Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 09:40 PM EDT

PDB ID	:	2B6A
Title	:	Crystal structure of HIV-1 reverse transcriptase (RT) in complex with THR-50
Authors	:	Morningstar, M.L.; Roth, T.; Smith, M.K.; Zajac, M.; Watson, K.; Buckheit, R.W.; Das, K.; Zhang, W.; Arnold, E.; Michejda, C.J.
Deposited on	:	2005-09-30
Resolution	:	2.65 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:

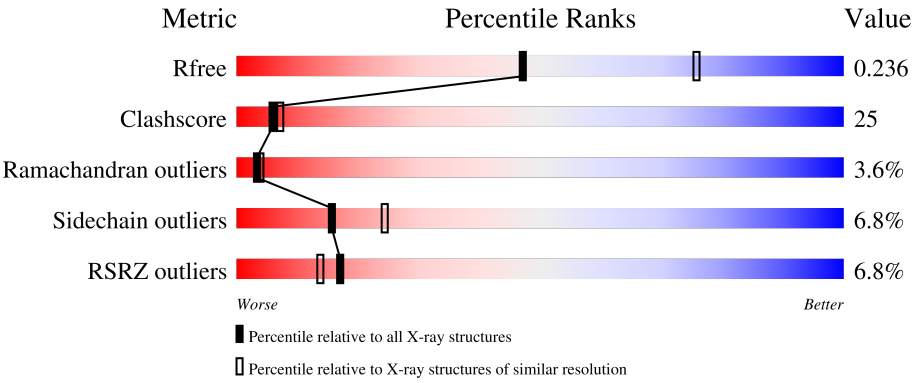
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	6% 54% 41%
2	B	430	8% 55% 37% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7921 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 p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	558	4451	2882	740	822	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366

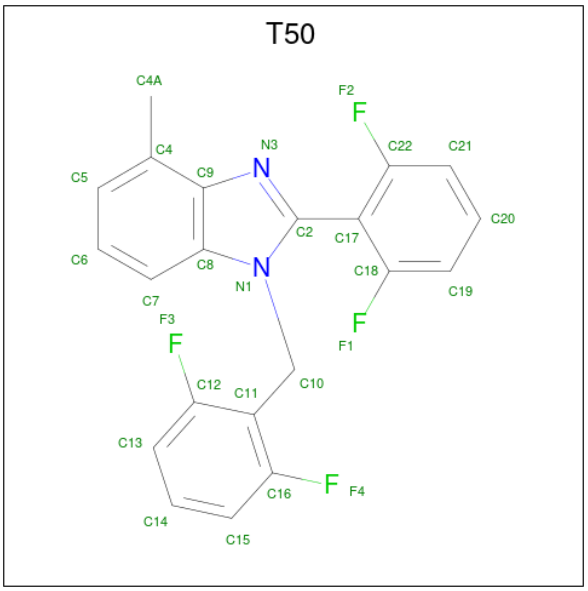
- Molecule 2 is a protein called Reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	427	3443	2241	567	630	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is 1-(2,6-DIFLUOROBENZYL)-2-(2,6-DIFLUOROPHENYL)-4-METHYL-1H-BENZIMIDAZOLE (three-letter code: T50) (formula: $C_{21}H_{14}F_4N_2$).

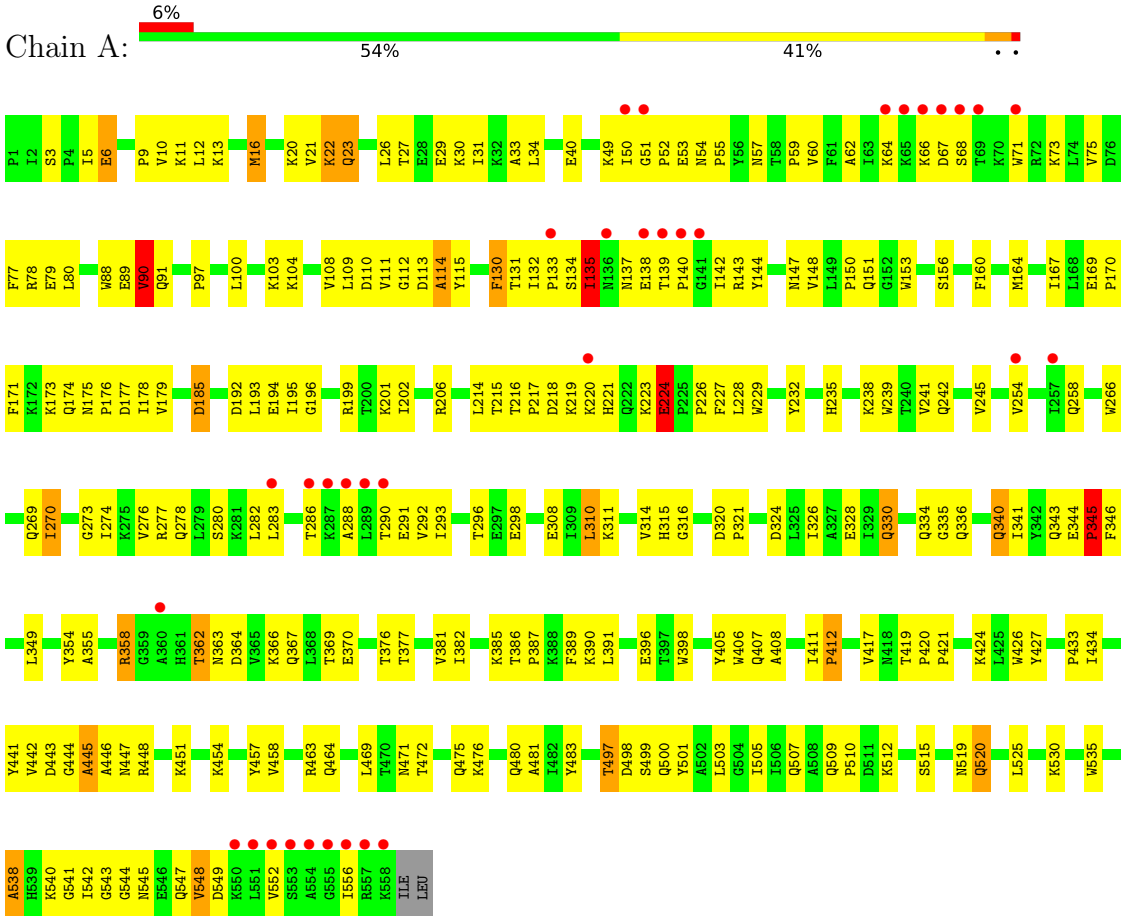


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	N		
3	A	1	27	21	4	2	0	0

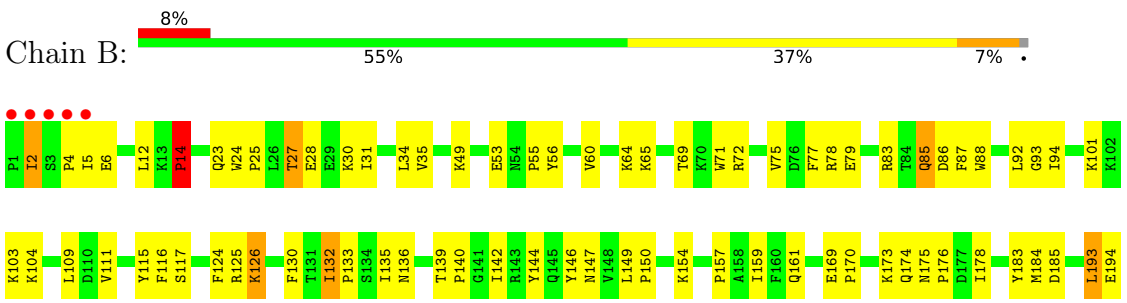
3 Residue-property plots (i)

