Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 05:06 am GMT

PDB ID	:	2V98
Title	:	Structure of the complex of TcAChE with 1-(2-nitrophenyl)-2,2,2- trifluoro ethyl-arsenocholine after a 9 seconds annealing to room temperature, during the first 5 seconds of which laser irradiation at 266nm took place
Authors	:	Colletier, J.-P.; Sanson, B.; Royant, A.; Specht, A.; Nachon, F.; Masson, P.; Zaccai, G.; Sussman, J.L.; Goeldner, M.; Silman, I.; Bourgeois, D.; Weik, M.
Deposited on	:	2007-08-22
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

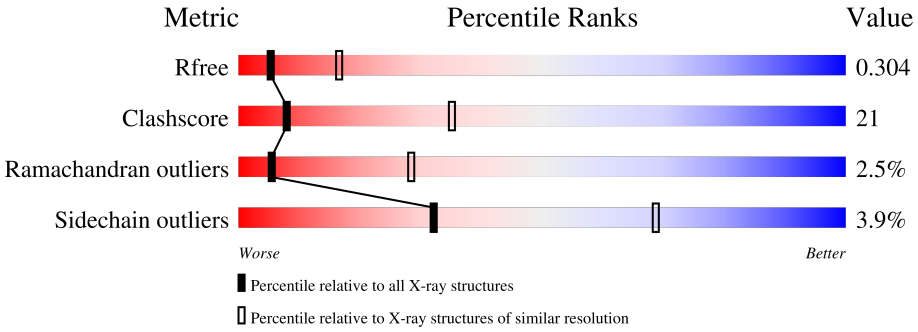
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.00 Å.

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



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

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%

Mol	Chain	Length	Quality of chain
1	A	537	40% 55%
1	B	537	44% 51%

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
2	CL	A	1536[A]	-	-	X	-
2	CL	A	1536[B]	-	-	X	-
3	CFQ	A	1538[A]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CFQ	B	1537[A]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18984 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.

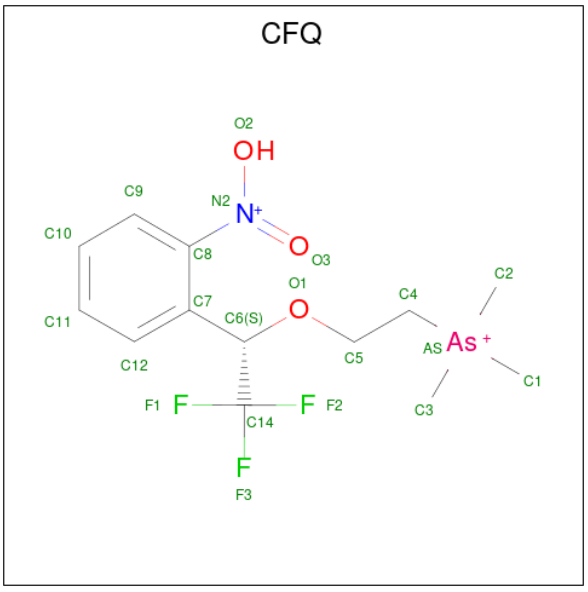
- Molecule 1 is a protein called ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	528	Total	C	N	O	S	0	528	0
			8362	5382	1406	1530	44			
1	B	532	Total	C	N	O	S	0	532	0
			8398	5406	1410	1538	44			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	1
			2	2		

- Molecule 3 is 1-(2-nitrophenyl)-2,2,2-trifluoroethyl]-arsenocholine (three-letter code: CFQ) (formula: $C_{13}H_{19}AsF_3NO_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	As	C	F	N	O	0	1
			42	2	26	6	2	6		

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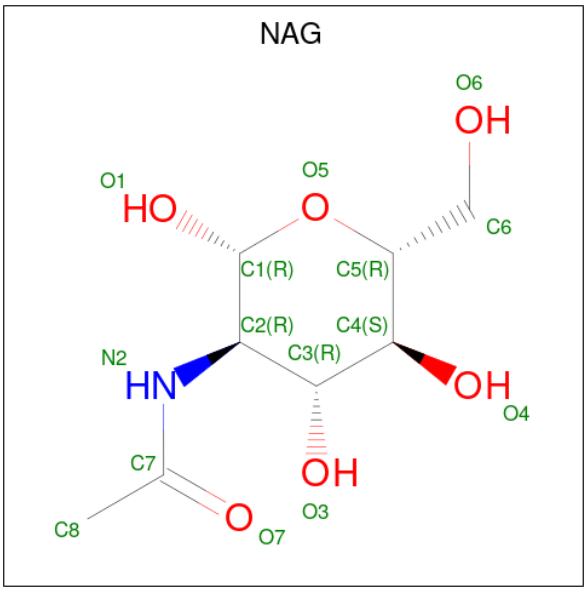
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	As	C	F	N	O	0	1
			42	2	26	6	2	6		
3	B	1	Total	As	C	F	N	O	0	1
			42	2	26	6	2	6		
3	B	1	Total	As	C	F	N	O	0	1
			42	2	26	6	2	6		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			28	16	2	10		
4	A	1	Total	C	N	O	0	1
			28	16	2	10		
4	B	1	Total	C	N	O	0	1
			28	16	2	10		
4	B	1	Total	C	N	O	0	1
			28	16	2	10		

- Molecule 5 is water.

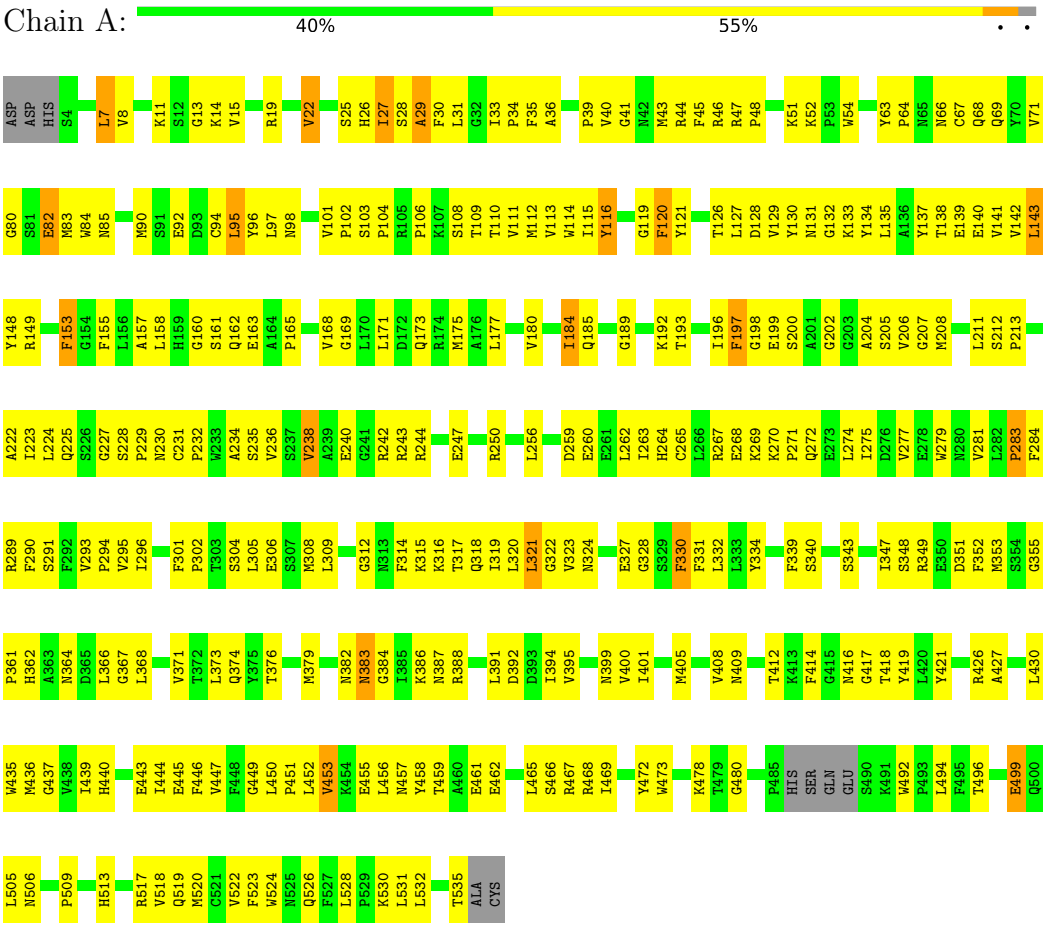
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	925	Total	O	0	814
			925	925		
5	B	1017	Total	O	0	919
			1017	1017		

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. 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. 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.

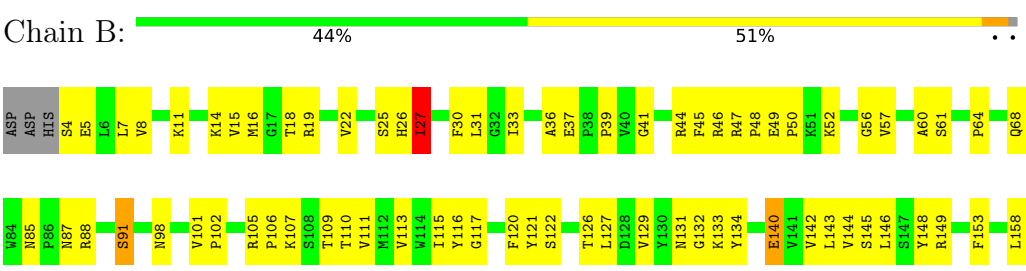
- Molecule 1: ACETYLCHOLINESTERASE

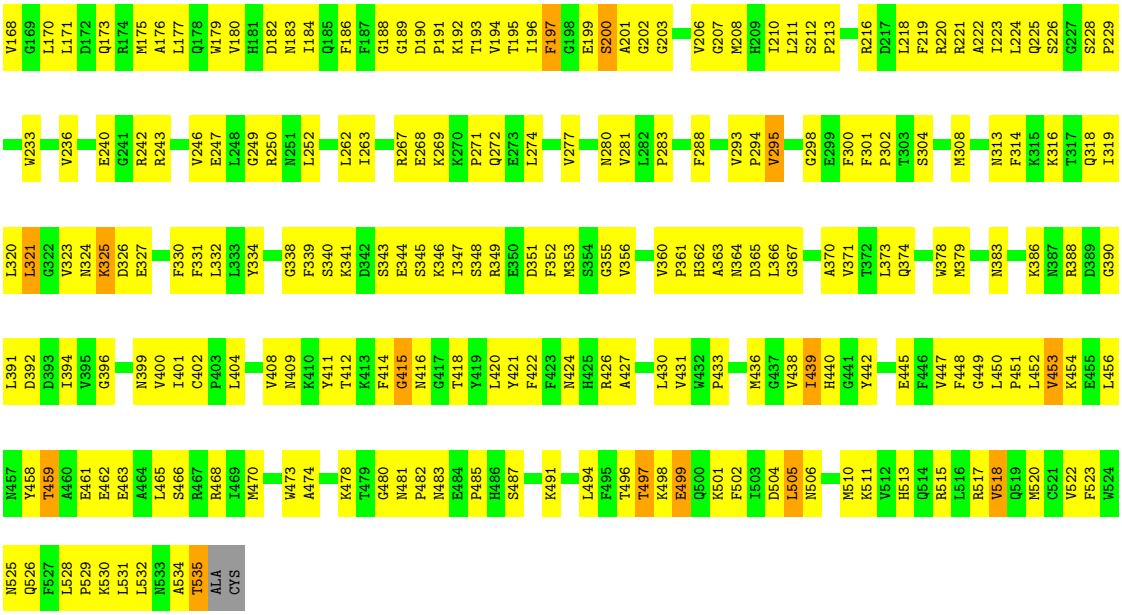
Chain A:



- Molecule 1: ACETYLCHOLINESTERASE

Chain B:




V168 G169 L170 L171 D172 Q173 R174 M175 A176 L177 Q178 W179 V180 H181 D182 N183 I184 Q185 F186 F187 G188 G189 D190 P191 K192 T193 V194 T195 I196 F197 G198 E199 S200 A201 G202 G203 V206 G207 M208 H209 I210 L211 S212 P213 R216 D217 L218 F219 R220 R221 A222 I223 L224 Q225 S226 G227 S228 P229
W233 V236 E240 G241 R242 R243 V246 E247 L248 G249 R250 N251 L252 L262 I263 R267 E268 K269 K270 P271 Q272 E273 L274 V277 N280 V281 L282 P283 F288 V293 P294 V295 G298 E299 F300 F301 P302 T303 S304 M308 N313 F314 K315 K316 T317 Q318 I319
L320 L321 G322 V323 N324 K325 D326 E327 F330 F331 L332 L333 Y334 G338 F339 S340 K341 D342 S343 E344 S345 K346 I347 S348 R349 E350 D351 F352 M353 S354 G355 V356 V360 P361 H362 A363 N364 D365 L366 G367 A370 V371 T372 L373 Q374 W378 M379 N383 K386 N387 R388 D389 G390
L391 D392 D393 I394 V395 G396 N399 V400 I401 C402 P403 L404 V408 N409 K410 Y411 T412 K413 F414 G415 N416 G417 T418 Y419 L420 Y421 F422 F423 N424 H425 R426 A427 L430 V431 W432 P433 M436 G437 V438 I439 H440 G441 Y442 E445 F446 V447 F448 G449 L450 P451 L452 V453 K454 E455 L456
N457 Y458 T459 A460 E461 E462 E463 A464 L465 S466 R467 R468 I469 M470 W473 A474 K478 T479 G480 M481 P482 M483 E484 P485 H486 S487 K491 L494 F495 T496 T497 K498 E499 Q500 K501 F502 I503 D504 L505 N506 M510 K511 V512 H513 Q514 R515 L516 R517 V518 Q519 M520 C521 V522 F523 W524
N525 Q526 F527 L528 P529 K530 L531 L532 N533 A534 T535 ALA CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.62Å 104.47Å 148.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.00 19.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (8.00-3.00) 99.3 (19.85-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.249 0.284 , 0.304	Depositor DCC
R_{free} test set	2672 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	52.7	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 66.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18984	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9698e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CFQ, NAG, CL

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	0.54	0/8604	0.71	2/11686 (0.0%)
1	B	0.54	0/8642	0.73	2/11738 (0.0%)
All	All	0.54	0/17246	0.72	4/23424 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	27[A]	ILE	CB-CA-C	-5.59	100.43	111.60
1	B	27[B]	ILE	CB-CA-C	-5.59	100.43	111.60
1	A	494[A]	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	494[B]	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8362	0	8036	354	0
1	B	8398	0	8068	324	0
2	A	2	0	0	6	0
3	A	84	0	32	31	0
3	B	84	0	32	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	56	0	52	1	0
4	B	56	0	52	0	0
5	A	925	0	0	69	0
5	B	1017	0	0	67	0
All	All	18984	0	16272	715	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 21.

