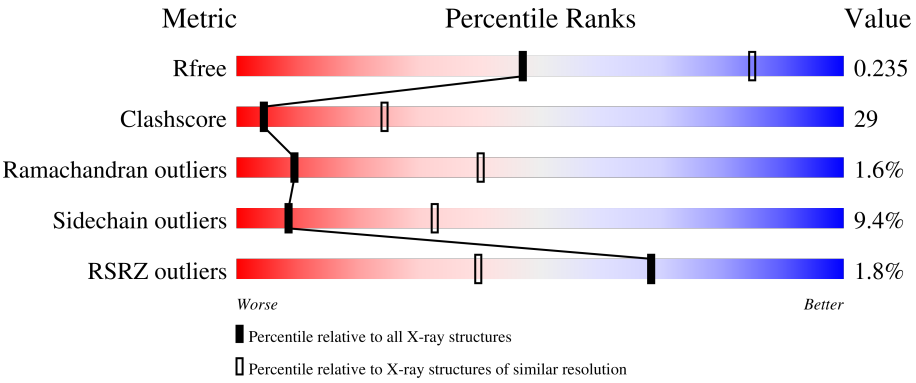
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	560	3% 44% 42% 7% 6%
2	B	440	45% 43% . 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7660 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 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4310	2792	714	796	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ILE	LEU	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

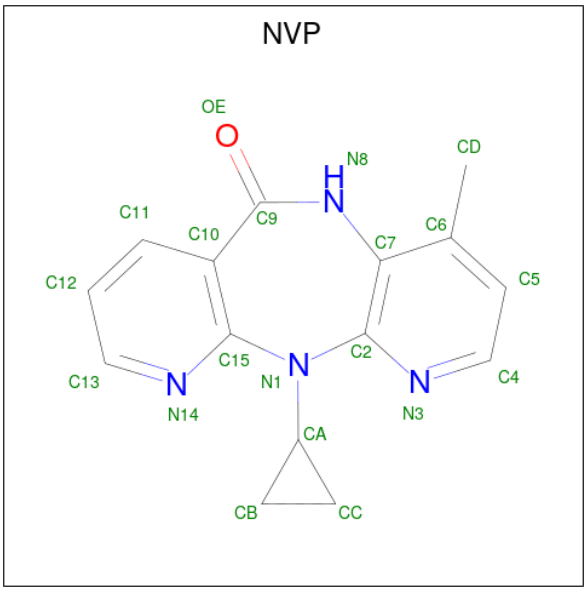
- Molecule 2 is a protein called Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3330	2173	549	601	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	100	ILE	LEU	engineered mutation	UNP P04585

- Molecule 3 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3' -E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: $C_{15}H_{14}N_4O$).



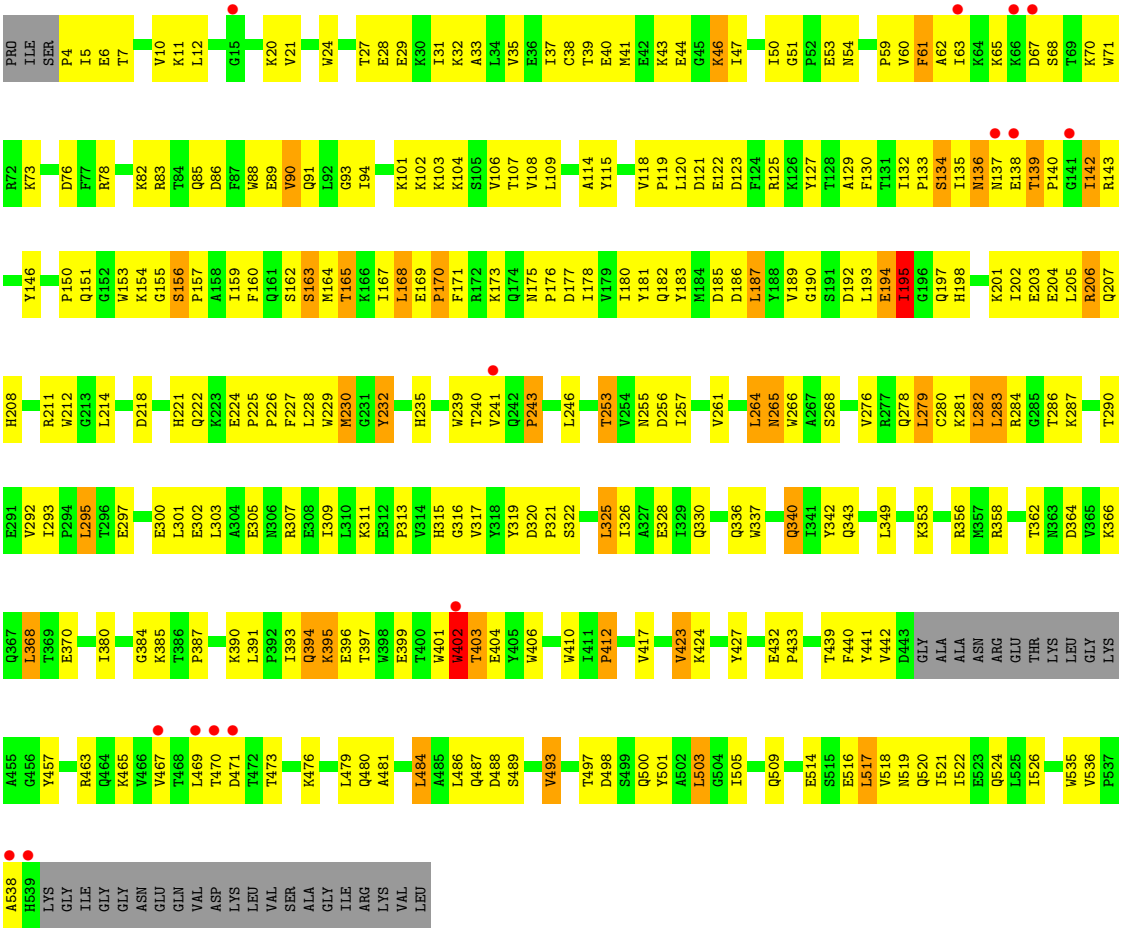
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	15	4	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