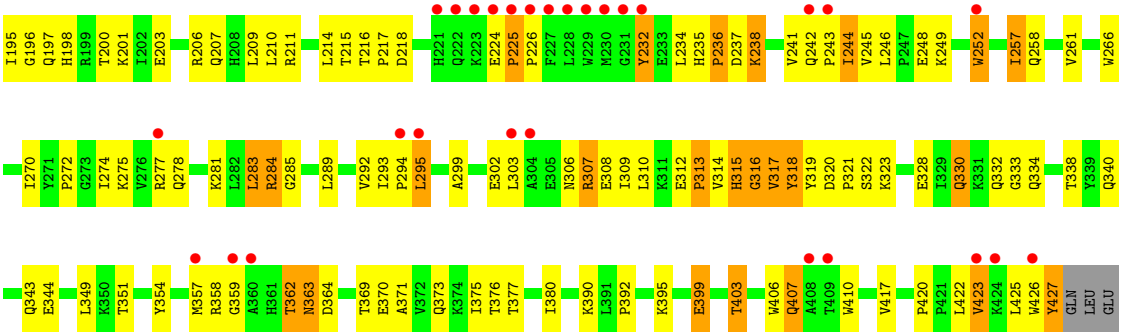
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Reverse transcriptase p66 subunit



• Molecule 2: Reverse transcriptase p51 subunit




I195 G196 Q197 H198 R199 T200 K201 I202 E203 R206 Q207 H208 L209 L210 R211 L214 T215 T216 P217 D218 H221 Q222 K223 E224 P225 P226 F227 L228 W229 M230 G231 Y232 E233 L234 H235 P236 D237 K238 V241 Q242 P243 I244 V245 L246 P247 E248 K249 W252 I257 Q258 V261 W266
I270 Y271 P272 G273 I274 K275 V276 R277 Q278 K281 L282 L283 R284 G285 L289 V292 I293 P294 L295 A299 E302 L303 A304 E305 N306 R307 E308 I309 L310 K311 E312 P313 V314 H315 G316 V317 Y318 Y319 D320 P321 S322 K323 E328 I329 Q330 K331 Q332 G333 Q334 T338 Y339 Q340
Q343 E344 L349 K350 T351 Y354 M357 R358 G359 A360 H361 T362 N363 D364 T369 E370 A371 V372 Q373 K374 I375 T376 T377 I380 K390 L391 P392 K395 E399 T403 W406 Q407 A408 T409 W410 V417 P420 P421 L422 V423 K424 L425 W426 Y427 GLN LEU GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	227.71Å 70.17Å 106.63Å 90.00° 105.82° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 36.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-2.65) 88.1 (36.51-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.277 0.228 , 0.236	Depositor DCC
R_{free} test set	2520 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	66.2	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 71.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7921	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: T50

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	0.55	0/4566	0.77	1/6209 (0.0%)
2	B	0.61	0/3541	0.85	2/4822 (0.0%)
All	All	0.58	0/8107	0.80	3/11031 (0.0%)

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
2	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	226	PRO	N-CA-CB	6.30	110.86	103.30
2	B	225	PRO	N-CA-CB	5.52	109.92	103.30
1	A	224	GLU	N-CA-C	5.30	125.30	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	146	TYR	Sidechain

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	4451	0	4430	234	0
2	B	3443	0	3415	171	0
3	A	27	0	14	2	0
All	All	7921	0	7859	395	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 25.

