Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 07:57 PM EST

PDB ID	:	3TAZ
Title	:	Crystal structure of NurA bound to dAMP and manganese
Authors	:	Chae, J.; Kim, Y.C.; Cho, Y.
Deposited on	:	2011-08-04
Resolution	:	3.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

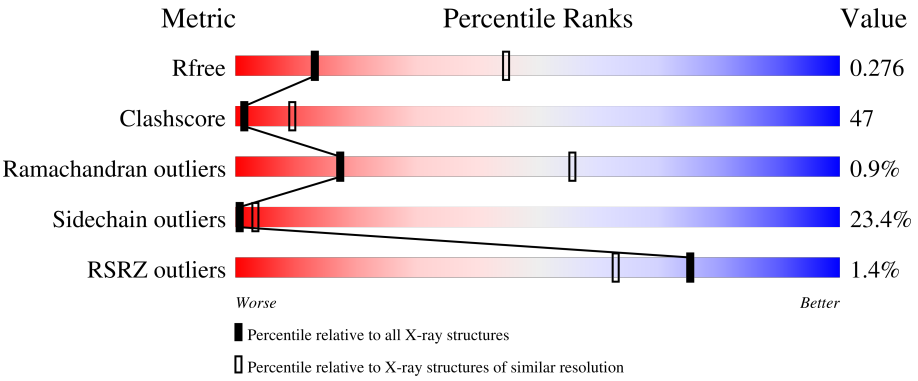
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	471	33% 44% 14% 8%
1	B	471	3% 31% 47% 13% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DA	B	453	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7020 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 DNA double-strand break repair protein nurA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3487	2235	597	648	7			
1	B	433	Total	C	N	O	S	0	0	0
			3494	2240	597	650	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8U1N8
A	-18	GLY	-	expression tag	UNP Q8U1N8
A	-17	SER	-	expression tag	UNP Q8U1N8
A	-16	SER	-	expression tag	UNP Q8U1N8
A	-15	HIS	-	expression tag	UNP Q8U1N8
A	-14	HIS	-	expression tag	UNP Q8U1N8
A	-13	HIS	-	expression tag	UNP Q8U1N8
A	-12	HIS	-	expression tag	UNP Q8U1N8
A	-11	HIS	-	expression tag	UNP Q8U1N8
A	-10	HIS	-	expression tag	UNP Q8U1N8
A	-9	SER	-	expression tag	UNP Q8U1N8
A	-8	SER	-	expression tag	UNP Q8U1N8
A	-7	GLY	-	expression tag	UNP Q8U1N8
A	-6	LEU	-	expression tag	UNP Q8U1N8
A	-5	VAL	-	expression tag	UNP Q8U1N8
A	-4	PRO	-	expression tag	UNP Q8U1N8
A	-3	ARG	-	expression tag	UNP Q8U1N8
A	-2	GLY	-	expression tag	UNP Q8U1N8
A	-1	SER	-	expression tag	UNP Q8U1N8
A	0	HIS	-	expression tag	UNP Q8U1N8
B	-19	MET	-	expression tag	UNP Q8U1N8
B	-18	GLY	-	expression tag	UNP Q8U1N8
B	-17	SER	-	expression tag	UNP Q8U1N8
B	-16	SER	-	expression tag	UNP Q8U1N8
B	-15	HIS	-	expression tag	UNP Q8U1N8

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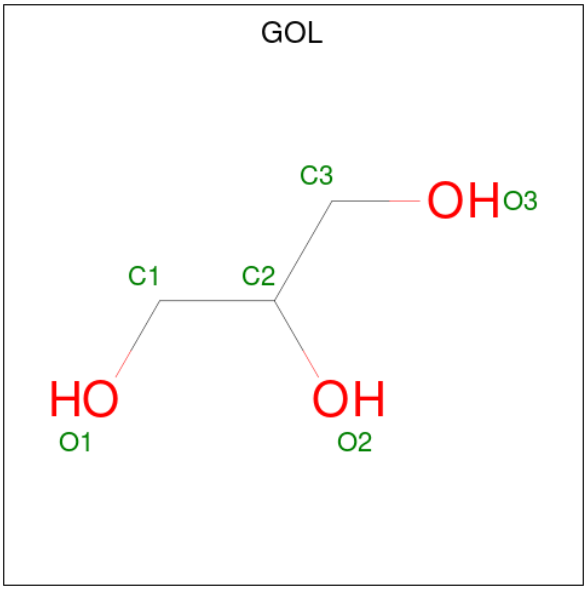
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8U1N8
B	-13	HIS	-	expression tag	UNP Q8U1N8
B	-12	HIS	-	expression tag	UNP Q8U1N8
B	-11	HIS	-	expression tag	UNP Q8U1N8
B	-10	HIS	-	expression tag	UNP Q8U1N8
B	-9	SER	-	expression tag	UNP Q8U1N8
B	-8	SER	-	expression tag	UNP Q8U1N8
B	-7	GLY	-	expression tag	UNP Q8U1N8
B	-6	LEU	-	expression tag	UNP Q8U1N8
B	-5	VAL	-	expression tag	UNP Q8U1N8
B	-4	PRO	-	expression tag	UNP Q8U1N8
B	-3	ARG	-	expression tag	UNP Q8U1N8
B	-2	GLY	-	expression tag	UNP Q8U1N8
B	-1	SER	-	expression tag	UNP Q8U1N8
B	0	HIS	-	expression tag	UNP Q8U1N8

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

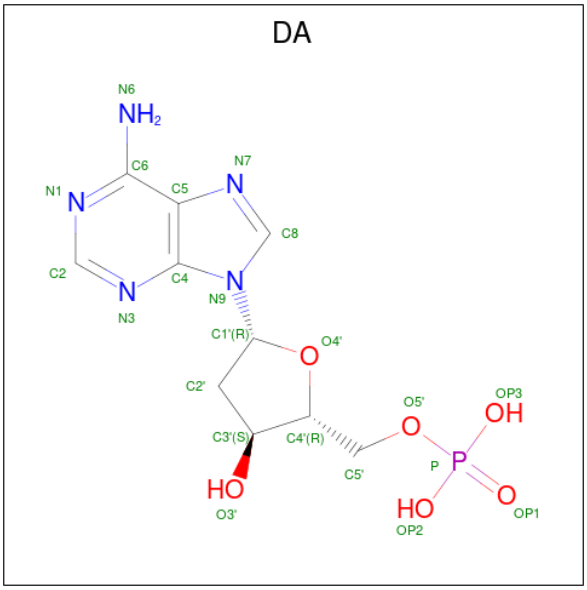
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is 2'-DEOXYADENOSINE-5'-MONOPHOSPHATE (three-letter code: DA) (formula: $C_{10}H_{14}N_5O_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 22 10 5 6 1	0	0

- Molecule 5 is water.

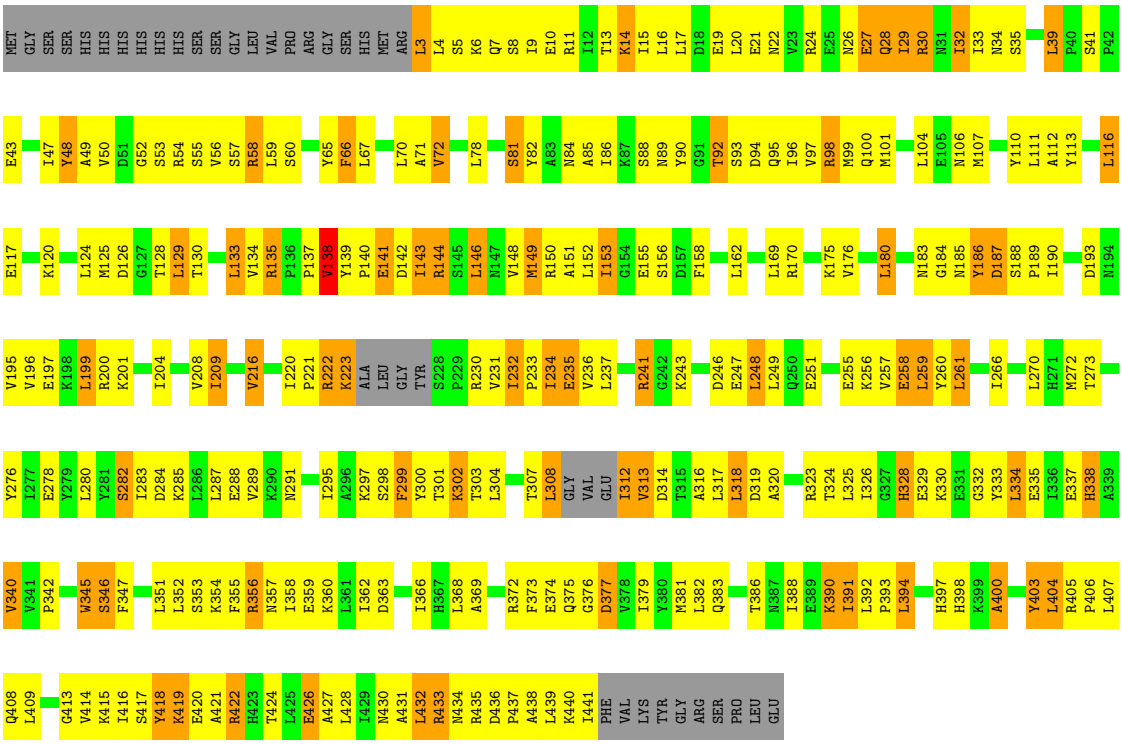
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	4	Total O 4 4	0	0

3 Residue-property plots (i)

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

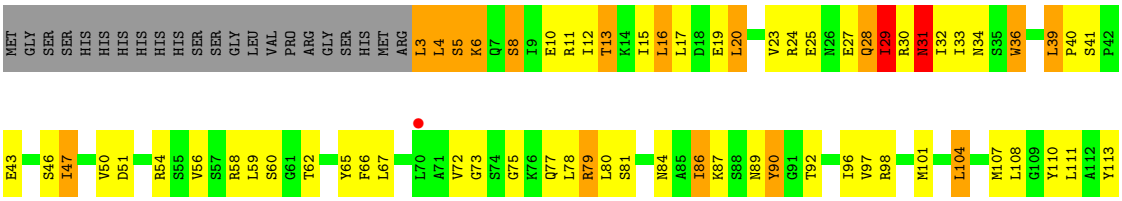
• Molecule 1: DNA double-strand break repair protein nurA