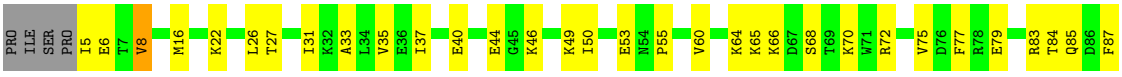
- Molecule 1: Reverse transcriptase

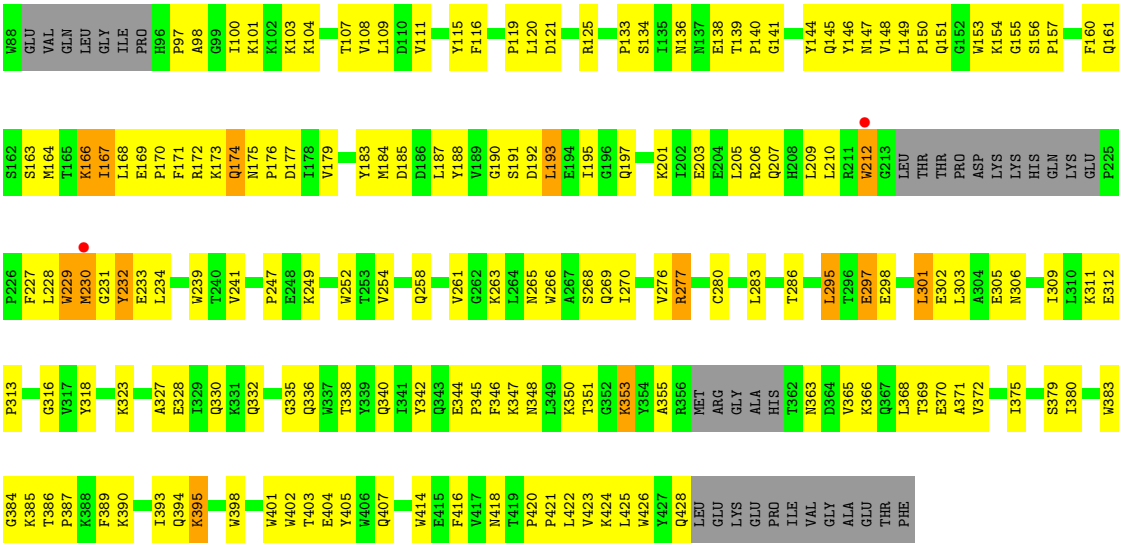
Chain A:



- Molecule 2: Reverse transcriptase

Chain B:




W88 E96 P97 A98 G99 I100 K101 K102 K103 K104 T107 V108 L109 D110 V111 Y115 F116 P119 L120 D121 R125 P133 S134 I135 N136 N137 E138 T139 P140 G141 Y144 Q145 Y146 N147 V148 L149 P150 Q151 G152 W153 K154 G155 S156 P157 F160 Q161
S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 R172 K173 Q174 N175 P176 D177 I178 V179 Y183 M184 D185 D186 L187 Y188 V189 G190 S191 D192 L193 E194 I195 G196 Q197 K201 I202 E203 E204 L205 R206 Q207 H208 L209 L210 R211 W212 G213 LEU THR THR PRO ASP LYS LYS HIS GLN LYS GLU P225
P226 F227 L228 W229 M230 G231 Y232 E233 L234 W239 T240 V241 P247 E248 K249 W252 T253 V254 Q258 V261 G262 K263 L264 N265 W266 A267 S268 Q269 I270 V276 R277 C280 L283 T286 L295 T296 E297 E298 L301 E302 L303 A304 E305 N306 I309 L310 K311 E312
P313 G316 V317 Y318 K323 A327 E328 I329 Q330 K331 Q332 G335 Q336 W337 T338 Y339 Q340 I341 Y342 Q343 E344 P345 F346 K347 N348 L349 K350 T351 G352 K353 Y354 A355 R356 MET ARG GLY ALA HIS T362 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 I375 S379 I380 W383
G384 K385 T386 P387 K388 F389 K390 I393 Q394 K395 W398 W401 W402 T403 E404 Y405 W406 Q407 W414 E415 F416 V417 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427 Q428 LEU GLU LYS GLU PRO ILE VAL GLY ALA GLU THR PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.80Å 115.50Å 66.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.00 29.90 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (29.90-3.00) 98.6 (29.90-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.285 0.217 , 0.235	Depositor DCC
R_{free} test set	1060 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	84.0	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 90.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7660	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: CSD, NVP

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	0.52	0/4417	0.75	1/6005 (0.0%)
2	B	0.51	0/3426	0.73	1/4653 (0.0%)
All	All	0.52	0/7843	0.74	2/10658 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	90	VAL	N-CA-C	-5.53	96.06	111.00
2	B	229	TRP	CA-CB-CG	-5.09	104.02	113.70

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	4310	0	4343	243	0
2	B	3330	0	3353	207	0
3	A	20	0	14	0	0
All	All	7660	0	7710	440	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 29.