All (395) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:ARG:HH11	2:B:284:ARG:HB2	1.08	1.18
2:B:31:ILE:HG23	2:B:132:ILE:HD11	1.40	1.03
1:A:454:LYS:HD2	1:A:552:VAL:HA	1.41	1.02
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.43	1.00
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.41	0.99
2:B:373:GLN:HE22	2:B:407:GLN:H	1.10	0.96
2:B:85:GLN:HG3	2:B:154:LYS:CB	1.95	0.96
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.47	0.94
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.47	0.94
1:A:447:ASN:HD22	1:A:556:ILE:HG12	1.30	0.93
1:A:542:ILE:HG22	1:A:543:GLY:H	1.32	0.93
1:A:132:ILE:HB	1:A:142:ILE:HG23	1.48	0.92
1:A:109:LEU:HD13	1:A:216:THR:HG21	1.52	0.91
2:B:2:ILE:O	2:B:2:ILE:HG13	1.69	0.91
1:A:3:SER:OG	1:A:5:ILE:HG13	1.71	0.90
1:A:51:GLY:H	1:A:52:PRO:HD2	1.38	0.87
2:B:292:VAL:HG12	2:B:294:PRO:HD3	1.59	0.83
2:B:284:ARG:HB2	2:B:284:ARG:NH1	1.92	0.82
1:A:254:VAL:HG13	1:A:283:LEU:HD22	1.60	0.82
2:B:278:GLN:O	2:B:281:LYS:HG2	1.81	0.81
1:A:51:GLY:H	1:A:52:PRO:CD	1.93	0.81
1:A:542:ILE:HG22	1:A:543:GLY:N	1.94	0.81
1:A:64:LYS:HD3	1:A:71:TRP:CE2	2.16	0.80
1:A:545:ASN:O	1:A:549:ASP:HB2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:TRP:NE1	2:B:420:PRO:HG3	1.98	0.78
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.67	0.77
1:A:542:ILE:H	1:A:545:ASN:HB2	1.49	0.77
2:B:24:TRP:CE3	2:B:25:PRO:HD2	2.20	0.76
2:B:363:ASN:HD22	2:B:364:ASP:H	1.34	0.76
2:B:242:GLN:N	2:B:243:PRO:HD3	2.01	0.76
2:B:249:LYS:HB2	2:B:252:TRP:CZ3	2.21	0.75
1:A:199:ARG:NH1	1:A:220:LYS:HE2	2.02	0.75
1:A:50:ILE:HG13	1:A:50:ILE:O	1.85	0.74
1:A:148:VAL:O	1:A:150:PRO:HD3	1.87	0.74
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.53	0.74
2:B:363:ASN:HD22	2:B:364:ASP:N	1.85	0.74
1:A:51:GLY:N	1:A:52:PRO:HD2	2.03	0.73
1:A:53:GLU:O	1:A:55:PRO:HD3	1.89	0.73
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.70	0.73
2:B:284:ARG:HH11	2:B:284:ARG:CB	1.96	0.73
1:A:288:ALA:HB1	1:A:291:GLU:HB3	1.72	0.72
2:B:241:VAL:HG12	2:B:351:THR:O	1.89	0.72
1:A:447:ASN:ND2	1:A:556:ILE:HG12	2.05	0.72
2:B:215:THR:HG22	2:B:216:THR:H	1.53	0.71
1:A:57:ASN:OD1	1:A:143:ARG:NH1	2.24	0.71
2:B:303:LEU:HD21	2:B:307:ARG:HH21	1.56	0.71
2:B:206:ARG:HH12	2:B:218:ASP:HA	1.55	0.71
1:A:542:ILE:CG2	1:A:543:GLY:H	2.02	0.71
2:B:252:TRP:CD1	2:B:295:LEU:HG	2.26	0.70
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.71	0.70
2:B:94:ILE:HG12	2:B:161:GLN:NE2	2.07	0.69
1:A:23:GLN:NE2	1:A:131:THR:O	2.25	0.69
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.28	0.69
1:A:454:LYS:CD	1:A:552:VAL:HA	2.20	0.69
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.74	0.69
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.75	0.68
2:B:206:ARG:NH1	2:B:218:ASP:HA	2.07	0.68
2:B:244:ILE:HD13	2:B:244:ILE:H	1.58	0.68
1:A:111:VAL:HG12	1:A:185:ASP:O	1.94	0.68
1:A:424:LYS:HE3	1:A:426:TRP:CH2	2.29	0.68
2:B:87:PHE:O	2:B:88:TRP:CD1	2.47	0.68
2:B:373:GLN:NE2	2:B:407:GLN:H	1.88	0.68
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.76	0.68
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.29	0.67
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:LYS:HE3	2:B:277:ARG:HD3	1.77	0.67
1:A:52:PRO:HG2	1:A:53:GLU:H	1.58	0.67
2:B:323:LYS:HB2	2:B:343:GLN:OE1	1.94	0.67
1:A:454:LYS:HD2	1:A:552:VAL:CA	2.20	0.67
2:B:257:ILE:O	2:B:261:VAL:HG23	1.95	0.66
1:A:417:VAL:HG12	1:A:419:THR:CG2	2.26	0.66
1:A:90:VAL:O	1:A:91:GLN:HG2	1.96	0.65
2:B:2:ILE:O	2:B:2:ILE:CG1	2.42	0.65
2:B:132:ILE:HD12	2:B:133:PRO:HD2	1.77	0.65
1:A:362:THR:HG21	1:A:367:GLN:HG3	1.79	0.65
1:A:97:PRO:HA	1:A:100:LEU:HD12	1.78	0.65
1:A:442:VAL:HG13	1:A:481:ALA:CB	2.23	0.65
2:B:24:TRP:HE3	2:B:25:PRO:HD2	1.61	0.64
1:A:406:TRP:HE1	2:B:420:PRO:HG3	1.62	0.64
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.79	0.64
1:A:26:LEU:CB	1:A:30:LYS:HE2	2.27	0.64
2:B:343:GLN:HE21	2:B:349:LEU:HD11	1.63	0.64
2:B:315:HIS:O	2:B:317:VAL:N	2.31	0.63
2:B:274:ILE:HB	2:B:306:ASN:OD1	1.98	0.63
2:B:215:THR:HG22	2:B:216:THR:N	2.13	0.63
2:B:425:LEU:HG	2:B:425:LEU:O	1.99	0.63
1:A:202:ILE:O	1:A:206:ARG:HG3	1.98	0.63
1:A:132:ILE:HB	1:A:142:ILE:CG2	2.27	0.62
1:A:427:TYR:CE2	1:A:525:LEU:HD13	2.34	0.62
2:B:358:ARG:HA	2:B:362:THR:HA	1.80	0.62
1:A:97:PRO:HA	1:A:100:LEU:CD1	2.29	0.62
1:A:345:PRO:O	1:A:346:PHE:CD2	2.52	0.62
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.80	0.62
1:A:542:ILE:CG2	1:A:543:GLY:N	2.62	0.62
2:B:315:HIS:CG	2:B:316:GLY:N	2.68	0.62
2:B:132:ILE:HD12	2:B:133:PRO:CD	2.29	0.62