All (715) 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)
3:B:1537[A]:CFQ:C4	3:B:1537[A]:CFQ:AS	2.21	1.49
3:A:1538[A]:CFQ:C4	3:A:1538[A]:CFQ:AS	2.23	1.47
3:B:1537[A]:CFQ:AS	3:B:1537[A]:CFQ:C1	2.23	1.47
3:B:1537[A]:CFQ:AS	3:B:1537[A]:CFQ:C2	2.23	1.46
3:A:1537[A]:CFQ:AS	3:A:1537[A]:CFQ:C4	2.24	1.46
3:A:1538[A]:CFQ:AS	3:A:1538[A]:CFQ:C1	2.23	1.46
3:B:1536[B]:CFQ:AS	3:B:1536[B]:CFQ:C1	2.24	1.46
3:B:1536[B]:CFQ:AS	3:B:1536[B]:CFQ:C4	2.24	1.45
3:B:1537[B]:CFQ:C2	3:B:1537[B]:CFQ:AS	2.24	1.45
3:A:1537[B]:CFQ:AS	3:A:1537[B]:CFQ:C3	2.24	1.45
3:A:1538[A]:CFQ:AS	3:A:1538[A]:CFQ:C2	2.24	1.45
3:B:1537[B]:CFQ:AS	3:B:1537[B]:CFQ:C3	2.25	1.45
3:B:1537[B]:CFQ:AS	3:B:1537[B]:CFQ:C4	2.25	1.45
3:A:1537[A]:CFQ:AS	3:A:1537[A]:CFQ:C1	2.24	1.45
3:A:1538[B]:CFQ:C3	3:A:1538[B]:CFQ:AS	2.24	1.45
3:B:1537[A]:CFQ:AS	3:B:1537[A]:CFQ:C3	2.25	1.45
3:A:1537[A]:CFQ:AS	3:A:1537[A]:CFQ:C3	2.25	1.45
3:A:1538[A]:CFQ:AS	3:A:1538[A]:CFQ:C3	2.23	1.45
3:A:1538[B]:CFQ:AS	3:A:1538[B]:CFQ:C2	2.25	1.45
3:B:1536[A]:CFQ:AS	3:B:1536[A]:CFQ:C4	2.24	1.45
3:A:1537[B]:CFQ:AS	3:A:1537[B]:CFQ:C1	2.24	1.44
3:B:1536[A]:CFQ:AS	3:B:1536[A]:CFQ:C2	2.25	1.44
3:B:1536[B]:CFQ:AS	3:B:1536[B]:CFQ:C2	2.25	1.44
3:B:1537[B]:CFQ:AS	3:B:1537[B]:CFQ:C1	2.24	1.44
3:B:1536[A]:CFQ:AS	3:B:1536[A]:CFQ:C1	2.25	1.44
3:B:1536[B]:CFQ:AS	3:B:1536[B]:CFQ:C3	2.25	1.44
3:A:1537[B]:CFQ:AS	3:A:1537[B]:CFQ:C2	2.25	1.44
3:A:1537[B]:CFQ:AS	3:A:1537[B]:CFQ:C4	2.24	1.44
3:A:1538[B]:CFQ:AS	3:A:1538[B]:CFQ:C1	2.25	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1538[B]:CFQ:AS	3:A:1538[B]:CFQ:C4	2.24	1.43
3:A:1537[A]:CFQ:AS	3:A:1537[A]:CFQ:C2	2.25	1.43
3:B:1536[A]:CFQ:AS	3:B:1536[A]:CFQ:C3	2.26	1.43
1:A:334[A]:TYR:CG	3:A:1538[A]:CFQ:H10	2.05	0.91
1:B:194[A]:VAL:HG12	5:B:2433[A]:HOH:O	1.71	0.91
1:B:30[B]:PHE:HA	1:B:60[B]:ALA:HB1	1.52	0.90
1:A:499[A]:GLU:HG2	1:A:501[A]:LYS:HE3	1.56	0.88
1:A:135[A]:LEU:HB3	5:A:2305[A]:HOH:O	1.74	0.86
1:A:102[B]:PRO:HG2	1:A:106[B]:PRO:HD3	1.58	0.85
1:B:194[B]:VAL:HG12	5:B:2432[B]:HOH:O	1.79	0.83
1:A:208[A]:MET:SD	5:A:2394[A]:HOH:O	2.38	0.82
1:B:140[A]:GLU:HG2	5:B:2373[A]:HOH:O	1.80	0.80
1:B:316[B]:LYS:HE3	1:B:414[B]:PHE:HB3	1.64	0.80
1:A:213[B]:PRO:HA	1:A:216[B]:ARG:HD3	1.63	0.78
1:B:221[B]:ARG:HD3	1:B:480[B]:GLY:HA2	1.65	0.78
1:B:194[A]:VAL:HG13	1:B:219[A]:PHE:HA	1.65	0.78
1:B:31[B]:LEU:HD23	1:B:98[B]:ASN:HB3	1.67	0.77
1:B:158[B]:LEU:HD12	1:B:263[B]:ILE:HD11	1.68	0.76
1:B:334[A]:TYR:CG	3:B:1537[A]:CFQ:H10	2.21	0.76
1:B:325[B]:LYS:HB3	1:B:438[B]:VAL:HB	1.68	0.75
1:B:268[A]:GLU:HG3	5:B:2521[A]:HOH:O	1.86	0.75
1:B:331[A]:PHE:HA	3:B:1537[A]:CFQ:H11	1.68	0.75
1:A:427[B]:ALA:HB3	1:A:430[B]:LEU:HG	1.67	0.75
1:B:82[A]:GLU:HG3	1:B:85[A]:ASN:HD22	1.51	0.75
1:A:227[A]:GLY:HA2	5:A:2421[A]:HOH:O	1.88	0.73
1:A:204[A]:ALA:C	5:A:2394[A]:HOH:O	2.26	0.73
1:A:39[B]:PRO:HD3	1:A:95[B]:LEU:HD12	1.71	0.72
1:B:252[B]:LEU:HD13	1:B:269[B]:LYS:HE3	1.70	0.72
1:B:391[A]:LEU:HA	1:B:394[A]:ILE:HD12	1.71	0.72
1:A:27[B]:ILE:HG13	1:A:28[B]:SER:H	1.55	0.72
1:A:430[A]:LEU:HD11	5:A:2734[A]:HOH:O	1.87	0.71
1:B:22[B]:VAL:HB	1:B:133[B]:LYS:HD2	1.72	0.71
1:A:207[A]:GLY:HA3	1:A:229[A]:PRO:HD3	1.72	0.71
1:B:332[B]:LEU:HD11	1:B:392[B]:ASP:HA	1.73	0.71
1:B:197[B]:PHE:HB3	1:B:223[B]:ILE:HB	1.74	0.70
1:B:263[B]:ILE:HG22	1:B:267[B]:ARG:HH12	1.57	0.69
1:A:366[B]:LEU:HD21	1:B:531[B]:LEU:HA	1.72	0.69
1:B:347[B]:ILE:HG23	1:B:351[B]:ASP:HB2	1.75	0.69
1:A:405[B]:MET:HA	1:A:408[B]:VAL:HG12	1.75	0.68
1:B:236[B]:VAL:HG23	1:B:295[B]:VAL:HG12	1.75	0.68
1:A:236[B]:VAL:HG23	1:A:295[B]:VAL:HG12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242[A]:ARG:HD3	5:B:2501[A]:HOH:O	1.93	0.68
1:A:28[B]:SER:HB2	1:A:101[B]:VAL:H	1.59	0.68
1:B:212[B]:SER:O	1:B:216[B]:ARG:HG3	1.93	0.68
1:B:374[A]:GLN:NE2	5:B:2688[A]:HOH:O	2.20	0.68
1:B:491[A]:LYS:HE3	5:B:2860[A]:HOH:O	1.93	0.68
1:B:107[A]:LYS:HE2	5:B:2318[A]:HOH:O	1.94	0.67
1:B:426[B]:ARG:HH21	1:B:430[B]:LEU:HD23	1.59	0.67
1:B:452[B]:LEU:HA	1:B:463[B]:GLU:HG3	1.75	0.67
1:B:182[A]:ASP:OD1	5:B:2411[A]:HOH:O	2.12	0.67
1:B:228[A]:SER:HB2	1:B:229[A]:PRO:HD2	1.74	0.67
1:B:323[B]:VAL:HG11	1:B:401[B]:ILE:HA	1.76	0.67
1:B:353[B]:MET:O	1:B:356[B]:VAL:HG22	1.94	0.67
1:A:391[B]:LEU:HD12	1:A:394[B]:ILE:HD12	1.77	0.67
1:A:439[A]:ILE:HG23	5:A:2739[A]:HOH:O	1.95	0.67
1:B:340[B]:SER:HB3	1:B:343[B]:SER:OG	1.95	0.66
1:A:162[A]:GLN:OE1	5:A:2341[A]:HOH:O	2.12	0.66
1:B:535[A]:THR:HG21	5:B:2990[A]:HOH:O	1.95	0.66
1:A:163[A]:GLU:HG3	2:A:1536[A]:CL:CL	2.32	0.66
1:A:204[A]:ALA:O	5:A:2394[A]:HOH:O	2.13	0.66
1:B:107[A]:LYS:HE2	5:B:2317:HOH:O	1.96	0.66
1:A:349[B]:ARG:HH22	1:A:376[B]:THR:HG21	1.60	0.65
1:B:183[B]:ASN:HD22	1:B:183[B]:ASN:N	1.93	0.65
1:B:110[B]:THR:HG21	1:B:478[B]:LYS:HA	1.78	0.65
1:B:111[B]:VAL:HB	1:B:194[B]:VAL:HG23	1.78	0.65
1:B:364[B]:ASN:ND2	1:B:366[B]:LEU:HB3	2.11	0.65
1:A:144[B]:VAL:HG12	1:A:145[B]:SER:H	1.62	0.65
1:A:260[A]:GLU:OE2	1:A:264[A]:HIS:NE2	2.26	0.65
1:B:396[A]:GLY:HA3	5:B:2718[A]:HOH:O	1.95	0.65
1:A:129[A]:VAL:HG12	1:A:450[A]:LEU:HD11	1.78	0.65
1:A:196[B]:ILE:HG13	1:A:206[B]:VAL:HG13	1.79	0.65
1:B:211[B]:LEU:HD23	1:B:314[B]:PHE:HB3	1.79	0.65
1:B:263[B]:ILE:HG22	1:B:267[B]:ARG:NH1	2.11	0.65
1:A:355[A]:GLY:HA3	1:A:391[A]:LEU:HD21	1.78	0.64
1:A:247[B]:GLU:HG2	1:A:281[B]:VAL:HA	1.79	0.64
1:B:223[A]:ILE:HG21	5:B:2463[A]:HOH:O	1.97	0.64
1:B:431[A]:VAL:HG22	5:B:2780[A]:HOH:O	1.97	0.64
5:A:2510[B]:HOH:O	1:B:107[B]:LYS:HB3	1.97	0.63
1:A:465[B]:LEU:O	1:A:469[B]:ILE:HG13	1.98	0.63
1:A:399[A]:ASN:ND2	5:A:2685[A]:HOH:O	2.13	0.63
1:A:115[A]:ILE:HG12	1:A:146[A]:LEU:HD11	1.80	0.63
1:B:212[A]:SER:O	1:B:216[A]:ARG:HG3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499[A]:GLU:HB3	5:B:2891[A]:HOH:O	1.97	0.63
1:A:395[A]:VAL:N	5:A:2675[A]:HOH:O	2.31	0.63
1:B:450[B]:LEU:O	1:B:453[B]:VAL:HG12	1.98	0.63
1:A:207[B]:GLY:HA3	1:A:229[B]:PRO:HD3	1.81	0.62
1:B:355[A]:GLY:HA3	1:B:391[A]:LEU:HD21	1.81	0.62
1:A:518[B]:VAL:HG12	1:B:379[B]:MET:SD	2.40	0.62
1:B:391[B]:LEU:HA	1:B:394[B]:ILE:HD12	1.80	0.62
1:A:268[A]:GLU:HG3	5:A:2137[A]:HOH:O	1.99	0.62
1:A:339[B]:PHE:HE1	1:A:388[B]:ARG:HG3	1.64	0.62
1:B:293[A]:VAL:HB	1:B:294[A]:PRO:HD2	1.82	0.62
3:B:1537[A]:CFQ:C1	5:B:2235:HOH:O	2.48	0.62
1:B:168[B]:VAL:HA	1:B:171[B]:LEU:HB2	1.81	0.62
1:B:364[B]:ASN:HD21	1:B:366[B]:LEU:HB3	1.65	0.61
1:B:25[B]:SER:HA	5:B:2104[B]:HOH:O	1.99	0.61
1:A:22[B]:VAL:HB	1:A:133[B]:LYS:HD2	1.81	0.61
1:A:383[B]:ASN:HD22	1:A:386[B]:LYS:HG3	1.64	0.61
1:B:27[A]:ILE:HD11	1:B:133[A]:LYS:HB2	1.82	0.61
1:B:459[B]:THR:OG1	1:B:462[B]:GLU:HG3	1.99	0.61
1:A:35[B]:PHE:O	1:A:175[B]:MET:HE1	2.00	0.61
1:A:212[A]:SER:O	1:A:216[A]:ARG:HG3	2.00	0.61
4:A:1540[B]:NAG:H82	5:A:2703:HOH:O	2.00	0.61
1:B:31[B]:LEU:O	1:B:60[B]:ALA:HA	2.01	0.61
1:B:36[B]:ALA:HB2	1:B:175[B]:MET:HE3	1.83	0.61
1:B:182[B]:ASP:C	1:B:183[B]:ASN:HD22	2.04	0.60
1:B:323[A]:VAL:HG21	1:B:401[A]:ILE:HG12	1.82	0.60
1:A:163[B]:GLU:HG2	2:A:1536[B]:CL:CL	2.37	0.60
1:B:195[B]:THR:HG21	1:B:223[B]:ILE:HG13	1.84	0.60
1:A:408[B]:VAL:HG23	1:A:418[B]:THR:HG21	1.83	0.60
1:A:36[A]:ALA:O	5:A:2078[A]:HOH:O	2.17	0.60
1:B:344[B]:GLU:HB2	5:B:2647[B]:HOH:O	2.02	0.60
1:A:459[B]:THR:HB	1:A:461[B]:GLU:OE2	2.02	0.60
1:B:391[B]:LEU:HD12	1:B:394[B]:ILE:HD12	1.83	0.60
1:A:131[A]:ASN:OD1	1:A:133[A]:LYS:HG2	2.01	0.59
1:A:302[B]:PRO:HD2	1:A:308[B]:MET:HE1	1.83	0.59
5:A:2349[A]:HOH:O	1:B:511[A]:LYS:HD2	2.00	0.59
1:B:7[B]:LEU:HD11	1:B:14[B]:LYS:HB3	1.83	0.59
1:B:110[B]:THR:HG22	1:B:193[B]:THR:HB	1.85	0.59
1:B:68[B]:GLN:HG2	1:B:91[B]:SER:O	2.02	0.59
1:B:101[B]:VAL:HG11	1:B:105[B]:ARG:HG3	1.83	0.59
1:A:135[B]:LEU:HB3	5:A:2306[B]:HOH:O	2.02	0.59
1:A:168[B]:VAL:HG22	5:A:2328:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40[B]:VAL:HG12	1:A:92[B]:GLU:HB3	1.83	0.59
1:A:293[A]:VAL:HB	1:A:294[A]:PRO:HD2	1.83	0.59
1:A:7[B]:LEU:HD11	1:A:14[B]:LYS:HD3	1.85	0.59
1:A:450[B]:LEU:O	1:A:453[B]:VAL:HG12	2.02	0.59
1:A:405[A]:MET:O	1:A:408[A]:VAL:HG12	2.03	0.59
1:A:36[A]:ALA:HB2	1:A:175[A]:MET:CE	2.33	0.59
1:A:27[B]:ILE:HG13	1:A:28[B]:SER:N	2.17	0.59
1:A:450[A]:LEU:N	1:A:451[A]:PRO:CD	2.66	0.59
1:B:247[B]:GLU:HB3	1:B:281[B]:VAL:HG12	1.85	0.59
1:B:323[B]:VAL:HG13	1:B:404[B]:LEU:HD22	1.85	0.59
1:A:29[B]:ALA:O	1:A:31[B]:LEU:HG	2.02	0.58
1:A:340[B]:SER:HB3	1:A:343[B]:SER:OG	2.04	0.58
1:B:183[B]:ASN:N	1:B:183[B]:ASN:ND2	2.51	0.58
1:A:208[A]:MET:HG2	1:A:301[A]:PHE:CZ	2.39	0.58
1:A:202[A]:GLY:O	1:A:206[A]:VAL:HG23	2.04	0.58
1:A:259[B]:ASP:O	1:A:263[B]:ILE:HG13	2.04	0.58
1:B:5[A]:GLU:HB2	5:B:2015[A]:HOH:O	2.03	0.58
1:B:30[A]:PHE:HB3	1:B:33[A]:ILE:HD11	1.86	0.58
1:A:496[B]:THR:HB	5:A:2815:HOH:O	2.04	0.57
1:A:469[B]:ILE:HG12	1:A:505[B]:LEU:HD11	1.86	0.57
1:B:247[B]:GLU:HG2	1:B:281[B]:VAL:HA	1.86	0.57
1:A:143[A]:LEU:HD13	5:A:2305[A]:HOH:O	2.03	0.57
1:B:115[B]:ILE:HG23	1:B:146[B]:LEU:HD11	1.86	0.57
1:B:367[B]:GLY:O	1:B:371[B]:VAL:HG23	2.04	0.57
1:A:206[B]:VAL:HB	1:A:224[B]:LEU:HG	1.85	0.57
3:B:1537[A]:CFQ:AS	3:B:1537[A]:CFQ:C5	3.08	0.57
1:A:331[A]:PHE:HA	3:A:1538[A]:CFQ:H11	1.87	0.57
1:B:510[B]:MET:HG2	1:B:511[B]:LYS:N	2.19	0.57
1:B:431[B]:VAL:HG22	5:B:2779[B]:HOH:O	2.05	0.56
1:A:163[A]:GLU:HB2	1:A:263[A]:ILE:HD13	1.87	0.56
1:A:426[A]:ARG:HG3	1:A:430[A]:LEU:HD12	1.87	0.56
1:A:72[B]:ASP:HB3	1:A:85[B]:ASN:OD1	2.05	0.56
1:A:227[B]:GLY:HA2	5:A:2687:HOH:O	2.04	0.56
1:A:405[A]:MET:HA	1:A:408[A]:VAL:HG12	1.86	0.56
1:B:451[A]:PRO:HA	1:B:458[A]:TYR:CD1	2.40	0.56
1:A:98[A]:ASN:HB2	1:A:145[A]:SER:OG	2.05	0.56
1:A:25[B]:SER:HA	5:A:2069[B]:HOH:O	2.05	0.56
3:A:1537[A]:CFQ:AS	3:A:1537[A]:CFQ:C5	3.11	0.56
1:B:142[B]:VAL:HG11	1:B:184[B]:ILE:HD11	1.87	0.56
1:A:102[A]:PRO:HG2	1:A:106[A]:PRO:HD3	1.88	0.56
1:B:360[B]:VAL:HG12	1:B:363[B]:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518[A]:VAL:HG13	5:B:2944[A]:HOH:O	2.05	0.56
3:A:1538[A]:CFQ:AS	3:A:1538[A]:CFQ:C5	3.11	0.56
1:A:352[A]:PHE:O	1:A:356[A]:VAL:HG13	2.06	0.55
1:A:161[A]:SER:HB2	2:A:1536[A]:CL:CL	2.43	0.55
1:B:374[B]:GLN:HA	1:B:374[B]:GLN:HE21	1.70	0.55
1:A:128[B]:ASP:HB3	5:A:2290[B]:HOH:O	2.06	0.55
1:A:334[A]:TYR:CD1	3:A:1538[A]:CFQ:H10	2.40	0.55
1:A:392[A]:ASP:C	5:A:2675[A]:HOH:O	2.45	0.55
1:B:450[A]:LEU:O	1:B:453[A]:VAL:HG13	2.06	0.55
1:A:119[A]:GLY:O	1:A:120[A]:PHE:HB2	2.05	0.55
1:A:116[A]:TYR:CE1	1:A:148[A]:TYR:CE1	2.94	0.55
1:B:221[A]:ARG:HD3	1:B:480[A]:GLY:HA2	1.87	0.55
1:B:426[B]:ARG:O	1:B:426[B]:ARG:HG3	2.04	0.55
1:A:518[A]:VAL:O	1:A:522[A]:VAL:HG23	2.07	0.55
1:B:468[B]:ARG:HH12	1:B:505[B]:LEU:HG	1.70	0.55
3:B:1536[A]:CFQ:AS	3:B:1536[A]:CFQ:C5	3.12	0.55
1:A:459[B]:THR:OG1	1:A:462[B]:GLU:HG3	2.07	0.55
1:B:184[B]:ILE:HG23	1:B:189[B]:GLY:O	2.07	0.55
1:B:132[B]:GLY:HA3	1:B:143[B]:LEU:HD23	1.89	0.55
1:A:34[B]:PRO:HB3	1:A:96[B]:TYR:CE2	2.42	0.54
1:A:216[A]:ARG:NH1	1:A:314[A]:PHE:HA	2.22	0.54
1:A:240[B]:GLU:O	1:A:244[B]:ARG:HG3	2.06	0.54
1:A:317[B]:THR:HG23	1:A:318[B]:GLN:N	2.23	0.54
1:B:213[A]:PRO:HD2	5:B:2584[A]:HOH:O	2.06	0.54
1:A:44[B]:ARG:HD2	1:A:267[B]:ARG:HA	1.89	0.54
1:B:190[B]:ASP:OD1	1:B:192[B]:LYS:HB2	2.08	0.54
1:B:331[A]:PHE:CE2	3:B:1537[A]:CFQ:H12	2.43	0.54
1:A:155[B]:PHE:CE1	1:A:294[B]:PRO:HG3	2.42	0.54
1:A:364[A]:ASN:HB2	5:A:2617[A]:HOH:O	2.06	0.54
1:A:531[B]:LEU:HD13	1:B:531[B]:LEU:HD13	1.89	0.54
1:B:179[B]:TRP:HA	5:B:2408:HOH:O	2.06	0.54
1:A:502[A]:PHE:CZ	1:A:513[A]:HIS:HB2	2.43	0.54
1:B:246[B]:VAL:O	1:B:250[B]:ARG:HB2	2.08	0.54
1:B:408[B]:VAL:HG23	1:B:418[B]:THR:HG21	1.90	0.53
1:B:504[A]:ASP:HB2	5:B:2921[A]:HOH:O	2.07	0.53
3:B:1536[B]:CFQ:AS	3:B:1536[B]:CFQ:C5	3.15	0.53
1:A:453[B]:VAL:HG13	1:A:453[B]:VAL:O	2.09	0.53
1:B:176[B]:ALA:O	1:B:180[B]:VAL:HG23	2.07	0.53
1:A:69[B]:GLN:O	1:A:275[B]:ILE:HD13	2.07	0.53
1:A:461[B]:GLU:H	1:A:461[B]:GLU:CD	2.11	0.53
1:B:197[A]:PHE:HB3	1:B:223[A]:ILE:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240[A]:GLU:OE2	1:B:243[A]:ARG:NH1	2.41	0.53
1:A:439[B]:ILE:HG22	1:A:440[B]:HIS:N	2.24	0.53
1:B:517[B]:ARG:HH11	1:B:517[B]:ARG:HG2	1.73	0.53
1:A:143[B]:LEU:HD22	5:A:2306[B]:HOH:O	2.08	0.53
1:B:331[A]:PHE:CZ	3:B:1537[A]:CFQ:H12	2.43	0.53
1:A:506[B]:ASN:HB2	5:A:2710[B]:HOH:O	2.07	0.53
1:B:447[A]:VAL:O	1:B:470[A]:MET:HG2	2.09	0.53
1:B:497[B]:THR:HG22	5:B:2730[B]:HOH:O	2.08	0.53
1:A:265[A]:CYS:HB2	5:A:2473[A]:HOH:O	2.08	0.52
1:B:487[B]:SER:HB3	5:B:2883[B]:HOH:O	2.08	0.52
1:A:82[B]:GLU:HA	1:A:85[B]:ASN:ND2	2.24	0.52
1:B:30[B]:PHE:HB3	1:B:33[B]:ILE:HD11	1.90	0.52
1:B:497[A]:THR:HB	5:B:2731[A]:HOH:O	2.09	0.52
1:B:194[A]:VAL:CG1	1:B:219[A]:PHE:HA	2.39	0.52
1:A:306[B]:GLU:HA	1:A:309[B]:LEU:HD12	1.91	0.52
1:A:445[B]:GLU:HG3	1:A:446[B]:PHE:HD1	1.74	0.52
1:B:313[A]:ASN:HB2	5:B:2601[A]:HOH:O	2.08	0.52
1:A:340[A]:SER:HB3	1:A:343[A]:SER:OG	2.10	0.52
1:A:450[A]:LEU:O	1:A:453[A]:VAL:HG13	2.09	0.52
1:B:117[B]:GLY:HA3	1:B:199[B]:GLU:O	2.10	0.52
1:B:453[B]:VAL:HG13	1:B:453[B]:VAL:O	2.10	0.52
1:A:321[B]:LEU:HD23	1:A:321[B]:LEU:H	1.75	0.52
1:B:26[B]:HIS:HB2	5:B:2299:HOH:O	2.10	0.52
1:B:39[B]:PRO:HG3	1:B:149[B]:ARG:HD3	1.92	0.52
1:B:349[B]:ARG:O	1:B:353[B]:MET:HG2	2.09	0.52
1:A:68[B]:GLN:HG3	1:A:271[B]:PRO:HB3	1.92	0.52
1:B:197[A]:PHE:CB	1:B:223[A]:ILE:HB	2.39	0.52
1:B:497[A]:THR:HG23	5:B:2895[A]:HOH:O	2.09	0.52
1:A:119[B]:GLY:C	1:A:121[B]:TYR:H	2.12	0.52
1:A:388[B]:ARG:NH2	1:A:435[B]:TRP:HB2	2.25	0.52
1:A:517[B]:ARG:HG2	1:A:517[B]:ARG:HH11	1.75	0.52
1:A:339[A]:PHE:HE1	1:A:388[A]:ARG:HG3	1.75	0.52
1:B:439[B]:ILE:HG22	1:B:440[B]:HIS:N	2.25	0.52
1:B:46[A]:ARG:HG3	1:B:267[A]:ARG:NH2	2.25	0.51
1:A:39[A]:PRO:HD3	1:A:95[A]:LEU:HD12	1.91	0.51
1:A:196[B]:ILE:HG13	1:A:196[B]:ILE:O	2.09	0.51
1:B:158[B]:LEU:HD23	1:B:242[B]:ARG:HA	1.93	0.51
1:B:318[B]:GLN:HE21	1:B:416[B]:ASN:HB3	1.76	0.51
1:A:43[B]:MET:HE3	5:A:2086[B]:HOH:O	2.10	0.51
1:A:518[B]:VAL:O	1:A:522[B]:VAL:HG23	2.09	0.51
1:A:520[B]:MET:O	1:A:523[B]:PHE:HB3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313[B]:ASN:HB2	5:B:2600[B]:HOH:O	2.10	0.51
1:B:528[B]:LEU:HB3	1:B:529[B]:PRO:HD3	1.93	0.51
1:B:11[B]:LYS:HE2	1:B:186[B]:PHE:HZ	1.76	0.51
1:A:119[B]:GLY:HA2	1:A:290[B]:PHE:CE2	2.45	0.51
1:A:234[B]:ALA:O	1:A:294[B]:PRO:HD2	2.09	0.51
1:A:395[B]:VAL:N	5:A:2676[B]:HOH:O	2.43	0.51
1:A:450[B]:LEU:N	1:A:451[B]:PRO:CD	2.73	0.51
1:B:158[B]:LEU:HD22	1:B:242[B]:ARG:NH2	2.26	0.51
1:B:373[B]:LEU:HD12	1:B:378[B]:TRP:HE1	1.76	0.51
1:A:131[B]:ASN:OD1	1:A:133[B]:LYS:HG2	2.11	0.51
1:A:440[A]:HIS:HD2	3:A:1538[A]:CFQ:H5C2	1.76	0.51
1:A:27[B]:ILE:CG1	1:A:28[B]:SER:H	2.18	0.51
1:B:27[A]:ILE:HG22	1:B:101[A]:VAL:O	2.11	0.51
1:B:263[A]:ILE:O	1:B:267[A]:ARG:HG3	2.11	0.51
1:B:453[A]:VAL:O	1:B:453[A]:VAL:HG22	2.10	0.51
1:A:46[B]:ARG:HG2	1:A:47[B]:ARG:N	2.26	0.51
1:A:161[B]:SER:HB2	2:A:1536[B]:CL:CL	2.48	0.51
1:A:162[B]:GLN:O	1:A:165[B]:PRO:HD3	2.11	0.51
1:A:355[B]:GLY:HA3	1:A:391[B]:LEU:HD21	1.92	0.51
1:A:440[B]:HIS:HD2	3:A:1538[B]:CFQ:H5C2	1.76	0.51
1:B:27[A]:ILE:CD1	1:B:133[A]:LYS:HB2	2.41	0.51
1:B:133[A]:LYS:HE3	1:B:134[A]:TYR:CZ	2.47	0.51
1:B:364[B]:ASN:H	1:B:532[B]:LEU:HD22	1.76	0.51
1:A:224[B]:LEU:N	1:A:224[B]:LEU:HD12	2.26	0.50
1:A:366[A]:LEU:HD23	1:A:535[A]:THR:HG21	1.93	0.50
1:A:36[A]:ALA:CB	1:A:175[A]:MET:CE	2.90	0.50
1:A:199[A]:GLU:HA	1:A:225[A]:GLN:O	2.11	0.50
1:A:453[A]:VAL:HG22	1:A:456[A]:LEU:HG	1.93	0.50
1:A:119[B]:GLY:O	1:A:121[B]:TYR:N	2.42	0.50
1:A:211[A]:LEU:HD23	1:A:314[A]:PHE:HB3	1.92	0.50
1:B:18[B]:THR:OG1	1:B:19[B]:ARG:N	2.44	0.50
1:B:192[B]:LYS:O	1:B:220[B]:ARG:HB2	2.11	0.50
1:B:408[A]:VAL:CG2	1:B:418[A]:THR:HG21	2.42	0.50
1:B:302[A]:PRO:HD2	1:B:308[A]:MET:CE	2.42	0.50
1:B:478[A]:LYS:HD3	5:B:2848[A]:HOH:O	2.11	0.50
1:A:289[B]:ARG:HH21	1:A:362[B]:HIS:HE1	1.58	0.50
1:A:293[A]:VAL:HB	1:A:294[A]:PRO:CD	2.41	0.50
1:B:461[B]:GLU:CD	1:B:461[B]:GLU:H	2.14	0.50
1:A:321[B]:LEU:HD23	1:A:321[B]:LEU:N	2.27	0.50
1:A:353[A]:MET:O	1:A:356[A]:VAL:HG22	2.12	0.50
1:B:121[B]:TYR:CE1	1:B:122[B]:SER:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8[B]:VAL:HG13	5:A:2023[B]:HOH:O	2.11	0.50
1:B:439[A]:ILE:HG22	1:B:440[A]:HIS:N	2.26	0.50
1:A:132[A]:GLY:HA3	1:A:143[A]:LEU:HD22	1.94	0.50
1:A:197[B]:PHE:CB	1:A:223[B]:ILE:HB	2.42	0.50
1:A:305[B]:LEU:O	1:A:309[B]:LEU:HG	2.12	0.50
1:A:30[A]:PHE:HB3	1:A:33[A]:ILE:HD11	1.93	0.49
1:B:30[B]:PHE:CA	1:B:60[B]:ALA:HB1	2.36	0.49
1:B:211[A]:LEU:HD23	1:B:314[A]:PHE:HB3	1.94	0.49
1:B:223[A]:ILE:CG2	5:B:2463[A]:HOH:O	2.55	0.49
1:A:236[A]:VAL:HG23	1:A:295[A]:VAL:HG12	1.93	0.49
1:A:283[B]:PRO:HG2	1:A:284[B]:PHE:H	1.76	0.49
1:A:347[B]:ILE:HG22	1:A:348[B]:SER:O	2.12	0.49
1:B:22[A]:VAL:O	1:B:22[A]:VAL:HG13	2.10	0.49
1:A:304[B]:SER:O	1:A:308[B]:MET:HG3	2.13	0.49
1:A:417[B]:GLY:HA2	5:A:2808[B]:HOH:O	2.13	0.49
1:A:535[B]:THR:HG22	1:B:534[B]:ALA:HB1	1.94	0.49
1:B:36[B]:ALA:HB2	1:B:175[B]:MET:CE	2.42	0.49
1:B:293[A]:VAL:HB	1:B:294[A]:PRO:CD	2.43	0.49
3:A:1537[A]:CFQ:AS	3:A:1537[A]:CFQ:O1	2.91	0.49
1:A:127[A]:LEU:HD12	1:A:130[A]:TYR:CE2	2.47	0.49
1:A:168[A]:VAL:HG22	5:A:2332[A]:HOH:O	2.12	0.49
1:A:197[A]:PHE:CB	1:A:223[A]:ILE:HB	2.42	0.49
1:A:242[A]:ARG:HD3	5:A:2451:HOH:O	2.11	0.49
1:A:247[B]:GLU:HB3	1:A:281[B]:VAL:HG12	1.93	0.49
1:A:316[B]:LYS:HG2	1:A:414[B]:PHE:O	2.13	0.49
1:A:388[B]:ARG:HD2	1:A:435[B]:TRP:CE3	2.47	0.49
1:A:531[B]:LEU:HA	1:B:366[B]:LEU:HD21	1.94	0.49
3:A:1537[A]:CFQ:H5C2	5:A:2524[A]:HOH:O	2.13	0.49
1:B:47[B]:ARG:HG3	5:B:2385[B]:HOH:O	2.12	0.49
1:B:365[B]:ASP:HB3	5:B:2673[B]:HOH:O	2.11	0.49
1:B:421[B]:TYR:HB2	1:B:505[B]:LEU:HD13	1.94	0.49
1:A:332[B]:LEU:HB3	1:A:339[B]:PHE:CD2	2.48	0.49
1:B:450[A]:LEU:N	1:B:451[A]:PRO:CD	2.75	0.49
1:B:518[B]:VAL:HG13	5:B:2943[B]:HOH:O	2.11	0.49
1:A:272[B]:GLN:NE2	1:A:275[B]:ILE:HB	2.27	0.49
1:A:453[B]:VAL:HA	5:A:2750:HOH:O	2.12	0.49
1:A:327[B]:GLU:OE2	1:A:400[B]:VAL:HG11	2.11	0.49
1:A:110[B]:THR:HB	1:A:141[B]:VAL:HG12	1.96	0.48
1:A:137[A]:TYR:HD1	5:A:2312[A]:HOH:O	1.96	0.48
1:A:319[B]:ILE:HG13	1:A:418[B]:THR:HG23	1.94	0.48
1:B:109[B]:THR:HG22	1:B:188[B]:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481[B]:ASN:HD21	1:B:483[B]:ASN:HB2	1.78	0.48