All (440) 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:469:LEU:HD21	1:A:480:GLN:HG3	1.17	1.10
2:B:66:LYS:HG2	2:B:230:MET:HA	1.35	1.07
1:A:195:ILE:HD13	1:A:195:ILE:H	1.25	1.01
1:A:295:LEU:HB3	1:A:300:GLU:HG3	1.46	0.96
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.30	0.95
2:B:167:ILE:HD12	2:B:212:TRP:HB3	1.46	0.94
2:B:227:PHE:HB2	2:B:231:GLY:HA2	1.49	0.94
1:A:228:LEU:H	1:A:228:LEU:HD23	1.32	0.93
2:B:227:PHE:CB	2:B:231:GLY:HA2	2.00	0.91
2:B:166:LYS:HE3	2:B:166:LYS:HA	1.51	0.91
1:A:167:ILE:O	1:A:170:PRO:HD2	1.73	0.88
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.04	0.87
1:A:171:PHE:CE1	1:A:205:LEU:HA	2.11	0.85
2:B:297:GLU:O	2:B:301:LEU:HD22	1.76	0.85
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.42	0.84
1:A:46:LYS:NZ	1:A:46:LYS:HB3	1.93	0.84
2:B:66:LYS:CG	2:B:230:MET:HA	2.08	0.83
2:B:66:LYS:HE3	2:B:230:MET:CG	2.08	0.83
1:A:65:LYS:HB3	1:A:68:SER:HB3	1.59	0.82
1:A:226:PRO:HG3	1:A:235:HIS:CE1	2.16	0.80
1:A:142:ILE:HD13	1:A:142:ILE:H	1.46	0.80
2:B:66:LYS:HG2	2:B:230:MET:CA	2.10	0.80
2:B:227:PHE:HB2	2:B:231:GLY:CA	2.12	0.79
2:B:230:MET:C	2:B:232:TYR:H	1.81	0.79
1:A:469:LEU:HD11	1:A:480:GLN:HE21	1.48	0.79
1:A:165:THR:HG21	2:B:140:PRO:HG2	1.65	0.79
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.07	0.78
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.33	0.77
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.66	0.77
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.66	0.76
2:B:175:ASN:HD21	2:B:201:LYS:HZ1	1.31	0.76
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.00	0.75
2:B:167:ILE:HD12	2:B:212:TRP:CB	2.16	0.75
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.67	0.75
2:B:175:ASN:HD21	2:B:201:LYS:NZ	1.84	0.75
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.68	0.75
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.69	0.75
2:B:103:LYS:NZ	2:B:191:SER:HA	2.02	0.74
2:B:169:GLU:N	2:B:170:PRO:HD2	2.02	0.74
1:A:27:THR:HG22	1:A:29:GLU:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LEU:H	2:B:295:LEU:HD12	1.53	0.73
2:B:395:LYS:HD2	2:B:416:PHE:CE1	2.23	0.73
2:B:420:PRO:O	2:B:423:VAL:HG12	1.88	0.73
1:A:325:LEU:HD22	1:A:385:LYS:HE3	1.70	0.73
2:B:353:LYS:NZ	2:B:428:GLN:HG3	2.03	0.73
2:B:136:ASN:HB3	2:B:138:GLU:HG3	1.71	0.72
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.54	0.72
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.24	0.72
1:A:101:LYS:H	1:A:101:LYS:HD2	1.55	0.71
2:B:254:VAL:O	2:B:258:GLN:HG3	1.92	0.70
2:B:229:TRP:HA	2:B:229:TRP:CE3	2.26	0.70
1:A:134:SER:CB	1:A:139:THR:O	2.40	0.69
2:B:154:LYS:O	2:B:157:PRO:HD2	1.92	0.69
1:A:228:LEU:H	1:A:228:LEU:CD2	2.04	0.69
1:A:295:LEU:HB3	1:A:300:GLU:CG	2.20	0.69
1:A:253:THR:HG22	1:A:256:ASP:H	1.55	0.69
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.75	0.69
1:A:101:LYS:HD2	1:A:101:LYS:N	2.07	0.69
2:B:295:LEU:HD12	2:B:295:LEU:N	2.08	0.69
1:A:325:LEU:CD2	1:A:385:LYS:HE3	2.22	0.68
1:A:295:LEU:HD12	1:A:300:GLU:HG2	1.75	0.68
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.75	0.68
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.76	0.67
2:B:175:ASN:CG	2:B:201:LYS:HZ2	1.96	0.67
1:A:134:SER:OG	1:A:140:PRO:HA	1.92	0.67
2:B:266:TRP:O	2:B:269:GLN:HG2	1.94	0.67
1:A:165:THR:HG23	1:A:182:GLN:OE1	1.94	0.67
1:A:194:GLU:OE1	1:A:197:GLN:HB2	1.95	0.67
1:A:115:TYR:OH	1:A:157:PRO:HG3	1.94	0.66
1:A:295:LEU:CB	1:A:300:GLU:HG3	2.23	0.66
2:B:66:LYS:HE3	2:B:230:MET:HA	1.77	0.66
1:A:228:LEU:HD23	1:A:228:LEU:N	2.09	0.66
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.31	0.66
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.76	0.66
1:A:142:ILE:H	1:A:142:ILE:CD1	1.99	0.66
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.30	0.66
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.60	0.66
2:B:97:PRO:O	2:B:100:ILE:HG22	1.96	0.65
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.78	0.65
2:B:31:ILE:CD1	2:B:133:PRO:HG2	2.26	0.65
2:B:393:ILE:HG12	2:B:394:GLN:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:PHE:CB	2:B:231:GLY:CA	2.73	0.65
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.78	0.64
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.79	0.64
2:B:103:LYS:HZ1	2:B:191:SER:HA	1.62	0.64
1:A:358:ARG:NH2	2:B:394:GLN:OE1	2.29	0.64
2:B:66:LYS:HE3	2:B:230:MET:CB	2.27	0.64
2:B:372:VAL:HA	2:B:389:PHE:CE2	2.33	0.64
2:B:5:ILE:HG22	2:B:6:GLU:N	2.11	0.64
1:A:395:LYS:H	1:A:395:LYS:CD	2.10	0.63
2:B:372:VAL:HA	2:B:389:PHE:HE2	1.63	0.63
1:A:181:TYR:CE1	1:A:183:TYR:HB2	2.34	0.63
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.64	0.63
1:A:171:PHE:HE1	1:A:205:LEU:HA	1.65	0.62
1:A:232:TYR:HD2	1:A:239:TRP:HZ3	1.47	0.62
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.34	0.62
1:A:201:LYS:HA	1:A:204:GLU:HG3	1.81	0.62
1:A:46:LYS:HB3	1:A:46:LYS:HZ2	1.62	0.62
2:B:66:LYS:CE	2:B:230:MET:HA	2.30	0.61
2:B:393:ILE:HG12	2:B:394:GLN:H	1.65	0.61
1:A:195:ILE:HD13	1:A:195:ILE:N	2.07	0.61
1:A:279:LEU:HD22	1:A:302:GLU:OE1	2.00	0.61
1:A:498:ASP:HA	1:A:536:VAL:O	1.99	0.61
2:B:301:LEU:HD13	2:B:301:LEU:N	2.16	0.61
2:B:203:GLU:O	2:B:206:ARG:HB2	2.00	0.61
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.83	0.60
2:B:5:ILE:HG22	2:B:6:GLU:H	1.66	0.60
2:B:134:SER:OG	2:B:139:THR:HB	2.01	0.60
2:B:348:ASN:HD22	2:B:351:THR:CG2	2.15	0.60
1:A:524:GLN:HA	1:A:524:GLN:OE1	2.00	0.60
1:A:393:ILE:HB	1:A:423:VAL:HG22	1.84	0.60
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.30	0.59
1:A:465:LYS:HD3	1:A:488:ASP:OD1	2.01	0.59
1:A:279:LEU:HA	1:A:282:LEU:CD2	2.32	0.59
2:B:100:ILE:HG23	2:B:101:LYS:N	2.17	0.59
2:B:193:LEU:HD23	2:B:197:GLN:HB3	1.82	0.59
1:A:171:PHE:CE1	1:A:205:LEU:CA	2.83	0.59
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.37	0.59
2:B:366:LYS:HD2	2:B:405:TYR:CE2	2.37	0.59
1:A:218:ASP:OD1	1:A:221:HIS:CD2	2.55	0.59
1:A:325:LEU:HD23	1:A:325:LEU:H	1.67	0.59
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:SER:OG	2:B:387:PRO:HG3	2.02	0.59
1:A:295:LEU:CB	1:A:300:GLU:CG	2.80	0.58
2:B:340:GLN:HB3	2:B:348:ASN:ND2	2.18	0.58
1:A:61:PHE:N	1:A:61:PHE:CD2	2.72	0.58
1:A:136:ASN:HB3	1:A:139:THR:OG1	2.04	0.58
1:A:253:THR:HG23	1:A:255:ASN:H	1.68	0.58
2:B:66:LYS:HE3	2:B:230:MET:HG3	1.84	0.58
1:A:516:GLU:O	1:A:520:GLN:HG3	2.03	0.58
1:A:342:TYR:HA	1:A:349:LEU:HD23	1.84	0.58
1:A:193:LEU:HD12	1:A:198:HIS:HA	1.86	0.58
1:A:195:ILE:H	1:A:195:ILE:CD1	1.93	0.58
2:B:175:ASN:CG	2:B:201:LYS:NZ	2.58	0.57
2:B:203:GLU:HG3	2:B:207:GLN:HE22	1.69	0.57
2:B:227:PHE:HB3	2:B:231:GLY:HA2	1.85	0.57
1:A:311:LYS:O	1:A:313:PRO:HD3	2.05	0.57
2:B:163:SER:O	2:B:167:ILE:HG22	2.04	0.57
2:B:305:GLU:O	2:B:309:ILE:HG13	2.04	0.57
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.69	0.57
2:B:234:LEU:HD23	2:B:239:TRP:CZ2	2.39	0.57
2:B:139:THR:HG23	2:B:140:PRO:CD	2.35	0.57