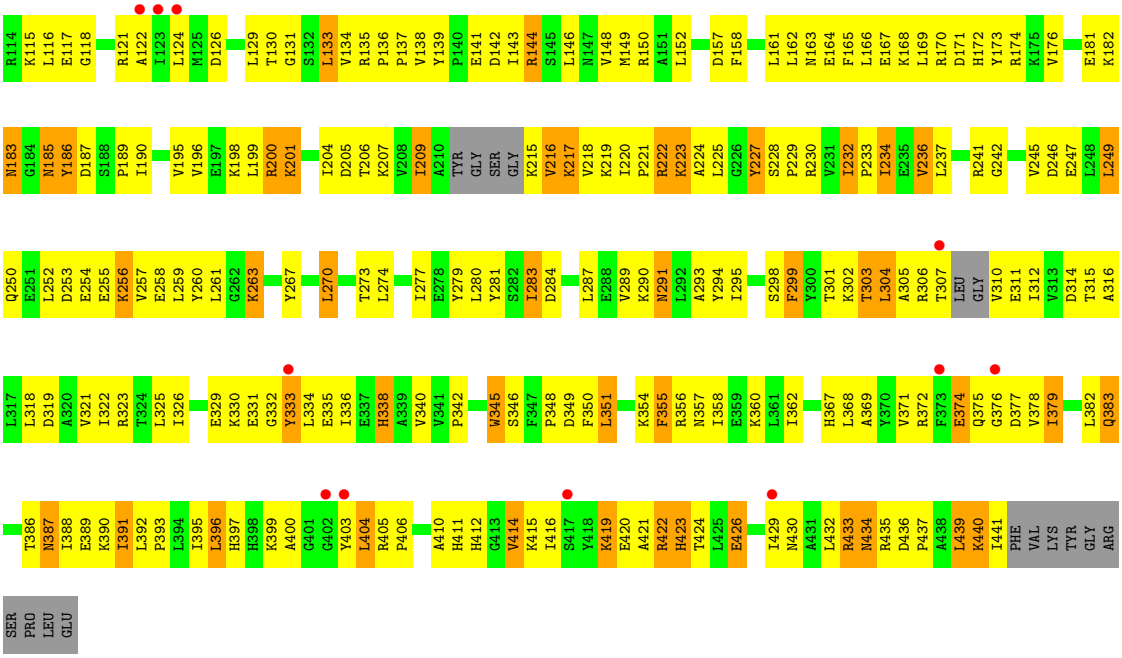
Chain A:



• Molecule 1: DNA double-strand break repair protein nurA

Chain B:




R114 K115 L116 E117 G118 R121 A122 I123 L124 M125 D126 L129 T130 G131 S132 L133 V134 R135 P136 P137 V138 Y139 P140 E141 D142 I143 R144 S145 L146 N147 V148 M149 R150 A151 L152 D157 F158 L161 L162 N163 E164 F165 L166 E167 K168 L169 R170 D171 H172 Y173 R174 K175 V176 E181 K182
N183 G184 N185 Y186 D187 S188 P189 I190 V195 V196 E197 K198 L199 R200 K201 I204 D205 T206 K207 V208 I209 A210 TYR GLY SER GLY K215 V216 K217 V218 K219 I220 P221 R222 K223 A224 L225 G226 Y227 S228 P229 R230 V231 I232 P233 I234 E235 V236 L237 R241 G242 V245 D246 E247 L248 L249
Q250 E251 L252 D253 E254 E255 K256 V257 E258 L259 Y260 L261 G262 K263 Y267 L270 T273 L274 I277 E278 Y279 L280 Y281 S282 I283 D284 L287 E288 V289 K290 N291 L292 A293 Y294 I295 S298 F299 Y300 T301 K302 T303 L304 A305 R306 T307 LEU GLY V310 E311 I312 V313 D314 T315 A316
L317 L318 D319 A320 V321 I322 R323 T324 L325 I326 E329 K330 E331 G332 Y333 L334 E335 I336 E337 H338 A339 V340 V341 P342 W345 S346 F347 P348 D349 F350 L351 K354 F355 R356 N357 I358 E359 K360 L361 I362 H367 L368 A369 Y370 V371 R372 F373 E374 Q375 G376 D377 V378 I379 L382 Q383
T386 N387 I388 E389 K390 I391 L392 P393 L394 I395 L396 H397 H398 K399 A400 G401 G402 Y403 L404 R405 P406 A410 H411 H412 G413 V414 K415 I416 S417 Y418 K419 E420 A421 R422 H423 T424 L425 E426 I429 N430 A431 L432 R433 N434 R435 D436 P437 A438 L439 K440 I441 PHE VAL LYS TYR GLY ARG
SER PRO LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.16Å 114.85Å 123.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.71 – 3.20 44.80 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (28.71-3.20) 97.1 (44.80-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.191 , 0.279 0.188 , 0.276	Depositor DCC
R_{free} test set	798 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	98.5	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 106.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7020	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: GOL, MN

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	0.53	0/3546	0.72	0/4784
1	B	0.46	0/3553	0.67	0/4796
All	All	0.50	0/7099	0.70	0/9580

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	LEU	Peptide
1	A	400	ALA	Peptide
1	A	417	SER	Peptide
1	B	374	GLU	Peptide
1	B	400	ALA	Peptide
1	B	8	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3487	0	3609	335	0
1	B	3494	0	3610	388	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	8	2	0
4	B	22	0	12	12	0
5	A	5	0	0	3	0
5	B	4	0	0	0	0
All	All	7020	0	7239	671	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 47.

