Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2021 – 11:14 PM EDT

PDB ID	:	1T9U
Title	:	Structural Basis of Multidrug Transport by the AcrB Multidrug Efflux Pump
Authors	:	Yu, E.W.; McDermott, G.; Nikaido, H.
Deposited on	:	2004-05-18
Resolution	:	3.11 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 following versions of software and data (see references (1)) were used in the production of this report:

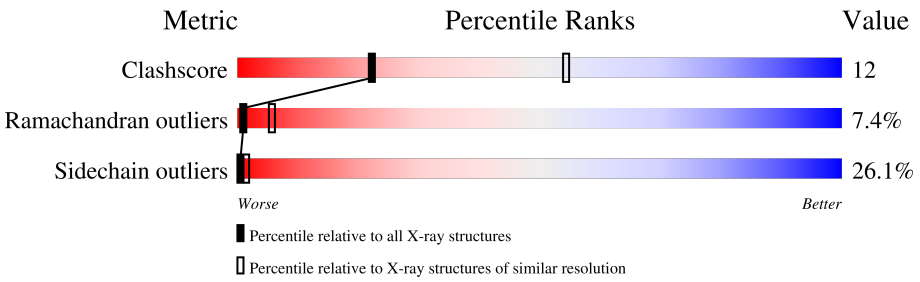
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.11 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))
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1049	56% 31% 8% • •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CPF	A	5002	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7739 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.

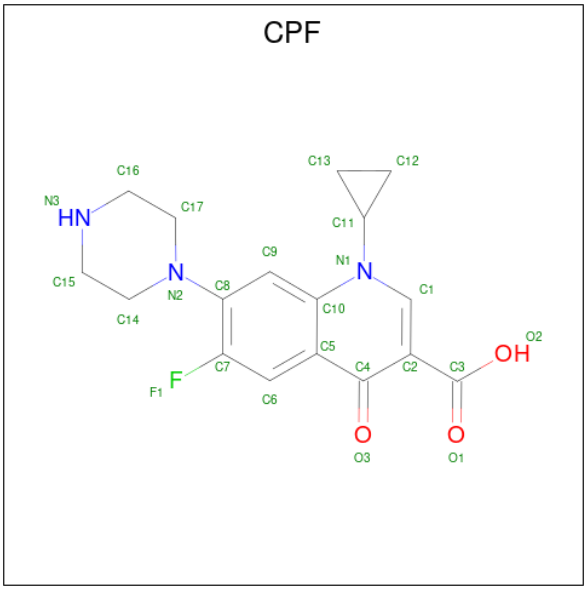
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1013	7691	4946	1272	1431	42	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ALA	ASN	engineered mutation	UNP P31224

- Molecule 2 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (three-letter code: CPF) (formula: $C_{17}H_{18}FN_3O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	24	17	1	3	3	0	0
			Total	C	F	N	O		
2	A	1	24	17	1	3	3	0	0