1:A:135:ILE:HG13	1:A:138:GLU:CD	2.21	0.61
1:A:66:LYS:C	1:A:68:SER:H	2.03	0.61
2:B:244:ILE:H	2:B:244:ILE:CD1	2.12	0.61
2:B:316:GLY:O	2:B:318:TYR:N	2.34	0.60
1:A:31:ILE:HD13	1:A:133:PRO:O	2.01	0.60
1:A:276:VAL:HG12	1:A:276:VAL:O	2.01	0.60
2:B:104:LYS:HG3	2:B:237:ASP:OD2	2.02	0.60
1:A:282:LEU:HD21	1:A:296:THR:HG23	1.83	0.60
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.38	0.59
1:A:552:VAL:HG12	1:A:552:VAL:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:GLU:O	2:B:310:LEU:N	2.35	0.59
2:B:320:ASP:OD1	2:B:322:SER:HB3	2.03	0.59
1:A:266:TRP:O	1:A:269:GLN:HG2	2.03	0.59
2:B:12:LEU:O	2:B:14:PRO:HD3	2.03	0.59
2:B:371:ALA:O	2:B:375:ILE:HG13	2.03	0.58
1:A:498:ASP:HB2	1:A:538:ALA:HA	1.86	0.58
2:B:244:ILE:HG12	2:B:244:ILE:O	2.04	0.58
1:A:138:GLU:O	1:A:140:PRO:HD3	2.04	0.57
1:A:239:TRP:CZ2	1:A:270:ILE:HD12	2.39	0.57
1:A:23:GLN:O	1:A:23:GLN:HG3	2.02	0.57
2:B:422:LEU:O	2:B:426:TRP:CZ3	2.57	0.57
2:B:209:LEU:HD22	2:B:214:LEU:HD12	1.87	0.57
2:B:423:VAL:HG13	2:B:423:VAL:O	2.03	0.57
2:B:132:ILE:HG23	2:B:142:ILE:HB	1.87	0.57
1:A:556:ILE:HD12	1:A:556:ILE:N	2.19	0.57
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.86	0.57
2:B:178:ILE:HD11	2:B:201:LYS:HD3	1.85	0.56
1:A:543:GLY:HA2	2:B:284:ARG:O	2.04	0.56
2:B:234:LEU:HD11	2:B:377:THR:HG21	1.85	0.56
2:B:330:GLN:HE22	2:B:340:GLN:HE22	1.51	0.56
2:B:132:ILE:HD12	2:B:132:ILE:C	2.25	0.56
1:A:411:ILE:HG13	1:A:411:ILE:O	2.05	0.56
1:A:5:ILE:HD11	1:A:167:ILE:HD11	1.87	0.56
1:A:10:VAL:HG12	1:A:11:LYS:N	2.20	0.56
1:A:108:VAL:HG13	1:A:223:LYS:CB	2.36	0.56
1:A:454:LYS:HD2	1:A:552:VAL:HG13	1.87	0.56
2:B:306:ASN:O	2:B:308:GLU:N	2.38	0.56
1:A:254:VAL:HG13	1:A:283:LEU:CD2	2.33	0.56
2:B:56:TYR:HE1	2:B:126:LYS:HE3	1.71	0.56
1:A:177:ASP:OD1	1:A:193:LEU:HD21	2.06	0.56
2:B:87:PHE:O	2:B:88:TRP:HD1	1.87	0.56
1:A:151:GLN:O	1:A:151:GLN:HG2	2.04	0.55
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.41	0.55
2:B:109:LEU:HD22	2:B:216:THR:HG21	1.88	0.55
2:B:293:ILE:HG12	2:B:293:ILE:O	2.06	0.55
2:B:257:ILE:HD13	2:B:283:LEU:HD13	1.87	0.55
1:A:33:ALA:HB1	1:A:71:TRP:CG	2.41	0.55
2:B:64:LYS:HE3	2:B:71:TRP:CH2	2.42	0.55
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.89	0.55
1:A:112:GLY:C	1:A:114:ALA:H	2.09	0.55
1:A:229:TRP:CH2	3:A:561:T50:H14	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:ILE:HD12	2:B:133:PRO:N	2.22	0.55
1:A:137:ASN:O	1:A:139:THR:N	2.37	0.55
2:B:363:ASN:ND2	2:B:364:ASP:N	2.54	0.54
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.40	0.54
2:B:139:THR:HB	2:B:140:PRO:HD2	1.89	0.54
1:A:199:ARG:HH11	1:A:220:LYS:HE2	1.73	0.54
1:A:362:THR:CG2	1:A:367:GLN:HG3	2.37	0.54
1:A:228:LEU:HB3	1:A:242:GLN:NE2	2.23	0.54
2:B:423:VAL:O	2:B:423:VAL:CG1	2.56	0.54
1:A:170:PRO:O	1:A:174:GLN:HG3	2.07	0.54
1:A:174:GLN:C	1:A:176:PRO:HD3	2.28	0.54
1:A:544:GLY:HA2	1:A:548:VAL:HG23	1.88	0.54
1:A:51:GLY:N	1:A:52:PRO:CD	2.62	0.54
1:A:543:GLY:HA3	2:B:285:GLY:O	2.07	0.54
1:A:324:ASP:O	1:A:343:GLN:HG2	2.08	0.53
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.37	0.53
2:B:197:GLN:O	2:B:200:THR:HB	2.09	0.53
1:A:556:ILE:HD12	1:A:556:ILE:H	1.74	0.53
1:A:345:PRO:O	1:A:346:PHE:CG	2.62	0.53
1:A:366:LYS:HE3	1:A:370:GLU:OE2	2.08	0.53
1:A:270:ILE:HD11	1:A:316:GLY:N	2.25	0.52
1:A:57:ASN:OD1	1:A:131:THR:HB	2.09	0.52
1:A:77:PHE:O	1:A:79:GLU:N	2.42	0.52
2:B:423:VAL:O	2:B:427:TYR:HE1	1.92	0.52
1:A:454:LYS:CG	1:A:552:VAL:HG13	2.40	0.52
2:B:319:TYR:O	2:B:321:PRO:HD3	2.10	0.52
2:B:241:VAL:HG23	2:B:241:VAL:O	2.09	0.52
2:B:103:LYS:HE2	2:B:103:LYS:HA	1.92	0.52
2:B:173:LYS:O	2:B:176:PRO:HD3	2.10	0.51
1:A:328:GLU:CG	1:A:390:LYS:HB2	2.40	0.51
1:A:108:VAL:CG1	1:A:223:LYS:CB	2.88	0.51
2:B:295:LEU:HB3	2:B:299:ALA:HB3	1.93	0.51
1:A:115:TYR:CE1	1:A:156:SER:HB3	2.44	0.51
1:A:219:LYS:O	1:A:220:LYS:HB3	2.10	0.51
2:B:306:ASN:C	2:B:308:GLU:N	2.62	0.51
1:A:5:ILE:HG22	1:A:6:GLU:O	2.11	0.51
1:A:13:LYS:HB2	1:A:16:MET:HG3	1.92	0.51
1:A:135:ILE:HG13	1:A:138:GLU:OE1	2.10	0.51
2:B:5:ILE:HG22	2:B:6:GLU:O	2.11	0.51
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.77	0.50
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:C	1:A:29:GLU:H	2.14	0.50
1:A:27:THR:C	1:A:29:GLU:N	2.64	0.50
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.47	0.50
1:A:215:THR:O	1:A:217:PRO:HD3	2.11	0.50
1:A:500:GLN:HE21	2:B:422:LEU:CD1	2.24	0.50
1:A:194:GLU:O	1:A:196:GLY:N	2.45	0.50
2:B:281:LYS:HA	2:B:284:ARG:NH1	2.26	0.50
2:B:244:ILE:HD13	2:B:244:ILE:N	2.26	0.50
2:B:64:LYS:HE3	2:B:71:TRP:CZ2	2.47	0.50
1:A:30:LYS:HD2	1:A:62:ALA:HB3	1.92	0.50
