Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 10:37 PM EDT

PDB ID	:	2QE2
Title	:	Structure of HCV NS5B Bound to an Anthranilic Acid Inhibitor
Authors	:	Chopra, R.; Svenson, K.; Bard, J.
Deposited on	:	2007-06-22
Resolution	:	2.90 Å(reported)

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

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

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

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

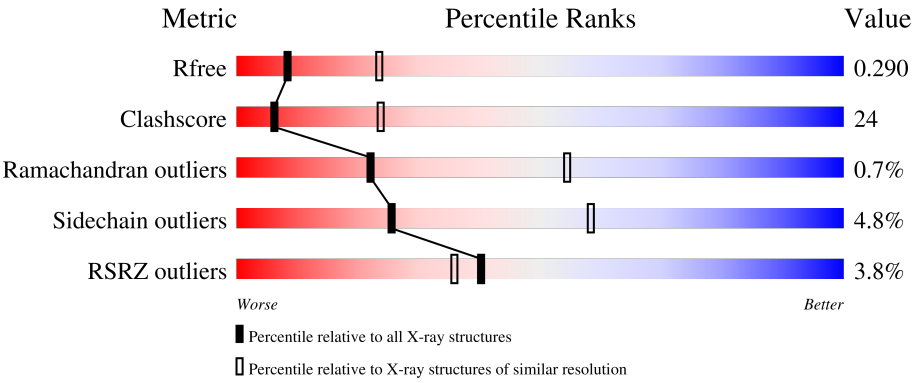
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	578	3% 52% 35% · 10%
1	B	578	4% 52% 34% · 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8193 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.

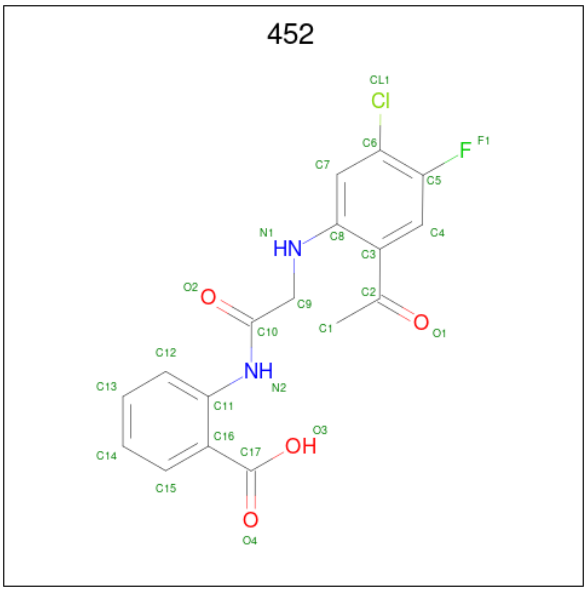
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	521	Total	C	N	O	S	0	0	0
			4065	2567	721	748	29			
1	B	523	Total	C	N	O	S	0	0	0
			4078	2573	725	751	29			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	GLY	-	expression tag	UNP Q99AU2
A	572	SER	-	expression tag	UNP Q99AU2
A	573	HIS	-	expression tag	UNP Q99AU2
A	574	HIS	-	expression tag	UNP Q99AU2
A	575	HIS	-	expression tag	UNP Q99AU2
A	576	HIS	-	expression tag	UNP Q99AU2
A	577	HIS	-	expression tag	UNP Q99AU2
A	578	HIS	-	expression tag	UNP Q99AU2
B	571	GLY	-	expression tag	UNP Q99AU2
B	572	SER	-	expression tag	UNP Q99AU2
B	573	HIS	-	expression tag	UNP Q99AU2
B	574	HIS	-	expression tag	UNP Q99AU2
B	575	HIS	-	expression tag	UNP Q99AU2
B	576	HIS	-	expression tag	UNP Q99AU2
B	577	HIS	-	expression tag	UNP Q99AU2
B	578	HIS	-	expression tag	UNP Q99AU2

- Molecule 2 is 2-{[N-(2-ACETYL-5-CHLORO-4-FLUOROPHENYL)GLYCYL]AMINO}BENZOIC ACID (three-letter code: 452) (formula: $C_{17}H_{14}ClFN_2O_4$).



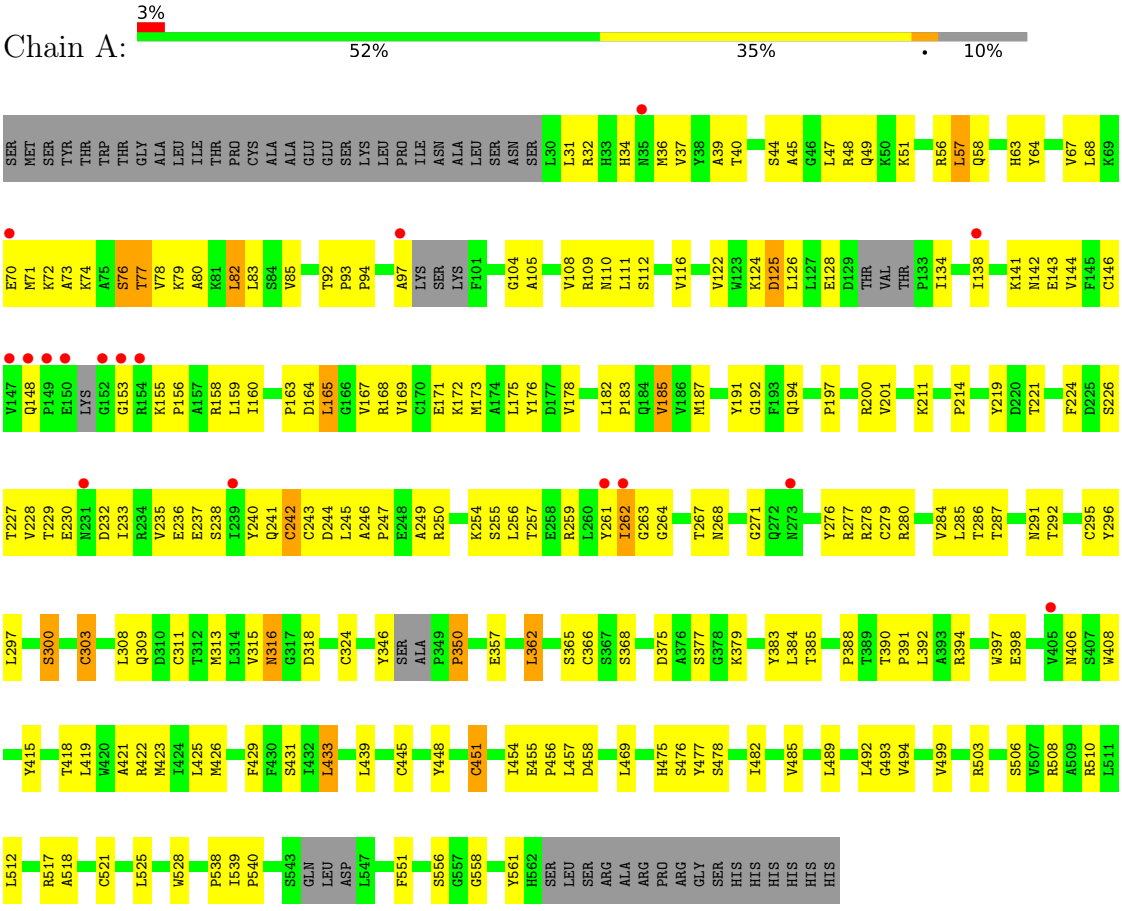
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			25	17	1	1	2	4		
2	B	1	Total	C	Cl	F	N	O	0	0
			25	17	1	1	2	4		

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.