1:A:229:TRP:O	1:A:232:TYR:HD1	1.87	0.56
2:B:175:ASN:OD1	2:B:201:LYS:NZ	2.36	0.56
1:A:91:GLN:NE2	2:B:140:PRO:O	2.37	0.56
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.87	0.56
1:A:10:VAL:HG12	1:A:11:LYS:N	2.21	0.56
1:A:106:VAL:HG22	1:A:190:GLY:HA3	1.87	0.56
1:A:305:GLU:O	1:A:309:ILE:HG13	2.05	0.56
1:A:115:TYR:HD1	1:A:151:GLN:HA	1.71	0.56
1:A:358:ARG:CZ	2:B:394:GLN:OE1	2.54	0.56
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.86	0.56
2:B:241:VAL:HG11	2:B:313:PRO:HG3	1.88	0.56
1:A:169:GLU:O	1:A:173:LYS:HG3	2.05	0.56
2:B:139:THR:HG22	2:B:141:GLY:H	1.70	0.56
1:A:257:ILE:O	1:A:261:VAL:HG23	2.06	0.55
1:A:5:ILE:CG1	1:A:6:GLU:N	2.69	0.55
1:A:390:LYS:O	1:A:391:LEU:HD23	2.06	0.55
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.36	0.55
2:B:295:LEU:H	2:B:295:LEU:CD1	2.19	0.55
1:A:61:PHE:N	1:A:61:PHE:HD2	2.04	0.55
2:B:371:ALA:O	2:B:375:ILE:HG13	2.06	0.55
2:B:169:GLU:N	2:B:170:PRO:CD	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:VAL:HG13	2:B:389:PHE:CE2	2.42	0.55
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.42	0.55
1:A:106:VAL:HA	1:A:190:GLY:HA2	1.87	0.55
1:A:320:ASP:O	1:A:343:GLN:NE2	2.37	0.55
1:A:228:LEU:O	1:A:228:LEU:HG	2.07	0.54
1:A:229:TRP:O	1:A:230:MET:C	2.45	0.54
1:A:229:TRP:O	1:A:232:TYR:CD1	2.60	0.54
1:A:138:GLU:O	1:A:138:GLU:HG3	2.07	0.54
1:A:39:THR:O	1:A:43:LYS:HG2	2.06	0.54
1:A:264:LEU:HD23	1:A:276:VAL:HG12	1.90	0.54
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.41	0.54
1:A:115:TYR:HE2	1:A:160:PHE:CD1	2.26	0.54
1:A:37:ILE:O	1:A:41:MET:HG3	2.08	0.54
2:B:65:LYS:CB	2:B:68:SER:HB3	2.37	0.54
2:B:230:MET:HB2	2:B:232:TYR:HB2	1.89	0.54
2:B:372:VAL:HG13	2:B:389:PHE:CZ	2.42	0.54
1:A:239:TRP:O	1:A:315:HIS:HA	2.07	0.54
1:A:27:THR:O	1:A:31:ILE:HG13	2.08	0.54
2:B:332:GLN:HB2	2:B:336:GLN:O	2.08	0.54
2:B:66:LYS:HE3	2:B:230:MET:CA	2.38	0.53
2:B:79:GLU:O	2:B:83:ARG:HG3	2.08	0.53
1:A:159:ILE:O	1:A:162:SER:HB3	2.09	0.53
1:A:268:SER:HB3	1:A:353:LYS:HE2	1.89	0.53
1:A:134:SER:HB3	1:A:139:THR:O	2.07	0.53
1:A:229:TRP:N	1:A:232:TYR:O	2.41	0.53
2:B:49:LYS:HG3	2:B:144:TYR:CE1	2.43	0.53
2:B:173:LYS:O	2:B:176:PRO:HD3	2.07	0.53
1:A:78:ARG:O	1:A:82:LYS:HG3	2.09	0.53
1:A:165:THR:HA	1:A:168:LEU:HD22	1.90	0.53
1:A:395:LYS:N	1:A:395:LYS:HD2	2.24	0.53
1:A:467:VAL:HG21	1:A:484:LEU:HD11	1.90	0.53
1:A:297:GLU:O	1:A:301:LEU:HB2	2.08	0.52
2:B:175:ASN:N	2:B:176:PRO:HD3	2.24	0.52
1:A:146:TYR:CG	1:A:150:PRO:HG3	2.44	0.52
1:A:38:CYS:O	1:A:47:ILE:HD11	2.10	0.52
1:A:417:VAL:O	1:A:417:VAL:HG13	2.09	0.52
2:B:385:LYS:HG2	2:B:386:THR:N	2.24	0.52
2:B:139:THR:HG22	2:B:141:GLY:N	2.25	0.52
1:A:11:LYS:O	1:A:85:GLN:HG2	2.10	0.51
2:B:302:GLU:O	2:B:306:ASN:ND2	2.43	0.51
2:B:366:LYS:O	2:B:370:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:HG12	1:A:133:PRO:HG2	1.91	0.51
1:A:319:TYR:CD2	1:A:320:ASP:N	2.78	0.51
2:B:249:LYS:HG3	2:B:252:TRP:CE2	2.45	0.51
1:A:63:ILE:N	1:A:63:ILE:HD12	2.25	0.51
2:B:31:ILE:HD11	2:B:133:PRO:HG2	1.91	0.51
1:A:5:ILE:HG12	1:A:6:GLU:N	2.25	0.51
1:A:94:ILE:HG23	1:A:229:TRP:CH2	2.45	0.51
1:A:142:ILE:HD13	1:A:142:ILE:N	2.20	0.51
1:A:503:LEU:HG	1:A:535:TRP:HB2	1.91	0.51
2:B:174:GLN:NE2	2:B:175:ASN:OD1	2.44	0.51
1:A:24:TRP:HZ3	1:A:61:PHE:CD2	2.28	0.51
1:A:46:LYS:HB3	1:A:46:LYS:HZ3	1.72	0.51
2:B:161:GLN:O	2:B:164:MET:HB3	2.10	0.51
1:A:76:ASP:OD2	1:A:78:ARG:HG3	2.11	0.51
2:B:139:THR:CG2	2:B:140:PRO:N	2.73	0.51
2:B:40:GLU:O	2:B:44:GLU:HG3	2.10	0.51
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.92	0.51
2:B:423:VAL:HG13	2:B:424:LYS:N	2.26	0.51
1:A:86:ASP:HA	1:A:154:LYS:HE2	1.93	0.51
1:A:240:THR:OG1	1:A:241:VAL:N	2.44	0.51
2:B:206:ARG:HD2	2:B:227:PHE:CE1	2.45	0.51
1:A:457:TYR:CE1	1:A:463:ARG:HG2	2.44	0.50
2:B:103:LYS:HE3	2:B:190:GLY:C	2.32	0.50
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.46	0.50
2:B:380:ILE:O	2:B:384:GLY:HA2	2.10	0.50
1:A:395:LYS:H	1:A:395:LYS:HD2	1.77	0.50
2:B:227:PHE:HB3	2:B:231:GLY:O	2.12	0.50
1:A:108:VAL:HG23	1:A:227:PHE:CZ	2.47	0.50
2:B:402:TRP:CE2	2:B:403:THR:HG23	2.47	0.50
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.92	0.50
2:B:350:LYS:HG3	2:B:351:THR:N	2.27	0.50
1:A:232:TYR:HD2	1:A:239:TRP:CZ3	2.29	0.50
1:A:337:TRP:CZ3	1:A:368:LEU:HD23	2.47	0.50
2:B:85:GLN:O	2:B:87:PHE:CE1	2.65	0.50
2:B:195:ILE:HD11	2:B:233:GLU:CD	2.32	0.50
1:A:481:ALA:O	1:A:484:LEU:HB2	2.11	0.50
2:B:206:ARG:O	2:B:210:LEU:HD23	2.11	0.50
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.94	0.49
2:B:298:GLU:OE1	2:B:298:GLU:N	2.44	0.49
2:B:134:SER:CB	2:B:139:THR:HB	2.42	0.49
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LYS:HE2	2:B:68:SER:O	2.12	0.49
1:A:358:ARG:NE	2:B:394:GLN:HE22	2.11	0.49
2:B:311:LYS:O	2:B:312:GLU:HG3	2.13	0.49
1:A:181:TYR:HE1	1:A:183:TYR:HB2	1.78	0.49
2:B:175:ASN:ND2	2:B:201:LYS:CE	2.75	0.49
2:B:301:LEU:N	2:B:301:LEU:CD1	2.76	0.49
2:B:353:LYS:HZ2	2:B:428:GLN:HG3	1.76	0.49
1:A:24:TRP:HZ3	1:A:61:PHE:CG	2.30	0.49
1:A:402:TRP:CG	1:A:403:THR:N	2.81	0.49
2:B:195:ILE:HD11	2:B:233:GLU:HG2	1.95	0.49
1:A:186:ASP:O	1:A:187:LEU:HD22	2.13	0.48
1:A:295:LEU:HB2	1:A:300:GLU:OE1	2.13	0.48
1:A:497:THR:O	1:A:535:TRP:HA	2.13	0.48
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.96	0.48
1:A:62:ALA:C	1:A:63:ILE:HD12	2.33	0.48
2:B:44:GLU:HB2	2:B:46:LYS:HG2	1.95	0.48
2:B:100:ILE:CG2	2:B:101:LYS:N	2.75	0.48
2:B:423:VAL:CG1	2:B:424:LYS:N	2.75	0.48
1:A:432:GLU:HB2	1:A:433:PRO:HD2	1.95	0.48
1:A:469:LEU:HD11	1:A:480:GLN:NE2	2.23	0.48
1:A:106:VAL:HG12	1:A:107:THR:N	2.29	0.48
1:A:380:ILE:O	1:A:384:GLY:HA2	2.13	0.48
1:A:107:THR:HG22	1:A:109:LEU:CD1	2.43	0.48
2:B:425:LEU:HD22	2:B:426:TRP:CD1	2.49	0.48
1:A:175:ASN:N	1:A:176:PRO:HD3	2.28	0.47
1:A:202:ILE:HG22	1:A:203:GLU:N	2.29	0.47
2:B:167:ILE:O	2:B:167:ILE:CG1	2.61	0.47
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.96	0.47
1:A:279:LEU:O	1:A:282:LEU:HB2	2.14	0.47
2:B:380:ILE:O	2:B:384:GLY:N	2.45	0.47
1:A:279:LEU:HA	1:A:282:LEU:HD22	1.94	0.47
2:B:87:PHE:CD1	2:B:87:PHE:N	2.81	0.47
2:B:175:ASN:ND2	2:B:201:LYS:HZ1	2.00	0.47
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.44	0.47
1:A:203:GLU:O	1:A:204:GLU:C	2.53	0.47
1:A:28:GLU:O	1:A:32:LYS:HG3	2.12	0.47
1:A:101:LYS:N	1:A:101:LYS:CD	2.77	0.47
1:A:155:GLY:O	1:A:156:SER:C	2.53	0.47
1:A:232:TYR:CD2	1:A:239:TRP:CZ3	3.03	0.47
1:A:168:LEU:HD13	1:A:168:LEU:N	2.29	0.47
1:A:303:LEU:O	1:A:303:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASP:OD2	1:A:322:SER:OG	2.28	0.47
2:B:234:LEU:HD23	2:B:239:TRP:CH2	2.50	0.47
2:B:379:SER:HA	2:B:383:TRP:CE3	2.49	0.47
2:B:422:LEU:O	2:B:425:LEU:HB3	2.14	0.47
1:A:28:GLU:HG3	1:A:135:ILE:HG21	1.96	0.47
1:A:325:LEU:CD2	1:A:325:LEU:H	2.28	0.47
2:B:167:ILE:HD11	2:B:209:LEU:HD23	1.97	0.47
1:A:427:TYR:OH	1:A:509:GLN:HA	2.15	0.47
1:A:522:ILE:O	1:A:526:ILE:HG13	2.14	0.47