1:A:192[B]:LYS:O	1:A:220[B]:ARG:HB2	2.14	0.48
1:B:27[B]:ILE:HD11	1:B:133[B]:LYS:HB2	1.94	0.48
1:B:196[B]:ILE:HG13	1:B:196[B]:ILE:O	2.13	0.48
1:B:302[B]:PRO:HD2	1:B:308[B]:MET:HE1	1.94	0.48
1:B:433[A]:PRO:HG2	1:B:436[A]:MET:HG3	1.95	0.48
1:A:330[A]:PHE:CD2	3:A:1538[A]:CFQ:H5C1	2.48	0.48
1:B:499[B]:GLU:HB3	1:B:501[B]:LYS:HG3	1.95	0.48
1:A:27[A]:ILE:HG21	1:A:137[A]:TYR:HB2	1.95	0.48
1:A:64[B]:PRO:HG3	1:A:96[B]:TYR:HB2	1.95	0.48
1:B:16[B]:MET:HB2	1:B:57[B]:VAL:CG1	2.44	0.48
1:B:520[B]:MET:O	1:B:523[B]:PHE:HB3	2.14	0.48
1:A:330[B]:PHE:HB2	1:A:439[B]:ILE:CG2	2.43	0.48
1:A:373[B]:LEU:HD21	1:B:523[B]:PHE:HD1	1.78	0.48
1:A:433[B]:PRO:HG2	1:A:436[B]:MET:SD	2.53	0.48
1:A:26[B]:HIS:O	1:A:27[B]:ILE:HG23	2.14	0.48
1:A:97[B]:LEU:O	1:A:97[B]:LEU:HD12	2.12	0.48
1:A:443[B]:GLU:O	1:A:447[B]:VAL:HG23	2.13	0.48
1:B:44[B]:ARG:O	1:B:45[B]:PHE:HB2	2.13	0.48
1:B:325[B]:LYS:HB2	1:B:424[B]:ASN:HA	1.96	0.48
1:B:277[B]:VAL:HA	1:B:280[B]:ASN:ND2	2.29	0.48
1:B:338[A]:GLY:N	5:B:2625[A]:HOH:O	2.47	0.48
1:B:110[B]:THR:CG2	1:B:478[B]:LYS:HG3	2.44	0.48
1:B:225[B]:GLN:HG2	1:B:421[B]:TYR:OH	2.14	0.48
1:B:528[A]:LEU:HB3	1:B:529[A]:PRO:HD3	1.95	0.48
1:A:27[B]:ILE:HD11	1:A:133[B]:LYS:HB3	1.96	0.48
1:A:163[B]:GLU:HB2	1:A:263[B]:ILE:HD13	1.96	0.48
1:B:202[B]:GLY:O	1:B:206[B]:VAL:HG23	2.13	0.48
1:B:339[B]:PHE:HE1	1:B:388[B]:ARG:HG3	1.79	0.48
1:B:433[B]:PRO:HG2	1:B:436[B]:MET:HG3	1.96	0.48
1:A:127[B]:LEU:HD12	1:A:130[B]:TYR:CE2	2.49	0.47
1:A:451[A]:PRO:HA	1:A:458[A]:TYR:CD1	2.48	0.47
1:B:249[B]:GLY:HA3	1:B:262[B]:LEU:HD11	1.95	0.47
1:A:240[A]:GLU:OE2	1:A:243[A]:ARG:NH1	2.46	0.47
1:A:520[A]:MET:O	1:A:523[A]:PHE:HB3	2.15	0.47
1:B:199[B]:GLU:OE2	1:B:226[B]:SER:HB2	2.14	0.47
1:A:453[A]:VAL:HG22	1:A:453[A]:VAL:O	2.15	0.47
3:A:1538[B]:CFQ:AS	3:A:1538[B]:CFQ:C5	3.17	0.47
1:B:474[B]:ALA:HB1	1:B:478[B]:LYS:NZ	2.29	0.47
1:A:27[B]:ILE:HG21	1:A:137[B]:TYR:HB2	1.96	0.47
1:A:277[B]:VAL:HG12	5:B:2321[B]:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110[B]:THR:HG21	1:B:478[B]:LYS:HG3	1.96	0.47
1:B:203[B]:GLY:O	1:B:224[B]:LEU:HD23	2.15	0.47
1:B:448[B]:PHE:O	1:B:450[B]:LEU:HD22	2.13	0.47
1:A:109[B]:THR:OG1	1:A:110[B]:THR:N	2.47	0.47
1:A:270[B]:LYS:HB3	5:A:2495[B]:HOH:O	2.14	0.47
1:B:506[A]:ASN:HB2	5:B:2930[A]:HOH:O	2.15	0.47
1:A:184[A]:ILE:HG23	1:A:189[A]:GLY:O	2.14	0.47
1:A:22[B]:VAL:O	1:A:22[B]:VAL:HG13	2.13	0.47
1:A:408[B]:VAL:HG13	1:A:409[B]:ASN:N	2.29	0.47
1:B:339[A]:PHE:HE1	1:B:388[A]:ARG:HG3	1.80	0.47
1:B:498[B]:LYS:HD3	5:B:2901[B]:HOH:O	2.14	0.47
1:B:502[A]:PHE:CZ	1:B:513[A]:HIS:HB2	2.49	0.47
1:A:27[B]:ILE:HD11	1:A:133[B]:LYS:CB	2.45	0.47
1:A:73[B]:GLU:HA	5:A:2179[B]:HOH:O	2.15	0.47
1:A:94[B]:CYS:O	1:A:96[B]:TYR:N	2.48	0.47
1:A:143[B]:LEU:HG	1:A:144[B]:VAL:N	2.30	0.47
1:A:193[B]:THR:HG23	1:A:221[B]:ARG:HH22	1.80	0.47
1:A:286[B]:SER:OG	1:A:361[B]:PRO:HB3	2.14	0.47
1:B:115[B]:ILE:HD13	1:B:173[B]:GLN:OE1	2.14	0.47
1:B:203[A]:GLY:O	1:B:224[A]:LEU:HD23	2.15	0.47
1:B:321[B]:LEU:HD23	1:B:321[B]:LEU:N	2.29	0.47
1:A:173[B]:GLN:O	1:A:177[B]:LEU:HG	2.15	0.47
1:A:193[B]:THR:HG23	1:A:221[B]:ARG:NH2	2.29	0.47
1:A:315[B]:LYS:HE3	1:A:317[B]:THR:HG21	1.97	0.47
1:A:323[B]:VAL:HG11	1:A:401[B]:ILE:HA	1.97	0.47
1:A:353[B]:MET:HA	1:A:356[B]:VAL:HG22	1.96	0.47
1:A:115[B]:ILE:HG12	1:A:146[B]:LEU:HD11	1.96	0.47
1:A:158[B]:LEU:HD22	1:A:242[B]:ARG:NH2	2.30	0.47
1:A:228[B]:SER:H	1:A:231[B]:CYS:HG	1.62	0.47
1:A:312[A]:GLY:HA2	1:A:314[A]:PHE:CE2	2.50	0.47
1:A:347[A]:ILE:HG22	1:A:348[A]:SER:O	2.15	0.47
1:B:170[B]:LEU:HD23	1:B:173[B]:GLN:NE2	2.30	0.47
1:A:302[B]:PRO:HD2	1:A:308[B]:MET:CE	2.44	0.46
1:A:419[B]:TYR:HB3	1:A:492[B]:TRP:NE1	2.30	0.46
1:B:242[B]:ARG:O	1:B:246[B]:VAL:HG23	2.15	0.46
1:B:272[B]:GLN:HB2	5:B:2535[B]:HOH:O	2.14	0.46
1:B:302[B]:PRO:HD2	1:B:308[B]:MET:CE	2.44	0.46
1:B:325[A]:LYS:HG2	1:B:326[A]:ASP:OD2	2.14	0.46
1:A:94[B]:CYS:O	1:A:96[B]:TYR:HD1	1.98	0.46
1:A:114[A]:TRP:CZ3	1:A:198[A]:GLY:HA2	2.51	0.46
1:B:16[A]:MET:HB2	1:B:57[A]:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16[B]:MET:HB2	1:B:57[B]:VAL:HG12	1.96	0.46
1:B:520[A]:MET:HG2	5:B:2954[A]:HOH:O	2.14	0.46
1:A:66[B]:ASN:O	1:A:90[B]:MET:HA	2.15	0.46
1:A:528[B]:LEU:O	1:A:532[B]:LEU:HG	2.16	0.46
1:B:14[B]:LYS:HB2	1:B:56[B]:GLY:O	2.15	0.46
1:B:224[A]:LEU:N	1:B:224[A]:LEU:HD12	2.30	0.46
1:B:362[B]:HIS:HA	5:B:2666[B]:HOH:O	2.15	0.46
1:B:474[B]:ALA:HB1	1:B:478[B]:LYS:HZ3	1.81	0.46
1:A:68[A]:GLN:NE2	1:A:68[A]:GLN:HA	2.31	0.46
1:A:80[B]:GLY:HA3	1:A:432[B]:TRP:NE1	2.31	0.46
1:B:412[B]:THR:HG23	5:B:2739[B]:HOH:O	2.15	0.46
1:B:510[A]:MET:HG2	1:B:511[A]:LYS:N	2.30	0.46
1:A:383[B]:ASN:ND2	1:A:386[B]:LYS:HG3	2.28	0.46
1:B:48[A]:PRO:HB2	1:B:175[A]:MET:HE1	1.96	0.46
1:B:332[B]:LEU:HB3	1:B:339[B]:PHE:CD2	2.51	0.46
1:A:108[A]:SER:N	5:A:2266[A]:HOH:O	2.47	0.46
1:A:366[A]:LEU:HD23	1:A:531[A]:LEU:HD11	1.98	0.46
1:B:132[A]:GLY:HA3	1:B:143[A]:LEU:HD22	1.97	0.46
1:A:111[B]:VAL:HG22	1:A:142[B]:VAL:HB	1.97	0.46
1:A:445[B]:GLU:HA	1:A:450[B]:LEU:HD12	1.98	0.46
1:A:499[B]:GLU:HB2	5:A:2806:HOH:O	2.16	0.46
1:B:427[B]:ALA:O	1:B:430[B]:LEU:HB2	2.16	0.46
1:B:465[B]:LEU:CD1	1:B:468[B]:ARG:HH11	2.29	0.46
1:A:317[B]:THR:HG23	1:A:318[B]:GLN:H	1.78	0.45
1:A:405[B]:MET:HA	1:A:408[B]:VAL:CG1	2.42	0.45
1:B:426[B]:ARG:HA	5:B:2766[B]:HOH:O	2.16	0.45
1:A:83[B]:MET:HG3	1:A:84[B]:TRP:CE3	2.51	0.45
1:A:221[A]:ARG:HD3	1:A:480[A]:GLY:HA2	1.98	0.45
1:A:412[B]:THR:HG23	5:A:2693[B]:HOH:O	2.16	0.45
1:B:132[A]:GLY:HA3	1:B:143[A]:LEU:CD2	2.46	0.45
1:B:298[B]:GLY:HA2	1:B:302[B]:PRO:O	2.16	0.45
1:A:208[A]:MET:HG3	5:A:2394[A]:HOH:O	2.16	0.45
3:B:1537[B]:CFQ:AS	3:B:1537[B]:CFQ:C5	3.19	0.45
1:B:49[B]:GLU:HG3	1:B:50[B]:PRO:HD2	1.99	0.45
1:A:163[A]:GLU:CG	2:A:1536[A]:CL:CL	3.00	0.45
1:A:444[B]:ILE:HB	5:A:2746[B]:HOH:O	2.16	0.45
1:B:153[B]:PHE:CE1	1:B:274[B]:LEU:HD22	2.51	0.45
1:B:438[B]:VAL:HA	5:B:2790[B]:HOH:O	2.17	0.45
1:B:496[B]:THR:HB	5:B:2896[B]:HOH:O	2.16	0.45
1:A:36[A]:ALA:HB2	1:A:175[A]:MET:HE2	1.98	0.45
1:A:168[A]:VAL:HG22	5:A:2328:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208[A]:MET:HG2	1:A:301[A]:PHE:HZ	1.80	0.45
1:A:208[A]:MET:CE	5:A:2394[A]:HOH:O	2.64	0.45
1:A:224[A]:LEU:HD12	1:A:224[A]:LEU:N	2.32	0.45
1:A:263[B]:ILE:HG22	1:A:267[B]:ARG:NH1	2.31	0.45
1:A:509[A]:PRO:HD2	5:A:2851[A]:HOH:O	2.17	0.45
1:B:87[A]:ASN:OD1	1:B:126[A]:THR:OG1	2.27	0.45
1:A:44[B]:ARG:O	1:A:45[B]:PHE:HB2	2.17	0.45
1:A:98[A]:ASN:HB2	1:A:145[A]:SER:HG	1.80	0.45
1:A:134[B]:TYR:HA	5:A:2313[B]:HOH:O	2.16	0.45
1:A:321[A]:LEU:HD23	1:A:321[A]:LEU:H	1.81	0.45
1:A:138[A]:THR:HG23	5:A:2779[A]:HOH:O	2.17	0.45
1:A:269[B]:LYS:HB2	1:A:274[B]:LEU:HD11	1.98	0.45
1:A:357[B]:LYS:HD2	1:A:357[B]:LYS:O	2.17	0.45
1:B:22[B]:VAL:HG13	1:B:22[B]:VAL:O	2.17	0.45
1:B:116[A]:TYR:CE1	1:B:148[A]:TYR:CE1	3.04	0.45
1:B:439[B]:ILE:H	1:B:439[B]:ILE:HG13	1.57	0.45
1:B:461[A]:GLU:CD	1:B:461[A]:GLU:H	2.18	0.45
5:A:2350[B]:HOH:O	1:B:511[B]:LYS:HD2	2.17	0.45
1:B:213[B]:PRO:HD2	5:B:2585[B]:HOH:O	2.17	0.45
1:B:390[B]:GLY:O	1:B:394[B]:ILE:HG13	2.17	0.45
1:B:439[A]:ILE:HG23	5:B:2620[A]:HOH:O	2.16	0.45
1:A:256[A]:LEU:HD23	1:A:262[A]:LEU:HD13	1.99	0.44
1:B:27[B]:ILE:HG22	1:B:102[B]:PRO:HA	1.98	0.44
1:B:197[B]:PHE:CB	1:B:223[B]:ILE:HB	2.45	0.44
1:B:347[B]:ILE:HG22	1:B:348[B]:SER:O	2.16	0.44
1:B:511[B]:LYS:HD3	5:B:2923:HOH:O	2.17	0.44
1:A:67[A]:CYS:O	1:A:69[A]:GLN:HG2	2.18	0.44
1:A:197[A]:PHE:HB3	1:A:223[A]:ILE:HB	1.99	0.44
1:A:334[A]:TYR:CD2	3:A:1538[A]:CFQ:H10	2.49	0.44
1:B:113[A]:VAL:O	1:B:197[A]:PHE:CD1	2.70	0.44
1:B:511[A]:LYS:HD3	5:B:2924[A]:HOH:O	2.16	0.44
1:A:47[B]:ARG:NH1	1:A:171[B]:LEU:HD11	2.31	0.44
1:A:153[B]:PHE:HB2	5:A:2323[B]:HOH:O	2.17	0.44
1:A:382[B]:ASN:N	5:A:2638:HOH:O	2.49	0.44
1:B:220[B]:ARG:HD3	5:B:2436[B]:HOH:O	2.18	0.44
1:A:46[A]:ARG:HD3	5:A:2345[A]:HOH:O	2.18	0.44
1:A:108[B]:SER:HA	1:A:189[B]:GLY:C	2.38	0.44
1:A:433[A]:PRO:HG2	1:A:436[A]:MET:HG3	2.00	0.44
1:A:452[B]:LEU:HD21	1:A:467[B]:ARG:HG3	1.99	0.44
1:B:41[B]:GLY:HA3	5:B:2128[B]:HOH:O	2.16	0.44
1:B:481[B]:ASN:ND2	1:B:483[B]:ASN:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259[A]:ASP:O	1:A:263[A]:ILE:HG13	2.16	0.44
1:A:324[A]:ASN:O	1:A:327[A]:GLU:HG2	2.18	0.44
1:B:162[B]:GLN:O	1:B:165[B]:PRO:HD3	2.17	0.44
1:B:321[B]:LEU:O	1:B:420[B]:LEU:HA	2.17	0.44
1:B:347[A]:ILE:HG22	1:B:348[A]:SER:O	2.17	0.44
1:A:180[B]:VAL:HG13	1:A:184[B]:ILE:HB	1.99	0.44
1:B:144[B]:VAL:HG12	1:B:145[B]:SER:N	2.33	0.44
1:B:224[B]:LEU:O	1:B:321[B]:LEU:HA	2.18	0.44
1:A:112[B]:MET:HB2	1:A:143[B]:LEU:HD12	1.99	0.44
1:A:202[B]:GLY:O	1:A:206[B]:VAL:HG23	2.18	0.44
1:A:347[B]:ILE:HA	5:A:2603:HOH:O	2.18	0.44
1:A:13[B]:GLY:HA3	1:A:54[B]:TRP:CE2	2.52	0.44
1:A:102[B]:PRO:HG2	1:A:106[B]:PRO:CD	2.41	0.44
1:B:18[B]:THR:HB	1:B:61[B]:SER:HB3	1.99	0.44
1:B:131[A]:ASN:OD1	1:B:133[A]:LYS:HG2	2.18	0.44
1:B:320[B]:LEU:HD23	1:B:321[B]:LEU:N	2.32	0.44
1:A:162[A]:GLN:HB2	5:A:2343[A]:HOH:O	2.18	0.43
1:A:379[B]:MET:HA	1:B:515[B]:ARG:HD2	2.00	0.43
1:A:449[A]:GLY:HA2	1:A:466[A]:SER:OG	2.17	0.43
1:B:341[A]:LYS:HA	1:B:433[A]:PRO:HG3	2.00	0.43
1:A:48[B]:PRO:HD3	1:A:149[B]:ARG:NH2	2.34	0.43
1:A:206[A]:VAL:CG1	1:A:222[A]:ALA:HB1	2.49	0.43
1:A:366[B]:LEU:HG	1:A:531[B]:LEU:HD11	2.00	0.43
1:B:111[B]:VAL:O	1:B:194[B]:VAL:HA	2.18	0.43
1:B:127[A]:LEU:HB3	5:B:2233[A]:HOH:O	2.18	0.43
1:B:324[A]:ASN:O	1:B:327[A]:GLU:HG2	2.18	0.43
1:A:35[A]:PHE:CD2	1:A:97[A]:LEU:HD23	2.53	0.43
1:A:149[A]:ARG:HG2	5:A:2231[A]:HOH:O	2.17	0.43
1:B:37[B]:GLU:HG2	1:B:50[B]:PRO:O	2.17	0.43
1:B:207[B]:GLY:O	1:B:210[B]:ILE:HB	2.18	0.43
1:B:445[A]:GLU:OE2	1:B:458[A]:TYR:OH	2.29	0.43
1:B:450[B]:LEU:N	1:B:451[B]:PRO:CD	2.81	0.43
1:B:451[B]:PRO:HD2	1:B:466[B]:SER:OG	2.18	0.43
1:B:515[A]:ARG:NE	5:B:2942[A]:HOH:O	2.51	0.43
1:A:364[B]:ASN:HB2	5:A:2622:HOH:O	2.17	0.43
1:B:88[A]:ARG:NE	5:B:2254[A]:HOH:O	2.40	0.43
1:B:146[A]:LEU:HD12	1:B:146[A]:LEU:C	2.39	0.43
1:A:235[B]:SER:HA	1:A:293[B]:VAL:HG23	2.01	0.43
1:A:264[A]:HIS:O	1:A:268[A]:GLU:HG2	2.18	0.43
1:A:439[A]:ILE:HG22	1:A:440[A]:HIS:N	2.32	0.43
1:B:173[B]:GLN:O	1:B:177[B]:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63[A]:TYR:CD1	1:A:126[A]:THR:HG22	2.53	0.43
1:A:204[B]:ALA:C	5:A:2395[B]:HOH:O	2.56	0.43
1:A:279[B]:TRP:HA	1:A:291[B]:SER:OG	2.19	0.43
1:A:384[B]:GLY:HA2	1:A:387[B]:ASN:HD22	1.83	0.43
1:A:437[B]:GLY:O	1:A:439[B]:ILE:HG13	2.19	0.43
1:A:458[B]:TYR:HB3	1:A:459[B]:THR:H	1.75	0.43
1:B:327[B]:GLU:OE2	1:B:400[B]:VAL:HG11	2.19	0.43
1:B:346[B]:LYS:NZ	5:B:2648:HOH:O	2.51	0.43
1:B:383[A]:ASN:HB3	1:B:386[A]:LYS:HB2	2.00	0.43
1:A:238[B]:VAL:HG13	1:A:296[B]:ILE:O	2.18	0.43
1:B:339[B]:PHE:HD1	1:B:345[B]:SER:HB3	1.83	0.43
1:B:426[B]:ARG:NH2	1:B:430[B]:LEU:HB3	2.34	0.43
1:A:27[B]:ILE:HG22	5:A:2256[B]:HOH:O	2.18	0.43
1:A:68[B]:GLN:HG3	1:A:271[B]:PRO:CB	2.49	0.43
1:A:157[B]:ALA:HB2	5:A:2330[B]:HOH:O	2.18	0.43
1:A:518[A]:VAL:HG13	1:A:519[A]:GLN:N	2.34	0.43
1:B:146[B]:LEU:HD22	1:B:173[B]:GLN:HA	2.01	0.43
1:B:450[B]:LEU:O	1:B:456[B]:LEU:HD12	2.18	0.43
1:A:168[B]:VAL:HG12	1:A:171[B]:LEU:HD12	2.00	0.43
1:B:222[B]:ALA:HB3	1:B:319[B]:ILE:HG22	2.01	0.43
1:A:469[A]:ILE:O	1:A:473[A]:TRP:CE3	2.71	0.43
1:B:27[A]:ILE:CG2	1:B:102[A]:PRO:HA	2.48	0.43
1:B:416[B]:ASN:HD22	1:B:416[B]:ASN:HA	1.56	0.43
1:B:447[B]:VAL:O	1:B:470[B]:MET:HG2	2.19	0.43
1:A:208[A]:MET:CG	5:A:2394[A]:HOH:O	2.63	0.42
1:A:530[B]:LYS:HB3	1:B:366[B]:LEU:HD13	1.99	0.42
1:B:120[A]:PHE:HD2	5:B:2478[A]:HOH:O	2.01	0.42
1:B:218[A]:LEU:O	5:B:2447[A]:HOH:O	2.21	0.42
1:B:421[A]:TYR:HB2	1:B:505[A]:LEU:HD22	2.02	0.42
1:A:222[B]:ALA:O	1:A:319[B]:ILE:HA	2.19	0.42
1:A:232[B]:PRO:HG3	1:A:399[B]:ASN:HA	2.02	0.42
1:A:287[B]:ILE:C	1:A:289[B]:ARG:H	2.22	0.42
1:A:293[B]:VAL:HB	1:A:294[B]:PRO:HD2	2.01	0.42
1:A:305[A]:LEU:O	1:A:309[A]:LEU:HG	2.19	0.42
3:A:1537[A]:CFQ:O3	3:A:1537[A]:CFQ:H6	2.19	0.42
1:B:37[A]:GLU:OE2	1:B:52[A]:LYS:HG2	2.19	0.42
1:B:370[B]:ALA:O	1:B:374[B]:GLN:HB2	2.18	0.42
1:A:92[B]:GLU:HG3	5:A:2230[B]:HOH:O	2.18	0.42
1:A:113[A]:VAL:O	1:A:197[A]:PHE:HD1	2.03	0.42
1:A:260[A]:GLU:HG3	1:A:264[A]:HIS:CD2	2.54	0.42
1:A:317[B]:THR:O	1:A:416[B]:ASN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439[B]:ILE:HB	1:B:442[B]:TYR:CD1	2.54	0.42
1:A:19[B]:ARG:HG2	1:A:19[B]:ARG:HH11	1.84	0.42
1:A:320[A]:LEU:C	1:A:320[A]:LEU:HD23	2.40	0.42
1:A:478[B]:LYS:O	1:A:478[B]:LYS:HD3	2.19	0.42
1:B:7[B]:LEU:HA	1:B:15[B]:VAL:O	2.20	0.42
1:B:367[A]:GLY:O	1:B:371[A]:VAL:HG23	2.19	0.42
1:A:467[B]:ARG:HD2	5:A:2781[B]:HOH:O	2.20	0.42
1:A:522[B]:VAL:HG13	1:A:526[B]:GLN:OE1	2.19	0.42
1:B:52[A]:LYS:HE2	1:B:52[A]:LYS:HB3	1.90	0.42
1:B:352[A]:PHE:O	1:B:356[A]:VAL:HG13	2.19	0.42
1:A:46[B]:ARG:HG3	5:A:2340[B]:HOH:O	2.18	0.42
1:A:131[B]:ASN:ND2	1:A:133[B]:LYS:HE2	2.34	0.42
1:A:364[B]:ASN:O	1:A:368[B]:LEU:HG	2.19	0.42
1:A:46[A]:ARG:CD	5:A:2347[A]:HOH:O	2.68	0.42
3:A:1537[B]:CFQ:AS	3:A:1537[B]:CFQ:C5	3.18	0.42
1:B:110[A]:THR:OG1	1:B:478[A]:LYS:HG2	2.20	0.42
1:B:502[B]:PHE:HA	5:B:2917:HOH:O	2.20	0.42
1:A:36[A]:ALA:CB	1:A:175[A]:MET:HE3	2.50	0.42
1:A:71[B]:VAL:O	1:A:73[B]:GLU:HG3	2.19	0.42
1:A:98[B]:ASN:O	1:A:144[B]:VAL:HA	2.20	0.42
1:A:347[A]:ILE:HG23	1:A:351[A]:ASP:HB2	2.01	0.42
1:A:367[B]:GLY:O	1:A:371[B]:VAL:HG23	2.20	0.42
1:A:36[A]:ALA:HB2	1:A:175[A]:MET:HE3	2.01	0.42
1:B:206[B]:VAL:CG1	1:B:222[B]:ALA:HB1	2.50	0.42
1:B:326[B]:ASP:HA	5:B:2613:HOH:O	2.20	0.42
1:A:44[A]:ARG:O	1:A:45[A]:PHE:HB2	2.20	0.42
1:A:250[B]:ARG:HA	1:A:256[B]:LEU:HD11	2.01	0.42
1:A:334[A]:TYR:CE2	3:A:1538[A]:CFQ:H9	2.55	0.42
1:A:366[B]:LEU:HD13	1:B:530[B]:LYS:HB3	2.02	0.42
1:A:445[A]:GLU:OE2	1:A:458[A]:TYR:OH	2.31	0.42
1:A:468[B]:ARG:HH12	1:A:472[B]:TYR:HE2	1.68	0.42
1:B:68[B]:GLN:HG3	1:B:271[B]:PRO:HB3	2.01	0.42
1:B:439[A]:ILE:H	1:B:439[A]:ILE:HG13	1.69	0.42
1:B:520[A]:MET:O	1:B:523[A]:PHE:HB3	2.20	0.42
1:A:51[B]:LYS:HG3	1:A:52[B]:LYS:N	2.35	0.41
1:A:467[B]:ARG:HG2	1:A:467[B]:ARG:HH11	1.85	0.41
1:B:320[A]:LEU:C	1:B:320[A]:LEU:HD23	2.40	0.41
1:B:83[A]:MET:CE	1:B:129[A]:VAL:HG11	2.50	0.41
1:B:179[A]:TRP:HA	5:B:2409[A]:HOH:O	2.19	0.41
1:B:408[A]:VAL:HG13	1:B:409[A]:ASN:N	2.34	0.41
1:B:422[B]:PHE:HD2	1:B:424[B]:ASN:HD22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211[B]:LEU:HD23	1:A:314[B]:PHE:HB3	2.02	0.41
1:B:208[A]:MET:HG2	1:B:301[A]:PHE:CZ	2.55	0.41
1:B:411[B]:TYR:CE2	1:B:415[B]:GLY:HA3	2.55	0.41
1:B:517[B]:ARG:HG2	1:B:517[B]:ARG:NH1	2.36	0.41
1:B:323[B]:VAL:CG1	1:B:404[B]:LEU:HD13	2.50	0.41
1:A:30[B]:PHE:HB3	1:A:33[B]:ILE:HD11	2.03	0.41
1:A:108[B]:SER:N	5:A:2267[B]:HOH:O	2.52	0.41
1:B:176[A]:ALA:O	1:B:180[A]:VAL:HG23	2.21	0.41
1:B:191[B]:PRO:HG3	5:B:2422[B]:HOH:O	2.21	0.41
1:B:212[A]:SER:HA	1:B:213[A]:PRO:HD3	1.89	0.41
1:A:115[B]:ILE:HG23	1:A:146[B]:LEU:HD11	2.02	0.41
1:A:453[B]:VAL:HG22	1:A:455[B]:GLU:HG2	2.02	0.41
1:B:4[B]:SER:HB3	5:B:2008:HOH:O	2.19	0.41
1:A:46[A]:ARG:HG2	1:A:163[A]:GLU:O	2.21	0.41
1:A:322[A]:GLY:HA3	1:A:421[A]:TYR:CD2	2.56	0.41
1:A:437[B]:GLY:HA2	5:A:2731[B]:HOH:O	2.20	0.41
1:B:206[B]:VAL:O	1:B:210[B]:ILE:HG13	2.20	0.41
1:B:347[B]:ILE:CG2	1:B:351[B]:ASP:HB2	2.49	0.41
1:A:40[B]:VAL:HG12	1:A:92[B]:GLU:CB	2.50	0.41
1:A:139[A]:GLU:O	1:A:140[A]:GLU:HB2	2.19	0.41
1:A:173[B]:GLN:OE1	1:A:205[B]:SER:HB3	2.20	0.41
1:A:185[B]:GLN:HB2	5:A:2375[B]:HOH:O	2.20	0.41
1:A:331[B]:PHE:CD1	1:A:331[B]:PHE:N	2.88	0.41
1:B:132[B]:GLY:HA3	1:B:143[B]:LEU:CD2	2.50	0.41
1:B:408[A]:VAL:CG1	1:B:409[A]:ASN:N	2.83	0.41
1:B:420[B]:LEU:HD12	1:B:421[B]:TYR:H	1.86	0.41
1:A:229[B]:PRO:O	1:A:305[B]:LEU:HD13	2.21	0.41
1:A:504[B]:ASP:HB2	5:A:2841[B]:HOH:O	2.20	0.41
1:B:36[A]:ALA:HB2	1:B:175[A]:MET:CE	2.51	0.41
1:B:83[B]:MET:CE	1:B:129[B]:VAL:HG11	2.50	0.41
1:B:116[B]:TYR:N	5:B:2328:HOH:O	2.53	0.41
1:B:210[B]:ILE:HG22	1:B:314[B]:PHE:HB2	2.02	0.41
1:B:304[B]:SER:O	1:B:308[B]:MET:HG3	2.21	0.41
1:B:327[B]:GLU:HB2	1:B:396[B]:GLY:HA2	2.03	0.41
1:B:402[B]:CYS:HB3	1:B:525[B]:ASN:HD21	1.85	0.41
1:B:450[B]:LEU:HB2	1:B:451[B]:PRO:HD3	2.01	0.41
1:B:481[B]:ASN:C	1:B:483[B]:ASN:H	2.25	0.41
1:A:148[B]:TYR:HB2	1:A:169[B]:GLY:O	2.21	0.41
1:A:395[B]:VAL:HG13	1:A:399[B]:ASN:ND2	2.36	0.41
1:A:505[A]:LEU:HD12	1:A:505[A]:LEU:HA	1.87	0.41
1:B:195[B]:THR:CG2	1:B:223[B]:ILE:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207[B]:GLY:HA3	1:B:229[B]:PRO:HD3	2.03	0.41
1:B:528[B]:LEU:O	1:B:532[B]:LEU:HG	2.21	0.41
3:B:1536[A]:CFQ:AS	3:B:1536[A]:CFQ:O1	2.98	0.41
1:A:108[B]:SER:HA	1:A:189[B]:GLY:O	2.20	0.40
1:A:184[B]:ILE:HG13	1:A:184[B]:ILE:O	2.21	0.40
1:A:197[B]:PHE:HB3	1:A:223[B]:ILE:HB	2.03	0.40
1:A:212[B]:SER:HA	1:A:213[B]:PRO:HD3	1.96	0.40
1:A:247[B]:GLU:CG	1:A:281[B]:VAL:HG12	2.50	0.40
1:A:361[B]:PRO:HG2	1:A:362[B]:HIS:ND1	2.36	0.40
1:B:200[B]:SER:HB3	1:B:201[B]:ALA:H	1.67	0.40
1:B:331[B]:PHE:CD1	1:B:331[B]:PHE:N	2.89	0.40
1:A:220[B]:ARG:HG3	1:A:221[B]:ARG:HG3	2.04	0.40
1:A:230[A]:ASN:O	1:A:231[A]:CYS:C	2.60	0.40
1:B:7[B]:LEU:HD12	1:B:15[B]:VAL:O	2.21	0.40
1:B:8[B]:VAL:HG13	5:B:2041[B]:HOH:O	2.22	0.40
1:B:105[B]:ARG:HA	1:B:106[B]:PRO:HD3	1.88	0.40
1:B:212[A]:SER:HB2	1:B:300[A]:PHE:CE1	2.56	0.40
1:B:298[B]:GLY:HA2	1:B:302[B]:PRO:HA	2.03	0.40
1:A:213[B]:PRO:CA	1:A:216[B]:ARG:HD3	2.43	0.40
1:A:321[B]:LEU:N	1:A:321[B]:LEU:CD2	2.85	0.40
1:B:522[A]:VAL:O	1:B:526[A]:GLN:HB2	2.21	0.40
1:A:103[B]:SER:HA	1:A:104[B]:PRO:C	2.41	0.40
1:B:113[A]:VAL:O	1:B:197[A]:PHE:HD1	2.05	0.40
1:B:233[B]:TRP:NE1	1:B:399[B]:ASN:HB3	2.37	0.40
1:A:163[B]:GLU:CG	2:A:1536[B]:CL:CL	3.06	0.40
1:A:366[A]:LEU:CD2	1:A:531[A]:LEU:HD11	2.51	0.40
1:A:374[A]:GLN:NE2	5:B:2688[A]:HOH:O	2.24	0.40
1:A:405[A]:MET:CA	1:A:408[A]:VAL:HG12	2.51	0.40
1:A:457[A]:ASN:ND2	5:A:2758[A]:HOH:O	2.55	0.40
1:A:524[B]:TRP:CZ3	1:A:528[B]:LEU:HD22	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	1048/537 (195%)	892 (85%)	128 (12%)	28 (3%)	5 26
1	B	1060/537 (197%)	910 (86%)	126 (12%)	24 (2%)	6 30
All	All	2108/1074 (196%)	1802 (86%)	254 (12%)	52 (2%)	5 28