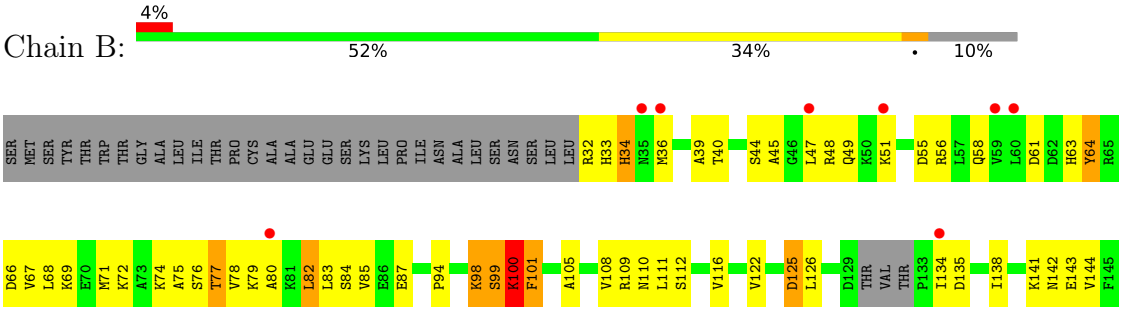
• Molecule 1: RNA-directed RNA polymerase

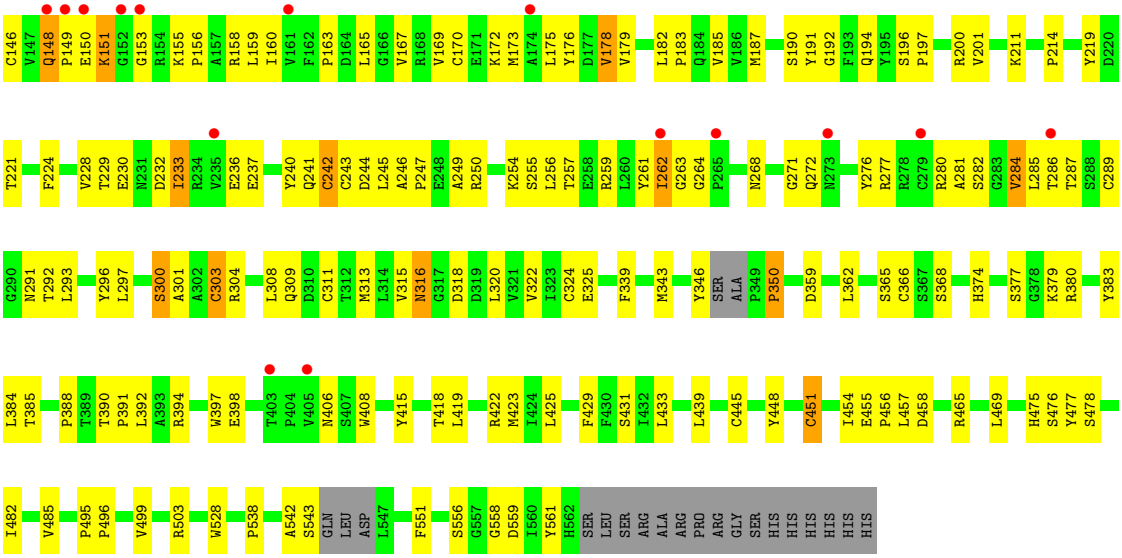
Chain A:



• Molecule 1: RNA-directed RNA polymerase

Chain B:




C146 V147 Q148 P149 E150 K151 G152 G153 R154 K155 P156 A157 R158 L159 I160 V161 F162 P163 D164 L165 G166 V167 R168 V169 C170 E171 K172 M173 A174 L175 Y176 D177 V178 V179 L182 P183 Q184 V185 V186 M187 S190 Y191 G192 F193 Q194 Y195 S196 P197 R200 V201 K211 P214 Y219 D220
T221 F224 V228 T229 E230 N231 D232 I233 R234 V235 E236 E237 Y240 Q241 C242 C243 D244 L245 A246 P247 E248 A249 R250 K254 S255 L256 T257 E258 R259 L260 Y261 I262 G263 G264 P265 N268 G271 Q272 N273 Y276 R277 R278 C279 R280 A281 S282 G283 V284 L285 T286 T287 S288 C289
G290 N291 T292 L293 Y296 L297 S300 A301 A302 C303 R304 L308 Q309 D310 C311 T312 M313 L314 V315 N316 G317 D318 D319 L320 V321 V322 I323 C324 E325 F339 M343 Y346 SER ALA P349 P350 D359 L362 S365 C366 S367 S368 H374 S377 G378 K379 R380 Y383
L384 T385 P388 T389 T390 P391 L392 A393 R394 W397 E398 T403 P404 V405 N406 S407 W408 Y415 T418 L419 R422 M423 I424 L425 F429 F430 S431 I432 L433 L439 C445 Y448 C451 I454 E455 P456 L457 D458 R465 L469 H475 S476 Y477 S478
I482 V485 P495 P496 V499 R503 W528 P538 A542 S543 GLN LEU ASP L547 F551 S556 G557 G558 D559 I560 Y561 H562 SER LEU SER ARG ALA ARG PRO ARG GLY SER HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.83Å 70.88Å 251.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 2.90 49.14 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.77-2.90) 99.0 (49.14-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.279 , 0.296 0.272 , 0.290	Depositor DCC
R_{free} test set	2495 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.707	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 21.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.488 for k,h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8193	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: 452

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	0.48	0/4151	0.77	2/5622 (0.0%)
1	B	0.51	1/4166 (0.0%)	0.80	9/5643 (0.2%)
All	All	0.49	1/8317 (0.0%)	0.78	11/11265 (0.1%)

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	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	LYS	C-O	-6.71	1.10	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	151	LYS	N-CA-C	6.45	128.42	111.00
1	A	558	GLY	N-CA-C	-5.78	98.66	113.10
1	B	558	GLY	N-CA-C	-5.67	98.92	113.10
1	B	99	SER	N-CA-C	-5.62	95.83	111.00
1	B	101	PHE	N-CA-C	5.62	126.17	111.00
1	B	100	LYS	CA-C-N	-5.49	105.12	117.20
1	B	101	PHE	C-N-CA	-5.37	111.02	122.30
1	B	98	LYS	N-CA-C	5.33	125.41	111.00
1	B	99	SER	C-N-CA	-5.26	108.55	121.70
1	B	148	GLN	N-CA-C	5.25	125.18	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	57	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	LYS	Mainchain

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	4065	0	4071	204	0
1	B	4078	0	4084	198	0
2	A	25	0	13	0	0
2	B	25	0	13	0	0
All	All	8193	0	8181	400	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 24.