1:A:111:VAL:O	1:A:111:VAL:HG13	2.12	0.50
1:A:290:THR:O	1:A:290:THR:HG22	2.11	0.50
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.34	0.50
1:A:112:GLY:O	1:A:114:ALA:N	2.34	0.50
2:B:183:TYR:CD2	2:B:380:ILE:HD13	2.47	0.50
2:B:308:GLU:C	2:B:310:LEU:N	2.64	0.50
2:B:242:GLN:N	2:B:243:PRO:CD	2.75	0.49
1:A:60:VAL:HG23	1:A:130:PHE:HB2	1.94	0.49
1:A:164:MET:HE1	1:A:214:LEU:HD13	1.93	0.49
1:A:215:THR:C	1:A:217:PRO:HD3	2.33	0.49
2:B:234:LEU:HD11	2:B:377:THR:CG2	2.42	0.49
2:B:395:LYS:O	2:B:399:GLU:CG	2.61	0.49
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.75	0.49
1:A:334:GLN:CD	1:A:512:LYS:HG3	2.33	0.49
2:B:65:LYS:HG3	2:B:72:ARG:HB2	1.94	0.49
1:A:50:ILE:HD11	1:A:54:ASN:HD22	1.78	0.48
2:B:157:PRO:HG3	2:B:184:MET:HA	1.95	0.48
2:B:169:GLU:HB2	2:B:170:PRO:HD3	1.96	0.48
2:B:403:THR:HG23	2:B:403:THR:O	2.12	0.48
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.95	0.48
2:B:306:ASN:C	2:B:308:GLU:H	2.17	0.48
2:B:178:ILE:CD1	2:B:201:LYS:HD3	2.44	0.48
1:A:354:TYR:OH	1:A:370:GLU:OE1	2.31	0.48
1:A:433:PRO:HB3	2:B:289:LEU:CD1	2.44	0.48
2:B:2:ILE:O	2:B:4:PRO:HD3	2.14	0.48
1:A:103:LYS:HE3	1:A:179:VAL:HG11	1.96	0.47
1:A:276:VAL:HG12	1:A:280:SER:HB2	1.95	0.47
2:B:115:TYR:O	2:B:117:SER:N	2.47	0.47
1:A:369:THR:HG23	1:A:398:TRP:HH2	1.79	0.47
2:B:49:LYS:HG3	2:B:144:TYR:CE1	2.49	0.47
1:A:49:LYS:O	1:A:50:ILE:CG2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TRP:O	1:A:89:GLU:C	2.52	0.47
2:B:27:THR:HG22	2:B:30:LYS:HG3	1.97	0.47
1:A:131:THR:HB	1:A:143:ARG:HH11	1.79	0.47
2:B:101:LYS:O	2:B:236:PRO:HB2	2.15	0.47
1:A:135:ILE:H	1:A:135:ILE:HG12	1.48	0.47
1:A:326:ILE:O	1:A:341:ILE:HA	2.15	0.47
1:A:457:TYR:CD1	1:A:457:TYR:C	2.88	0.47
1:A:49:LYS:HG3	1:A:144:TYR:CE2	2.50	0.47
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.44	0.47
2:B:88:TRP:CZ3	2:B:92:LEU:HD12	2.49	0.47
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.50	0.47
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.97	0.47
2:B:88:TRP:HZ3	2:B:159:ILE:HG13	1.80	0.47
1:A:358:ARG:HH12	1:A:366:LYS:HE2	1.80	0.46
2:B:308:GLU:C	2:B:310:LEU:H	2.18	0.46
2:B:423:VAL:O	2:B:427:TYR:CE1	2.68	0.46
1:A:314:VAL:HG12	1:A:315:HIS:N	2.29	0.46
1:A:344:GLU:HB3	1:A:345:PRO:HD2	1.97	0.46
1:A:472:THR:OG1	1:A:476:LYS:HB2	2.16	0.46
1:A:177:ASP:OD2	1:A:177:ASP:N	2.48	0.46
1:A:278:GLN:OE1	1:A:298:GLU:HB3	2.14	0.46
1:A:483:TYR:CZ	1:A:520:GLN:HG2	2.49	0.46
1:A:164:MET:CE	1:A:214:LEU:HD13	2.46	0.46
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.50	0.46
1:A:290:THR:O	1:A:291:GLU:C	2.54	0.46
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.16	0.46
1:A:219:LYS:O	1:A:220:LYS:CB	2.63	0.46
2:B:245:VAL:HG12	2:B:246:LEU:N	2.31	0.46
1:A:220:LYS:O	1:A:221:HIS:CB	2.63	0.46
1:A:433:PRO:HB3	2:B:289:LEU:HD13	1.98	0.46
1:A:5:ILE:HG22	1:A:6:GLU:N	2.31	0.46
2:B:392:PRO:HA	2:B:417:VAL:HG22	1.96	0.46
1:A:111:VAL:CG1	1:A:185:ASP:O	2.62	0.46
1:A:451:LYS:O	1:A:471:ASN:N	2.49	0.46
2:B:175:ASN:OD1	2:B:201:LYS:HE2	2.15	0.46
2:B:214:LEU:N	2:B:214:LEU:HD23	2.31	0.46
1:A:497:THR:HG22	1:A:499:SER:H	1.81	0.45
1:A:500:GLN:HE21	2:B:422:LEU:HD13	1.81	0.45
1:A:49:LYS:O	1:A:50:ILE:HG23	2.16	0.45
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.37	0.45
1:A:411:ILE:O	1:A:412:PRO:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:THR:CG2	1:A:363:ASN:N	2.79	0.45
1:A:441:TYR:HB3	1:A:548:VAL:HG21	1.98	0.45
2:B:194:GLU:O	2:B:196:GLY:N	2.49	0.45
1:A:66:LYS:C	1:A:68:SER:N	2.70	0.45
1:A:134:SER:HB3	1:A:139:THR:HA	1.99	0.45
1:A:420:PRO:HA	1:A:421:PRO:C	2.37	0.45
2:B:407:GLN:HE21	2:B:407:GLN:HB3	1.59	0.45
1:A:50:ILE:CD1	1:A:54:ASN:HD22	2.30	0.45
2:B:395:LYS:O	2:B:399:GLU:HG2	2.17	0.45
2:B:238:LYS:HG2	2:B:238:LYS:O	2.16	0.45
2:B:332:GLN:HB3	2:B:333:GLY:H	1.51	0.45
1:A:111:VAL:O	1:A:185:ASP:HB2	2.17	0.45
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.82	0.45
1:A:291:GLU:O	1:A:293:ILE:N	2.50	0.45
2:B:270:ILE:O	2:B:272:PRO:HD3	2.17	0.45
2:B:232:TYR:CE2	2:B:234:LEU:HD21	2.52	0.45
1:A:112:GLY:C	1:A:114:ALA:N	2.70	0.44
1:A:382:ILE:O	2:B:136:ASN:HB2	2.16	0.44
2:B:206:ARG:CZ	2:B:217:PRO:O	2.66	0.44
2:B:369:THR:HG23	2:B:406:TRP:CE3	2.52	0.44
1:A:142:ILE:HG23	1:A:142:ILE:O	2.17	0.44
1:A:175:ASN:N	1:A:176:PRO:HD3	2.33	0.44
1:A:398:TRP:CD1	1:A:398:TRP:C	2.91	0.44
2:B:258:GLN:HG3	2:B:283:LEU:HD21	1.98	0.44
1:A:10:VAL:CG1	1:A:11:LYS:N	2.81	0.44
1:A:52:PRO:HG2	1:A:53:GLU:N	2.31	0.44
1:A:217:PRO:O	1:A:219:LYS:N	2.51	0.44
2:B:257:ILE:HG12	2:B:283:LEU:HD22	1.99	0.44