All (671) 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:441:ILE:CG2	1:B:378:VAL:HG21	1.69	1.21
1:A:441:ILE:HG21	1:B:378:VAL:CG2	1.71	1.19
1:B:310:VAL:HG22	1:B:311:GLU:H	1.09	1.11
1:B:229:PRO:HA	1:B:230:ARG:HB2	1.27	1.10
1:A:419:LYS:H	1:A:419:LYS:HD2	1.13	1.10
1:A:347:PHE:HB3	1:A:352:LEU:HD11	1.26	1.09
1:A:314:ASP:OD1	1:B:60:SER:HB3	1.54	1.08
1:B:378:VAL:HG22	1:B:379:ILE:N	1.72	1.04
1:A:230:ARG:HB3	1:B:234:ILE:HB	1.37	1.04
1:B:378:VAL:HG22	1:B:379:ILE:H	0.88	1.01
1:B:130:THR:HG23	1:B:383:GLN:HE22	1.29	0.98
1:B:378:VAL:CG2	1:B:379:ILE:H	1.75	0.97
1:B:162:LEU:HD21	1:B:354:LYS:HG3	1.47	0.96
1:A:435:ARG:HE	1:A:439:LEU:HD21	1.26	0.95
1:A:421:ALA:HA	1:A:424:THR:OG1	1.68	0.93
1:B:284:ASP:HB2	1:B:355:PHE:HB3	1.50	0.92
1:A:236:VAL:HG23	1:A:259:LEU:HD11	1.56	0.87
1:A:441:ILE:HG21	1:B:378:VAL:HG21	0.89	0.87
1:B:138:VAL:HG22	1:B:141:GLU:HB3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:CD	1:A:27:GLU:H	1.78	0.87
1:A:302:LYS:HG2	1:B:89:ASN:ND2	1.90	0.87
1:B:259:LEU:HD23	1:B:260:TYR:N	1.89	0.87
1:B:310:VAL:HG22	1:B:311:GLU:N	1.89	0.86
1:B:419:LYS:HD2	1:B:422:ARG:HG3	1.56	0.86
1:A:320:ALA:HB1	1:B:434:ASN:ND2	1.91	0.86
1:A:302:LYS:HG2	1:B:89:ASN:HD21	1.39	0.85
1:B:131:GLY:HA3	4:B:453:DA:H3'	1.58	0.85
1:A:27:GLU:HG2	1:A:28:GLN:H	1.41	0.84
1:A:435:ARG:NE	1:A:439:LEU:HD21	1.91	0.83
1:B:144:ARG:O	1:B:148:VAL:HG23	1.79	0.83
1:B:422:ARG:NH1	1:B:423:HIS:HE1	1.76	0.83
1:A:295:ILE:HD11	1:A:382:LEU:HD13	1.61	0.82
1:B:135:ARG:NH2	1:B:306:ARG:HH12	1.76	0.82
1:B:229:PRO:HA	1:B:230:ARG:CB	2.10	0.82
1:A:419:LYS:HD2	1:A:419:LYS:N	1.95	0.81
1:B:130:THR:HG23	1:B:383:GLN:NE2	1.94	0.81
1:A:220:ILE:O	1:A:220:ILE:HD12	1.81	0.81
1:B:67:LEU:HD22	1:B:101:MET:HE2	1.63	0.81
1:A:325:LEU:HB3	1:A:326:ILE:HD12	1.64	0.79
1:B:29:ILE:HG12	1:B:33:ILE:HD13	1.65	0.79
1:A:162:LEU:HD21	1:A:354:LYS:HG3	1.65	0.79
1:B:27:GLU:OE2	1:B:30:ARG:HD2	1.83	0.78
1:A:129:LEU:HD13	1:A:366:ILE:HG12	1.65	0.78
1:A:144:ARG:HA	1:B:229:PRO:HG3	1.64	0.77
1:A:153:ILE:HD11	1:A:158:PHE:HA	1.67	0.77
1:B:421:ALA:HA	1:B:424:THR:OG1	1.85	0.77
1:B:222:ARG:HG3	1:B:223:LYS:HD3	1.67	0.77
1:B:419:LYS:H	1:B:419:LYS:HE2	1.50	0.76
1:B:241:ARG:HG2	1:B:242:GLY:H	1.49	0.76
1:B:29:ILE:HD11	1:B:326:ILE:HD11	1.68	0.75
1:B:342:PRO:HD2	1:B:362:ILE:HA	1.66	0.75
1:A:419:LYS:H	1:A:419:LYS:CD	1.95	0.75
1:B:12:ILE:O	1:B:15:ILE:HG22	1.85	0.75
1:A:427:ALA:O	1:A:430:ASN:HB2	1.86	0.75
1:B:86:ILE:CD1	1:B:87:LYS:HG2	2.16	0.75
1:B:150:ARG:NH2	1:B:350:PHE:CG	2.54	0.75
1:B:170:ARG:HH21	1:B:174:ARG:HH22	1.35	0.75
1:A:9:ILE:O	1:A:13:THR:HG23	1.86	0.74
1:A:170:ARG:HD2	1:A:170:ARG:O	1.87	0.74
1:B:229:PRO:CA	1:B:230:ARG:HB2	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:TYR:CD1	1:A:140:PRO:HA	2.23	0.74
1:A:302:LYS:CE	1:B:87:LYS:HG3	2.17	0.74
1:B:375:GLN:HG3	1:B:376:GLY:H	1.52	0.74
1:B:137:PRO:HG3	4:B:453:DA:H61	1.51	0.74
1:B:30:ARG:O	1:B:32:ILE:HG12	1.88	0.73
1:B:144:ARG:HD3	1:B:225:LEU:HD11	1.70	0.73
1:A:230:ARG:HB3	1:B:234:ILE:CB	2.16	0.73
1:A:39:LEU:HD13	1:A:332:GLY:HA2	1.71	0.73
1:A:320:ALA:HA	1:B:436:ASP:OD2	1.89	0.73
1:A:441:ILE:O	1:A:441:ILE:HG22	1.87	0.73
1:B:144:ARG:HB2	1:B:225:LEU:CD1	2.19	0.72
1:B:130:THR:H	1:B:383:GLN:HE22	1.36	0.72
1:A:302:LYS:HE2	1:B:87:LYS:HG3	1.71	0.72
1:B:419:LYS:O	1:B:422:ARG:HB2	1.89	0.72
1:A:303:THR:HG22	1:A:307:THR:OG1	1.89	0.72
1:A:302:LYS:HE2	1:B:87:LYS:HZ3	1.54	0.71
1:B:176:VAL:HG22	1:B:186:TYR:HE2	1.54	0.71
1:A:16:LEU:O	1:A:19:GLU:HB2	1.91	0.71
1:A:300:TYR:CG	1:A:301:THR:N	2.58	0.71
1:A:104:LEU:HD22	1:A:189:PRO:HB2	1.73	0.70
1:B:319:ASP:HA	1:B:379:ILE:CD1	2.21	0.70
1:A:6:LYS:HA	1:A:9:ILE:HB	1.74	0.70
1:B:342:PRO:CD	1:B:362:ILE:HA	2.21	0.70
1:A:232:ILE:HG13	1:B:232:ILE:HG23	1.73	0.70
1:B:217:LYS:HD3	1:B:260:TYR:CE2	2.27	0.70
1:B:176:VAL:HG13	1:B:186:TYR:HD2	1.55	0.69
1:B:137:PRO:HG3	4:B:453:DA:N1	2.08	0.69
1:A:320:ALA:HB1	1:B:434:ASN:HD21	1.55	0.69
1:B:336:ILE:HG12	1:B:368:LEU:HB2	1.75	0.69
1:A:358:ILE:O	1:A:362:ILE:HG12	1.92	0.69
1:B:162:LEU:CD2	1:B:166:LEU:HD11	2.23	0.68
1:B:67:LEU:CD2	1:B:101:MET:HE2	2.23	0.68
1:B:426:GLU:CD	1:B:426:GLU:H	1.96	0.68
1:B:392:LEU:HB3	1:B:393:PRO:HD3	1.75	0.68
1:B:220:ILE:HB	1:B:221:PRO:HD2	1.75	0.68
1:A:135:ARG:HH22	1:B:90:TYR:H	1.41	0.68
1:A:8:SER:CB	1:A:11:ARG:NH2	2.57	0.68
1:A:325:LEU:CB	1:A:326:ILE:HD12	2.23	0.68
1:B:333:TYR:HB2	1:B:371:VAL:HG22	1.77	0.67
1:B:118:GLY:H	1:B:121:ARG:NH2	1.91	0.67
1:B:86:ILE:HD12	1:B:87:LYS:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:OD1	1:B:60:SER:CB	2.39	0.67
1:A:375:GLN:HG3	1:A:376:GLY:H	1.58	0.67
1:B:342:PRO:HG2	1:B:362:ILE:HD13	1.77	0.67
1:B:377:ASP:OD1	1:B:378:VAL:N	2.26	0.67
1:B:335:GLU:HG3	1:B:388:ILE:HG13	1.77	0.67
1:B:176:VAL:HG13	1:B:186:TYR:CD2	2.30	0.66
1:A:241:ARG:O	1:B:246:ASP:OD2	2.13	0.66
1:B:196:VAL:HG23	1:B:274:LEU:HD12	1.76	0.66
1:B:310:VAL:CG2	1:B:311:GLU:H	1.93	0.66
1:A:249:LEU:HD21	1:B:237:LEU:HB3	1.78	0.66
1:B:30:ARG:HG2	1:B:32:ILE:HG12	1.76	0.66
1:B:138:VAL:HG13	1:B:138:VAL:O	1.95	0.66
1:B:375:GLN:HG3	1:B:376:GLY:N	2.09	0.66
1:A:435:ARG:HH21	1:A:439:LEU:HD11	1.59	0.66
4:B:453:DA:H2'	4:B:453:DA:N3	2.10	0.65
1:B:323:ARG:NH1	1:B:329:GLU:HG3	2.11	0.65
1:A:49:ALA:HA	1:A:124:LEU:HB3	1.78	0.65
1:A:302:LYS:CG	1:B:89:ASN:HD21	2.09	0.65
1:B:162:LEU:CD2	1:B:354:LYS:HG3	2.23	0.65
1:B:299:PHE:HD1	1:B:299:PHE:H	1.43	0.65
1:B:137:PRO:O	1:B:138:VAL:HG12	1.96	0.65
1:A:39:LEU:HD13	1:A:332:GLY:CA	2.27	0.65
1:B:325:LEU:HB3	1:B:326:ILE:HD12	1.78	0.65
1:A:300:TYR:C	1:A:304:LEU:HD12	2.17	0.64
1:B:56:VAL:HG12	1:B:65:TYR:HB3	1.78	0.64
1:B:436:ASP:O	1:B:439:LEU:HB2	1.97	0.64
1:B:4:LEU:C	1:B:6:LYS:H	1.99	0.64
1:B:135:ARG:HH21	1:B:306:ARG:HH12	1.45	0.64
1:B:420:GLU:O	1:B:424:THR:HG23	1.98	0.64
1:A:381:MET:HE3	1:A:383:GLN:HG2	1.79	0.64
1:B:392:LEU:O	1:B:396:LEU:HD12	1.97	0.64
1:B:176:VAL:HG22	1:B:186:TYR:CE2	2.32	0.64
1:A:120:LYS:NZ	1:A:390:LYS:HE2	2.12	0.64
1:A:176:VAL:HG22	1:A:186:TYR:CE2	2.33	0.64
1:B:152:LEU:HG	1:B:207:LYS:HE2	1.79	0.63
1:B:440:LYS:HE3	1:B:440:LYS:HA	1.79	0.63
1:B:173:TYR:CE1	1:B:281:TYR:HE2	2.17	0.63
1:A:104:LEU:CD2	1:A:189:PRO:HB2	2.28	0.63
1:B:322:ILE:CD1	1:B:323:ARG:HG3	2.28	0.63
1:A:53:SER:O	1:A:101:MET:HE3	1.99	0.63
1:B:144:ARG:HB2	1:B:225:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:VAL:HG12	1:B:249:LEU:HD12	1.80	0.62
1:A:372:ARG:HD3	1:A:375:GLN:O	1.99	0.62
1:A:295:ILE:CD1	1:A:382:LEU:HD13	2.29	0.62
1:A:124:LEU:HD21	1:A:404:LEU:HD12	1.81	0.62
1:B:86:ILE:HD12	1:B:87:LYS:H	1.64	0.62
1:B:228:SER:H	1:B:230:ARG:HG2	1.64	0.62
1:A:3:LEU:HD11	1:B:66:PHE:CZ	2.34	0.62
1:A:426:GLU:CD	1:A:426:GLU:H	2.03	0.62
1:B:8:SER:HB2	1:B:11:ARG:NH2	2.15	0.62
1:B:355:PHE:CB	1:B:358:ILE:HD12	2.30	0.62
1:A:135:ARG:HH22	1:B:90:TYR:HB2	1.65	0.61
1:A:222:ARG:HA	1:A:230:ARG:NH1	2.15	0.61
1:A:142:ASP:OD2	1:A:143:ILE:HD13	1.99	0.61
1:B:115:LYS:HE2	1:B:181:GLU:OE2	2.00	0.61
1:B:98:ARG:HG2	4:B:453:DA:H62	1.63	0.61
1:B:342:PRO:HG2	1:B:362:ILE:HA	1.83	0.61
1:A:104:LEU:HD22	1:A:189:PRO:CB	2.30	0.61
1:B:399:LYS:HA	1:B:404:LEU:HA	1.81	0.61
1:B:422:ARG:HH11	1:B:423:HIS:HE1	1.48	0.61
1:B:436:ASP:HA	1:B:439:LEU:HD12	1.80	0.61
1:A:11:ARG:O	1:A:15:ILE:HG13	1.99	0.61
1:B:165:PHE:HD2	1:B:277:ILE:HG21	1.66	0.61
1:B:374:GLU:HB3	1:B:375:GLN:HG2	1.82	0.61
1:A:32:ILE:HG22	1:A:33:ILE:HD13	1.83	0.61
1:A:241:ARG:HD3	1:B:246:ASP:OD1	2.00	0.61
1:B:86:ILE:HD11	1:B:87:LYS:HG2	1.82	0.61
1:B:284:ASP:CB	1:B:355:PHE:HB3	2.25	0.61
1:A:144:ARG:O	1:A:148:VAL:HG23	2.01	0.61
1:A:313:VAL:HG23	1:A:314:ASP:N	2.16	0.61
1:A:89:ASN:HB2	1:A:92:THR:HB	1.83	0.61
1:A:24:ARG:HH21	1:A:325:LEU:HD21	1.65	0.61
1:B:137:PRO:HG3	4:B:453:DA:N6	2.14	0.60
1:A:419:LYS:HB2	1:A:422:ARG:HB2	1.83	0.60
1:A:60:SER:HB2	1:B:314:ASP:OD1	2.01	0.60
1:A:106:ASN:HB2	1:A:282:SER:OG	2.01	0.60
1:B:412:HIS:HA	1:B:415:LYS:HE2	1.83	0.60
1:B:310:VAL:O	1:B:312:ILE:HG23	2.02	0.60
1:B:440:LYS:HA	1:B:440:LYS:CE	2.31	0.60
1:A:308:LEU:HD23	1:A:308:LEU:H	1.67	0.60
1:A:392:LEU:HB3	1:A:393:PRO:HD3	1.82	0.60
1:B:195:VAL:HG12	1:B:199:LEU:HD23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ILE:C	1:A:313:VAL:HG12	2.22	0.60
1:B:58:ARG:O	1:B:59:LEU:HD23	2.01	0.60
1:A:439:LEU:O	1:A:440:LYS:HB3	2.01	0.59
1:B:258:GLU:O	1:B:259:LEU:HB2	2.02	0.59
1:B:80:LEU:HG	1:B:108:LEU:HD13	1.84	0.59
1:A:3:LEU:O	1:A:4:LEU:HG	2.01	0.59
1:A:104:LEU:HA	1:A:107:MET:HE2	1.83	0.59
1:B:16:LEU:O	1:B:19:GLU:HB2	2.02	0.59
1:B:336:ILE:HG13	1:B:368:LEU:O	2.03	0.59
1:A:85:ALA:O	1:B:15:ILE:HD13	2.03	0.59
1:A:308:LEU:HD23	1:A:308:LEU:N	2.18	0.59
1:B:29:ILE:O	1:B:33:ILE:HD12	2.02	0.59
1:A:291:ASN:HB3	1:A:391:ILE:HD11	1.85	0.59
1:A:369:ALA:HB2	1:A:388:ILE:HG13	1.85	0.59
1:B:319:ASP:HA	1:B:379:ILE:HD11	1.83	0.59
1:B:135:ARG:HH21	1:B:306:ARG:NH1	2.00	0.59
1:A:195:VAL:HG22	1:A:199:LEU:HD22	1.84	0.59
1:A:441:ILE:CG1	1:B:378:VAL:HG11	2.33	0.59
1:A:5:SER:C	1:A:7:GLN:H	2.05	0.58
1:A:170:ARG:NH1	5:A:458:HOH:O	2.22	0.58
1:A:53:SER:C	1:A:101:MET:HE3	2.24	0.58
1:A:259:LEU:HD23	1:A:261:LEU:HD21	1.85	0.58
1:A:96:ILE:HD11	1:A:272:MET:CE	2.33	0.58
1:A:152:LEU:HD21	1:A:266:ILE:CD1	2.32	0.58
1:A:313:VAL:HG23	1:A:314:ASP:O	2.03	0.58
1:A:318:LEU:HD23	1:A:319:ASP:N	2.18	0.58
1:B:17:LEU:HA	1:B:20:LEU:HG	1.85	0.58
1:B:259:LEU:HD23	1:B:260:TYR:H	1.69	0.58
1:A:120:LYS:NZ	1:A:394:LEU:HD11	2.19	0.58
1:B:54:ARG:HB3	1:B:101:MET:CE	2.34	0.58
1:B:319:ASP:HA	1:B:379:ILE:HD12	1.85	0.58
1:B:28:GLN:O	1:B:29:ILE:HG22	2.04	0.58
1:A:169:LEU:HD21	1:A:278:GLU:HG3	1.85	0.58
1:B:345:TRP:CD1	1:B:345:TRP:C	2.77	0.58
1:A:146:LEU:HD11	1:A:273:THR:HG23	1.86	0.57
1:A:149:MET:HE1	1:A:204:ILE:HD11	1.86	0.57
1:B:17:LEU:O	1:B:20:LEU:HG	2.04	0.57
1:B:4:LEU:O	1:B:6:LYS:N	2.37	0.57
1:B:4:LEU:C	1:B:6:LYS:N	2.57	0.57
1:B:113:TYR:CG	1:B:289:VAL:HG22	2.40	0.57
1:B:131:GLY:HA3	4:B:453:DA:C3'	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LYS:HA	1:B:205:ASP:HB2	1.87	0.57