2:B:366:LYS:HD2	2:B:405:TYR:CD2	2.49	0.47
1:A:265:ASN:O	1:A:266:TRP:C	2.52	0.47
2:B:206:ARG:HD2	2:B:227:PHE:HE1	1.80	0.46
2:B:66:LYS:CD	2:B:230:MET:HA	2.45	0.46
2:B:365:VAL:O	2:B:366:LYS:C	2.52	0.46
2:B:66:LYS:HE3	2:B:230:MET:HG2	1.96	0.46
2:B:332:GLN:HB3	2:B:428:GLN:NE2	2.27	0.46
2:B:345:PRO:C	2:B:347:LYS:H	2.18	0.46
1:A:208:HIS:O	1:A:212:TRP:CD1	2.69	0.46
1:A:486:LEU:CD1	1:A:521:ILE:HG23	2.45	0.46
2:B:116:PHE:CZ	2:B:151:GLN:HG3	2.51	0.46
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.51	0.46
2:B:33:ALA:O	2:B:37:ILE:HG13	2.16	0.46
2:B:175:ASN:ND2	2:B:201:LYS:HE3	2.31	0.46
1:A:246:LEU:O	1:A:307:ARG:NH1	2.44	0.46
2:B:104:LYS:HG3	2:B:192:ASP:OD2	2.16	0.46
2:B:385:LYS:HG2	2:B:386:THR:H	1.81	0.46
1:A:132:ILE:HB	1:A:142:ILE:CG1	2.44	0.46
1:A:218:ASP:O	1:A:222:GLN:HG3	2.16	0.46
2:B:125:ARG:NH1	2:B:147:ASN:HD22	2.13	0.46
1:A:51:GLY:C	1:A:53:GLU:H	2.18	0.46
1:A:395:LYS:CD	1:A:395:LYS:N	2.77	0.46
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.51	0.45
2:B:31:ILE:O	2:B:35:VAL:HG23	2.16	0.45
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.98	0.45
2:B:5:ILE:CG2	2:B:6:GLU:N	2.78	0.45
1:A:156:SER:CB	1:A:157:PRO:HD3	2.44	0.45
2:B:401:TRP:O	2:B:404:GLU:HB2	2.17	0.45
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.51	0.45
2:B:103:LYS:HD2	2:B:191:SER:CA	2.47	0.45
2:B:168:LEU:C	2:B:170:PRO:HD2	2.36	0.45
2:B:276:VAL:O	2:B:277:ARG:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:VAL:CG2	1:A:484:LEU:HD11	2.47	0.44
1:A:101:LYS:H	1:A:101:LYS:CD	2.28	0.44
2:B:125:ARG:HH11	2:B:147:ASN:HD22	1.66	0.44
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.52	0.44
2:B:46:LYS:O	2:B:147:ASN:HB2	2.17	0.44
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.00	0.44
1:A:380:ILE:HG12	2:B:27:THR:HG22	1.98	0.44
2:B:316:GLY:O	2:B:318:TYR:HD1	2.01	0.44
1:A:268:SER:CB	1:A:353:LYS:HE2	2.47	0.44
1:A:366:LYS:O	1:A:370:GLU:HG3	2.18	0.44
2:B:111:VAL:HG22	2:B:185:ASP:O	2.18	0.44
2:B:344:GLU:O	2:B:347:LYS:HB2	2.18	0.44
1:A:232:TYR:HB3	1:A:240:THR:O	2.17	0.44
1:A:90:VAL:O	1:A:91:GLN:C	2.56	0.43
1:A:94:ILE:HG23	1:A:229:TRP:HH2	1.82	0.43
1:A:102:LYS:O	1:A:103:LYS:HD3	2.18	0.43
1:A:170:PRO:O	1:A:171:PHE:C	2.56	0.43
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.53	0.43
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.53	0.43
2:B:167:ILE:O	2:B:167:ILE:HG12	2.18	0.43
2:B:172:ARG:O	2:B:176:PRO:HG3	2.18	0.43
2:B:353:LYS:HZ3	2:B:428:GLN:HG3	1.78	0.43
1:A:54:ASN:O	1:A:143:ARG:NH2	2.51	0.43
1:A:283:LEU:O	1:A:286:THR:HG23	2.18	0.43
1:A:325:LEU:HD21	1:A:385:LYS:HE3	2.01	0.43
1:A:108:VAL:C	1:A:109:LEU:HD12	2.39	0.43
1:A:169:GLU:N	1:A:170:PRO:CD	2.81	0.43
2:B:66:LYS:HA	2:B:407:GLN:HE22	1.84	0.43
2:B:160:PHE:O	2:B:160:PHE:CD1	2.72	0.43
1:A:207:GLN:O	1:A:211:ARG:HG3	2.19	0.43
1:A:153:TRP:CG	1:A:154:LYS:N	2.86	0.43
2:B:107:THR:HG22	2:B:109:LEU:CD1	2.49	0.43
1:A:41:MET:HB3	1:A:46:LYS:HG3	2.00	0.43
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.54	0.43
1:A:518:VAL:O	1:A:519:ASN:C	2.58	0.43
2:B:265:ASN:O	2:B:268:SER:OG	2.28	0.43
2:B:330:GLN:HB2	2:B:338:THR:HG1	1.82	0.43
2:B:393:ILE:CG1	2:B:394:GLN:N	2.80	0.43
2:B:98:ALA:O	2:B:101:LYS:HG2	2.18	0.42
2:B:207:GLN:HA	2:B:210:LEU:HB2	2.01	0.42
1:A:93:GLY:C	1:A:94:ILE:HD12	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD12	1:A:307:ARG:CA	2.50	0.42
2:B:247:PRO:O	2:B:252:TRP:CH2	2.72	0.42
1:A:83:ARG:HH11	1:A:83:ARG:CG	2.27	0.42
1:A:163:SER:O	1:A:164:MET:C	2.57	0.42
1:A:320:ASP:HA	1:A:321:PRO:HD2	1.83	0.42
1:A:401:TRP:O	1:A:404:GLU:HG2	2.20	0.42
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.55	0.42
2:B:85:GLN:CG	2:B:87:PHE:CZ	3.02	0.42
1:A:33:ALA:HB2	1:A:71:TRP:CD1	2.54	0.42
1:A:281:LYS:O	1:A:284:ARG:HG3	2.19	0.42
2:B:8:VAL:O	2:B:121:ASP:HB2	2.19	0.42
2:B:103:LYS:NZ	2:B:177:ASP:O	2.53	0.42
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.45	0.42
1:A:364:ASP:O	1:A:368:LEU:HB2	2.20	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.02	0.42
2:B:64:LYS:HD2	2:B:70:LYS:O	2.19	0.42
2:B:115:TYR:OH	2:B:157:PRO:HG3	2.20	0.42
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.00	0.42
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.49	0.42
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.35	0.42
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.93	0.42
1:A:201:LYS:O	1:A:204:GLU:HB2	2.19	0.42
1:A:340:GLN:HE21	1:A:340:GLN:HB3	1.67	0.42
1:A:108:VAL:HG23	1:A:227:PHE:CE1	2.54	0.41
1:A:303:LEU:HD23	1:A:303:LEU:C	2.40	0.41
2:B:394:GLN:O	2:B:395:LYS:C	2.58	0.41
1:A:54:ASN:ND2	1:A:129:ALA:HB2	2.35	0.41
1:A:83:ARG:CG	1:A:83:ARG:NH1	2.82	0.41
2:B:263:LYS:O	2:B:266:TRP:HB3	2.21	0.41
1:A:479:LEU:HB3	1:A:517:LEU:HD13	2.03	0.41
2:B:393:ILE:CG1	2:B:394:GLN:H	2.32	0.41
1:A:4:PRO:HG2	1:A:212:TRP:HE3	1.85	0.41
1:A:31:ILE:O	1:A:35:VAL:HG23	2.20	0.41
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.54	0.41
2:B:193:LEU:HB3	2:B:197:GLN:HB2	2.01	0.41
2:B:210:LEU:HD13	2:B:210:LEU:HA	1.87	0.41
1:A:10:VAL:HG12	1:A:11:LYS:H	1.85	0.41
1:A:178:ILE:N	1:A:178:ILE:HD13	2.35	0.41
1:A:224:GLU:HA	1:A:225:PRO:HD3	1.96	0.41
1:A:325:LEU:HG	1:A:387:PRO:HB3	2.03	0.41
1:A:399:GLU:HG3	1:A:402:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:N	1:A:70:LYS:O	2.46	0.41
1:A:40:GLU:HG3	1:A:44:GLU:OE1	2.20	0.41
1:A:295:LEU:N	1:A:295:LEU:CD2	2.83	0.41
1:A:394:GLN:O	1:A:397:THR:N	2.53	0.41
2:B:5:ILE:CG2	2:B:6:GLU:H	2.31	0.41
2:B:26:LEU:HB2	2:B:31:ILE:HD11	2.03	0.41
2:B:153:TRP:CH2	2:B:155:GLY:HA3	2.56	0.41
2:B:234:LEU:HD23	2:B:239:TRP:HZ2	1.85	0.41
1:A:487:GLN:HA	1:A:524:GLN:NE2	2.36	0.41
2:B:119:PRO:HA	2:B:148:VAL:HA	2.01	0.41
2:B:151:GLN:HB3	2:B:185:ASP:OD1	2.21	0.41
1:A:5:ILE:HD13	1:A:163:SER:HB3	2.02	0.40
1:A:167:ILE:C	1:A:170:PRO:HD2	2.39	0.40
1:A:239:TRP:O	1:A:315:HIS:CA	2.69	0.40
1:A:489:SER:HB2	1:A:493:VAL:HG13	2.03	0.40
2:B:134:SER:HB2	2:B:139:THR:HB	2.02	0.40
2:B:327:ALA:O	2:B:389:PHE:HA	2.21	0.40
1:A:279:LEU:HA	1:A:282:LEU:HD23	2.03	0.40
2:B:335:GLY:O	2:B:355:ALA:HA	2.22	0.40
2:B:380:ILE:O	2:B:384:GLY:CA	2.69	0.40
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.87	0.40
1:A:292:VAL:C	1:A:293:ILE:HD12	2.41	0.40
1:A:441:TYR:O	1:A:457:TYR:HA	2.22	0.40
1:A:120:LEU:O	1:A:121:ASP:C	2.60	0.40
2:B:84:THR:HB	2:B:154:LYS:HE2	2.02	0.40
2:B:107:THR:HG22	2:B:109:LEU:HD12	2.03	0.40
2:B:195:ILE:HD11	2:B:233:GLU:CG	2.52	0.40
1:A:60:VAL:HG21	1:A:130:PHE:CD1	2.56	0.40
1:A:168:LEU:C	1:A:170:PRO:HD2	2.42	0.40
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.56	0.40
2:B:323:LYS:HE3	2:B:323:LYS:HB3	1.94	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	520/560 (93%)	464 (89%)	45 (9%)	11 (2%)	7 33
2	B	393/440 (89%)	346 (88%)	43 (11%)	4 (1%)	15 53
All	All	913/1000 (91%)	810 (89%)	88 (10%)	15 (2%)	9 40