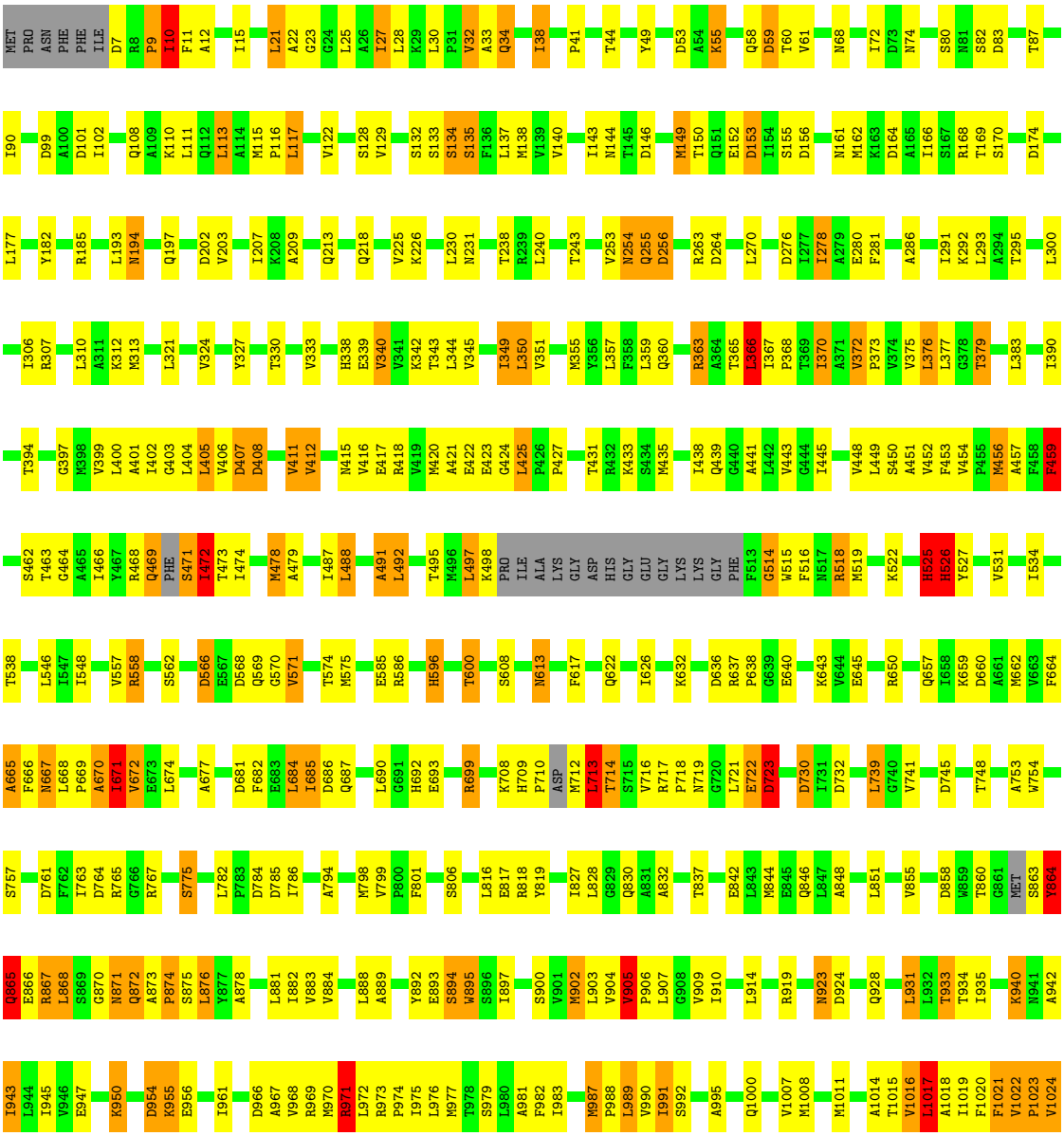
3 Residue-property plots (i)

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

Note EDS was not executed.

- Molecule 1: Acriflavine resistance protein B

Chain A: 56% 31% 8%



F1025
F1026
Y1027
V1028
V1029
R1030
R1031
R1032
F1033
S1034
R1035
K1036
ASN
GLU
ASP
ILE
GLU
HIS
SER
HIS
THR
VAL
ASP
HIS
HIS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	144.09Å 144.09Å 518.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	182.57 – 3.11	Depositor
% Data completeness (in resolution range)	(Not available) (182.57-3.11)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.265 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7739	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CPF

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	0.36	0/7830	0.73	35/10630 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	4

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1032	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	722	GLU	N-CA-C	6.12	127.53	111.00
1	A	568	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	924	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	966	ASP	CB-CG-OD2	5.77	123.49	118.30
1	A	7	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	407	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	53	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	276	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	408	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	732	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	99	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	174	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	153	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	764	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	83	ASP	CB-CG-OD2	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	660	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	745	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	101	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	858	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	954	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	686	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	146	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	784	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	723	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	256	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	761	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	566	ASP	CB-CG-OD2	5.09	122.89	118.30
1	A	730	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	785	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	264	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	636	ASP	CB-CG-OD2	5.03	122.82	118.30
1	A	59	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	202	ASP	CB-CG-OD2	5.01	122.81	118.30
1	A	156	ASP	CB-CG-OD2	5.00	122.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	722	GLU	CA
1	A	954	ASP	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	525	HIS	Peptide
1	A	712	MET	Peptide
1	A	864	TYR	Peptide
1	A	867	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7691	0	7851	181	0
2	A	48	0	34	10	0
All	All	7739	0	7885	181	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 12.