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27[A]	ILE
1	A	27[B]	ILE
1	A	95[A]	LEU
1	A	95[B]	LEU
1	B	27[A]	ILE
1	B	27[B]	ILE
1	A	41[A]	GLY
1	A	41[B]	GLY
1	A	283[A]	PRO
1	A	283[B]	PRO
1	B	283[A]	PRO
1	B	283[B]	PRO
1	B	454[A]	LYS
1	B	454[B]	LYS
1	A	29[A]	ALA
1	A	29[B]	ALA
1	A	184[A]	ILE
1	A	184[B]	ILE
1	B	415[A]	GLY
1	B	415[B]	GLY
1	A	22[A]	VAL
1	A	22[B]	VAL
1	A	145[A]	SER
1	A	145[B]	SER
1	B	459[A]	THR
1	B	459[B]	THR
1	A	120[A]	PHE
1	A	120[B]	PHE
1	A	153[A]	PHE
1	A	153[B]	PHE
1	B	91[A]	SER
1	B	91[B]	SER
1	A	11[A]	LYS

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Mol	Chain	Res	Type
1	A	11[B]	LYS
1	A	160[A]	GLY
1	A	160[B]	GLY
1	A	328[A]	GLY
1	A	328[B]	GLY
1	B	485[A]	PRO
1	B	485[B]	PRO
1	B	439[A]	ILE
1	B	439[B]	ILE
1	B	482[A]	PRO
1	B	482[B]	PRO
1	B	64[A]	PRO
1	B	64[B]	PRO
1	B	361[A]	PRO
1	B	361[B]	PRO
1	A	238[A]	VAL
1	A	238[B]	VAL
1	B	449[A]	GLY
1	B	449[B]	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	900/469 (192%)	868 (96%)	32 (4%)	35	70
1	B	902/469 (192%)	864 (96%)	38 (4%)	30	66
All	All	1802/938 (192%)	1732 (96%)	70 (4%)	32	69