1:A:43:GLU:O	1:A:397:HIS:HB2	2.04	0.57
1:B:215:LYS:O	1:B:216:VAL:HG13	2.04	0.57
1:A:5:SER:HB2	1:A:8:SER:H	1.69	0.57
1:A:95:GLN:HB3	1:A:138:VAL:HG22	1.86	0.56
1:A:24:ARG:HH21	1:A:325:LEU:CD2	2.17	0.56
1:B:8:SER:HA	1:B:11:ARG:NH1	2.19	0.56
1:B:113:TYR:OH	1:B:290:LYS:HB2	2.04	0.56
1:A:66:PHE:CZ	1:A:421:ALA:HB3	2.40	0.56
1:A:342:PRO:HD2	1:A:362:ILE:HA	1.87	0.56
1:B:200:ARG:O	1:B:204:ILE:HB	2.06	0.56
1:B:323:ARG:HH11	1:B:329:GLU:HG3	1.70	0.56
1:A:413:GLY:O	1:A:416:ILE:HB	2.06	0.56
1:B:287:LEU:HB2	1:B:357:ASN:HB3	1.86	0.56
1:A:3:LEU:HD12	1:A:4:LEU:HA	1.88	0.56
1:B:279:TYR:CE2	1:B:283:ILE:HD11	2.41	0.56
1:B:130:THR:H	1:B:383:GLN:NE2	2.01	0.56
1:B:169:LEU:O	1:B:172:HIS:HB3	2.06	0.56
1:B:302:LYS:N	1:B:302:LYS:HD2	2.20	0.56
1:B:342:PRO:CG	1:B:362:ILE:HA	2.35	0.55
1:B:6:LYS:HD3	1:B:6:LYS:C	2.26	0.55
1:B:322:ILE:HD12	1:B:323:ARG:HG3	1.87	0.55
1:B:348:PRO:HB3	1:B:350:PHE:CE2	2.41	0.55
1:A:67:LEU:O	1:A:81:SER:HA	2.07	0.55
1:B:19:GLU:O	1:B:23:VAL:HG23	2.07	0.55
1:B:29:ILE:O	1:B:33:ILE:CD1	2.55	0.55
1:B:414:VAL:O	1:B:416:ILE:HD12	2.06	0.55
1:A:24:ARG:HE	1:A:325:LEU:HD21	1.72	0.55
1:A:151:ALA:HB1	1:A:233:PRO:HD3	1.87	0.55
1:A:323:ARG:HD3	1:A:329:GLU:OE1	2.06	0.55
1:B:107:MET:HG2	1:B:173:TYR:CE2	2.41	0.55
1:B:130:THR:O	1:B:133:LEU:HD23	2.06	0.55
1:B:224:ALA:O	1:B:225:LEU:HD12	2.06	0.55
1:A:375:GLN:HG3	1:A:376:GLY:N	2.20	0.55
1:A:435:ARG:HG3	1:A:439:LEU:HD23	1.89	0.55
1:B:310:VAL:CG2	1:B:311:GLU:N	2.62	0.55
1:B:374:GLU:C	1:B:375:GLN:HG2	2.27	0.55
1:A:223:LYS:HD3	1:A:223:LYS:H	1.72	0.54
1:B:319:ASP:OD2	1:B:378:VAL:HG23	2.07	0.54
1:A:10:GLU:O	1:A:14:LYS:HD3	2.06	0.54
1:A:146:LEU:CD1	1:A:273:THR:HG23	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:HG22	1:A:302:LYS:N	2.22	0.54
1:B:375:GLN:CG	1:B:376:GLY:N	2.66	0.54
1:A:373:PHE:CZ	1:A:404:LEU:HD21	2.42	0.54
1:A:434:ASN:ND2	1:A:437:PRO:HD3	2.23	0.54
1:A:435:ARG:HG3	1:A:439:LEU:CD2	2.38	0.54
1:B:183:ASN:N	1:B:183:ASN:ND2	2.55	0.54
1:B:137:PRO:CG	4:B:453:DA:H61	2.19	0.54
1:B:173:TYR:CE1	1:B:281:TYR:CE2	2.94	0.54
1:A:135:ARG:HH22	1:B:90:TYR:N	2.04	0.54
1:A:283:ILE:O	1:A:287:LEU:HG	2.07	0.54
1:A:326:ILE:HG21	1:A:328:HIS:CD2	2.42	0.54
1:B:43:GLU:O	1:B:397:HIS:HB2	2.07	0.54
1:B:326:ILE:HG22	1:B:326:ILE:O	2.08	0.54
1:A:243:LYS:O	1:B:245:VAL:HG23	2.07	0.54
1:A:398:HIS:HE1	3:A:453:GOL:H2	1.73	0.54
1:B:158:PHE:O	1:B:161:LEU:HB3	2.08	0.54
1:B:209:ILE:HD13	1:B:209:ILE:N	2.23	0.54
1:B:326:ILE:HD12	1:B:326:ILE:N	2.23	0.54
1:A:54:ARG:HB3	1:A:101:MET:CE	2.38	0.54
1:A:436:ASP:O	1:A:439:LEU:HB2	2.08	0.54
1:A:3:LEU:HD11	1:B:66:PHE:HZ	1.73	0.53
1:B:54:ARG:HD2	1:B:97:VAL:HG12	1.90	0.53
1:B:170:ARG:NH2	1:B:174:ARG:HH22	2.05	0.53
1:B:336:ILE:CD1	1:B:338:HIS:O	2.56	0.53
1:A:96:ILE:HD11	1:A:272:MET:HE2	1.91	0.53
1:A:188:SER:N	1:A:189:PRO:HD3	2.23	0.53
1:A:297:LYS:NZ	1:B:441:ILE:HA	2.23	0.53
1:B:17:LEU:HD22	1:B:20:LEU:HD11	1.89	0.53
1:B:117:GLU:HA	1:B:121:ARG:HH21	1.73	0.53
1:A:421:ALA:O	1:A:426:GLU:OE2	2.25	0.53
1:B:86:ILE:HD12	1:B:87:LYS:N	2.24	0.53
1:B:144:ARG:HB2	1:B:225:LEU:HD12	1.89	0.53
1:B:321:VAL:O	1:B:325:LEU:HB2	2.08	0.53
1:B:54:ARG:HB3	1:B:101:MET:HE3	1.89	0.53
1:A:72:VAL:HG21	1:A:409:LEU:CB	2.38	0.53
1:B:165:PHE:CD2	1:B:277:ILE:HG21	2.42	0.53
1:A:439:LEU:C	1:A:441:ILE:H	2.11	0.53
1:A:230:ARG:HG2	1:B:234:ILE:HG13	1.90	0.53
1:A:54:ARG:HB3	1:A:101:MET:HE1	1.90	0.53
1:B:89:ASN:HB2	1:B:92:THR:HB	1.89	0.53
1:B:430:ASN:HA	1:B:435:ARG:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:PHE:HB2	1:B:358:ILE:HD12	1.90	0.53
1:B:134:VAL:HG23	1:B:135:ARG:N	2.25	0.52
1:B:162:LEU:HD23	1:B:166:LEU:HD11	1.91	0.52
1:B:227:TYR:H	1:B:230:ARG:NH1	2.07	0.52
1:A:441:ILE:HG13	1:B:378:VAL:HG11	1.90	0.52
1:B:150:ARG:NH2	1:B:350:PHE:CB	2.72	0.52
1:B:323:ARG:HG2	1:B:329:GLU:H	1.74	0.52
1:A:180:LEU:O	1:A:184:GLY:HA2	2.09	0.52
1:A:170:ARG:NH2	5:A:458:HOH:O	2.36	0.52
1:A:88:SER:HA	1:A:93:SER:OG	2.10	0.52
1:B:137:PRO:HG3	4:B:453:DA:C6	2.44	0.52
1:A:113:TYR:O	1:A:116:LEU:HB2	2.10	0.52
1:A:314:ASP:HB3	1:A:317:LEU:HD12	1.90	0.52
1:A:324:THR:O	1:A:325:LEU:HD23	2.10	0.52
1:B:77:GLN:C	1:B:78:LEU:HD23	2.30	0.52
1:A:316:ALA:HB2	1:B:440:LYS:HZ3	1.75	0.52
1:A:347:PHE:HD1	1:A:362:ILE:HD11	1.74	0.52
1:B:129:LEU:HG	1:B:294:TYR:CZ	2.45	0.52
1:B:47:ILE:HG13	1:B:122:ALA:O	2.10	0.52
1:B:280:LEU:HA	1:B:283:ILE:HG13	1.92	0.52
1:B:305:ALA:HA	1:B:310:VAL:O	2.09	0.52
1:B:422:ARG:HH11	1:B:423:HIS:CE1	2.28	0.52
1:A:120:LYS:HZ3	1:A:390:LYS:HE2	1.72	0.52
1:A:328:HIS:HB3	1:A:330:LYS:H	1.75	0.52
1:B:136:PRO:HG3	1:B:346:SER:HB2	1.92	0.52
1:B:245:VAL:HG12	1:B:249:LEU:CD1	2.39	0.52
1:A:176:VAL:HG22	1:A:186:TYR:HE2	1.74	0.51
1:A:299:PHE:O	1:A:300:TYR:HB2	2.10	0.51
1:B:65:TYR:CZ	1:B:84:ASN:HB3	2.45	0.51
1:B:86:ILE:HG13	1:B:87:LYS:O	2.10	0.51
1:B:29:ILE:HG23	1:B:31:ASN:H	1.75	0.51
1:B:195:VAL:HG12	1:B:195:VAL:O	2.08	0.51
1:A:53:SER:O	1:A:101:MET:CE	2.57	0.51
1:A:288:GLU:HG3	1:A:357:ASN:HD21	1.75	0.51
1:A:326:ILE:CG2	1:A:328:HIS:CD2	2.93	0.51
1:A:72:VAL:HG21	1:A:409:LEU:HB2	1.93	0.51
1:A:82:TYR:OH	1:A:193:ASP:HB2	2.10	0.51
1:A:139:TYR:CG	1:A:140:PRO:HA	2.45	0.51
1:A:209:ILE:O	1:A:216:VAL:HG12	2.11	0.51
1:B:8:SER:HA	1:B:11:ARG:HH12	1.74	0.51
1:B:216:VAL:O	1:B:260:TYR:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:SER:H	1:B:230:ARG:HH11	1.59	0.51
1:B:322:ILE:HD11	1:B:323:ARG:HG3	1.91	0.51
1:A:110:TYR:CD2	1:A:111:LEU:HD23	2.46	0.51
1:B:29:ILE:CG2	1:B:31:ASN:H	2.24	0.50
1:B:182:LYS:HB2	1:B:183:ASN:ND2	2.25	0.50
1:B:283:ILE:O	1:B:287:LEU:HG	2.12	0.50
1:B:104:LEU:CD2	1:B:189:PRO:HB2	2.40	0.50
1:B:204:ILE:HG22	1:B:205:ASP:N	2.26	0.50
1:A:223:LYS:H	1:A:223:LYS:CD	2.25	0.50
1:B:323:ARG:HG2	1:B:329:GLU:N	2.26	0.50
1:B:426:GLU:CD	1:B:426:GLU:N	2.63	0.50
1:B:81:SER:O	1:B:189:PRO:HD3	2.11	0.50
1:A:433:ARG:HE	1:A:434:ASN:HB2	1.77	0.50
1:B:30:ARG:O	1:B:32:ILE:N	2.44	0.50
1:A:8:SER:HB3	1:A:11:ARG:NH2	2.27	0.50
1:A:120:LYS:HZ2	1:A:394:LEU:HD11	1.76	0.50
1:B:17:LEU:HA	1:B:20:LEU:CG	2.42	0.50
1:A:24:ARG:NH2	1:A:325:LEU:HD21	2.26	0.50
1:A:200:ARG:O	1:A:204:ILE:HB	2.12	0.50
1:A:287:LEU:HB3	1:A:357:ASN:HB3	1.93	0.50
1:A:312:ILE:HD12	1:A:313:VAL:N	2.27	0.50
1:B:30:ARG:C	1:B:32:ILE:H	2.15	0.50
1:B:133:LEU:CD1	1:B:342:PRO:HB3	2.42	0.49
1:A:135:ARG:NH2	1:B:90:TYR:H	2.09	0.49
1:A:398:HIS:CE1	3:A:453:GOL:H2	2.47	0.49
1:A:196:VAL:HG13	1:A:197:GLU:N	2.27	0.49
1:A:312:ILE:C	1:A:313:VAL:CG1	2.81	0.49
1:B:98:ARG:CG	4:B:453:DA:H62	2.25	0.49
1:B:319:ASP:O	1:B:322:ILE:HG13	2.13	0.49
1:A:302:LYS:HE2	1:B:87:LYS:NZ	2.26	0.49
1:A:316:ALA:HB2	1:B:440:LYS:NZ	2.27	0.49
1:A:67:LEU:HD21	1:A:97:VAL:HG13	1.95	0.49
1:B:333:TYR:HE2	1:B:335:GLU:HB2	1.78	0.49
1:A:53:SER:C	1:A:101:MET:CE	2.81	0.49
1:A:65:TYR:CZ	1:A:84:ASN:HB3	2.48	0.49
1:A:113:TYR:CG	1:A:289:VAL:HG22	2.48	0.49
1:A:436:ASP:HB2	1:A:437:PRO:HD3	1.94	0.49
1:B:20:LEU:HD23	1:B:20:LEU:N	2.27	0.49
1:B:247:GLU:O	1:B:250:GLN:HB3	2.13	0.49
1:A:433:ARG:HE	1:A:434:ASN:CB	2.26	0.49
1:B:245:VAL:O	1:B:249:LEU:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:HD3	1:A:329:GLU:CG	2.43	0.49
1:A:220:ILE:CG1	1:A:257:VAL:HB	2.42	0.48
1:A:333:TYR:HE2	1:A:335:GLU:HB2	1.78	0.48
1:A:441:ILE:HG12	1:B:378:VAL:HG11	1.94	0.48
1:B:217:LYS:HD3	1:B:260:TYR:HE2	1.76	0.48
1:B:323:ARG:HH21	1:B:372:ARG:HH11	1.60	0.48
1:A:170:ARG:HD2	1:A:170:ARG:C	2.31	0.48
1:A:319:ASP:HA	1:A:379:ILE:HD12	1.95	0.48
1:A:340:VAL:HG13	1:A:366:ILE:O	2.14	0.48
1:A:400:ALA:HB2	1:A:405:ARG:HB2	1.95	0.48
1:A:258:GLU:HG3	1:A:260:TYR:OH	2.14	0.48
1:B:355:PHE:HB3	1:B:358:ILE:HD12	1.95	0.48
1:B:422:ARG:NH1	1:B:423:HIS:CE1	2.67	0.48
1:A:124:LEU:HD21	1:A:404:LEU:CD1	2.44	0.48
1:A:234:ILE:HG12	1:B:227:TYR:CE2	2.48	0.48
1:B:13:THR:O	1:B:17:LEU:HG	2.14	0.48
1:B:116:LEU:HD23	1:B:121:ARG:HB3	1.96	0.48
1:A:8:SER:HB2	1:A:11:ARG:NH2	2.28	0.48
1:B:422:ARG:HD3	1:B:423:HIS:ND1	2.29	0.48
1:A:48:TYR:CD1	1:A:112:ALA:HB1	2.49	0.48
1:B:30:ARG:O	1:B:30:ARG:HG2	2.13	0.48
1:B:149:MET:HE1	1:B:270:LEU:HD22	1.94	0.48
1:B:386:THR:CG2	1:B:391:ILE:HG12	2.44	0.48
1:A:139:TYR:HA	1:A:141:GLU:N	2.29	0.48
1:A:221:PRO:O	1:A:230:ARG:NH1	2.44	0.48
1:A:342:PRO:CD	1:A:362:ILE:HA	2.44	0.48
1:A:433:ARG:HH21	1:A:434:ASN:HA	1.79	0.48
1:B:250:GLN:O	1:B:254:GLU:HB2	2.14	0.48
1:A:144:ARG:HD2	1:B:228:SER:HB3	1.95	0.47
1:A:441:ILE:C	1:B:316:ALA:CB	2.81	0.47
1:A:433:ARG:NH2	1:A:434:ASN:HA	2.29	0.47
1:B:3:LEU:HD22	1:B:4:LEU:HG	1.95	0.47
1:B:330:LYS:O	1:B:372:ARG:HD2	2.14	0.47
1:B:411:HIS:C	1:B:411:HIS:CD2	2.87	0.47
1:A:222:ARG:HD2	1:A:255:GLU:OE1	2.14	0.47
1:B:241:ARG:HG2	1:B:242:GLY:N	2.22	0.47
1:A:138:VAL:HG11	1:A:272:MET:HE1	1.95	0.47
1:A:169:LEU:HD11	1:A:278:GLU:HA	1.95	0.47
1:B:146:LEU:HG	1:B:273:THR:HG23	1.97	0.47
1:B:375:GLN:CG	1:B:376:GLY:H	2.16	0.47
1:A:39:LEU:HD13	1:A:332:GLY:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LYS:HD2	1:A:230:ARG:CD	2.44	0.47
1:A:28:GLN:O	1:A:32:ILE:HG12	2.15	0.47
1:A:129:LEU:O	1:A:133:LEU:HD22	2.15	0.47
1:A:320:ALA:HB2	1:B:436:ASP:HB2	1.95	0.47
1:B:28:GLN:C	1:B:30:ARG:H	2.18	0.47
1:B:345:TRP:CD1	1:B:346:SER:N	2.83	0.47
1:B:433:ARG:HG3	1:B:434:ASN:N	2.29	0.47
1:A:426:GLU:CD	1:A:426:GLU:N	2.67	0.47
1:B:201:LYS:HB3	1:B:205:ASP:OD2	2.15	0.47
1:B:382:LEU:HD12	1:B:383:GLN:N	2.30	0.47
1:A:95:GLN:HB3	1:A:138:VAL:HG13	1.97	0.47
1:A:129:LEU:HD13	1:A:366:ILE:CG1	2.42	0.47
1:B:51:ASP:OD2	1:B:126:ASP:OD2	2.33	0.47
1:B:124:LEU:HD12	1:B:293:ALA:HB3	1.96	0.47
1:B:437:PRO:O	1:B:440:LYS:HB2	2.15	0.47
1:A:431:ALA:O	1:A:432:LEU:C	2.54	0.47
1:A:175:LYS:HB2	1:A:175:LYS:HE3	1.71	0.46
1:A:176:VAL:HG22	1:A:186:TYR:CD2	2.50	0.46
1:A:297:LYS:HB3	1:A:297:LYS:HE3	1.46	0.46
1:A:209:ILE:H	1:A:209:ILE:HG12	1.65	0.46
1:B:124:LEU:HD12	1:B:293:ALA:CB	2.45	0.46
1:B:367:HIS:HB2	1:B:388:ILE:HD11	1.97	0.46
1:A:107:MET:HE2	1:A:107:MET:HB2	1.69	0.46
1:B:392:LEU:HG	1:B:396:LEU:CD1	2.45	0.46
1:B:118:GLY:H	1:B:121:ARG:CZ	2.28	0.46