All (400) 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:261:TYR:HE1	1:A:284:VAL:HG11	1.17	1.06
1:B:230:GLU:HB3	1:B:262:ILE:HD11	1.39	1.03
1:A:254:LYS:HE3	1:B:254:LYS:HE3	1.42	0.97
1:B:377:SER:HB2	1:B:379:LYS:HG3	1.45	0.96
1:A:230:GLU:HB3	1:A:262:ILE:HD11	1.48	0.94
1:B:175:LEU:HD11	1:B:261:TYR:HE2	1.32	0.92
1:A:221:THR:HG1	1:A:224:PHE:HD1	0.93	0.91
1:A:261:TYR:CE1	1:A:284:VAL:HG11	2.09	0.87
1:B:44:SER:HB2	1:B:47:LEU:HD12	1.57	0.86
1:A:377:SER:HB2	1:A:379:LYS:HG3	1.59	0.85
1:A:309:GLN:O	1:A:324:CYS:HB2	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:TYR:O	1:A:194:GLN:HG2	1.79	0.82
1:A:163:PRO:HB2	1:A:167:VAL:HB	1.64	0.79
1:B:191:TYR:O	1:B:194:GLN:HG2	1.82	0.79
1:B:74:LYS:O	1:B:77:THR:HB	1.83	0.79
1:B:163:PRO:HB2	1:B:167:VAL:HB	1.64	0.79
1:B:71:MET:CE	1:B:297:LEU:HB2	2.13	0.78
1:A:76:SER:HA	1:A:242:CYS:O	1.83	0.78
1:A:79:LYS:HA	1:A:244:ASP:HB3	1.65	0.78
1:A:44:SER:HB2	1:A:47:LEU:HD12	1.66	0.77
1:A:74:LYS:O	1:A:77:THR:HB	1.84	0.77
1:A:394:ARG:O	1:A:398:GLU:HG3	1.84	0.77
1:B:175:LEU:HD13	1:B:286:THR:CG2	2.14	0.77
1:B:230:GLU:HB3	1:B:262:ILE:CD1	2.14	0.76
1:B:221:THR:HG1	1:B:224:PHE:HD1	1.30	0.76
1:B:309:GLN:O	1:B:324:CYS:HB2	1.86	0.76
1:A:171:GLU:OE1	1:A:284:VAL:HG12	1.84	0.76
1:B:303:CYS:SG	1:B:308:LEU:HD11	2.26	0.75
1:A:230:GLU:HB3	1:A:262:ILE:CD1	2.16	0.75
1:B:79:LYS:HA	1:B:244:ASP:HB3	1.68	0.75
1:A:303:CYS:SG	1:A:308:LEU:HD11	2.28	0.74
1:A:126:LEU:HA	1:A:259:ARG:NH1	2.02	0.74
1:B:245:LEU:HB2	1:B:250:ARG:HE	1.53	0.74
1:B:63:HIS:O	1:B:67:VAL:HG23	1.87	0.74
1:A:141:LYS:HG3	1:A:160:ILE:CG1	2.18	0.73
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.70	0.73
1:A:232:ASP:O	1:A:236:GLU:HG3	1.89	0.73
1:B:175:LEU:HD13	1:B:286:THR:HG23	1.68	0.73
1:A:175:LEU:HD13	1:A:286:THR:CG2	2.18	0.72
1:A:175:LEU:HD11	1:A:261:TYR:HE2	1.55	0.72
1:B:230:GLU:CB	1:B:262:ILE:HD11	2.17	0.72
1:B:71:MET:HE2	1:B:297:LEU:HB2	1.71	0.72
1:A:261:TYR:HE1	1:A:284:VAL:CG1	1.99	0.71
1:B:80:ALA:HB3	1:B:245:LEU:CD2	2.20	0.71
1:B:122:VAL:O	1:B:126:LEU:HB2	1.89	0.71
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.73	0.70
1:A:230:GLU:CB	1:A:262:ILE:HD11	2.19	0.70
1:A:201:VAL:HG22	1:A:384:LEU:HG	1.73	0.70
1:B:141:LYS:HG3	1:B:160:ILE:CG1	2.21	0.69
1:A:182:LEU:HB3	1:A:183:PRO:HD3	1.74	0.69
1:B:448:TYR:CE2	1:B:551:PHE:HD1	2.11	0.69
1:A:80:ALA:HB3	1:A:245:LEU:CD2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:HB3	1:B:183:PRO:HD3	1.74	0.69
1:B:126:LEU:HA	1:B:259:ARG:NH1	2.07	0.69
1:B:175:LEU:CD1	1:B:261:TYR:HE2	2.06	0.69
1:B:76:SER:HA	1:B:242:CYS:O	1.93	0.68
1:A:175:LEU:HD13	1:A:286:THR:HG23	1.73	0.68
1:B:94:PRO:HG3	1:B:109:ARG:HH11	1.58	0.67
1:B:149:PRO:O	1:B:150:GLU:HB2	1.93	0.67
1:B:232:ASP:O	1:B:236:GLU:HG3	1.94	0.67
1:B:237:GLU:HG3	1:B:257:THR:HG21	1.76	0.67
1:A:485:VAL:O	1:A:489:LEU:HG	1.95	0.67
1:A:141:LYS:CG	1:A:160:ILE:HD11	2.25	0.66
1:B:148:GLN:O	1:B:151:LYS:HA	1.95	0.66
1:A:122:VAL:O	1:A:126:LEU:HB2	1.96	0.66
1:B:67:VAL:HG21	1:B:301:ALA:HB2	1.76	0.66
1:B:175:LEU:HD11	1:B:261:TYR:CE2	2.23	0.66
1:A:264:GLY:HA2	1:A:276:TYR:CZ	2.31	0.66
1:B:365:SER:O	1:B:366:CYS:HB2	1.96	0.66
1:B:388:PRO:O	1:B:392:LEU:HG	1.95	0.66
1:A:128:GLU:OE2	1:B:69:LYS:HE2	1.96	0.65
1:A:141:LYS:HG2	1:A:160:ILE:HD11	1.76	0.65
1:A:245:LEU:HB2	1:A:250:ARG:HE	1.61	0.65
1:A:171:GLU:OE1	1:A:284:VAL:CG1	2.44	0.65
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.30	0.65
1:B:67:VAL:O	1:B:71:MET:HG2	1.97	0.64
1:B:445:CYS:HB3	1:B:454:ILE:HD12	1.78	0.64
1:B:68:LEU:CD1	1:B:72:LYS:HE3	2.26	0.64
1:B:68:LEU:HD11	1:B:72:LYS:HE3	1.79	0.64
1:B:170:CYS:HA	1:B:173:MET:HE3	1.79	0.64
1:B:126:LEU:HD21	1:B:256:LEU:HG	1.80	0.64
1:B:394:ARG:O	1:B:398:GLU:HG3	1.98	0.63
1:A:71:MET:CE	1:A:297:LEU:HB2	2.28	0.63
1:B:94:PRO:HG3	1:B:109:ARG:NH1	2.12	0.63
1:A:63:HIS:O	1:A:67:VAL:HG23	1.98	0.63
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.81	0.62
1:B:263:GLY:HA2	1:B:277:ARG:NH1	2.14	0.62
1:A:237:GLU:HG3	1:A:257:THR:HG21	1.82	0.62
1:B:296:TYR:O	1:B:300:SER:HB2	2.00	0.62
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.80	0.62
1:A:68:LEU:HG	1:A:72:LYS:HE3	1.82	0.61
1:A:197:PRO:O	1:A:201:VAL:HG23	2.00	0.61
1:A:263:GLY:HA3	1:A:277:ARG:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:TRP:HB2	1:A:429:PHE:CE2	2.36	0.60
1:B:99:SER:C	1:B:101:PHE:N	2.49	0.60
1:B:141:LYS:CG	1:B:160:ILE:HD11	2.31	0.60
1:A:388:PRO:O	1:A:392:LEU:HG	2.01	0.60
1:B:141:LYS:HG2	1:B:160:ILE:HD11	1.83	0.59
1:B:419:LEU:HD23	1:B:477:TYR:CG	2.37	0.59
1:A:235:VAL:O	1:A:238:SER:HB3	2.03	0.59