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ALA
1	A	195	ILE
1	A	402	TRP
1	A	170	PRO
1	A	230	MET
1	A	403	THR
1	A	538	ALA
2	B	232	TYR
1	A	137	ASN
1	A	243	PRO
1	A	412	PRO
2	B	193	LEU
2	B	277	ARG
2	B	395	LYS
1	A	156	SER

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	473/499 (95%)	419 (89%)	54 (11%)	5 24
2	B	366/400 (92%)	341 (93%)	25 (7%)	16 48
All	All	839/899 (93%)	760 (91%)	79 (9%)	8 32

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	20	LYS
1	A	46	LYS
1	A	61	PHE
1	A	67	ASP
1	A	89	GLU
1	A	123	ASP
1	A	134	SER
1	A	136	ASN
1	A	139	THR
1	A	142	ILE
1	A	163	SER
1	A	165	THR
1	A	168	LEU
1	A	177	ASP
1	A	185	ASP
1	A	187	LEU
1	A	194	GLU
1	A	195	ILE
1	A	206	ARG
1	A	232	TYR
1	A	243	PRO
1	A	253	THR
1	A	264	LEU
1	A	265	ASN
1	A	279	LEU
1	A	282	LEU
1	A	283	LEU
1	A	287	LYS
1	A	290	THR
1	A	295	LEU
1	A	317	VAL
1	A	325	LEU
1	A	336	GLN
1	A	340	GLN
1	A	356	ARG
1	A	362	THR
1	A	368	LEU
1	A	394	GLN
1	A	395	LYS
1	A	396	GLU
1	A	402	TRP
1	A	423	VAL