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7[A]	LEU
1	A	7[B]	LEU
1	A	15[A]	VAL
1	A	15[B]	VAL

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Mol	Chain	Res	Type
1	A	74[A]	GLN
1	A	74[B]	GLN
1	A	82[A]	GLU
1	A	82[B]	GLU
1	A	116[A]	TYR
1	A	116[B]	TYR
1	A	143[A]	LEU
1	A	143[B]	LEU
1	A	197[A]	PHE
1	A	197[B]	PHE
1	A	200[A]	SER
1	A	200[B]	SER
1	A	285[A]	ASP
1	A	285[B]	ASP
1	A	288[A]	PHE
1	A	288[B]	PHE
1	A	321[A]	LEU
1	A	321[B]	LEU
1	A	330[A]	PHE
1	A	330[B]	PHE
1	A	358[A]	LEU
1	A	358[B]	LEU
1	A	383[A]	ASN
1	A	383[B]	ASN
1	A	453[A]	VAL
1	A	453[B]	VAL
1	A	499[A]	GLU
1	A	499[B]	GLU
1	B	27[A]	ILE
1	B	27[B]	ILE
1	B	74[A]	GLN
1	B	74[B]	GLN
1	B	82[A]	GLU
1	B	82[B]	GLU
1	B	140[A]	GLU
1	B	140[B]	GLU
1	B	197[A]	PHE
1	B	197[B]	PHE
1	B	200[A]	SER
1	B	200[B]	SER
1	B	288[A]	PHE
1	B	288[B]	PHE

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Mol	Chain	Res	Type
1	B	295[A]	VAL
1	B	295[B]	VAL
1	B	321[A]	LEU
1	B	321[B]	LEU
1	B	325[A]	LYS
1	B	325[B]	LYS
1	B	330[A]	PHE
1	B	330[B]	PHE
1	B	453[A]	VAL
1	B	453[B]	VAL
1	B	473[A]	TRP
1	B	473[B]	TRP
1	B	494[A]	LEU
1	B	494[B]	LEU
1	B	497[A]	THR
1	B	497[B]	THR
1	B	499[A]	GLU
1	B	499[B]	GLU
1	B	505[A]	LEU
1	B	505[B]	LEU
1	B	518[A]	VAL
1	B	518[B]	VAL
1	B	535[A]	THR
1	B	535[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
3	CFQ	B	1536[A]	-	16,21,21	3.24	5 (31%)	20,31,31	1.65	5 (25%)
3	CFQ	A	1537[A]	-	16,21,21	3.11	6 (37%)	20,31,31	1.53	5 (25%)
3	CFQ	B	1537[B]	-	16,21,21	3.17	5 (31%)	20,31,31	1.77	7 (35%)
4	NAG	B	1538[B]	-	14,14,15	0.54	0	17,19,21	0.71	0
3	CFQ	B	1536[B]	-	16,21,21	3.03	5 (31%)	20,31,31	1.70	5 (25%)
3	CFQ	A	1537[B]	-	16,21,21	2.92	6 (37%)	20,31,31	1.58	4 (20%)
4	NAG	B	1539[A]	-	14,14,15	0.77	0	17,19,21	0.62	0
3	CFQ	A	1538[A]	-	16,21,21	2.89	5 (31%)	20,31,31	1.93	6 (30%)
4	NAG	B	1539[B]	-	14,14,15	0.53	0	17,19,21	0.65	0
3	CFQ	A	1538[B]	-	16,21,21	3.20	6 (37%)	20,31,31	1.78	6 (30%)
4	NAG	A	1539[A]	-	14,14,15	0.68	0	17,19,21	1.07	2 (11%)
4	NAG	A	1540[A]	-	14,14,15	0.57	0	17,19,21	0.53	0
4	NAG	A	1539[B]	-	14,14,15	0.55	0	17,19,21	0.76	0
4	NAG	A	1540[B]	-	14,14,15	0.61	0	17,19,21	0.65	0
3	CFQ	B	1537[A]	-	16,21,21	3.02	6 (37%)	20,31,31	1.85	6 (30%)
4	NAG	B	1538[A]	-	14,14,15	0.70	0	17,19,21	0.85	1 (5%)

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	CFQ	B	1536[A]	-	-	1/18/21/21	0/1/1/1
3	CFQ	A	1537[A]	-	-	4/18/21/21	0/1/1/1
3	CFQ	B	1537[B]	-	-	1/18/21/21	0/1/1/1
4	NAG	B	1538[B]	-	-	2/6/23/26	0/1/1/1
3	CFQ	B	1536[B]	-	-	2/18/21/21	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CFQ	A	1537[B]	-	-	7/18/21/21	0/1/1/1
4	NAG	B	1539[A]	-	-	0/6/23/26	0/1/1/1
3	CFQ	A	1538[A]	-	-	8/18/21/21	0/1/1/1
4	NAG	B	1539[B]	-	-	2/6/23/26	0/1/1/1
3	CFQ	A	1538[B]	-	-	4/18/21/21	0/1/1/1
4	NAG	A	1539[A]	-	-	2/6/23/26	0/1/1/1
4	NAG	A	1540[A]	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1539[B]	-	-	4/6/23/26	0/1/1/1
4	NAG	A	1540[B]	-	-	2/6/23/26	0/1/1/1
3	CFQ	B	1537[A]	-	-	9/18/21/21	0/1/1/1
4	NAG	B	1538[A]	-	-	4/6/23/26	0/1/1/1