1:B:201:LYS:HA	1:B:205:ASP:CB	2.46	0.46
1:A:326:ILE:HD12	1:A:326:ILE:N	2.31	0.46
1:B:142:ASP:OD2	1:B:143:ILE:N	2.45	0.46
1:B:302:LYS:O	1:B:303:THR:HG22	2.16	0.46
1:B:411:HIS:O	1:B:415:LYS:HG3	2.16	0.46
1:A:392:LEU:O	1:A:392:LEU:HD12	2.15	0.46
1:B:92:THR:HG22	1:B:96:ILE:HD11	1.96	0.46
1:B:168:LYS:HE3	1:B:198:LYS:NZ	2.30	0.46
1:B:227:TYR:HB3	1:B:230:ARG:N	2.30	0.46
1:B:301:THR:O	1:B:304:LEU:HB2	2.16	0.46
1:A:337:GLU:HB2	1:A:338:HIS:CE1	2.51	0.46
1:A:316:ALA:HB3	1:B:60:SER:OG	2.16	0.46
1:A:368:LEU:HB3	1:A:381:MET:CE	2.46	0.46
1:B:27:GLU:O	1:B:30:ARG:N	2.49	0.46
1:A:8:SER:HB2	1:A:11:ARG:HH21	1.80	0.46
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ILE:C	1:B:316:ALA:HB1	2.36	0.46
1:B:17:LEU:CD2	1:B:20:LEU:HD11	2.46	0.46
1:B:338:HIS:ND1	1:B:338:HIS:N	2.63	0.46
1:A:47:ILE:HG22	1:A:398:HIS:CE1	2.51	0.45
1:B:80:LEU:HB3	1:B:189:PRO:CG	2.46	0.45
1:A:55:SER:HB3	1:A:66:PHE:HD2	1.79	0.45
1:A:152:LEU:HD21	1:A:266:ILE:HD11	1.98	0.45
1:A:5:SER:C	1:A:7:GLN:N	2.70	0.45
1:A:403:TYR:C	1:A:403:TYR:CD2	2.89	0.45
1:B:10:GLU:HA	1:B:13:THR:OG1	2.16	0.45
1:A:392:LEU:N	1:A:393:PRO:HD2	2.32	0.45
1:A:414:VAL:C	1:A:416:ILE:H	2.18	0.45
1:B:232:ILE:HG13	1:B:233:PRO:HD2	1.96	0.45
1:A:70:LEU:HD12	1:A:78:LEU:O	2.15	0.45
1:B:60:SER:OG	1:B:440:LYS:CD	2.64	0.45
1:B:233:PRO:HB2	1:B:236:VAL:HG22	1.98	0.45
1:A:284:ASP:OD2	1:A:355:PHE:HB3	2.16	0.45
1:B:287:LEU:HD13	1:B:357:ASN:O	2.17	0.45
1:A:180:LEU:HD22	1:A:180:LEU:HA	1.61	0.45
1:B:217:LYS:CD	1:B:260:TYR:CE2	2.99	0.45
1:A:54:ARG:HH22	1:A:98:ARG:NH2	2.14	0.45
1:A:230:ARG:CG	1:B:234:ILE:HG13	2.47	0.45
1:A:300:TYR:OH	1:A:302:LYS:HD3	2.17	0.45
1:A:352:LEU:O	1:A:353:SER:C	2.56	0.45
1:A:374:GLU:O	1:A:377:ASP:HB2	2.18	0.45
1:B:39:LEU:HA	1:B:40:PRO:HD3	1.85	0.45
1:B:305:ALA:HB1	1:B:311:GLU:HA	1.99	0.45
1:A:26:ASN:HB3	1:A:30:ARG:HG2	1.99	0.44
1:A:100:GLN:HG2	1:A:190:ILE:HG13	1.99	0.44
1:A:135:ARG:NH2	1:B:90:TYR:HB2	2.31	0.44
1:A:334:LEU:C	1:A:334:LEU:HD12	2.38	0.44
1:B:39:LEU:HG	1:B:332:GLY:HA2	1.99	0.44
1:B:148:VAL:HG13	1:B:261:LEU:HD11	1.99	0.44
1:A:27:GLU:HG2	1:A:28:GLN:N	2.21	0.44
1:A:302:LYS:HD3	1:A:302:LYS:HA	1.53	0.44
1:B:98:ARG:CD	4:B:453:DA:H62	2.29	0.44
1:A:29:ILE:O	1:A:33:ILE:HG12	2.18	0.44
1:A:139:TYR:HA	1:A:140:PRO:C	2.37	0.44
1:A:333:TYR:C	1:A:333:TYR:CD2	2.91	0.44
1:A:421:ALA:HA	1:A:424:THR:HG1	1.73	0.44
1:B:79:ARG:O	1:B:185:ASN:HA	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ILE:HD13	1:A:32:ILE:HA	1.83	0.44
1:A:120:LYS:HZ1	1:A:390:LYS:HE2	1.81	0.44
1:A:368:LEU:HB3	1:A:381:MET:HE1	1.98	0.44
1:A:24:ARG:NE	1:A:325:LEU:HD21	2.33	0.44
1:A:29:ILE:HA	1:A:29:ILE:HD12	1.75	0.44
1:A:141:GLU:HA	1:A:144:ARG:HD3	2.00	0.44
1:B:149:MET:HE1	1:B:204:ILE:HD11	1.99	0.44
1:B:215:LYS:HA	1:B:261:LEU:O	2.17	0.44
1:B:426:GLU:HA	1:B:429:ILE:HG13	1.99	0.44
1:A:8:SER:HA	1:A:11:ARG:CZ	2.48	0.44
1:B:32:ILE:HG22	1:B:334:LEU:HD21	2.00	0.44
1:B:162:LEU:O	1:B:166:LEU:HG	2.18	0.44
1:B:209:ILE:HD13	1:B:209:ILE:H	1.81	0.44
1:A:72:VAL:HG22	1:A:406:PRO:O	2.18	0.44
1:A:106:ASN:HD22	1:A:282:SER:HG	1.66	0.44
1:A:130:THR:O	1:A:134:VAL:HG13	2.18	0.44
1:A:170:ARG:CZ	5:A:458:HOH:O	2.63	0.44
1:A:220:ILE:HG12	1:A:257:VAL:HB	1.98	0.44
1:B:81:SER:O	1:B:189:PRO:CD	2.66	0.44
1:B:135:ARG:NH2	1:B:306:ARG:NH1	2.52	0.44
1:B:419:LYS:HB2	1:B:422:ARG:HB2	1.99	0.44
1:A:146:LEU:HD12	1:A:146:LEU:HA	1.76	0.43
1:B:219:LYS:HE2	1:B:256:LYS:HZ1	1.82	0.43
1:B:232:ILE:HG12	1:B:233:PRO:O	2.17	0.43
1:B:367:HIS:ND1	1:B:387:ASN:HA	2.33	0.43
1:B:410:ALA:O	1:B:414:VAL:CG1	2.65	0.43
1:A:52:GLY:HA2	1:A:414:VAL:HG21	2.00	0.43
1:A:59:LEU:CD2	1:A:440:LYS:HA	2.48	0.43
1:A:249:LEU:HD21	1:B:237:LEU:CB	2.46	0.43
1:A:302:LYS:CG	1:B:89:ASN:ND2	2.69	0.43
1:B:133:LEU:HD11	1:B:342:PRO:HB3	1.99	0.43
1:B:139:TYR:C	1:B:141:GLU:H	2.22	0.43
1:A:106:ASN:CB	1:A:282:SER:OG	2.65	0.43
1:A:405:ARG:N	1:A:406:PRO:HD2	2.32	0.43
1:B:419:LYS:O	1:B:422:ARG:CB	2.64	0.43
1:A:404:LEU:H	1:A:404:LEU:HG	1.45	0.43
1:A:53:SER:N	1:A:101:MET:HE3	2.32	0.43
1:A:366:ILE:HG22	1:A:368:LEU:HD23	2.00	0.43
1:A:195:VAL:HG22	1:A:199:LEU:CD2	2.49	0.43
1:B:350:PHE:CD1	1:B:351:LEU:HD23	2.53	0.43
1:B:107:MET:O	1:B:111:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:LEU:HD13	1:B:395:ILE:HD12	2.00	0.43
1:B:252:LEU:HA	1:B:252:LEU:HD23	1.85	0.43
1:B:294:TYR:O	1:B:295:ILE:HD13	2.18	0.43
1:B:163:ASN:HA	1:B:166:LEU:HD12	2.01	0.43
1:A:70:LEU:HD12	1:A:71:ALA:H	1.84	0.43
1:A:314:ASP:CG	1:B:60:SER:HB3	2.30	0.43
1:A:72:VAL:HG21	1:A:409:LEU:HB3	2.00	0.42
1:A:299:PHE:O	1:A:300:TYR:CB	2.66	0.42
1:A:420:GLU:OE1	1:A:420:GLU:N	2.52	0.42
1:B:130:THR:OG1	1:B:131:GLY:N	2.51	0.42
1:B:342:PRO:CG	1:B:362:ILE:HD13	2.48	0.42
1:A:357:ASN:HA	1:A:360:LYS:HB3	2.01	0.42
1:B:116:LEU:O	1:B:121:ARG:NE	2.52	0.42
1:B:351:LEU:HD22	1:B:351:LEU:HA	1.76	0.42
1:B:372:ARG:HH12	1:B:379:ILE:HD11	1.84	0.42
1:A:302:LYS:NZ	1:B:87:LYS:HG3	2.35	0.42
1:B:33:ILE:O	1:B:36:TRP:HB3	2.19	0.42
1:B:51:ASP:OD2	1:B:126:ASP:CG	2.57	0.42
1:B:73:GLY:C	1:B:75:GLY:H	2.21	0.42
1:B:134:VAL:CG2	1:B:135:ARG:N	2.82	0.42
1:B:163:ASN:O	1:B:164:GLU:C	2.58	0.42
1:A:247:GLU:O	1:A:251:GLU:HG3	2.20	0.42
1:A:390:LYS:C	1:A:390:LYS:HD3	2.40	0.42
1:A:433:ARG:HG3	1:A:434:ASN:H	1.84	0.42
1:B:115:LYS:HD2	1:B:115:LYS:HA	1.78	0.42
1:B:227:TYR:N	1:B:230:ARG:NH1	2.67	0.42
1:A:144:ARG:H	1:A:144:ARG:HG2	1.58	0.42
1:A:237:LEU:HD23	1:A:248:LEU:HD11	2.01	0.42
1:A:342:PRO:HG2	1:A:362:ILE:HD13	2.02	0.42
1:A:351:LEU:HD23	1:A:351:LEU:HA	1.75	0.42
1:B:36:TRP:CZ2	1:B:332:GLY:HA3	2.54	0.42
1:B:263:LYS:HD3	1:B:267:TYR:CZ	2.54	0.42
1:A:149:MET:SD	1:A:270:LEU:HA	2.60	0.42
1:B:342:PRO:HB2	1:B:362:ILE:CD1	2.50	0.42
1:A:148:VAL:O	1:A:152:LEU:HB2	2.19	0.42
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.82	0.42
1:A:345:TRP:CD1	1:A:345:TRP:C	2.93	0.42
1:B:150:ARG:HH22	1:B:350:PHE:CB	2.32	0.42
1:B:233:PRO:O	1:B:236:VAL:HG23	2.20	0.42
1:B:310:VAL:HG12	1:B:338:HIS:CD2	2.55	0.42
1:B:323:ARG:NH2	1:B:372:ARG:HH11	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:VAL:O	1:B:414:VAL:CG2	2.68	0.42
1:A:223:LYS:HD2	1:A:230:ARG:HD2	2.02	0.41
1:A:345:TRP:CD1	1:A:346:SER:N	2.88	0.41
1:B:104:LEU:HD22	1:B:189:PRO:HB2	2.01	0.41
1:B:301:THR:CG2	1:B:312:ILE:HG13	2.50	0.41
1:A:17:LEU:HD23	1:A:20:LEU:HD12	2.02	0.41
1:A:313:VAL:CG2	1:A:314:ASP:O	2.66	0.41
1:A:392:LEU:N	1:A:393:PRO:CD	2.84	0.41
1:A:58:ARG:HE	1:A:58:ARG:HB2	1.65	0.41
1:A:418:TYR:CD2	1:A:419:LYS:N	2.89	0.41
1:A:441:ILE:HD12	1:A:441:ILE:N	2.35	0.41
1:B:223:LYS:HD2	1:B:223:LYS:HA	1.81	0.41
1:B:340:VAL:HG11	1:B:368:LEU:HD11	2.03	0.41
1:B:420:GLU:H	1:B:420:GLU:HG2	1.60	0.41
1:A:299:PHE:N	1:A:299:PHE:CD1	2.89	0.41
1:A:400:ALA:HB3	1:A:403:TYR:O	2.21	0.41
1:B:104:LEU:HD11	1:B:189:PRO:HG2	2.01	0.41
1:B:162:LEU:HD23	1:B:166:LEU:CD1	2.49	0.41
1:B:227:TYR:CD1	1:B:229:PRO:O	2.74	0.41
1:B:299:PHE:CD1	1:B:299:PHE:N	2.84	0.41
1:B:303:THR:O	1:B:306:ARG:HB3	2.21	0.41
1:A:99:MET:HE2	1:A:276:TYR:HD1	1.85	0.41
1:A:99:MET:CE	1:A:276:TYR:HD1	2.34	0.41
1:A:137:PRO:C	1:A:138:VAL:HG23	2.39	0.41
1:A:347:PHE:CD1	1:A:362:ILE:HD11	2.55	0.41
1:B:144:ARG:CB	1:B:225:LEU:HD11	2.49	0.41
1:A:300:TYR:O	1:A:301:THR:OG1	2.26	0.41
1:A:329:GLU:O	1:A:329:GLU:HG2	2.21	0.41
1:A:439:LEU:O	1:A:440:LYS:CB	2.67	0.41
1:B:65:TYR:HE2	1:B:86:ILE:HG22	1.86	0.41
1:B:201:LYS:HA	1:B:205:ASP:CG	2.40	0.41
1:B:412:HIS:O	1:B:415:LYS:HE2	2.20	0.41
1:A:403:TYR:OH	1:A:407:LEU:HG	2.21	0.41
1:B:46:SER:O	1:B:116:LEU:HD21	2.21	0.41
1:B:121:ARG:O	1:B:291:ASN:ND2	2.49	0.41
1:B:315:THR:O	1:B:316:ALA:C	2.57	0.41
1:A:138:VAL:O	1:A:142:ASP:OD1	2.39	0.41
1:B:20:LEU:HD23	1:B:20:LEU:H	1.85	0.41
1:B:335:GLU:HA	1:B:369:ALA:HB2	2.02	0.41
1:B:360:LYS:HB2	1:B:360:LYS:HE3	1.73	0.41
1:A:52:GLY:CA	1:A:414:VAL:HG21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:HD2	1:B:228:SER:CB	2.51	0.41
1:A:195:VAL:HG22	1:A:195:VAL:O	2.21	0.41
1:A:285:LYS:HD2	1:A:285:LYS:HA	1.77	0.41
1:A:312:ILE:C	1:A:312:ILE:HD12	2.41	0.41
1:A:366:ILE:HG22	1:A:368:LEU:CD2	2.51	0.41
1:B:92:THR:HG22	1:B:96:ILE:CD1	2.51	0.41
1:B:124:LEU:HD12	1:B:124:LEU:HA	1.91	0.41
1:B:219:LYS:HD2	1:B:256:LYS:HE3	2.03	0.41
1:B:331:GLU:HB3	1:B:375:GLN:H	1.85	0.41
1:B:419:LYS:H	1:B:419:LYS:CE	2.26	0.41
1:A:400:ALA:HB2	1:A:405:ARG:CB	2.51	0.41
1:B:405:ARG:HG2	1:B:406:PRO:HD3	2.02	0.41
1:A:235:GLU:H	1:A:235:GLU:CD	2.24	0.40
1:B:195:VAL:O	1:B:195:VAL:CG1	2.68	0.40
1:A:26:ASN:CB	1:A:30:ARG:HG2	2.52	0.40
1:A:49:ALA:HA	1:A:124:LEU:O	2.22	0.40
1:A:98:ARG:HE	1:A:98:ARG:HB2	1.78	0.40
1:A:187:ASP:C	1:A:189:PRO:HD3	2.41	0.40
1:A:223:LYS:HD3	1:A:223:LYS:N	2.34	0.40
1:A:234:ILE:HG22	1:A:235:GLU:OE2	2.21	0.40
1:B:80:LEU:HB3	1:B:189:PRO:HG3	2.03	0.40
1:B:98:ARG:HG2	4:B:453:DA:N6	2.34	0.40
1:A:16:LEU:HD21	1:B:62:THR:HG21	2.03	0.40
1:A:298:SER:HB2	1:B:60:SER:HA	2.04	0.40
1:A:356:ARG:HD3	1:A:356:ARG:HA	1.55	0.40
1:A:435:ARG:O	1:A:438:ALA:HB3	2.20	0.40
1:B:199:LEU:HD13	1:B:199:LEU:HA	1.76	0.40
1:B:315:THR:OG1	1:B:316:ALA:N	2.54	0.40
1:A:20:LEU:O	1:A:24:ARG:HG3	2.22	0.40
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.77	0.40
1:A:116:LEU:HA	1:A:116:LEU:HD12	1.55	0.40
1:A:301:THR:CG2	1:A:302:LYS:N	2.85	0.40
1:B:144:ARG:CD	1:B:225:LEU:HD11	2.44	0.40
1:B:287:LEU:CB	1:B:357:ASN:HB3	2.49	0.40
1:B:374:GLU:HB3	1:B:375:GLN:CG	2.51	0.40
1:A:356:ARG:O	1:A:359:GLU:N	2.54	0.40
1:B:65:TYR:CD2	1:B:65:TYR:N	2.89	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	426/471 (90%)	382 (90%)	41 (10%)	3 (1%)	22 61
1	B	427/471 (91%)	370 (87%)	52 (12%)	5 (1%)	13 49
All	All	853/942 (91%)	752 (88%)	93 (11%)	8 (1%)	17 56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	ILE
1	B	4	LEU
1	B	5	SER
1	B	31	ASN
1	A	328	HIS
1	A	231	VAL
1	B	439	LEU
1	A	138	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	387/419 (92%)	292 (76%)	95 (24%)	0 2
1	B	387/419 (92%)	301 (78%)	86 (22%)	1 4
All	All	774/838 (92%)	593 (77%)	181 (23%)	1 3