1:A:448:TYR:CE2	1:A:551:PHE:HD1	2.20	0.59
1:A:224:PHE:CG	1:A:318:ASP:HB3	2.38	0.59
1:B:263:GLY:HA3	1:B:277:ARG:O	2.03	0.58
1:A:68:LEU:CG	1:A:72:LYS:HE3	2.32	0.58
1:A:68:LEU:HD11	1:A:72:LYS:HE3	1.83	0.58
1:B:201:VAL:HG22	1:B:384:LEU:HG	1.84	0.58
1:A:31:LEU:HA	1:A:494:VAL:HG12	1.85	0.58
1:A:175:LEU:O	1:A:178:VAL:N	2.26	0.58
1:B:309:GLN:HG2	1:B:325:GLU:HB2	1.85	0.58
1:A:68:LEU:CD1	1:A:72:LYS:HE3	2.34	0.58
1:A:72:LYS:HB3	1:A:242:CYS:SG	2.44	0.58
1:A:126:LEU:HD21	1:A:256:LEU:HG	1.85	0.58
1:A:219:TYR:CZ	1:A:350:PRO:HB3	2.38	0.58
1:B:408:TRP:HB2	1:B:429:PHE:CE2	2.39	0.58
1:A:105:ALA:O	1:A:109:ARG:HG3	2.03	0.58
1:A:56:ARG:NH1	1:A:279:CYS:HB3	2.19	0.57
1:A:175:LEU:HD11	1:A:261:TYR:CE2	2.38	0.57
1:A:257:THR:HA	1:A:261:TYR:HB2	1.86	0.57
1:A:264:GLY:HA2	1:A:276:TYR:CE1	2.39	0.57
1:A:246:ALA:O	1:A:249:ALA:HB3	2.05	0.57
1:A:78:VAL:HG21	1:A:185:VAL:HG21	1.86	0.57
1:B:237:GLU:HA	1:B:240:TYR:CD2	2.40	0.57
1:A:211:LYS:HB2	1:A:214:PRO:HB3	1.87	0.57
1:A:230:GLU:HB3	1:A:262:ILE:CG1	2.35	0.57
1:B:141:LYS:HE3	1:B:158:ARG:HB2	1.87	0.57
1:B:246:ALA:O	1:B:249:ALA:HB3	2.04	0.57
1:B:261:TYR:HE1	1:B:284:VAL:HG11	1.69	0.57
1:A:445:CYS:HB3	1:A:454:ILE:HD12	1.87	0.57
1:A:78:VAL:CG2	1:A:185:VAL:HG21	2.35	0.56
1:B:78:VAL:HG21	1:B:185:VAL:HG21	1.87	0.56
1:B:191:TYR:CD1	1:B:292:THR:HG21	2.39	0.56
1:B:264:GLY:HA2	1:B:276:TYR:CZ	2.41	0.56
1:A:192:GLY:HA3	1:A:316:ASN:OD1	2.05	0.56
1:B:175:LEU:HD13	1:B:286:THR:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ILE:HG13	1:B:259:ARG:HB3	1.87	0.56
1:A:71:MET:HE3	1:A:297:LEU:HB2	1.88	0.56
1:A:58:GLN:HG2	1:A:346:TYR:O	2.06	0.56
1:A:83:LEU:HB2	1:A:173:MET:HA	1.88	0.56
1:A:263:GLY:HA2	1:A:277:ARG:NH1	2.21	0.56
1:A:56:ARG:HH12	1:A:279:CYS:HB3	1.70	0.56
1:B:415:TYR:O	1:B:418:THR:HG23	2.06	0.56
1:B:175:LEU:CD1	1:B:261:TYR:CE2	2.87	0.55
1:A:108:VAL:HG21	1:A:165:LEU:HD21	1.88	0.55
1:A:134:ILE:HG13	1:A:259:ARG:HB3	1.89	0.55
1:B:149:PRO:C	1:B:151:LYS:H	2.08	0.55
1:B:99:SER:O	1:B:100:LYS:C	2.44	0.55
1:B:398:GLU:OE1	1:B:408:TRP:HD1	1.89	0.55
1:A:433:LEU:HB3	1:A:439:LEU:HD23	1.88	0.55
1:A:489:LEU:HD22	1:A:494:VAL:CG2	2.37	0.55
1:B:191:TYR:HD1	1:B:292:THR:HG21	1.70	0.54
1:B:221:THR:OG1	1:B:224:PHE:HD1	1.88	0.54
1:B:224:PHE:CG	1:B:318:ASP:HB3	2.42	0.54
1:B:245:LEU:HD12	1:B:250:ARG:HG2	1.89	0.54
1:A:365:SER:O	1:A:366:CYS:HB2	2.07	0.54
1:A:144:VAL:HG21	1:A:397:TRP:CD2	2.43	0.54
1:A:237:GLU:HA	1:A:240:TYR:CD2	2.42	0.54
1:B:40:THR:O	1:B:142:ASN:HA	2.06	0.54
1:B:108:VAL:HG21	1:B:165:LEU:HD21	1.89	0.54
1:A:40:THR:O	1:A:142:ASN:HA	2.06	0.54
1:B:48:ARG:HA	1:B:51:LYS:HD3	1.90	0.54
1:B:80:ALA:HB3	1:B:245:LEU:HD23	1.90	0.54
1:A:419:LEU:HD23	1:A:477:TYR:CG	2.42	0.53
1:B:423:MET:HG2	1:B:528:TRP:CZ3	2.44	0.53
1:A:165:LEU:O	1:A:169:VAL:HG23	2.09	0.53
1:B:170:CYS:HA	1:B:173:MET:CE	2.38	0.53
1:A:32:ARG:HB2	1:A:493:GLY:O	2.09	0.53
1:A:200:ARG:HD3	1:A:384:LEU:CD1	2.39	0.53
1:A:284:VAL:O	1:A:287:THR:HG22	2.08	0.52
1:B:58:GLN:HG2	1:B:346:TYR:O	2.09	0.52
1:B:48:ARG:CG	1:B:159:LEU:HG	2.40	0.52
1:B:144:VAL:HG21	1:B:397:TRP:CD2	2.45	0.52
1:A:241:GLN:HE22	1:A:250:ARG:HA	1.73	0.52
1:B:469:LEU:HD11	1:B:538:PRO:HA	1.91	0.52
1:A:241:GLN:HE22	1:A:250:ARG:CA	2.23	0.52
1:B:219:TYR:CZ	1:B:350:PRO:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:SER:CB	1:B:47:LEU:HD12	2.34	0.52
1:B:72:LYS:HB3	1:B:242:CYS:SG	2.49	0.52
1:B:83:LEU:O	1:B:173:MET:HG2	2.10	0.52
1:A:423:MET:HG2	1:A:528:TRP:CZ3	2.45	0.51
1:A:499:VAL:HG12	1:A:503:ARG:NE	2.26	0.51
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.75	0.51
1:A:219:TYR:HE2	1:A:221:THR:HG22	1.73	0.51
1:A:303:CYS:SG	1:A:308:LEU:HD21	2.50	0.51
1:A:475:HIS:O	1:A:476:SER:HB2	2.09	0.51
1:A:56:ARG:NH1	1:A:226:SER:O	2.44	0.51
1:A:236:GLU:OE2	1:A:280:ARG:NH2	2.39	0.51
1:B:85:VAL:HG11	1:B:116:VAL:HG13	1.93	0.51
1:B:141:LYS:HG3	1:B:160:ILE:HG12	1.91	0.51
1:B:224:PHE:HE2	1:B:291:ASN:HA	1.76	0.51
1:A:224:PHE:CB	1:A:318:ASP:HB3	2.41	0.51
1:A:141:LYS:HG3	1:A:160:ILE:HG12	1.92	0.51
1:B:39:ALA:HB2	1:B:144:VAL:HG22	1.93	0.51
1:B:105:ALA:O	1:B:109:ARG:HG3	2.11	0.50
1:A:255:SER:O	1:A:259:ARG:HG3	2.11	0.50
1:B:478:SER:O	1:B:482:ILE:HG13	2.11	0.50
1:B:237:GLU:OE1	1:B:241:GLN:HG3	2.11	0.50
1:B:211:LYS:HB2	1:B:214:PRO:HB3	1.94	0.50
1:A:406:ASN:H	1:A:406:ASN:HD22	1.60	0.50
1:A:48:ARG:CG	1:A:159:LEU:HG	2.41	0.50
1:B:200:ARG:HD3	1:B:384:LEU:CD1	2.42	0.49
1:A:44:SER:CB	1:A:47:LEU:HD12	2.41	0.49
1:B:68:LEU:HA	1:B:71:MET:HG3	1.93	0.49
1:B:78:VAL:CG2	1:B:185:VAL:HG21	2.42	0.49
1:A:56:ARG:HD3	1:A:226:SER:O	2.11	0.49