All (181) 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:830:GLN:NE2	2:A:5002:CPF:H121	1.53	1.22
1:A:830:GLN:HE22	2:A:5002:CPF:C12	1.59	1.09
1:A:667:ASN:OD1	2:A:5002:CPF:H152	1.53	1.06
1:A:830:GLN:HE22	2:A:5002:CPF:H121	0.80	0.96
1:A:667:ASN:OD1	2:A:5002:CPF:C15	2.19	0.90
1:A:950:LYS:NZ	1:A:1028:VAL:HG11	1.94	0.83
1:A:525:HIS:HB2	1:A:526:HIS:HB2	1.65	0.78
1:A:1023:PRO:HB3	1:A:1027:VAL:HG13	1.65	0.78
1:A:471:SER:O	1:A:473:THR:N	2.20	0.74
1:A:830:GLN:NE2	2:A:5002:CPF:H122	2.04	0.73
1:A:399:VAL:HA	1:A:402:ILE:HD12	1.76	0.67
1:A:990:VAL:HG21	1:A:1008:MET:SD	2.36	0.65
1:A:904:VAL:HA	1:A:907:LEU:HD13	1.78	0.65
1:A:892:TYR:CD2	1:A:897:ILE:HG21	2.33	0.64
1:A:365:THR:O	1:A:365:THR:HG23	1.97	0.64
1:A:950:LYS:HZ3	1:A:1028:VAL:HG11	1.62	0.64
1:A:459:PHE:CD1	1:A:468:ARG:HG3	2.33	0.64
1:A:830:GLN:CD	2:A:5002:CPF:H122	2.17	0.64
1:A:950:LYS:HZ2	1:A:1028:VAL:HG11	1.60	0.63
1:A:830:GLN:CD	2:A:5002:CPF:C12	2.65	0.63
1:A:383:LEU:HD11	1:A:473:THR:HG23	1.81	0.63
1:A:681:ASP:O	1:A:860:THR:O	2.16	0.63
1:A:33:ALA:O	1:A:34:GLN:O	2.16	0.63
1:A:905:VAL:HG23	1:A:906:PRO:HD3	1.82	0.61
1:A:400:LEU:HD11	1:A:933:THR:HG21	1.82	0.61
1:A:709:HIS:CD2	1:A:709:HIS:O	2.55	0.60
1:A:1024:VAL:O	1:A:1025:PHE:CG	2.56	0.59
1:A:525:HIS:HB2	1:A:526:HIS:CB	2.31	0.59
1:A:1023:PRO:HA	1:A:1026:PHE:HB2	1.86	0.57
1:A:372:VAL:H	1:A:373:PRO:HD2	1.69	0.57
1:A:117:LEU:HD23	1:A:117:LEU:N	2.20	0.57
1:A:10:ILE:CD1	1:A:10:ILE:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLY:O	1:A:401:ALA:HB2	2.06	0.55
1:A:525:HIS:CB	1:A:526:HIS:HB2	2.34	0.55
1:A:527:TYR:O	1:A:531:VAL:HG23	2.06	0.55
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.89	0.55
1:A:717:ARG:HD2	1:A:719:ASN:HD21	1.72	0.55
1:A:1015:THR:O	1:A:1019:ILE:HG22	2.07	0.55
1:A:21:LEU:O	1:A:23:GLY:N	2.41	0.54
1:A:55:LYS:HD2	1:A:816:LEU:HD11	1.89	0.54
1:A:525:HIS:HB2	1:A:526:HIS:CG	2.43	0.53
1:A:1032:ARG:CG	1:A:1032:ARG:HH11	2.20	0.53
1:A:463:THR:HG23	1:A:466:ILE:HG21	1.91	0.52
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.91	0.52
1:A:366:LEU:O	1:A:370:ILE:HG13	2.09	0.52
1:A:425:LEU:C	1:A:427:PRO:HD2	2.29	0.52
1:A:872:GLN:HG2	1:A:876:LEU:HD11	1.91	0.52
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.90	0.52
1:A:90:ILE:N	1:A:90:ILE:HD12	2.24	0.52
1:A:349:ILE:HG22	1:A:350:LEU:HD23	1.91	0.52