1:A:77:PHE:O	1:A:80:LEU:N	2.50	0.44
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.53	0.44
1:A:27:THR:OG1	1:A:29:GLU:HB3	2.16	0.44
1:A:134:SER:CB	1:A:139:THR:HA	2.48	0.44
2:B:31:ILE:HG23	2:B:132:ILE:CD1	2.29	0.44
1:A:108:VAL:HG12	1:A:227:PHE:HE1	1.82	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.53	0.43
2:B:241:VAL:CG1	2:B:351:THR:H	2.30	0.43
2:B:242:GLN:H	2:B:243:PRO:HD3	1.81	0.43
1:A:273:GLY:O	1:A:274:ILE:C	2.56	0.43
2:B:203:GLU:O	2:B:203:GLU:CG	2.65	0.43
2:B:125:ARG:HD3	2:B:147:ASN:HA	2.00	0.43
2:B:315:HIS:ND1	2:B:316:GLY:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.53	0.43
2:B:395:LYS:O	2:B:399:GLU:HG3	2.18	0.43
1:A:169:GLU:O	1:A:173:LYS:HB2	2.18	0.43
1:A:334:GLN:NE2	1:A:512:LYS:HG3	2.33	0.43
2:B:34:LEU:HD23	2:B:34:LEU:HA	1.81	0.43
1:A:515:SER:O	1:A:519:ASN:ND2	2.50	0.43
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.53	0.43
1:A:64:LYS:HD3	1:A:71:TRP:CZ2	2.53	0.43
1:A:130:PHE:CD1	1:A:130:PHE:N	2.86	0.43
1:A:224:GLU:H	1:A:224:GLU:HG3	1.55	0.43
1:A:310:LEU:HD12	1:A:310:LEU:HA	1.88	0.43
1:A:335:GLY:O	1:A:355:ALA:HA	2.18	0.43
2:B:323:LYS:NZ	2:B:344:GLU:OE2	2.49	0.43
2:B:422:LEU:HD23	2:B:422:LEU:HA	1.70	0.43
1:A:443:ASP:HB3	1:A:548:VAL:HG12	2.00	0.43
2:B:23:GLN:OE1	2:B:60:VAL:HG22	2.18	0.43
2:B:85:GLN:CG	2:B:154:LYS:HB2	2.45	0.43
2:B:139:THR:CB	2:B:140:PRO:HD2	2.46	0.43
2:B:198:HIS:C	2:B:200:THR:N	2.72	0.43
1:A:417:VAL:CG1	1:A:419:THR:HG23	2.33	0.43
1:A:444:GLY:O	1:A:445:ALA:HB2	2.19	0.43
1:A:377:THR:O	1:A:381:VAL:HG23	2.18	0.43
1:A:53:GLU:C	1:A:55:PRO:HD3	2.39	0.42
1:A:73:LYS:CE	1:A:130:PHE:CE2	3.03	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.42
2:B:77:PHE:O	2:B:78:ARG:C	2.58	0.42
1:A:406:TRP:CZ3	1:A:407:GLN:HG2	2.54	0.42
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.01	0.42
2:B:53:GLU:OE1	2:B:53:GLU:N	2.41	0.42
1:A:178:ILE:HD11	1:A:201:LYS:HB3	2.02	0.42
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.54	0.42
2:B:266:TRP:CG	2:B:426:TRP:CE3	3.07	0.42
1:A:131:THR:HA	1:A:143:ARG:HG2	2.01	0.42
2:B:193:LEU:HD11	2:B:201:LYS:HD2	2.02	0.42
2:B:216:THR:HA	2:B:217:PRO:HD3	1.89	0.42
2:B:423:VAL:HG13	2:B:427:TYR:OH	2.19	0.42
1:A:21:VAL:HG12	1:A:22:LYS:N	2.35	0.42
1:A:115:TYR:N	1:A:115:TYR:CD2	2.88	0.42
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.75	0.42
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.55	0.42
1:A:540:LYS:O	1:A:542:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:O	1:A:9:PRO:HG2	2.20	0.42
2:B:115:TYR:HE1	2:B:185:ASP:OD1	2.02	0.42
2:B:194:GLU:O	2:B:197:GLN:N	2.50	0.41
1:A:199:ARG:HH12	1:A:220:LYS:HE2	1.79	0.41
1:A:398:TRP:CH2	1:A:411:ILE:HD13	2.55	0.41
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.50	0.41
2:B:426:TRP:O	2:B:427:TYR:CB	2.69	0.41
1:A:308:GLU:O	1:A:311:LYS:CB	2.68	0.41
1:A:417:VAL:CG1	1:A:419:THR:CG2	2.97	0.41
2:B:85:GLN:O	2:B:86:ASP:C	2.56	0.41
2:B:277:ARG:NH2	2:B:302:GLU:OE1	2.53	0.41
1:A:147:ASN:C	1:A:148:VAL:HG13	2.41	0.41
1:A:503:LEU:HD11	1:A:507:GLN:OE1	2.20	0.41
1:A:12:LEU:O	1:A:13:LYS:C	2.58	0.41
1:A:179:VAL:HG22	3:A:561:T50:H20	2.02	0.41
1:A:276:VAL:O	1:A:276:VAL:CG1	2.68	0.41
2:B:85:GLN:CB	2:B:154:LYS:HB2	2.50	0.41
2:B:215:THR:CG2	2:B:216:THR:H	2.28	0.41
2:B:312:GLU:HA	2:B:313:PRO:HD2	1.81	0.41
1:A:398:TRP:CZ2	1:A:411:ILE:HD13	2.55	0.41
1:A:446:ALA:HB2	1:A:472:THR:HG23	2.02	0.41
1:A:509:GLN:N	1:A:510:PRO:CD	2.83	0.41
2:B:115:TYR:C	2:B:117:SER:H	2.24	0.41
2:B:210:LEU:HD12	2:B:214:LEU:O	2.20	0.41
2:B:235:HIS:C	2:B:237:ASP:H	2.23	0.41
2:B:124:PHE:O	2:B:125:ARG:C	2.59	0.41
1:A:20:LYS:HE2	1:A:55:PRO:O	2.21	0.41
1:A:270:ILE:HD11	1:A:316:GLY:CA	2.50	0.41
2:B:2:ILE:O	2:B:4:PRO:CD	2.69	0.41
2:B:369:THR:HG23	2:B:406:TRP:HE3	1.86	0.41
1:A:49:LYS:CG	1:A:144:TYR:CE2	3.05	0.40
1:A:424:LYS:HE3	1:A:426:TRP:CZ2	2.56	0.40
1:A:320:ASP:HA	1:A:321:PRO:HD3	1.79	0.40
1:A:398:TRP:CH2	1:A:411:ILE:HG21	2.57	0.40
1:A:254:VAL:O	1:A:258:GLN:HG3	2.21	0.40
2:B:354:TYR:OH	2:B:370:GLU:HB3	2.21	0.40
1:A:131:THR:CB	1:A:143:ARG:HG2	2.51	0.40
1:A:171:PHE:CD2	1:A:171:PHE:C	2.94	0.40
2:B:207:GLN:O	2:B:211:ARG:HB2	2.21	0.40
2:B:266:TRP:HB2	2:B:426:TRP:CZ3	2.56	0.40
1:A:137:ASN:C	1:A:139:THR:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:THR:HG23	1:A:386:THR:HG22	2.02	0.40
2:B:75:VAL:HG11	2:B:77:PHE:CZ	2.56	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	556/560 (99%)	480 (86%)	60 (11%)	16 (3%)	4 6
2	B	425/430 (99%)	347 (82%)	59 (14%)	19 (4%)	2 2
All	All	981/990 (99%)	827 (84%)	119 (12%)	35 (4%)	3 4