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1536[A]	CFQ	C7-C6	7.58	1.60	1.51
3	A	1538[B]	CFQ	C7-C6	7.42	1.60	1.51
3	A	1537[A]	CFQ	C7-C6	7.32	1.60	1.51
3	B	1537[A]	CFQ	C8-C7	7.06	1.49	1.39
3	B	1537[B]	CFQ	C8-C7	7.04	1.49	1.39
3	B	1536[B]	CFQ	C7-C6	7.03	1.59	1.51
3	A	1538[B]	CFQ	C8-C7	6.98	1.48	1.39
3	A	1538[A]	CFQ	C8-C7	6.97	1.48	1.39
3	B	1537[B]	CFQ	C7-C6	6.92	1.59	1.51
3	B	1537[A]	CFQ	C7-C6	6.50	1.59	1.51
3	B	1536[A]	CFQ	C8-C7	6.43	1.48	1.39
3	A	1537[B]	CFQ	C8-C7	6.00	1.47	1.39
3	A	1537[B]	CFQ	C7-C6	5.99	1.58	1.51
3	B	1536[B]	CFQ	C8-C7	5.94	1.47	1.39
3	A	1538[A]	CFQ	C7-C6	5.92	1.58	1.51
3	B	1536[A]	CFQ	C8-N2	5.67	1.56	1.45
3	A	1537[A]	CFQ	C8-C7	5.54	1.47	1.39
3	A	1538[A]	CFQ	C8-N2	5.50	1.55	1.45
3	B	1537[B]	CFQ	C8-N2	5.43	1.55	1.45
3	A	1538[B]	CFQ	C8-N2	5.41	1.55	1.45
3	B	1537[A]	CFQ	C8-N2	5.35	1.55	1.45
3	A	1537[B]	CFQ	C8-N2	5.28	1.55	1.45
3	B	1536[B]	CFQ	C8-N2	5.14	1.55	1.45
3	A	1537[A]	CFQ	C12-C7	4.87	1.46	1.39
3	A	1537[A]	CFQ	C8-N2	4.38	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1536[A]	CFQ	C12-C7	3.80	1.44	1.39
3	B	1536[B]	CFQ	C12-C7	3.70	1.44	1.39
3	A	1537[B]	CFQ	C12-C7	3.69	1.44	1.39
3	B	1537[B]	CFQ	C12-C7	3.41	1.44	1.39
3	A	1538[B]	CFQ	C12-C7	3.15	1.43	1.39
3	A	1537[A]	CFQ	C9-C8	3.06	1.44	1.39
3	B	1536[A]	CFQ	C9-C8	2.97	1.44	1.39
3	A	1538[A]	CFQ	C12-C7	2.91	1.43	1.39
3	A	1537[B]	CFQ	C9-C8	2.90	1.44	1.39
3	B	1536[B]	CFQ	C9-C8	2.88	1.44	1.39
3	B	1537[B]	CFQ	C9-C8	2.88	1.44	1.39
3	A	1538[B]	CFQ	C9-C8	2.73	1.44	1.39
3	A	1538[A]	CFQ	C14-C6	2.63	1.58	1.51
3	B	1537[A]	CFQ	C12-C7	2.43	1.42	1.39
3	B	1537[A]	CFQ	C9-C8	2.38	1.43	1.39
3	B	1537[A]	CFQ	O1-C6	2.37	1.46	1.43
3	A	1538[B]	CFQ	C14-C6	2.16	1.56	1.51
3	A	1537[A]	CFQ	C11-C10	2.08	1.43	1.38
3	A	1537[B]	CFQ	O1-C6	2.04	1.45	1.43

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1538[A]	CFQ	C9-C8-C7	-4.63	116.80	121.35
3	B	1537[A]	CFQ	C9-C8-C7	-4.52	116.92	121.35
3	B	1537[B]	CFQ	C9-C8-C7	-3.99	117.43	121.35
3	A	1537[A]	CFQ	C5-O1-C6	3.79	119.17	114.01
3	B	1536[A]	CFQ	C9-C8-C7	-3.68	117.74	121.35
3	A	1537[B]	CFQ	C9-C8-C7	-3.64	117.77	121.35
3	A	1538[B]	CFQ	C9-C8-C7	-3.56	117.85	121.35
3	B	1537[A]	CFQ	C12-C7-C6	-3.47	115.65	120.43
3	B	1536[B]	CFQ	O1-C6-C7	-3.46	105.98	110.93
3	B	1536[B]	CFQ	C9-C8-C7	-3.45	117.96	121.35
3	A	1538[A]	CFQ	C12-C7-C6	-3.40	115.74	120.43
3	B	1536[B]	CFQ	C14-C6-C7	3.24	118.16	112.14
3	B	1537[B]	CFQ	C12-C7-C6	-3.11	116.15	120.43
3	A	1538[B]	CFQ	C14-C6-C7	3.07	117.83	112.14
3	A	1538[B]	CFQ	O1-C6-C7	-3.04	106.58	110.93
3	A	1537[B]	CFQ	O1-C6-C7	-2.88	106.81	110.93
3	A	1538[A]	CFQ	O1-C6-C14	2.87	112.79	105.57
3	B	1536[B]	CFQ	C5-O1-C6	2.82	117.85	114.01
3	B	1536[A]	CFQ	O1-C6-C7	-2.81	106.90	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1538[B]	CFQ	C5-O1-C6	2.79	117.80	114.01
3	B	1536[A]	CFQ	C14-C6-C7	2.77	117.29	112.14
3	A	1538[B]	CFQ	C12-C7-C6	-2.74	116.65	120.43
3	B	1537[A]	CFQ	O3-N2-C8	2.66	123.59	119.03
3	A	1537[A]	CFQ	O1-C6-C7	-2.66	107.12	110.93
3	B	1537[B]	CFQ	C5-O1-C6	2.62	117.58	114.01
3	A	1538[A]	CFQ	O1-C6-C7	-2.61	107.20	110.93
3	A	1537[A]	CFQ	C9-C8-C7	-2.58	118.82	121.35
3	B	1536[A]	CFQ	O3-N2-C8	2.58	123.44	119.03
3	B	1537[A]	CFQ	C5-O1-C6	2.54	117.47	114.01
3	B	1537[B]	CFQ	O1-C6-C7	-2.51	107.33	110.93
3	A	1537[B]	CFQ	C5-O1-C6	2.47	117.37	114.01
3	B	1537[B]	CFQ	C14-C6-C7	2.37	116.54	112.14
3	A	1537[B]	CFQ	C14-C6-C7	2.34	116.49	112.14
3	B	1536[A]	CFQ	C5-O1-C6	2.32	117.17	114.01
3	B	1537[B]	CFQ	O3-N2-C8	2.30	122.97	119.03
3	A	1538[A]	CFQ	O3-N2-C8	2.25	122.89	119.03
3	B	1537[A]	CFQ	O1-C6-C7	-2.24	107.72	110.93
4	B	1538[A]	NAG	C2-N2-C7	-2.24	119.72	122.90
3	A	1537[A]	CFQ	C14-C6-C7	2.23	116.27	112.14
3	A	1538[B]	CFQ	O3-N2-C8	2.21	122.81	119.03
3	B	1536[B]	CFQ	O3-N2-C8	2.20	122.80	119.03
4	A	1539[A]	NAG	C3-C4-C5	-2.19	106.32	110.24
3	A	1538[A]	CFQ	C9-C8-N2	-2.19	114.13	116.47
3	B	1537[B]	CFQ	C9-C8-N2	-2.08	114.26	116.47
3	B	1537[A]	CFQ	O1-C6-C14	2.07	110.77	105.57
3	A	1537[A]	CFQ	O3-N2-C8	2.06	122.56	119.03
4	A	1539[A]	NAG	O5-C5-C6	2.01	110.35	107.20

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1537[A]	CFQ	O1-C6-C7-C8
3	A	1537[A]	CFQ	C14-C6-C7-C12
3	A	1537[B]	CFQ	F1-C14-C6-O1
3	A	1537[B]	CFQ	F2-C14-C6-O1
3	A	1538[A]	CFQ	F2-C14-C6-O1
3	A	1538[A]	CFQ	F3-C14-C6-O1
3	A	1538[B]	CFQ	C1-AS-C4-C5
3	A	1538[B]	CFQ	C2-AS-C4-C5
3	A	1538[B]	CFQ	C3-AS-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	1537[A]	CFQ	C2-AS-C4-C5
3	B	1537[A]	CFQ	C3-AS-C4-C5
3	B	1537[A]	CFQ	F1-C14-C6-O1
3	B	1537[A]	CFQ	F2-C14-C6-O1
3	B	1537[A]	CFQ	F3-C14-C6-O1
3	B	1537[A]	CFQ	F1-C14-C6-C7
3	B	1537[A]	CFQ	F2-C14-C6-C7
3	B	1537[A]	CFQ	F3-C14-C6-C7
4	A	1539[A]	NAG	C8-C7-N2-C2
4	A	1539[A]	NAG	O7-C7-N2-C2
4	A	1539[B]	NAG	C8-C7-N2-C2
4	A	1539[B]	NAG	O7-C7-N2-C2
4	A	1540[B]	NAG	C8-C7-N2-C2
4	A	1540[B]	NAG	O7-C7-N2-C2
4	B	1538[A]	NAG	C8-C7-N2-C2
4	B	1538[A]	NAG	O7-C7-N2-C2
4	B	1538[B]	NAG	C8-C7-N2-C2
4	B	1538[B]	NAG	O7-C7-N2-C2
4	B	1539[B]	NAG	O7-C7-N2-C2
4	B	1539[B]	NAG	C8-C7-N2-C2
4	A	1539[B]	NAG	C4-C5-C6-O6
4	B	1538[A]	NAG	O5-C5-C6-O6
4	B	1538[A]	NAG	C4-C5-C6-O6
3	A	1537[A]	CFQ	O1-C6-C7-C12
4	A	1539[B]	NAG	O5-C5-C6-O6
3	A	1537[B]	CFQ	F1-C14-C6-C7
3	A	1537[B]	CFQ	F2-C14-C6-C7
3	A	1537[B]	CFQ	F3-C14-C6-C7
3	A	1537[B]	CFQ	C7-C6-O1-C5
3	B	1537[B]	CFQ	C7-C6-O1-C5
3	A	1537[B]	CFQ	F3-C14-C6-O1
3	A	1538[A]	CFQ	F1-C14-C6-O1
3	A	1537[A]	CFQ	C7-C6-O1-C5
3	B	1536[A]	CFQ	C7-C6-O1-C5
3	B	1536[B]	CFQ	C7-C6-O1-C5
3	B	1536[B]	CFQ	O1-C6-C7-C12
3	A	1538[A]	CFQ	O1-C6-C7-C8
3	B	1537[A]	CFQ	O1-C6-C7-C8
3	A	1538[A]	CFQ	F1-C14-C6-C7
3	A	1538[A]	CFQ	C7-C6-O1-C5
3	A	1538[B]	CFQ	C7-C6-O1-C5
3	A	1538[A]	CFQ	F2-C14-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	1538[A]	CFQ	F3-C14-C6-C7

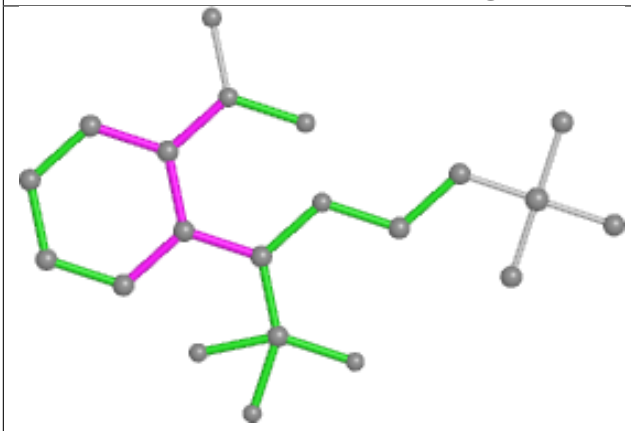
There are no ring outliers.

9 monomers are involved in 58 short contacts:

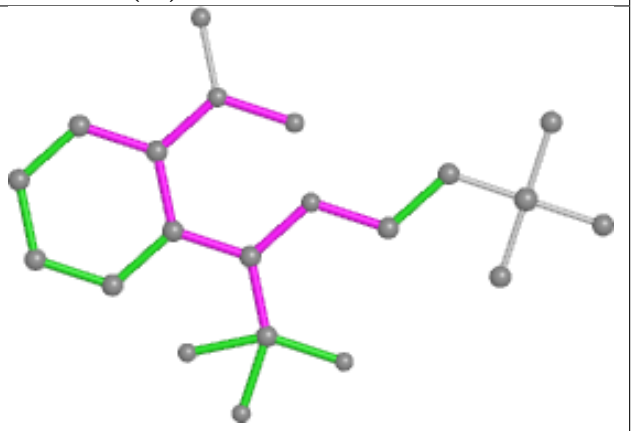
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1536[A]	CFQ	6	0
3	A	1537[A]	CFQ	8	0
3	B	1537[B]	CFQ	5	0
3	B	1536[B]	CFQ	5	0
3	A	1537[B]	CFQ	5	0
3	A	1538[A]	CFQ	12	0
3	A	1538[B]	CFQ	6	0
4	A	1540[B]	NAG	1	0
3	B	1537[A]	CFQ	10	0

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.

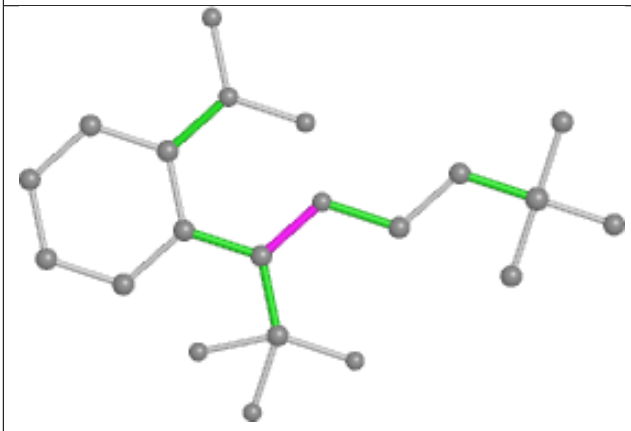
Ligand CFQ B 1536 (A)



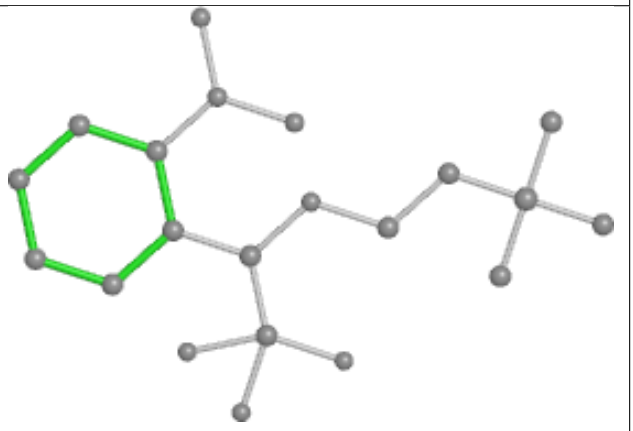
Bond lengths



Bond angles

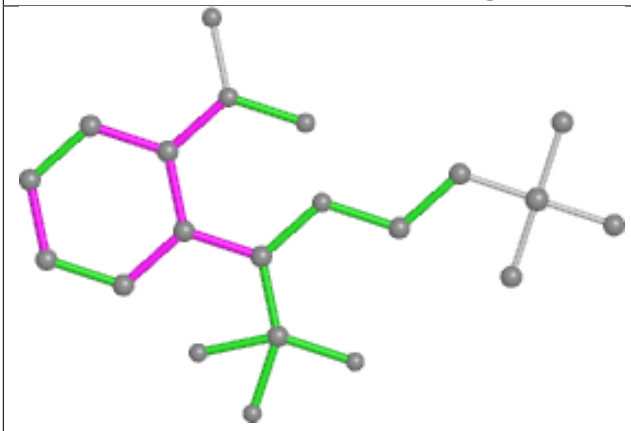


Torsions

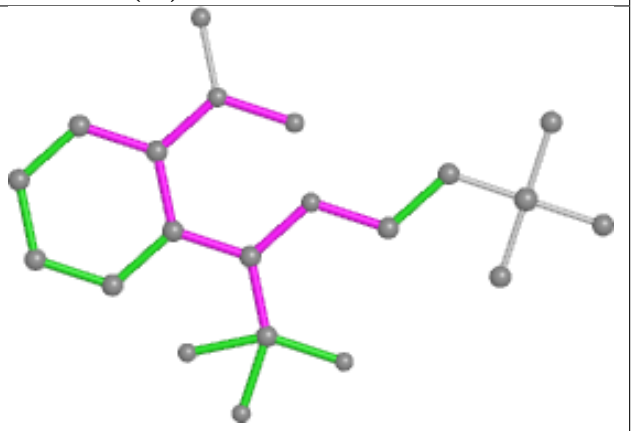


Rings

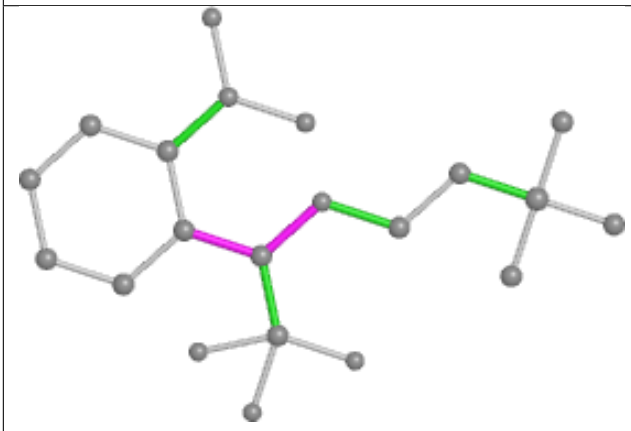
Ligand CFQ A 1537 (A)



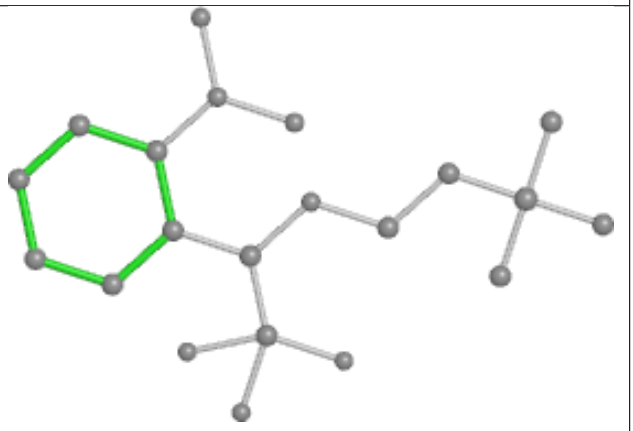
Bond lengths



Bond angles

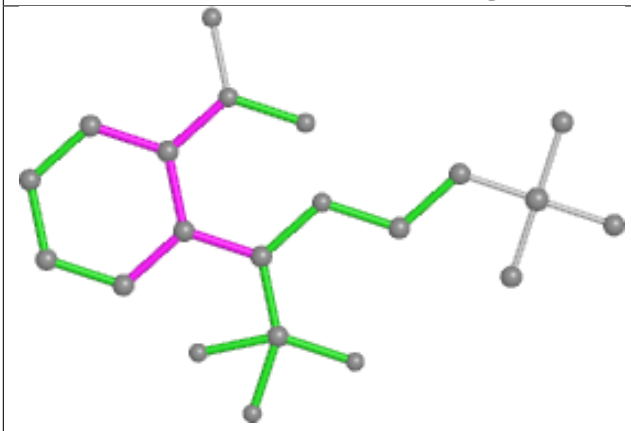


Torsions

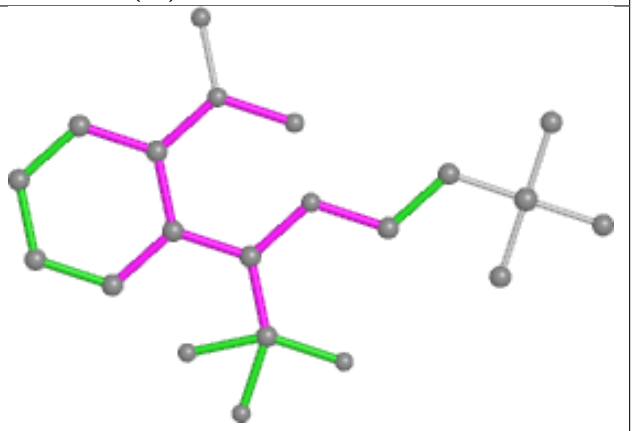


Rings

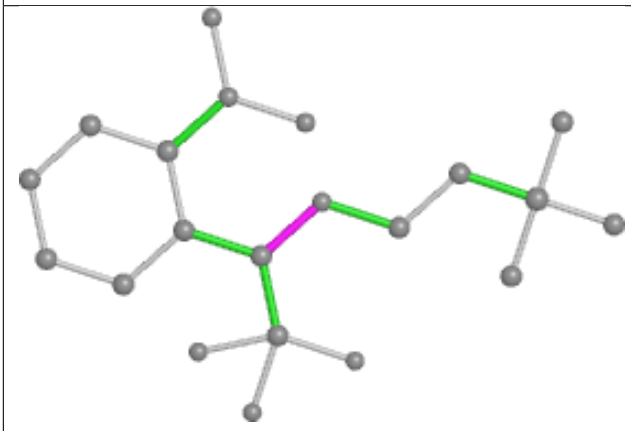
Ligand CFQ B 1537 (B)