1:A:894:SER:O	1:A:895:TRP:CE3	2.63	0.51
1:A:881:LEU:HD13	1:A:902:MET:CE	2.40	0.51
1:A:710:PRO:HB2	1:A:713:LEU:CB	2.40	0.51
1:A:897:ILE:O	1:A:900:SER:OG	2.23	0.51
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.58	0.51
1:A:870:GLY:O	1:A:872:GLN:N	2.43	0.51
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.93	0.51
1:A:9:PRO:HA	1:A:491:ALA:HB1	1.92	0.51
1:A:945:ILE:HA	1:A:971:ARG:CZ	2.41	0.51
1:A:10:ILE:HD13	1:A:11:PHE:H	1.77	0.50
1:A:905:VAL:HG12	1:A:935:ILE:HG12	1.94	0.50
1:A:459:PHE:CD1	1:A:459:PHE:N	2.80	0.50
1:A:971:ARG:HD2	1:A:971:ARG:C	2.32	0.50
1:A:1016:VAL:O	1:A:1017:LEU:HB2	2.12	0.50
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.94	0.50
1:A:415:ASN:HB3	1:A:438:ILE:HD11	1.94	0.50
1:A:338:HIS:O	1:A:338:HIS:ND1	2.45	0.49
1:A:667:ASN:OD1	2:A:5002:CPF:H151	2.08	0.49
1:A:534:ILE:HB	1:A:1026:PHE:CZ	2.48	0.49
1:A:709:HIS:N	1:A:710:PRO:HD3	2.27	0.49
1:A:451:ALA:CB	1:A:883:VAL:HG11	2.42	0.49
1:A:664:PHE:O	1:A:665:ALA:HB2	2.13	0.49
1:A:41:PRO:HB3	1:A:295:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:VAL:O	1:A:416:VAL:HG23	2.12	0.49
1:A:133:SER:O	1:A:135:SER:N	2.46	0.49
1:A:721:LEU:O	1:A:723:ASP:N	2.45	0.48
1:A:456:MET:HA	1:A:876:LEU:HB3	1.96	0.48
1:A:596:HIS:O	1:A:600:THR:HG22	2.13	0.48
1:A:10:ILE:N	1:A:10:ILE:HD12	2.28	0.48
1:A:1027:VAL:HG23	1:A:1028:VAL:H	1.78	0.48
1:A:68:ASN:HD21	1:A:113:LEU:HB2	1.78	0.48
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.96	0.48
1:A:613:ASN:HD22	1:A:613:ASN:C	2.17	0.48
1:A:987:MET:N	1:A:988:PRO:HD2	2.29	0.48
1:A:394:THR:HG22	1:A:469:GLN:HB3	1.95	0.47
1:A:518:ARG:O	1:A:522:LYS:HD2	2.14	0.47
1:A:973:ARG:HB3	1:A:974:PRO:CD	2.44	0.47
1:A:448:VAL:HG11	1:A:888:LEU:HG	1.97	0.47
1:A:457:ALA:HB2	1:A:471:SER:HB3	1.96	0.47
1:A:463:THR:CB	1:A:868:LEU:HD22	2.45	0.47
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.44	0.46
1:A:344:LEU:HD21	1:A:376:LEU:HD11	1.96	0.46
1:A:570:GLY:O	1:A:571:VAL:HG23	2.15	0.46
1:A:682:PHE:HB3	1:A:827:ILE:HB	1.97	0.46
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.96	0.46
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.98	0.46
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.44	0.46
1:A:923:ASN:C	1:A:923:ASN:HD22	2.19	0.46
1:A:363:ARG:HG3	1:A:497:LEU:O	2.16	0.46
1:A:873:ALA:HA	1:A:876:LEU:HD12	1.98	0.46