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	PRO
1	A	538	ALA
2	B	225	PRO
2	B	295	LEU
2	B	316	GLY
2	B	317	VAL
2	B	357	MET
1	A	78	ARG
1	A	218	ASP
1	A	345	PRO
1	A	358	ARG
1	A	541	GLY
2	B	85	GLN
2	B	93	GLY
2	B	116	PHE
2	B	307	ARG

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Mol	Chain	Res	Type
2	B	309	ILE
2	B	359	GLY
1	A	90	VAL
1	A	113	ASP
1	A	114	ALA
1	A	135	ILE
1	A	270	ILE
2	B	238	LYS
2	B	14	PRO
2	B	362	THR
1	A	195	ILE
2	B	126	LYS
2	B	313	PRO
1	A	67	ASP
1	A	292	VAL
1	A	445	ALA
2	B	195	ILE
2	B	224	GLU
2	B	236	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	472/500 (94%)	443 (94%)	29 (6%)	18	29
2	B	368/392 (94%)	340 (92%)	28 (8%)	13	21
All	All	840/892 (94%)	783 (93%)	57 (7%)	16	24

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	16	MET
1	A	22	LYS
1	A	23	GLN

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Mol	Chain	Res	Type
1	A	40	GLU
1	A	75	VAL
1	A	90	VAL
1	A	110	ASP
1	A	130	PHE
1	A	135	ILE
1	A	185	ASP
1	A	224	GLU
1	A	241	VAL
1	A	245	VAL
1	A	286	THR
1	A	310	LEU
1	A	330	GLN
1	A	340	GLN
1	A	345	PRO
1	A	362	THR
1	A	364	ASP
1	A	385	LYS
1	A	387	PRO
1	A	396	GLU
1	A	463	ARG
1	A	497	THR
1	A	520	GLN
1	A	547	GLN
1	A	548	VAL
2	B	2	ILE
2	B	14	PRO
2	B	27	THR
2	B	35	VAL
2	B	55	PRO
2	B	69	THR
2	B	111	VAL
2	B	132	ILE
2	B	174	GLN
2	B	193	LEU
2	B	232	TYR
2	B	244	ILE
2	B	248	GLU
2	B	252	TRP
2	B	257	ILE
2	B	283	LEU
2	B	284	ARG

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Mol	Chain	Res	Type
2	B	314	VAL
2	B	315	HIS
2	B	318	TYR
2	B	330	GLN
2	B	334	GLN
2	B	363	ASN
2	B	399	GLU
2	B	403	THR
2	B	407	GLN
2	B	423	VAL
2	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	91	GLN
1	A	151	GLN
1	A	242	GLN
1	A	373	GLN
1	A	428	GLN
1	A	471	ASN
1	A	487	GLN
1	A	500	GLN
2	B	91	GLN
2	B	96	HIS
2	B	145	GLN
2	B	147	ASN
2	B	161	GLN
2	B	235	HIS
2	B	258	GLN
2	B	330	GLN
2	B	340	GLN
2	B	343	GLN
2	B	348	ASN
2	B	363	ASN
2	B	373	GLN
2	B	407	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	T50	A	561	-	27,30,30	2.78	16 (59%)	31,44,44	1.41	6 (19%)

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	T50	A	561	-	-	0/4/8/8	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	T50	C21-C22	6.66	1.44	1.36
3	A	561	T50	C19-C18	4.79	1.41	1.36
3	A	561	T50	C2-N3	-4.14	1.29	1.33
3	A	561	T50	C5-C4	3.97	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	561	T50	C6-C5	3.97	1.47	1.38
3	A	561	T50	C6-C7	3.62	1.45	1.36
3	A	561	T50	C20-C19	2.90	1.45	1.38
3	A	561	T50	C20-C21	2.78	1.44	1.38
3	A	561	T50	F1-C18	-2.60	1.31	1.36
3	A	561	T50	F2-C22	-2.55	1.31	1.36
3	A	561	T50	C11-C12	2.53	1.42	1.38
3	A	561	T50	C13-C12	2.49	1.43	1.37
3	A	561	T50	C4A-C4	2.45	1.55	1.51
3	A	561	T50	C15-C16	2.31	1.42	1.37
3	A	561	T50	C7-C8	2.26	1.45	1.41
3	A	561	T50	C14-C13	2.03	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	561	T50	C16-C11-C12	3.43	119.28	114.51
3	A	561	T50	C19-C18-C17	-3.21	121.58	124.18
3	A	561	T50	C21-C22-C17	-3.07	121.69	124.18
3	A	561	T50	F3-C12-C11	2.18	120.23	117.63
3	A	561	T50	C10-C11-C16	-2.09	117.63	122.50
3	A	561	T50	C13-C12-C11	-2.01	120.37	124.02

There are no chirality outliers.

There are no torsion outliers.

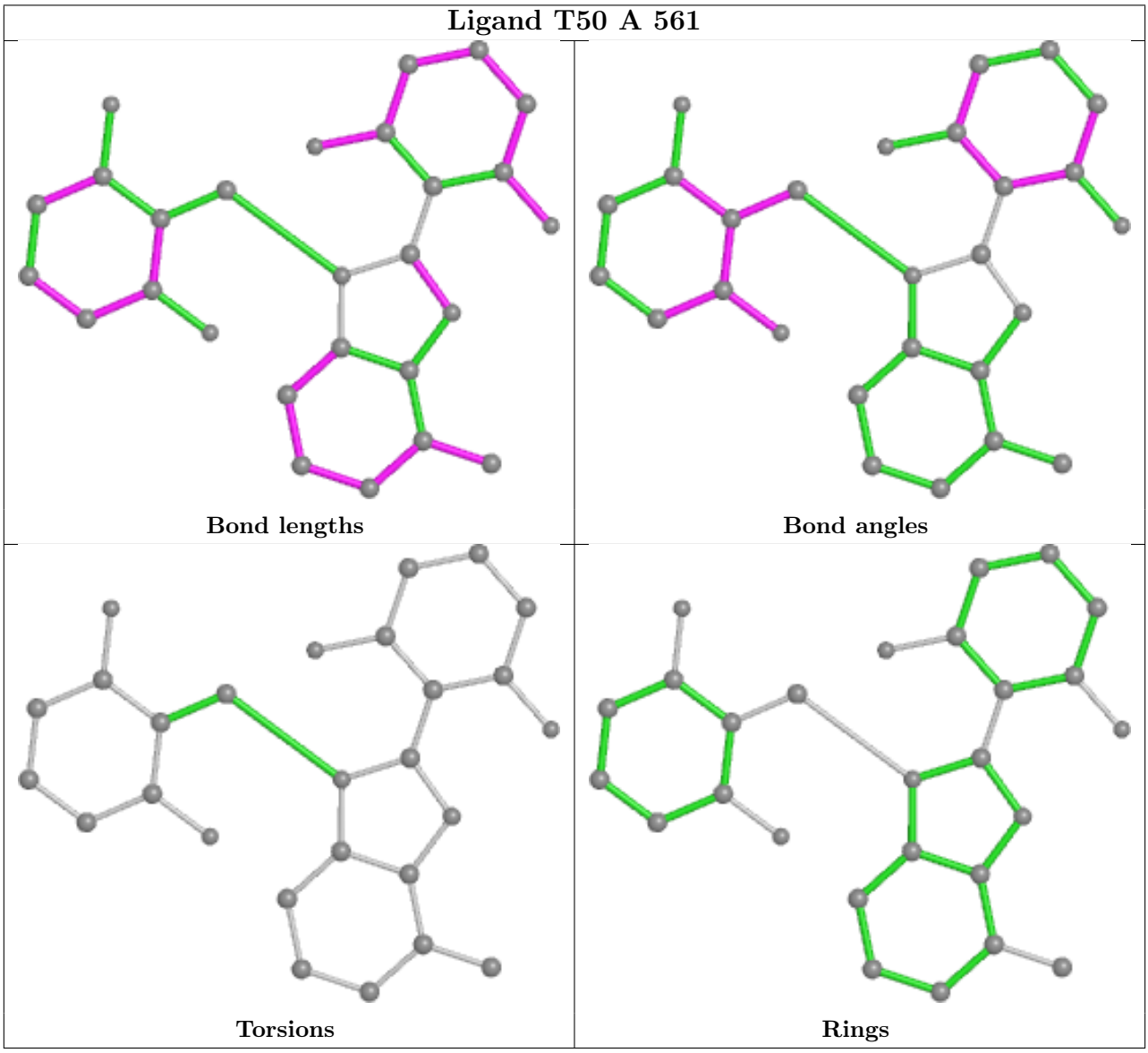
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	561	T50	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.