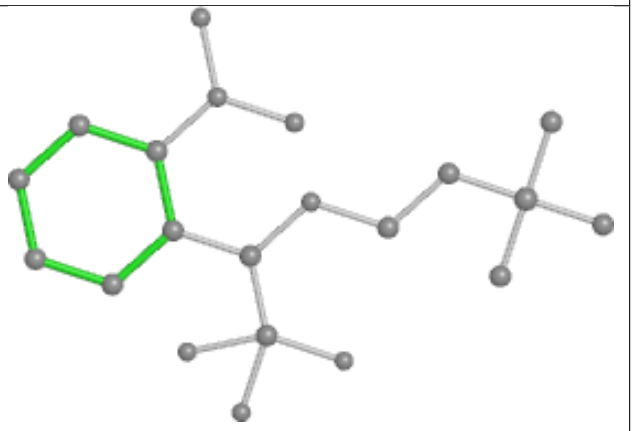
Bond lengths



Bond angles

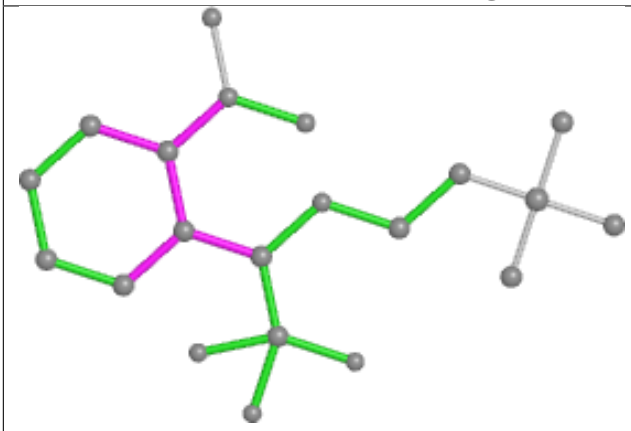


Torsions

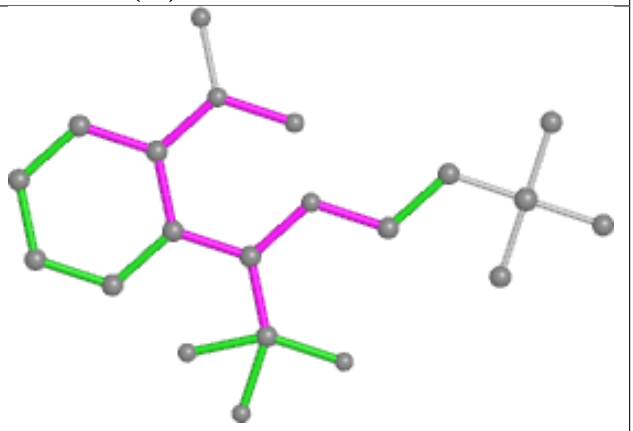


Rings

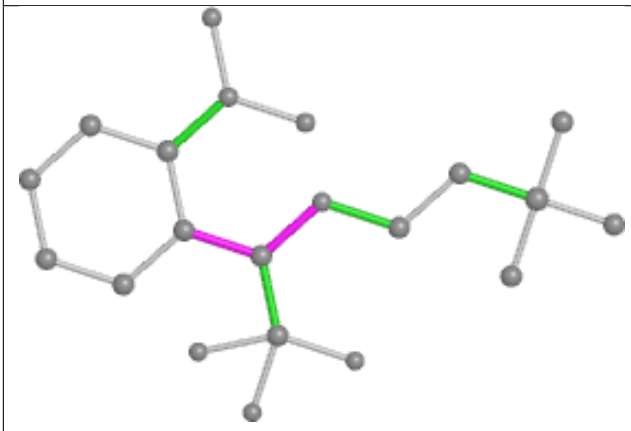
Ligand CFQ B 1536 (B)



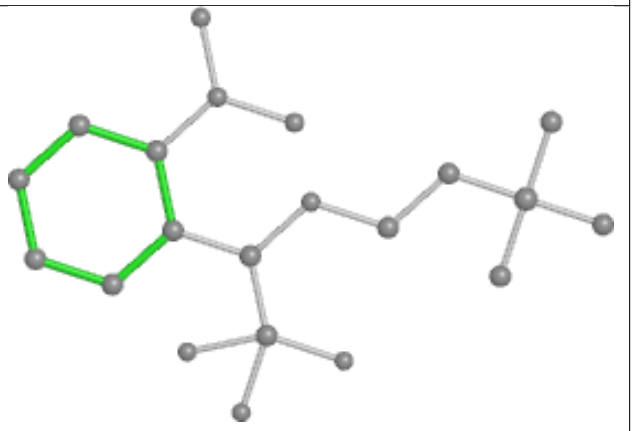
Bond lengths



Bond angles

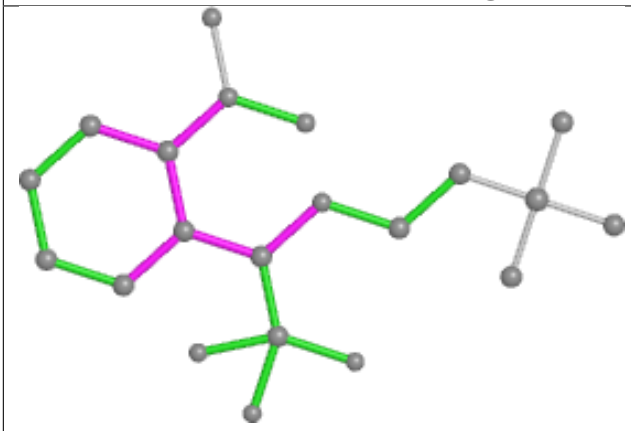


Torsions

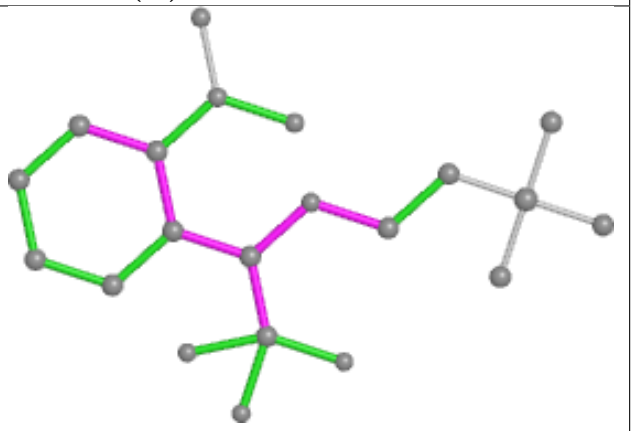


Rings

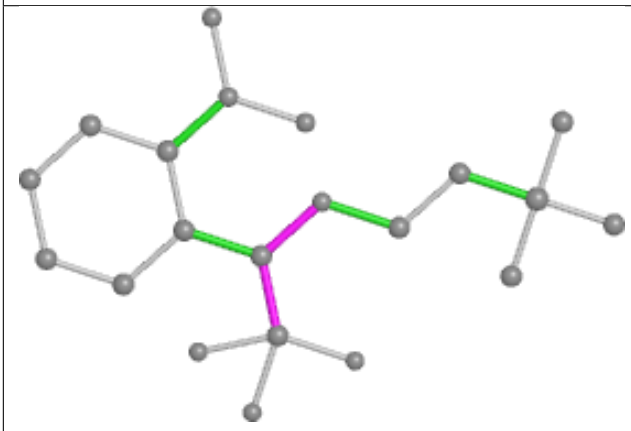
Ligand CFQ A 1537 (B)



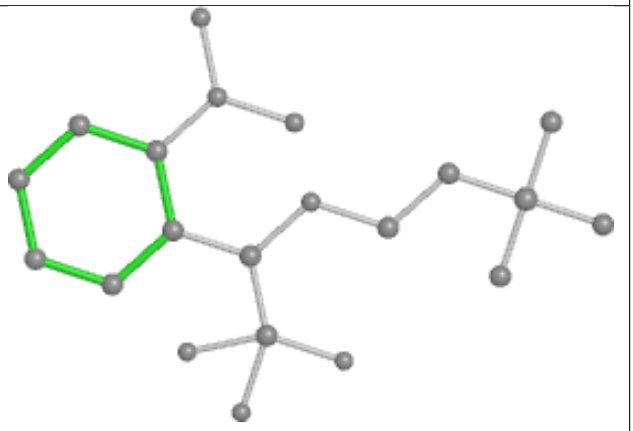
Bond lengths



Bond angles

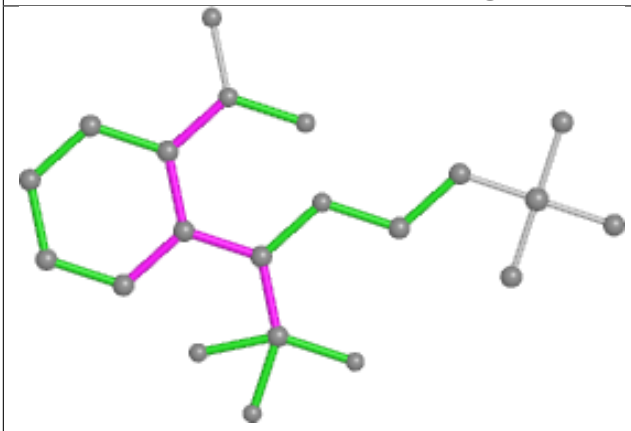


Torsions

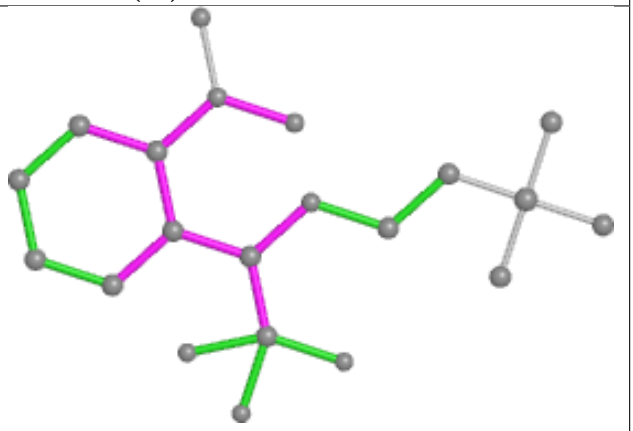


Rings

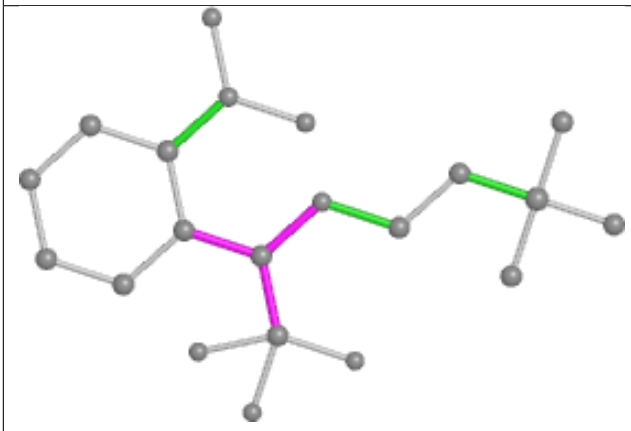
Ligand CFQ A 1538 (A)



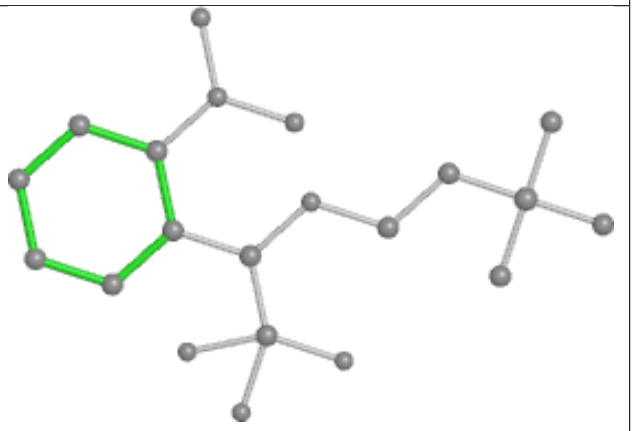
Bond lengths



Bond angles

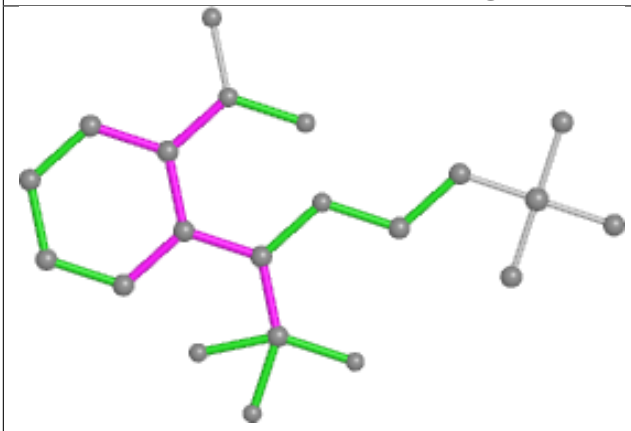


Torsions

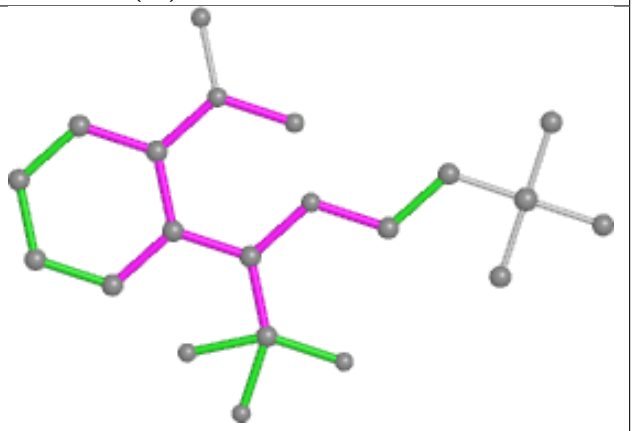


Rings

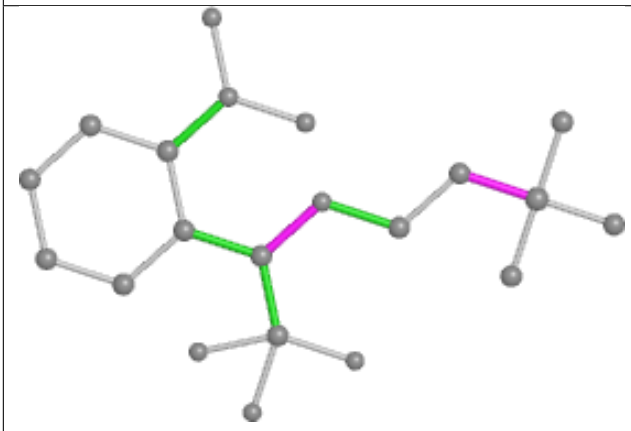
Ligand CFQ A 1538 (B)



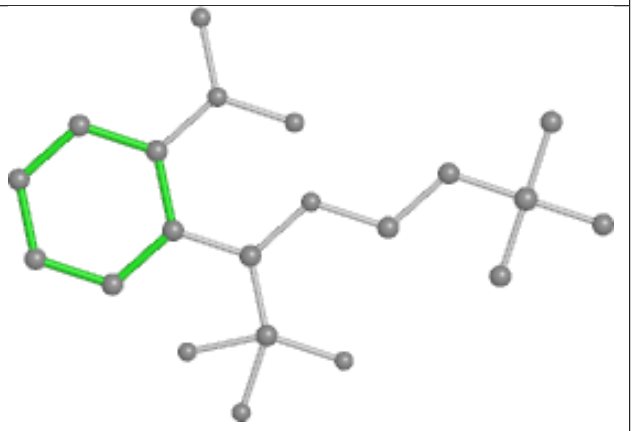
Bond lengths



Bond angles

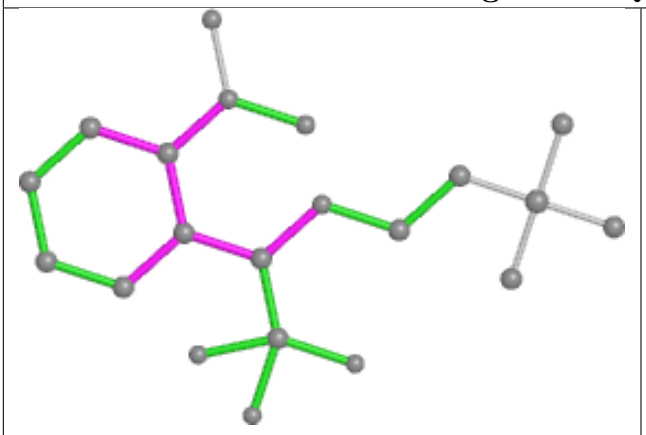


Torsions

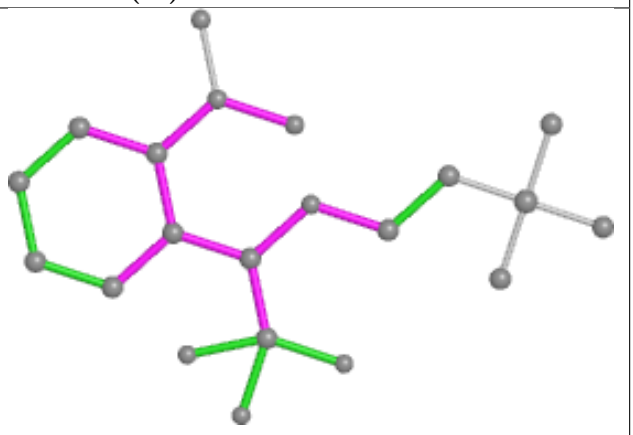


Rings

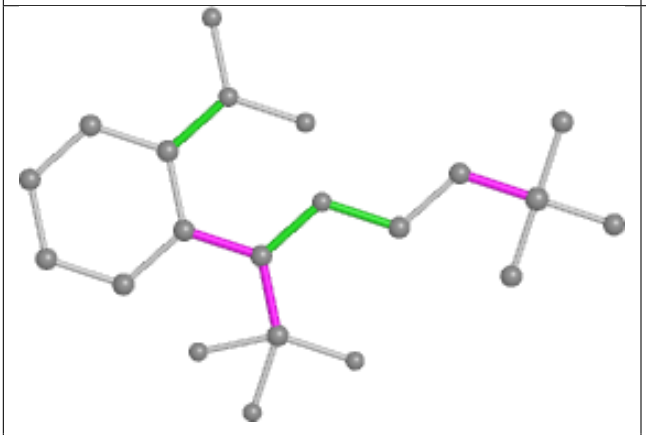
Ligand CFQ B 1537 (A)