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	21	GLU
1	A	22	ASN
1	A	27	GLU
1	A	28	GLN
1	A	29	ILE
1	A	30	ARG
1	A	32	ILE
1	A	34	ASN
1	A	35	SER
1	A	39	LEU
1	A	41	SER
1	A	48	TYR
1	A	50	VAL
1	A	56	VAL
1	A	57	SER
1	A	58	ARG
1	A	66	PHE
1	A	72	VAL
1	A	81	SER
1	A	86	ILE
1	A	90	TYR
1	A	92	THR
1	A	94	ASP
1	A	98	ARG
1	A	116	LEU
1	A	117	GLU
1	A	125	MET
1	A	126	ASP
1	A	128	THR
1	A	129	LEU
1	A	133	LEU
1	A	135	ARG
1	A	138	VAL
1	A	141	GLU
1	A	143	ILE
1	A	144	ARG
1	A	146	LEU
1	A	149	MET
1	A	150	ARG
1	A	153	ILE
1	A	155	GLU
1	A	156	SER

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Mol	Chain	Res	Type
1	A	180	LEU
1	A	183	ASN
1	A	185	ASN
1	A	186	TYR
1	A	187	ASP
1	A	199	LEU
1	A	201	LYS
1	A	208	VAL
1	A	209	ILE
1	A	216	VAL
1	A	222	ARG
1	A	223	LYS
1	A	232	ILE
1	A	234	ILE
1	A	235	GLU
1	A	241	ARG
1	A	246	ASP
1	A	248	LEU
1	A	256	LYS
1	A	258	GLU
1	A	259	LEU
1	A	261	LEU
1	A	282	SER
1	A	299	PHE
1	A	302	LYS
1	A	308	LEU
1	A	312	ILE
1	A	313	VAL
1	A	318	LEU
1	A	334	LEU
1	A	338	HIS
1	A	340	VAL
1	A	345	TRP
1	A	346	SER
1	A	356	ARG
1	A	363	ASP
1	A	377	ASP
1	A	386	THR
1	A	390	LYS
1	A	391	ILE
1	A	394	LEU
1	A	403	TYR