1:B:475:HIS:O	1:B:476:SER:HB2	2.11	0.49
1:A:246:ALA:HB3	1:A:249:ALA:HB2	1.94	0.49
1:B:408:TRP:CB	1:B:429:PHE:CE2	2.95	0.49
1:A:191:TYR:HD1	1:A:292:THR:HG21	1.78	0.49
1:A:224:PHE:O	1:A:228:VAL:HG23	2.12	0.49
1:A:82:LEU:CD1	1:A:249:ALA:HB2	2.43	0.49
1:A:31:LEU:HD21	1:A:34:HIS:HA	1.93	0.49
1:A:126:LEU:HA	1:A:259:ARG:HH12	1.74	0.49
1:A:451:CYS:HB3	1:A:561:TYR:HD1	1.78	0.49
1:B:422:ARG:NH2	1:B:528:TRP:HB3	2.28	0.49
1:B:264:GLY:HA2	1:B:276:TYR:CE1	2.47	0.49
1:A:39:ALA:HB2	1:A:144:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HA	1:A:240:TYR:HD2	1.78	0.48
1:B:390:THR:HB	1:B:391:PRO:HD3	1.95	0.48
1:A:224:PHE:HE2	1:A:291:ASN:HA	1.78	0.48
1:B:377:SER:C	1:B:379:LYS:H	2.17	0.48
1:A:200:ARG:HD3	1:A:384:LEU:HD11	1.95	0.48
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.94	0.48
1:B:237:GLU:OE1	1:B:241:GLN:CG	2.62	0.48
1:A:141:LYS:HG3	1:A:160:ILE:HD11	1.94	0.48
1:A:47:LEU:HB2	1:A:156:PRO:HB3	1.95	0.48
1:A:408:TRP:CB	1:A:429:PHE:CE2	2.96	0.48
1:B:182:LEU:HD21	1:B:293:LEU:HD21	1.95	0.48
1:A:233:ILE:O	1:A:236:GLU:HB2	2.14	0.48
1:A:48:ARG:HA	1:A:51:LYS:HD3	1.95	0.48
1:A:246:ALA:O	1:A:249:ALA:N	2.46	0.48
1:A:455:GLU:O	1:A:458:ASP:HB2	2.13	0.48
1:B:66:ASP:HB3	1:B:304:ARG:HH12	1.78	0.48
1:B:125:ASP:OD1	1:B:259:ARG:NH2	2.43	0.48
1:B:175:LEU:O	1:B:178:VAL:HG12	2.13	0.48
1:A:383:TYR:HE2	1:A:385:THR:HB	1.79	0.48
1:A:398:GLU:OE1	1:A:408:TRP:HD1	1.97	0.48
1:B:230:GLU:HB3	1:B:262:ILE:CG1	2.42	0.48
1:B:419:LEU:HD11	1:B:485:VAL:HG11	1.96	0.48
1:A:80:ALA:HB3	1:A:245:LEU:HD23	1.95	0.48
1:A:303:CYS:SG	1:A:308:LEU:CD1	3.01	0.48
1:A:415:TYR:O	1:A:418:THR:HG23	2.13	0.48
1:A:56:ARG:HE	1:A:229:THR:HG22	1.78	0.47
1:A:296:TYR:O	1:A:300:SER:HB2	2.13	0.47
1:A:191:TYR:CD1	1:A:292:THR:HG21	2.49	0.47
1:B:284:VAL:HG23	1:B:287:THR:HB	1.94	0.47
1:A:243:CYS:O	1:A:245:LEU:HG	2.14	0.47
1:A:85:VAL:HG11	1:A:116:VAL:HG13	1.97	0.47
1:B:47:LEU:HB2	1:B:156:PRO:HB3	1.97	0.47
1:B:56:ARG:HH11	1:B:56:ARG:HG3	1.80	0.47
1:B:339:PHE:O	1:B:343:MET:HG2	2.15	0.47
1:B:126:LEU:HA	1:B:259:ARG:HH11	1.80	0.47
1:B:141:LYS:HG3	1:B:160:ILE:HD11	1.97	0.47
1:B:284:VAL:O	1:B:287:THR:HG22	2.15	0.47
1:A:124:LYS:O	1:A:128:GLU:HG3	2.15	0.46
1:A:398:GLU:OE2	1:A:406:ASN:HA	2.15	0.46
1:B:257:THR:HA	1:B:261:TYR:HB2	1.96	0.46
1:A:383:TYR:CE2	1:A:385:THR:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:PRO:HB2	1:B:167:VAL:CB	2.40	0.46
1:B:233:ILE:O	1:B:236:GLU:HB2	2.15	0.46
1:B:398:GLU:OE2	1:B:406:ASN:HA	2.16	0.46
1:A:422:ARG:NH2	1:A:528:TRP:HB3	2.30	0.46
1:B:176:TYR:HA	1:B:285:LEU:HD21	1.96	0.46
1:B:149:PRO:C	1:B:151:LYS:N	2.67	0.46
1:A:97:ALA:O	1:A:168:ARG:NH2	2.48	0.46
1:A:110:ASN:O	1:A:111:LEU:HB2	2.15	0.46
1:A:141:LYS:HG3	1:A:160:ILE:CD1	2.45	0.46
1:A:31:LEU:HD22	1:A:37:VAL:HG21	1.98	0.46
1:B:192:GLY:HA3	1:B:316:ASN:OD1	2.15	0.46
1:A:94:PRO:HG3	1:A:109:ARG:NH1	2.31	0.46
1:A:506:SER:O	1:A:510:ARG:HG3	2.16	0.46
1:A:78:VAL:HB	1:A:243:CYS:SG	2.56	0.45
1:B:303:CYS:SG	1:B:308:LEU:CD1	3.02	0.45
1:A:94:PRO:HG3	1:A:109:ARG:HH11	1.81	0.45
1:B:84:SER:OG	1:B:87:GLU:HG3	2.16	0.45
1:B:237:GLU:CG	1:B:257:THR:HG21	2.45	0.45
1:A:56:ARG:HD3	1:A:227:THR:HA	1.97	0.45
1:A:377:SER:C	1:A:379:LYS:H	2.19	0.45
1:A:366:CYS:C	1:A:368:SER:H	2.20	0.45
1:A:377:SER:CB	1:A:379:LYS:HG3	2.36	0.45
1:A:489:LEU:HD22	1:A:494:VAL:HG21	1.97	0.45
1:A:499:VAL:CG1	1:A:503:ARG:HE	2.29	0.45
1:B:39:ALA:HA	1:B:143:GLU:O	2.16	0.45
1:A:245:LEU:HD12	1:A:250:ARG:HG2	1.99	0.45
1:A:263:GLY:HA2	1:A:277:ARG:CZ	2.47	0.45
1:B:75:ALA:C	1:B:77:THR:H	2.20	0.45
1:B:165:LEU:O	1:B:169:VAL:HG23	2.17	0.45
1:A:126:LEU:HA	1:A:259:ARG:HH11	1.78	0.45
1:B:78:VAL:HB	1:B:243:CYS:SG	2.57	0.45
1:B:108:VAL:CG2	1:B:165:LEU:HD21	2.46	0.45
1:B:469:LEU:HD11	1:B:538:PRO:CA	2.46	0.45
1:A:292:THR:HG23	1:A:315:VAL:HG12	1.97	0.45
1:A:313:MET:HB2	1:A:313:MET:HE3	1.82	0.45
1:A:56:ARG:NH2	1:A:278:ARG:O	2.49	0.45
1:A:70:GLU:O	1:A:73:ALA:HB3	2.17	0.44
1:A:141:LYS:HE3	1:A:158:ARG:HB2	1.99	0.44
1:A:221:THR:OG1	1:A:224:PHE:HD1	1.75	0.44
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.52	0.44
1:B:175:LEU:O	1:B:179:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:O	1:B:249:ALA:N	2.48	0.44
1:A:176:TYR:HA	1:A:285:LEU:HD21	1.99	0.44
1:B:465:ARG:NH1	1:B:543:SER:HA	2.32	0.44
1:A:92:THR:HA	1:A:93:PRO:HD3	1.80	0.44
1:B:125:ASP:OD1	1:B:125:ASP:C	2.56	0.44
1:B:313:MET:HB2	1:B:313:MET:HE3	1.68	0.44
1:A:303:CYS:SG	1:A:308:LEU:CG	3.05	0.44
1:B:419:LEU:C	1:B:419:LEU:HD12	2.38	0.44
1:A:36:MET:O	1:A:146:CYS:HA	2.17	0.44
1:A:175:LEU:HD13	1:A:286:THR:HG21	1.94	0.44