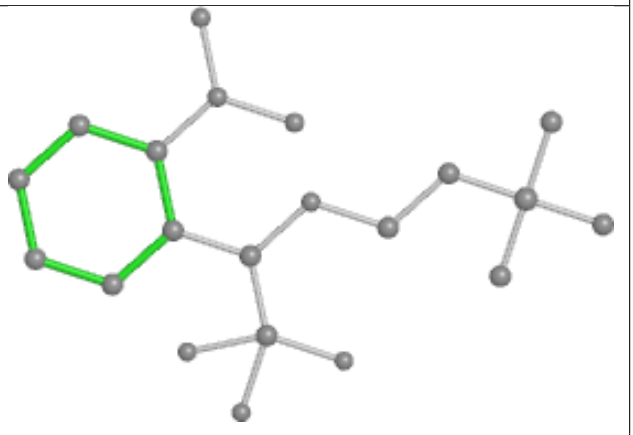
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

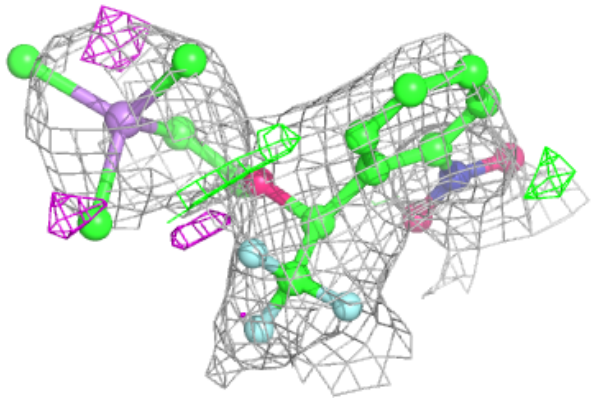
6.4 Ligands

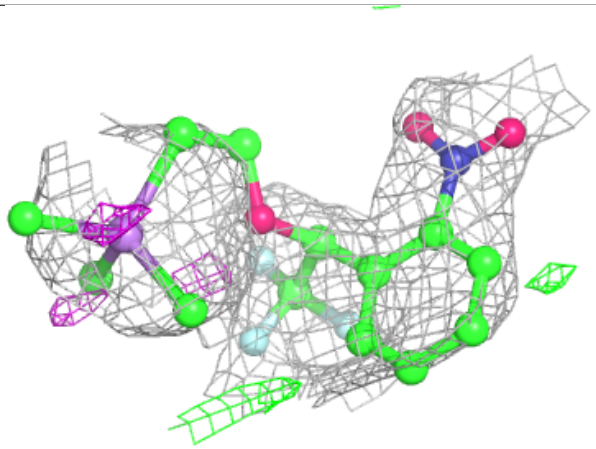
Unable to reproduce the depositors R factor - this section is therefore empty.

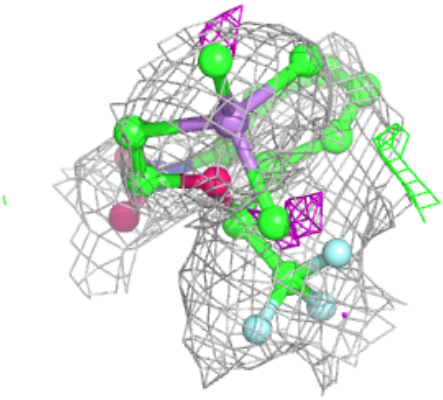
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CFQ A 1537 (A):

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

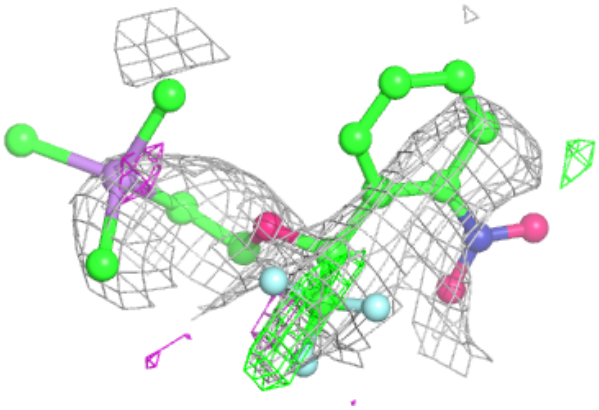


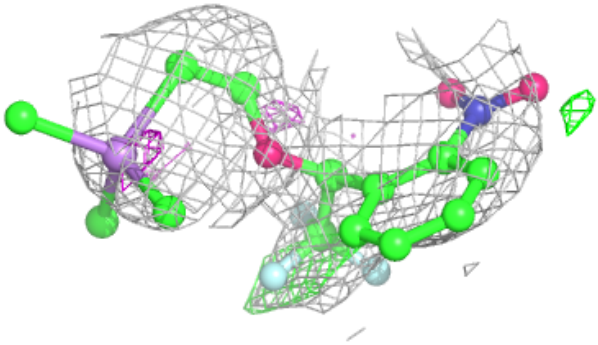


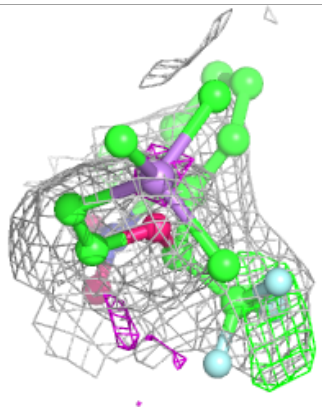


Electron density around CFQ A 1537 (B):

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

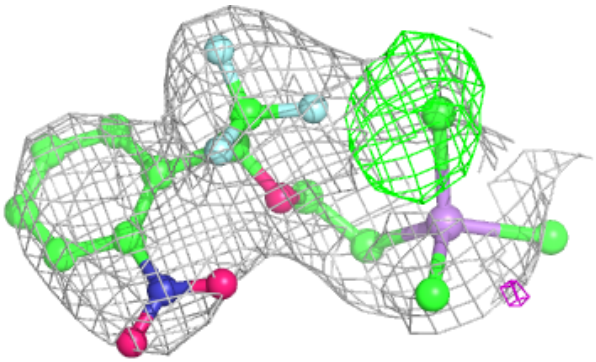


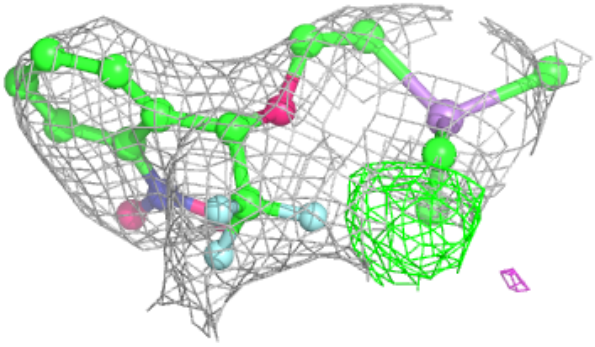


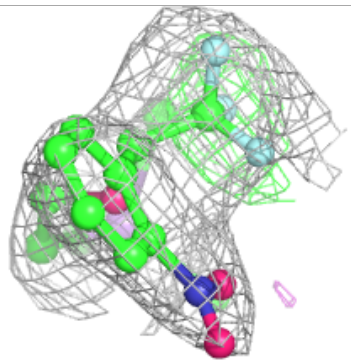


Electron density around CFQ A 1538 (A):

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

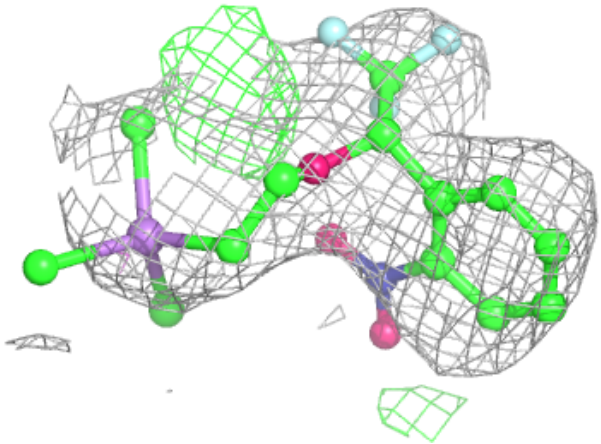


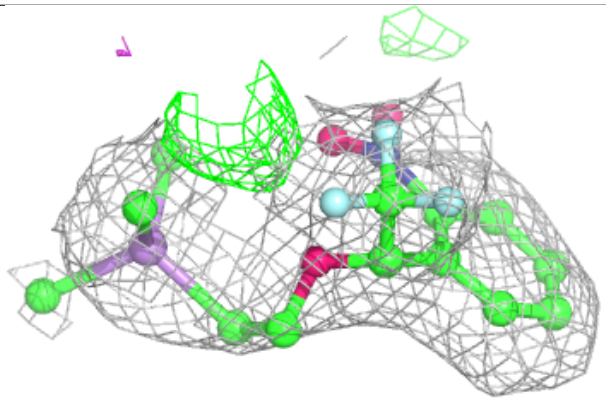


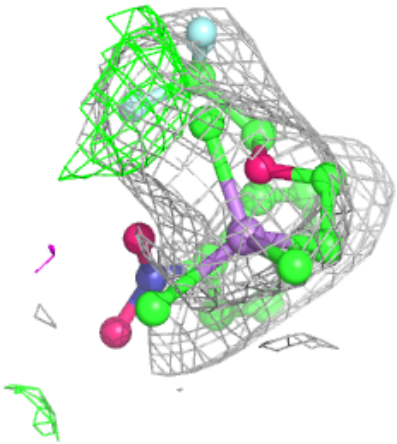


Electron density around CFQ A 1538 (B):

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

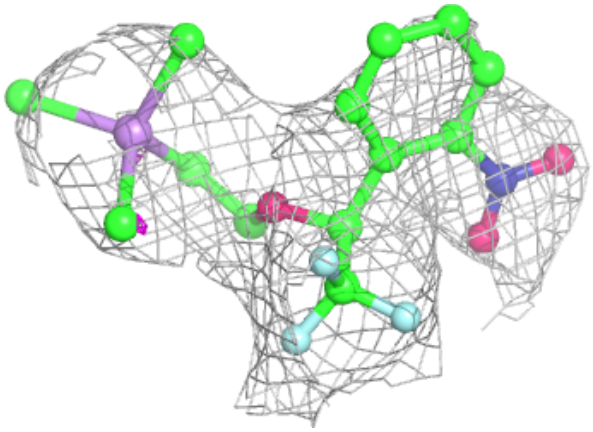


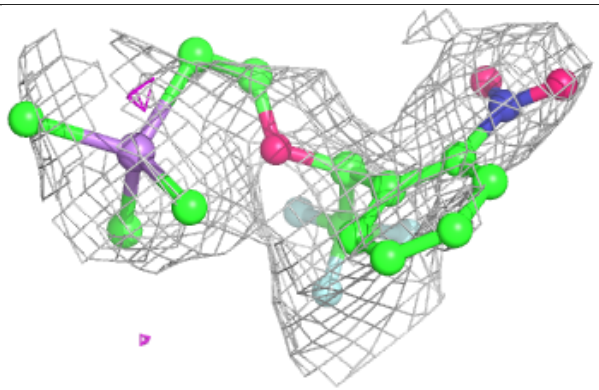


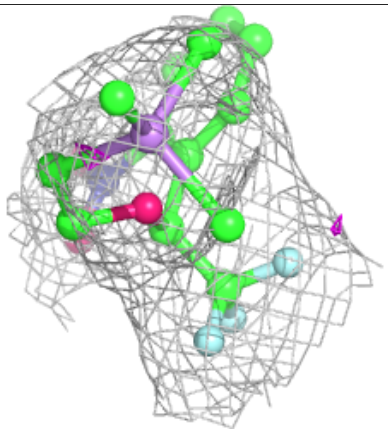


Electron density around CFQ B 1536 (A):

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

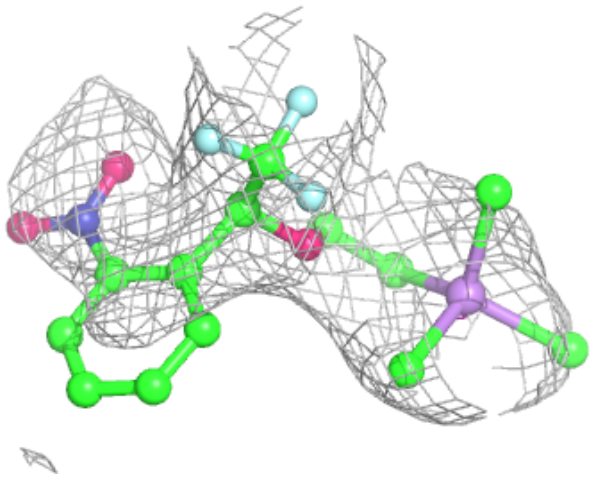


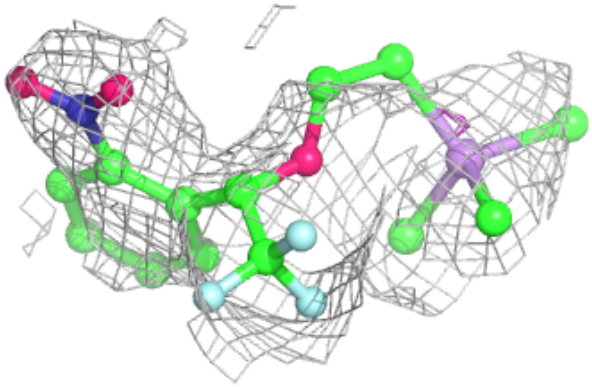


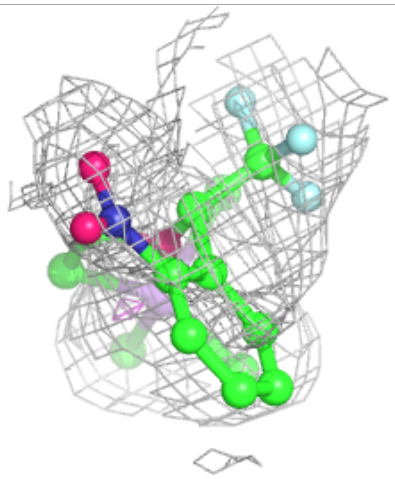


Electron density around CFQ B 1536 (B):

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

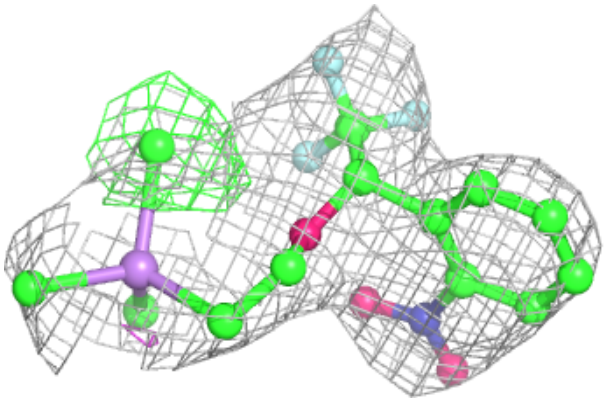


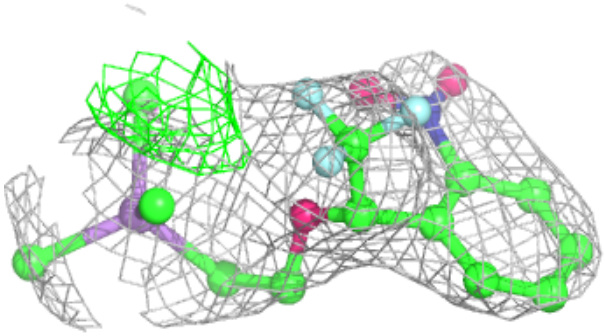


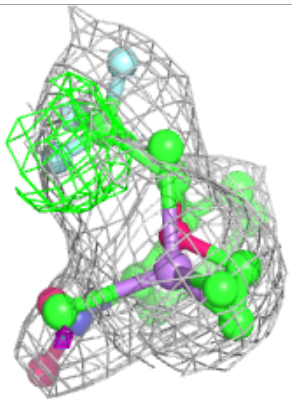


Electron density around CFQ B 1537 (A):

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

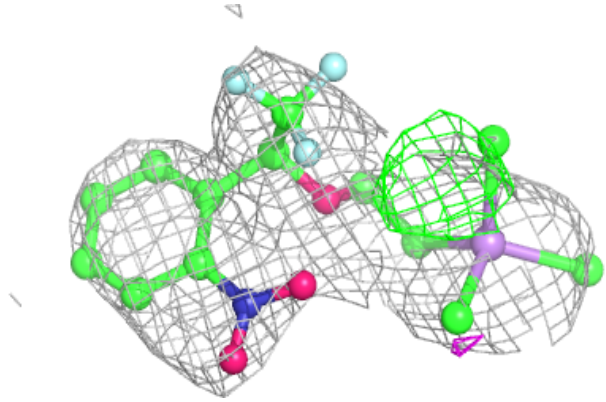


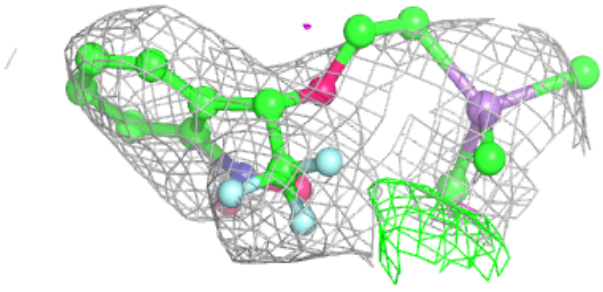


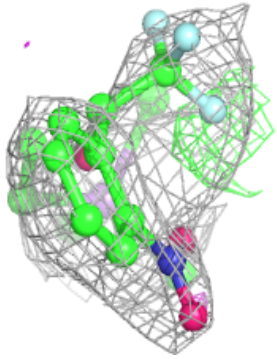


Electron density around CFQ B 1537 (B):

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.