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Mol	Chain	Res	Type
1	A	424	LYS
1	A	470	THR
1	A	471	ASP
1	A	473	THR
1	A	476	LYS
1	A	484	LEU
1	A	493	VAL
1	A	500	GLN
1	A	503	LEU
1	A	514	GLU
1	A	517	LEU
2	B	8	VAL
2	B	16	MET
2	B	22	LYS
2	B	53	GLU
2	B	55	PRO
2	B	60	VAL
2	B	72	ARG
2	B	166	LYS
2	B	167	ILE
2	B	171	PHE
2	B	174	GLN
2	B	205	LEU
2	B	212	TRP
2	B	228	LEU
2	B	230	MET
2	B	280	CYS
2	B	283	LEU
2	B	286	THR
2	B	295	LEU
2	B	297	GLU
2	B	301	LEU
2	B	303	LEU
2	B	353	LYS
2	B	368	LEU
2	B	414	TRP

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

Mol	Chain	Res	Type
1	A	174	GLN
1	A	207	GLN

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Mol	Chain	Res	Type
1	A	221	HIS
1	A	222	GLN
1	A	235	HIS
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	336	GLN
1	A	407	GLN
1	A	475	GLN
1	A	480	GLN
1	A	507	GLN
1	A	509	GLN
1	A	520	GLN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	174	GLN
2	B	175	ASN
2	B	207	GLN
2	B	242	GLN
2	B	269	GLN
2	B	278	GLN
2	B	336	GLN
2	B	348	ASN
2	B	407	GLN
2	B	428	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)

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\|>2$
1	CSD	A	280	1	3,7,8	0.80	0	1,8,10	6.79	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

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	A	280	CSD	OD1-SG-CB	6.79	118.46	105.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

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	NVP	A	999	-	15,23,23	1.66	5 (33%)	13,34,34	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NVP	A	999	-	-	0/0/6/6	0/3/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	NVP	C7-C2	3.24	1.42	1.38
3	A	999	NVP	C10-C15	2.84	1.44	1.41
3	A	999	NVP	C4-N3	2.25	1.37	1.32
3	A	999	NVP	C12-C11	2.20	1.41	1.36
3	A	999	NVP	C13-N14	2.15	1.36	1.32

There are no bond angle outliers.

There are no chirality outliers.

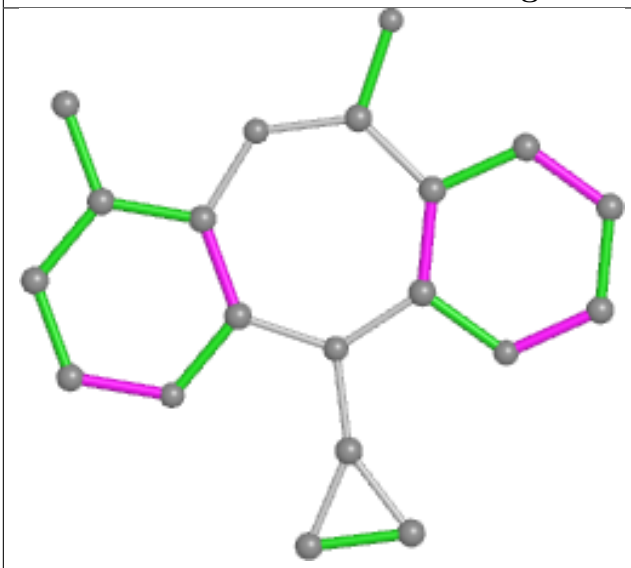
There are no torsion outliers.

There are no ring outliers.

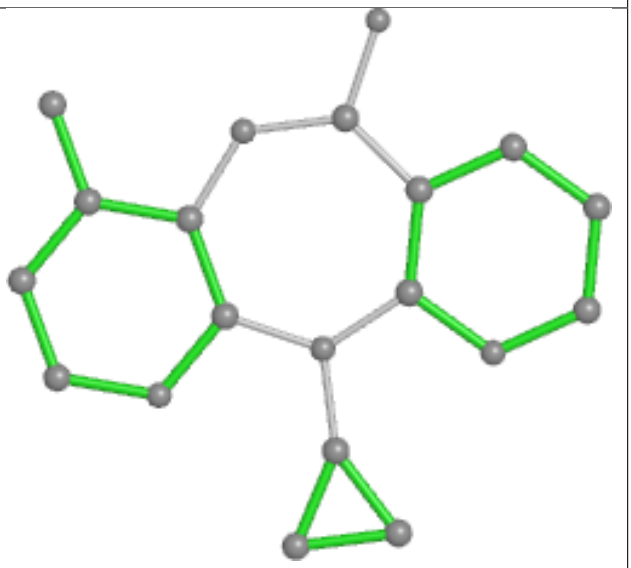
No monomer is involved in short contacts.

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.