1:A:182:LEU:O	1:A:185:VAL:N	2.47	0.44
1:A:421:ALA:O	1:A:426:MET:HG3	2.18	0.44
1:A:457:LEU:HB3	1:A:517:ARG:HB3	2.00	0.44
1:B:56:ARG:HD2	1:B:229:THR:HG22	2.00	0.44
1:A:224:PHE:CB	1:A:318:ASP:CB	2.96	0.44
1:B:155:LYS:HA	1:B:156:PRO:HD3	1.82	0.44
1:B:163:PRO:HB3	1:B:167:VAL:HG21	1.99	0.44
1:B:179:VAL:HG12	1:B:289:CYS:CB	2.47	0.44
1:B:383:TYR:CE2	1:B:385:THR:HB	2.53	0.44
1:B:55:ASP:OD1	1:B:56:ARG:N	2.51	0.44
1:B:224:PHE:CB	1:B:318:ASP:HB3	2.48	0.44
1:A:163:PRO:CB	1:A:167:VAL:HB	2.42	0.44
1:B:179:VAL:HG12	1:B:289:CYS:HB2	2.00	0.44
1:B:261:TYR:HE1	1:B:284:VAL:CG1	2.31	0.44
1:B:255:SER:O	1:B:259:ARG:HG3	2.18	0.43
1:A:182:LEU:HB3	1:A:183:PRO:CD	2.47	0.43
1:B:45:ALA:O	1:B:49:GLN:HG3	2.18	0.43
1:A:469:LEU:HD11	1:A:538:PRO:HA	2.00	0.43
1:B:406:ASN:HD22	1:B:406:ASN:H	1.66	0.43
1:A:518:ALA:O	1:A:521:CYS:HB2	2.19	0.43
1:B:183:PRO:HB3	1:B:187:MET:CE	2.48	0.43
1:B:433:LEU:HB3	1:B:439:LEU:HD23	1.99	0.43
1:A:408:TRP:HB2	1:A:429:PHE:CD2	2.54	0.43
1:B:542:ALA:O	1:B:543:SER:HB2	2.18	0.43
1:A:31:LEU:CD2	1:A:34:HIS:HA	2.49	0.43
1:A:439:LEU:HB3	1:A:457:LEU:HD21	2.01	0.43
1:A:56:ARG:HH21	1:A:229:THR:HA	1.83	0.43
1:A:478:SER:O	1:A:482:ILE:HG13	2.18	0.43
1:B:282:SER:O	1:B:287:THR:HG21	2.19	0.43
1:A:469:LEU:HD23	1:A:469:LEU:HA	1.88	0.43
1:B:141:LYS:HG3	1:B:160:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:PHE:CB	1:B:318:ASP:CB	2.97	0.43
1:B:408:TRP:HB2	1:B:429:PHE:CD2	2.53	0.43
1:A:267:THR:HG22	1:A:268:ASN:O	2.19	0.42
1:B:366:CYS:C	1:B:368:SER:H	2.21	0.42
1:A:419:LEU:C	1:A:419:LEU:HD12	2.39	0.42
1:B:126:LEU:HA	1:B:259:ARG:HH12	1.82	0.42
1:B:359:ASP:HB3	1:B:362:LEU:HD22	2.00	0.42
1:B:499:VAL:HG12	1:B:503:ARG:NE	2.34	0.42
1:A:71:MET:HE1	1:A:297:LEU:HB2	2.00	0.42
1:B:32:ARG:O	1:B:34:HIS:N	2.48	0.42
1:A:164:ASP:O	1:A:167:VAL:N	2.53	0.42
1:A:308:LEU:HD11	1:A:311:CYS:SG	2.59	0.42
1:A:155:LYS:HA	1:A:156:PRO:HD3	1.83	0.42
1:B:66:ASP:HB3	1:B:304:ARG:NH1	2.34	0.42
1:B:134:ILE:HG22	1:B:135:ASP:N	2.35	0.42
1:B:56:ARG:HE	1:B:229:THR:HG22	1.85	0.42
1:B:178:VAL:CG1	1:B:179:VAL:N	2.82	0.42
1:B:495:PRO:HA	1:B:496:PRO:HD3	1.90	0.42
1:A:39:ALA:HA	1:A:143:GLU:O	2.20	0.42
1:A:183:PRO:HB3	1:A:187:MET:CE	2.50	0.42
1:B:190:SER:HA	1:B:313:MET:O	2.19	0.42
1:B:315:VAL:HG22	1:B:320:LEU:CD1	2.50	0.42
1:A:390:THR:HB	1:A:391:PRO:HD3	2.02	0.42
1:A:237:GLU:OE1	1:A:241:GLN:CG	2.68	0.41
1:B:197:PRO:O	1:B:201:VAL:HG23	2.20	0.41
1:B:313:MET:HG2	1:B:322:VAL:HG22	2.02	0.41
1:A:148:GLN:HG3	1:A:153:GLY:O	2.20	0.41
1:B:196:SER:HA	1:B:551:PHE:CD1	2.55	0.41
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.90	0.41
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.82	0.41
1:A:224:PHE:CZ	1:A:295:CYS:HB2	2.56	0.41
1:A:45:ALA:O	1:A:49:GLN:HG3	2.21	0.41
1:B:237:GLU:HG2	1:B:257:THR:OG1	2.20	0.41
1:A:125:ASP:C	1:A:125:ASP:OD1	2.59	0.41
1:A:539:ILE:HG23	1:A:540:PRO:HD2	2.01	0.41
1:B:172:LYS:HE2	1:B:559:ASP:O	2.20	0.41
1:A:104:GLY:O	1:A:108:VAL:HG23	2.21	0.41
1:A:146:CYS:SG	1:A:492:LEU:HD21	2.60	0.41
1:A:164:ASP:O	1:A:165:LEU:C	2.57	0.41
1:B:221:THR:OG1	1:B:224:PHE:CD1	2.69	0.41
1:B:456:PRO:C	1:B:458:ASP:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:GLU:OE2	1:A:362:LEU:HD23	2.21	0.41
1:B:36:MET:O	1:B:146:CYS:HA	2.21	0.41
1:B:64:TYR:C	1:B:64:TYR:CD2	2.94	0.41
1:B:374:HIS:CE1	1:B:380:ARG:HG3	2.56	0.41
1:A:82:LEU:HA	1:A:82:LEU:HD12	1.86	0.41
1:A:172:LYS:HA	1:A:176:TYR:HB2	2.02	0.41
1:B:61:ASP:C	1:B:63:HIS:N	2.73	0.41
1:B:237:GLU:HA	1:B:240:TYR:HD2	1.84	0.41
1:B:451:CYS:HB3	1:B:561:TYR:HD1	1.85	0.41
1:B:455:GLU:O	1:B:458:ASP:HB2	2.21	0.41
1:B:56:ARG:HG3	1:B:56:ARG:NH1	2.35	0.40
1:A:508:ARG:O	1:A:512:LEU:HG	2.21	0.40
1:B:71:MET:HE2	1:B:297:LEU:CB	2.46	0.40
1:B:277:ARG:CZ	1:B:281:ALA:HB2	2.52	0.40
1:B:148:GLN:HG3	1:B:153:GLY:O	2.22	0.40
1:B:311:CYS:HA	1:B:324:CYS:HB3	2.03	0.40
1:A:375:ASP:OD1	1:A:377:SER:N	2.47	0.40
1:B:228:VAL:HG21	1:B:280:ARG:HB2	2.01	0.40
1:A:521:CYS:O	1:A:525:LEU:HB2	2.22	0.40
1:B:110:ASN:O	1:B:111:LEU:HB2	2.21	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	509/578 (88%)	466 (92%)	41 (8%)	2 (0%)	34	66
1	B	515/578 (89%)	464 (90%)	46 (9%)	5 (1%)	15	45
All	All	1024/1156 (89%)	930 (91%)	87 (8%)	7 (1%)	22	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	98	LYS
1	A	165	LEU
1	B	34	HIS
1	B	33	HIS
1	A	271	GLY
1	B	457	LEU
1	B	271	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	443/492 (90%)	420 (95%)	23 (5%)	23 55
1	B	444/492 (90%)	424 (96%)	20 (4%)	27 61
All	All	887/984 (90%)	844 (95%)	43 (5%)	25 58