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Mol	Chain	Res	Type
1	A	404	LEU
1	A	408	GLN
1	A	415	LYS
1	A	418	TYR
1	A	419	LYS
1	A	422	ARG
1	A	426	GLU
1	A	428	LEU
1	A	432	LEU
1	A	433	ARG
1	B	3	LEU
1	B	5	SER
1	B	6	LYS
1	B	13	THR
1	B	16	LEU
1	B	20	LEU
1	B	24	ARG
1	B	25	GLU
1	B	28	GLN
1	B	29	ILE
1	B	31	ASN
1	B	34	ASN
1	B	36	TRP
1	B	39	LEU
1	B	41	SER
1	B	47	ILE
1	B	50	VAL
1	B	72	VAL
1	B	79	ARG
1	B	86	ILE
1	B	90	TYR
1	B	104	LEU
1	B	110	TYR
1	B	133	LEU
1	B	144	ARG
1	B	157	ASP
1	B	167	GLU
1	B	171	ASP
1	B	183	ASN
1	B	185	ASN
1	B	186	TYR
1	B	187	ASP

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Mol	Chain	Res	Type
1	B	190	ILE
1	B	200	ARG
1	B	201	LYS
1	B	206	THR
1	B	209	ILE
1	B	216	VAL
1	B	217	LYS
1	B	218	VAL
1	B	222	ARG
1	B	223	LYS
1	B	227	TYR
1	B	232	ILE
1	B	234	ILE
1	B	236	VAL
1	B	249	LEU
1	B	253	ASP
1	B	255	GLU
1	B	256	LYS
1	B	257	VAL
1	B	263	LYS
1	B	270	LEU
1	B	283	ILE
1	B	291	ASN
1	B	298	SER
1	B	299	PHE
1	B	303	THR
1	B	304	LEU
1	B	307	THR
1	B	318	LEU
1	B	333	TYR
1	B	338	HIS
1	B	345	TRP
1	B	349	ASP
1	B	351	LEU
1	B	355	PHE
1	B	356	ARG
1	B	379	ILE
1	B	383	GLN
1	B	387	ASN
1	B	389	GLU
1	B	390	LYS
1	B	391	ILE