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	558/560 (99%)	0.16	34 (6%)	21	18	47, 87, 121, 121	0
2	B	427/430 (99%)	0.33	33 (7%)	13	10	41, 74, 121, 121	0
All	All	985/990 (99%)	0.24	67 (6%)	17	14	41, 83, 121, 121	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	8.1
2	B	1	PRO	6.1
1	A	554	ALA	5.9
2	B	222	GLN	5.7
2	B	3	SER	5.5
2	B	221	HIS	5.5
2	B	2	ILE	5.5
2	B	232	TYR	5.4
1	A	553	SER	5.3
1	A	286	THR	5.0
1	A	552	VAL	4.8
1	A	289	LEU	4.8
1	A	140	PRO	4.8
1	A	287	LYS	4.7
2	B	304	ALA	4.6
2	B	224	GLU	4.4
2	B	243	PRO	4.3
2	B	225	PRO	4.3
2	B	226	PRO	4.3
1	A	558	LYS	4.1
1	A	550	LYS	4.0
2	B	295	LEU	4.0
2	B	227	PHE	3.9
1	A	551	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	556	ILE	3.7
2	B	4	PRO	3.6
2	B	294	PRO	3.5
1	A	557	ARG	3.4
1	A	133	PRO	3.3
1	A	65	LYS	3.3
1	A	66	LYS	3.3
1	A	141	GLY	3.2
2	B	230	MET	3.1
1	A	68	SER	3.1
1	A	67	ASP	3.1
2	B	426	TRP	3.0
1	A	290	THR	3.0
2	B	5	ILE	3.0
2	B	223	LYS	2.9
1	A	139	THR	2.9
2	B	424	LYS	2.8
2	B	229	TRP	2.7
2	B	277	ARG	2.7
1	A	288	ALA	2.7
2	B	359	GLY	2.7
2	B	409	THR	2.7
2	B	357	MET	2.6
1	A	51	GLY	2.6
1	A	220	LYS	2.6
2	B	242	GLN	2.6
2	B	303	LEU	2.6
1	A	555	GLY	2.6
1	A	71	TRP	2.4
1	A	50	ILE	2.4
1	A	254	VAL	2.4
2	B	423	VAL	2.4
1	A	283	LEU	2.3
2	B	408	ALA	2.2
1	A	136	ASN	2.2
1	A	360	ALA	2.2
1	A	138	GLU	2.1
1	A	64	LYS	2.1
1	A	69	THR	2.1
2	B	252	TRP	2.1
2	B	360	ALA	2.1
2	B	228	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	257	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

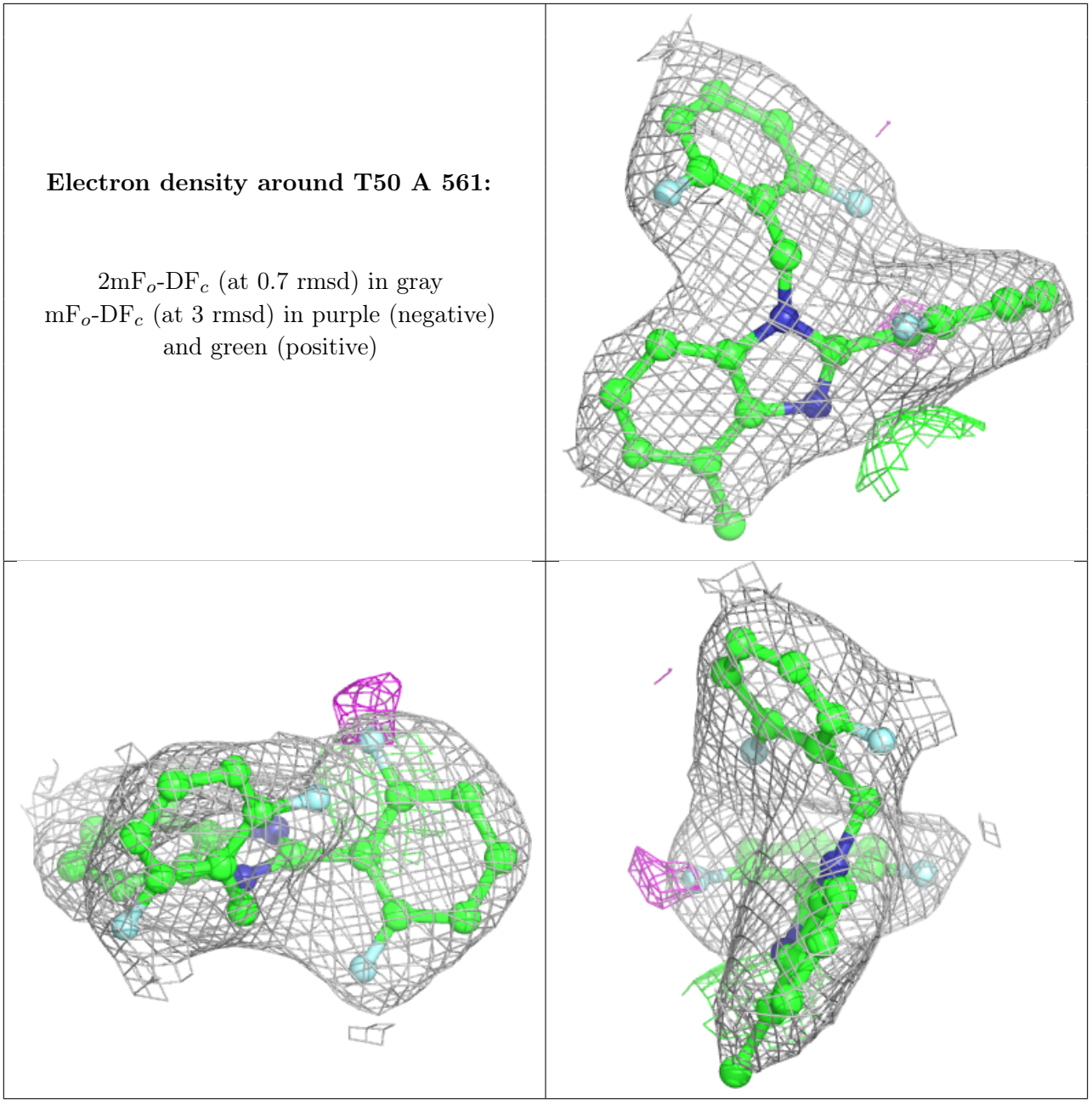
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	T50	A	561	27/27	0.96	0.14	47,53,66,72	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 T50 A 561:

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



6.5 Other polymers

There are no such residues in this entry.