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	64	TYR
1	A	76	SER
1	A	77	THR
1	A	82	LEU
1	A	112	SER
1	A	125	ASP
1	A	138	ILE
1	A	185	VAL
1	A	242	CYS
1	A	247	PRO
1	A	262	ILE
1	A	300	SER
1	A	303	CYS
1	A	316	ASN
1	A	350	PRO
1	A	362	LEU

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Mol	Chain	Res	Type
1	A	425	LEU
1	A	431	SER
1	A	433	LEU
1	A	451	CYS
1	A	456	PRO
1	A	556	SER
1	B	64	TYR
1	B	77	THR
1	B	82	LEU
1	B	112	SER
1	B	125	ASP
1	B	138	ILE
1	B	178	VAL
1	B	233	ILE
1	B	242	CYS
1	B	247	PRO
1	B	262	ILE
1	B	284	VAL
1	B	300	SER
1	B	303	CYS
1	B	316	ASN
1	B	350	PRO
1	B	425	LEU
1	B	431	SER
1	B	451	CYS
1	B	556	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
1	A	241	GLN
1	B	194	GLN

5.3.3 RNA

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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	452	A	579	-	26,26,26	2.28	12 (46%)	35,36,36	1.28	4 (11%)
2	452	B	579	-	26,26,26	2.40	12 (46%)	35,36,36	1.31	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	452	A	579	-	-	0/17/17/17	0/2/2/2
2	452	B	579	-	-	0/17/17/17	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	579	452	C7-C8	4.78	1.47	1.39
2	A	579	452	C7-C8	4.18	1.46	1.39
2	B	579	452	C3-C8	4.15	1.47	1.41
2	A	579	452	C4-C5	4.13	1.44	1.37
2	B	579	452	C4-C3	3.96	1.46	1.39
2	B	579	452	C4-C5	3.70	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	579	452	C16-C11	3.68	1.46	1.41
2	A	579	452	C4-C3	3.65	1.45	1.39
2	B	579	452	C6-C5	3.33	1.43	1.38
2	B	579	452	C16-C11	3.29	1.46	1.41
2	A	579	452	C12-C11	3.29	1.45	1.39
2	A	579	452	C6-C5	3.23	1.43	1.38
2	B	579	452	C12-C11	2.88	1.44	1.39
2	A	579	452	C15-C16	2.86	1.44	1.39
2	B	579	452	C3-C2	2.73	1.54	1.48
2	B	579	452	C15-C16	2.70	1.44	1.39
2	A	579	452	C3-C8	2.70	1.45	1.41
2	B	579	452	C8-N1	2.66	1.44	1.37
2	B	579	452	C9-N1	2.44	1.49	1.45
2	B	579	452	C7-C6	2.41	1.42	1.38
2	A	579	452	C3-C2	2.24	1.53	1.48
2	A	579	452	C10-N2	2.22	1.40	1.35
2	A	579	452	C8-N1	2.19	1.43	1.37
2	A	579	452	C11-N2	2.09	1.45	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	579	452	C9-N1-C8	3.27	128.66	123.98
2	A	579	452	C9-N1-C8	2.99	128.26	123.98
2	B	579	452	F1-C5-C6	2.53	121.31	118.98
2	A	579	452	F1-C5-C6	2.34	121.14	118.98
2	B	579	452	O2-C10-N2	2.21	127.66	123.63
2	A	579	452	C8-C7-C6	2.16	123.50	120.05
2	B	579	452	C8-C7-C6	2.11	123.42	120.05
2	A	579	452	C4-C5-C6	-2.03	119.76	121.72

There are no chirality outliers.

There are no torsion outliers.

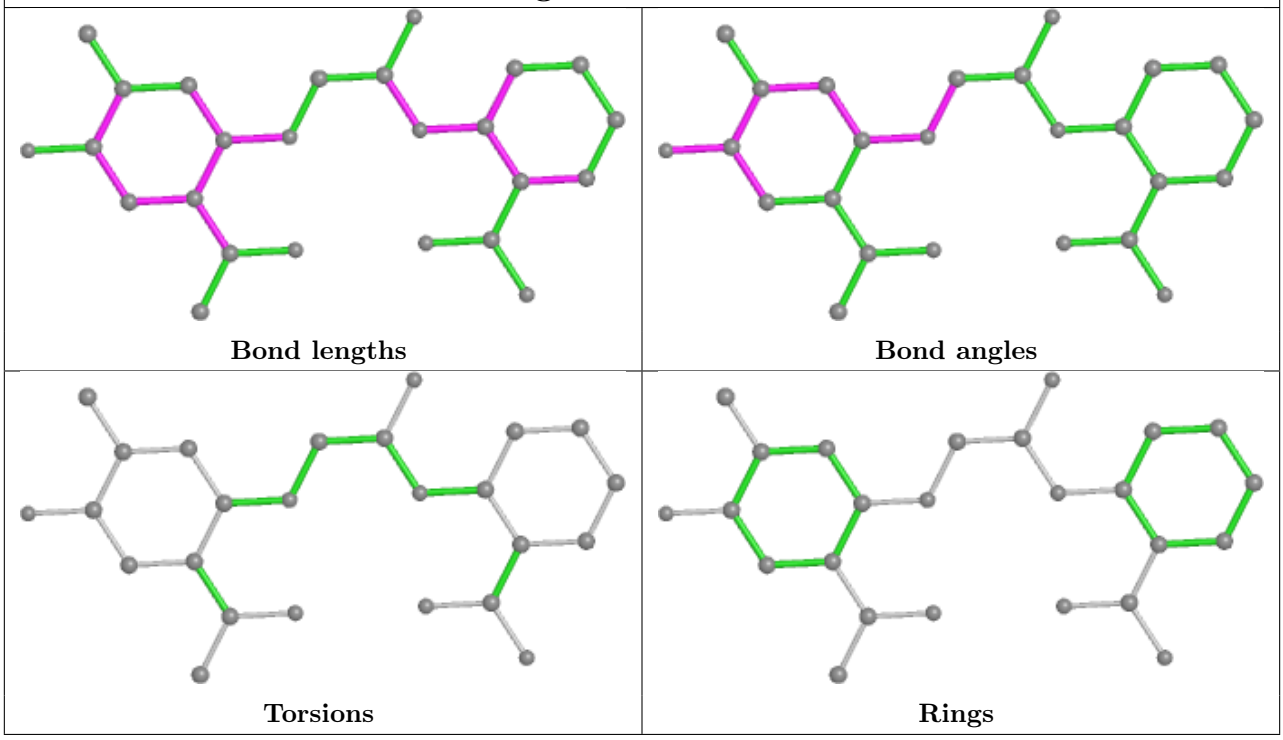
There are no ring outliers.

No monomer is involved in short contacts.

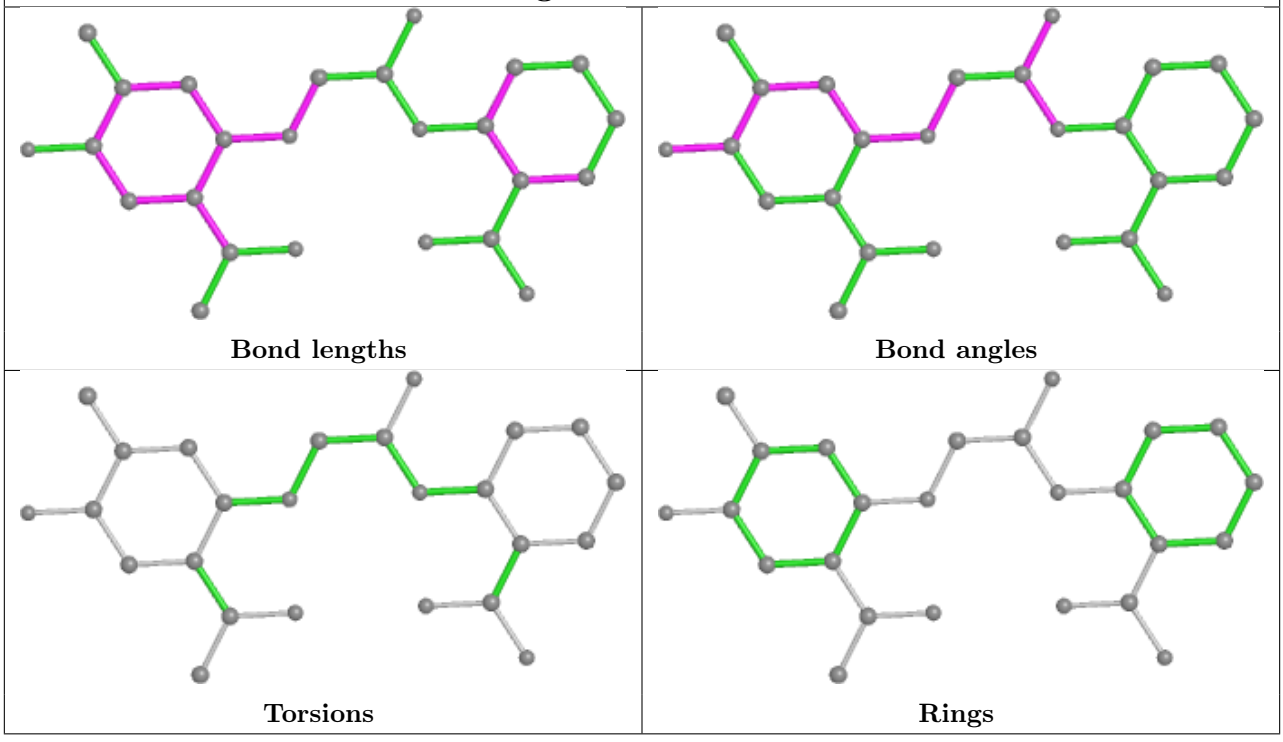
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 452 A 579