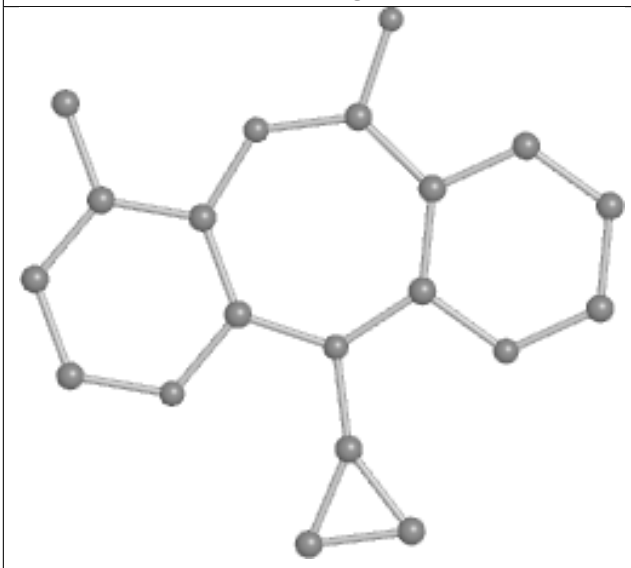
Ligand NVP A 999



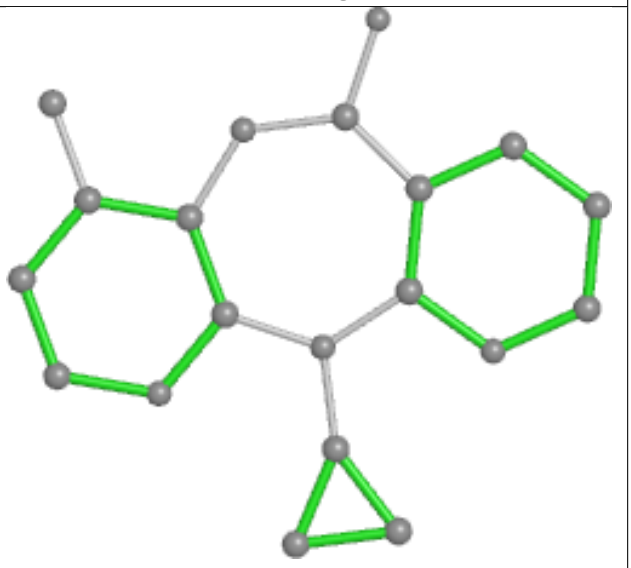
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	524/560 (93%)	-0.36	15 (2%) 51 23	36, 87, 141, 150	0
2	B	401/440 (91%)	-0.34	2 (0%) 91 75	40, 88, 133, 149	0
All	All	925/1000 (92%)	-0.35	17 (1%) 68 40	36, 88, 136, 150	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	ASP	4.7
1	A	470	THR	3.8
1	A	471	ASP	3.6
1	A	15	GLY	2.9
1	A	137	ASN	2.8
2	B	212	TRP	2.6
2	B	230	MET	2.5
1	A	141	GLY	2.5
1	A	402	TRP	2.5
1	A	467	VAL	2.4
1	A	66	LYS	2.4
1	A	469	LEU	2.4
1	A	63	ILE	2.3
1	A	241	VAL	2.3
1	A	138	GLU	2.2
1	A	539	HIS	2.1
1	A	538	ALA	2.0

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

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
1	CSD	A	280	8/9	0.93	0.16	78,81,85,89	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

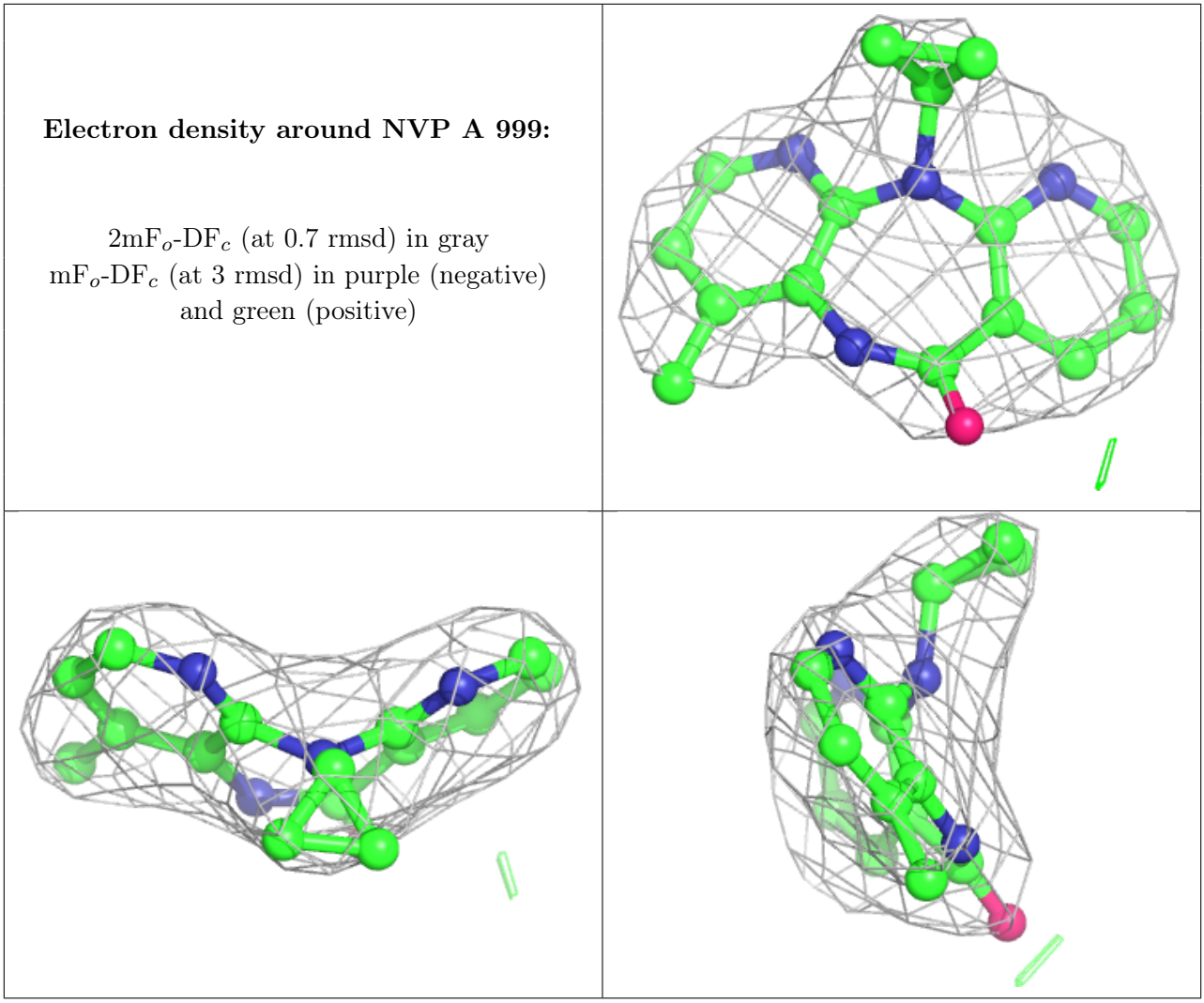
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NVP	A	999	20/20	0.97	0.23	58,63,77,78	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 NVP A 999:

$2mF_o$-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.