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Mol	Chain	Res	Type
1	B	396	LEU
1	B	403	TYR
1	B	404	LEU
1	B	414	VAL
1	B	419	LYS
1	B	422	ARG
1	B	423	HIS
1	B	426	GLU
1	B	432	LEU
1	B	433	ARG
1	B	434	ASN
1	B	440	LYS

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	291	ASN
1	A	338	HIS
1	A	397	HIS
1	A	398	HIS
1	B	89	ASN
1	B	183	ASN
1	B	383	GLN
1	B	387	ASN
1	B	411	HIS
1	B	423	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	DA	B	453	-	22,24,24	0.77	0	24,36,36	0.86	1 (4%)
3	GOL	A	453	-	5,5,5	0.55	0	5,5,5	0.71	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
4	DA	B	453	-	-	2/6/22/22	0/3/3/3
3	GOL	A	453	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	453	DA	OP2-P-OP1	2.09	118.88	110.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	453	GOL	O1-C1-C2-C3
4	B	453	DA	C5'-O5'-P-OP1
3	A	453	GOL	O1-C1-C2-O2
3	A	453	GOL	C1-C2-C3-O3
4	B	453	DA	C5'-O5'-P-OP3
3	A	453	GOL	O2-C2-C3-O3

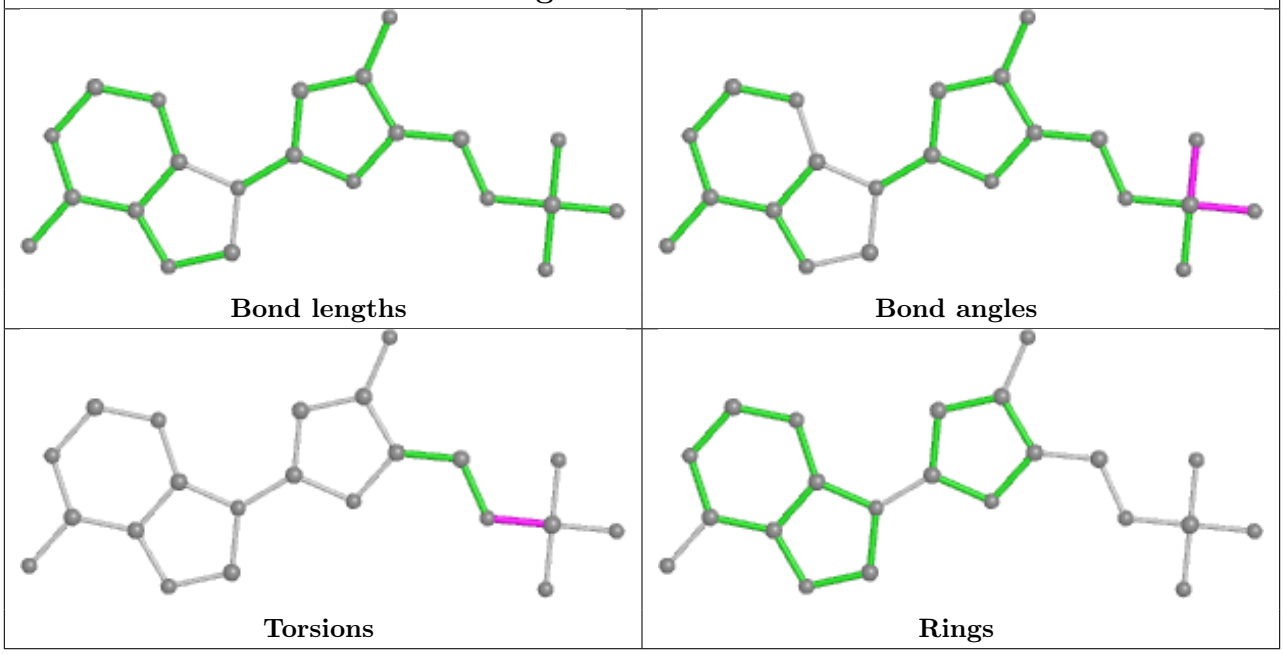
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	453	DA	12	0
3	A	453	GOL	2	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 DA B 453



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	432/471 (91%)	-0.29	0 100 100	51, 94, 153, 179	0
1	B	433/471 (91%)	-0.02	12 (2%) 53 37	62, 114, 169, 227	0
All	All	865/942 (91%)	-0.15	12 (1%) 75 63	51, 106, 163, 227	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	402	GLY	3.3
1	B	373	PHE	2.9
1	B	122	ALA	2.9
1	B	307	THR	2.8
1	B	403	TYR	2.6
1	B	376	GLY	2.5
1	B	333	TYR	2.4
1	B	124	LEU	2.4
1	B	70	LEU	2.3
1	B	123	ILE	2.2
1	B	429	ILE	2.1
1	B	417	SER	2.1

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

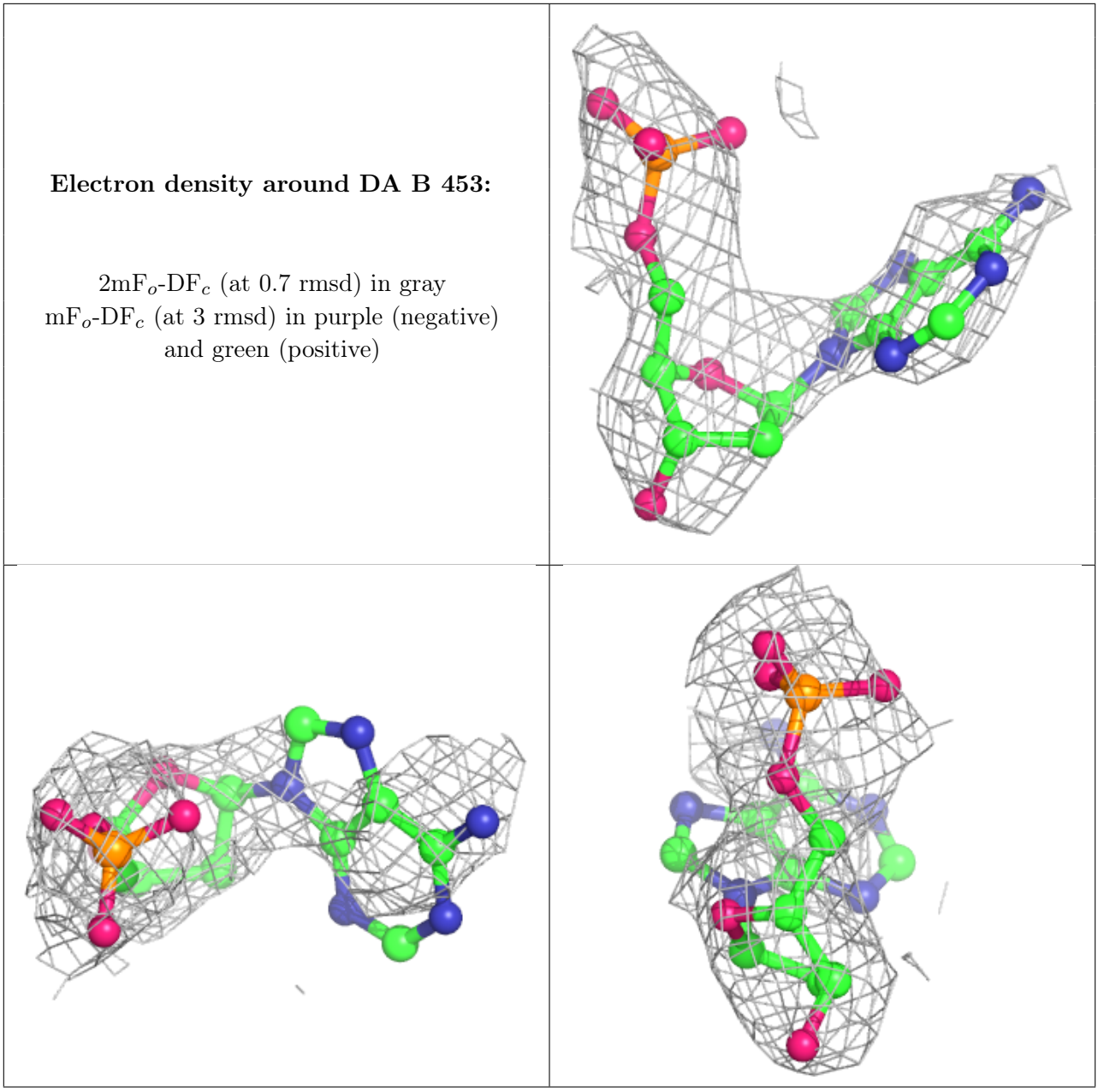
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	DA	B	453	22/22	0.83	0.25	137,179,188,189	0
3	GOL	A	453	6/6	0.84	0.39	69,90,110,113	0
2	MN	B	452	1/1	0.95	0.20	91,91,91,91	0
2	MN	A	452	1/1	0.98	0.22	73,73,73,73	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 DA B 453:

$2mF_o$-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.