Ligand 452 B 579



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	521/578 (90%)	0.00	17 (3%)	46	41	18, 43, 77, 119	0
1	B	523/578 (90%)	0.03	23 (4%)	34	30	19, 43, 79, 115	0
All	All	1044/1156 (90%)	0.01	40 (3%)	40	36	18, 43, 78, 119	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	GLY	9.7
1	A	150	GLU	7.3
1	B	150	GLU	6.4
1	B	149	PRO	5.3
1	B	152	GLY	4.9
1	A	153	GLY	4.2
1	A	261	TYR	3.7
1	A	147	VAL	3.6
1	A	273	ASN	3.5
1	A	138	ILE	3.4
1	A	35	ASN	3.4
1	B	405	VAL	3.3
1	A	148	GLN	3.2
1	B	60	LEU	3.2
1	B	153	GLY	3.1
1	B	35	ASN	3.1
1	B	262	ILE	3.0
1	B	51	LYS	2.8
1	B	286	THR	2.7
1	B	235	VAL	2.7
1	B	80	ALA	2.6
1	A	262	ILE	2.6
1	B	273	ASN	2.6
1	A	70	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	174	ALA	2.5
1	A	154	ARG	2.4
1	B	161	VAL	2.4
1	B	403	THR	2.4
1	A	405	VAL	2.3
1	A	97	ALA	2.3
1	B	134	ILE	2.3
1	B	265	PRO	2.2
1	B	279	CYS	2.2
1	A	239	ILE	2.1
1	A	149	PRO	2.1
1	B	47	LEU	2.1
1	B	148	GLN	2.1
1	B	36	MET	2.0
1	B	59	VAL	2.0
1	A	231	ASN	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)

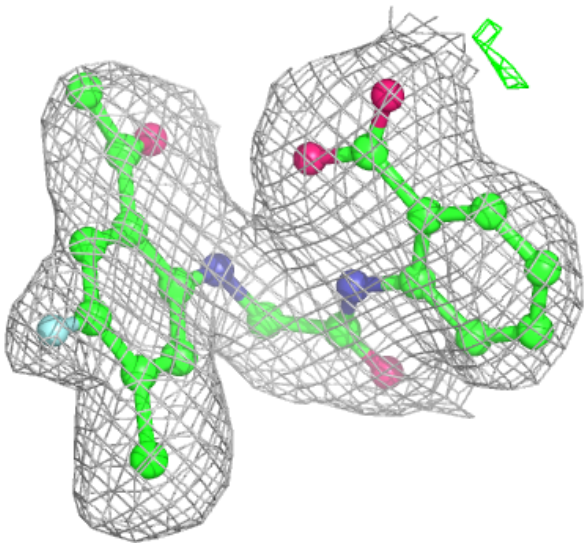
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

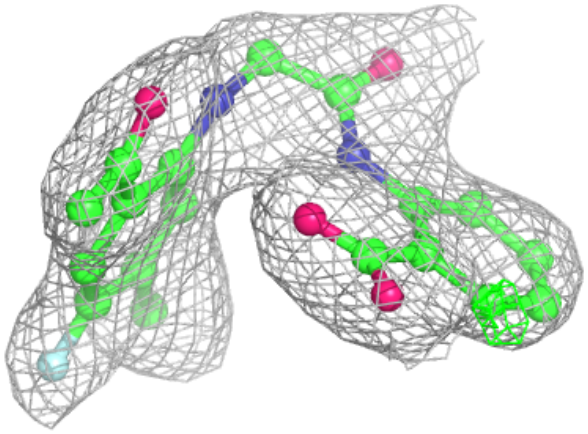
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	452	A	579	25/25	0.93	0.16	22,32,37,42	0
2	452	B	579	25/25	0.93	0.15	22,31,37,39	0

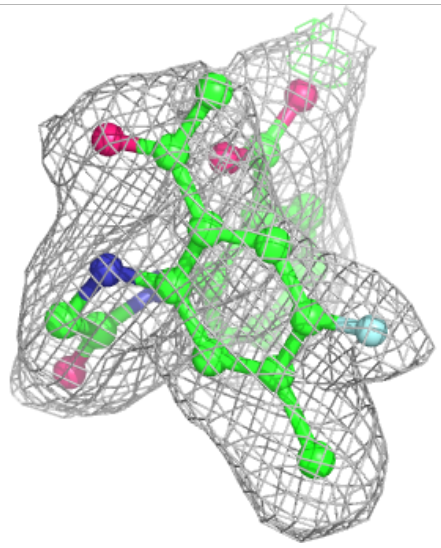
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 452 A 579:

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

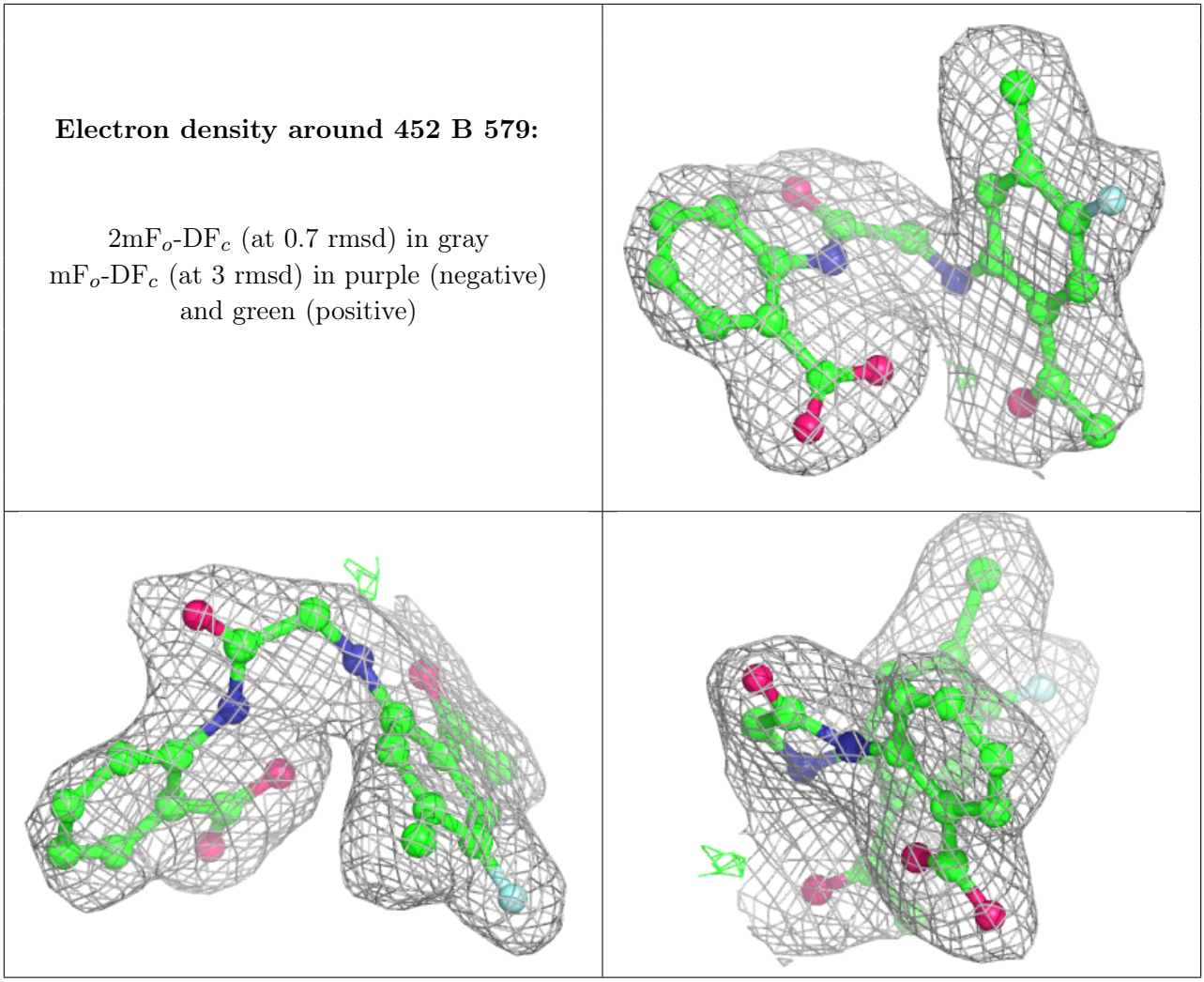






Electron density around 452 B 579:

$2mF_o$-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.