1:A:664:PHE:O	1:A:665:ALA:CB	2.63	0.46
1:A:967:ALA:O	1:A:971:ARG:HG3	2.17	0.45
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.98	0.45
1:A:134:SER:O	1:A:135:SER:HB3	2.16	0.45
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.99	0.45
1:A:531:VAL:O	1:A:534:ILE:HG13	2.16	0.45
1:A:140:VAL:HG11	1:A:310:LEU:HD11	1.99	0.45
1:A:942:ALA:O	1:A:945:ILE:N	2.50	0.45
1:A:1021:PHE:O	1:A:1026:PHE:CE1	2.70	0.45
1:A:367:ILE:HG12	1:A:492:LEU:HD22	1.98	0.44
1:A:710:PRO:HB2	1:A:713:LEU:HB3	1.99	0.44
1:A:848:ALA:HA	1:A:851:LEU:HD12	1.99	0.44
1:A:867:ARG:C	1:A:868:LEU:HD23	2.37	0.44
1:A:365:THR:O	1:A:365:THR:CG2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:979:SER:CB	1:A:1015:THR:HG21	2.47	0.44
1:A:383:LEU:HD21	1:A:473:THR:HA	1.99	0.44
1:A:905:VAL:O	1:A:909:VAL:HG23	2.17	0.44
1:A:478:MET:HG2	1:A:479:ALA:N	2.32	0.44
1:A:1024:VAL:H	1:A:1027:VAL:HG22	1.82	0.44
1:A:487:ILE:HG22	1:A:488:LEU:N	2.33	0.44
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.52	0.44
1:A:971:ARG:HD2	1:A:971:ARG:O	2.18	0.44
1:A:471:SER:OG	1:A:472:ILE:N	2.51	0.43
1:A:487:ILE:HG22	1:A:488:LEU:H	1.83	0.43
1:A:1018:ALA:O	1:A:1024:VAL:HB	2.18	0.43
1:A:111:LEU:O	1:A:111:LEU:HD23	2.18	0.43
1:A:669:PRO:O	1:A:670:ALA:CB	2.65	0.43
1:A:115:MET:N	1:A:116:PRO:CD	2.82	0.43
1:A:464:GLY:O	1:A:468:ARG:HB2	2.19	0.43
1:A:453:PHE:CD2	1:A:471:SER:HA	2.53	0.43
1:A:514:GLY:O	1:A:516:PHE:N	2.52	0.43
1:A:989:LEU:HD22	1:A:1000:GLN:HE21	1.84	0.43
1:A:144:ASN:ND2	1:A:149:MET:SD	2.92	0.43
1:A:379:THR:O	1:A:383:LEU:HG	2.18	0.43
1:A:739:LEU:HD12	1:A:799:VAL:HG11	2.00	0.43
1:A:1011:MET:HA	1:A:1014:ALA:HB3	1.99	0.43
1:A:32:VAL:HA	1:A:390:ILE:HB	2.00	0.43
1:A:684:LEU:HD11	1:A:855:VAL:HG13	1.99	0.43
1:A:713:LEU:O	1:A:832:ALA:HB2	2.19	0.43
1:A:27:ILE:HG22	1:A:28:LEU:HD12	2.01	0.42
1:A:1029:VAL:O	1:A:1033:PHE:HB2	2.19	0.42
1:A:339:GLU:O	1:A:340:VAL:HG23	2.19	0.42
1:A:684:LEU:HD23	1:A:699:ARG:HB2	2.01	0.42
1:A:684:LEU:C	1:A:684:LEU:HD12	2.40	0.42
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.53	0.42
1:A:904:VAL:O	1:A:907:LEU:HB2	2.18	0.42
1:A:441:ALA:HB2	1:A:947:GLU:HG2	2.02	0.42
1:A:666:PHE:HB3	2:A:5002:CPF:F1	2.10	0.42
1:A:373:PRO:O	1:A:377:LEU:HG	2.20	0.42
1:A:895:TRP:CE3	1:A:895:TRP:HA	2.55	0.42
1:A:970:MET:O	1:A:971:ARG:HB3	2.19	0.42
1:A:450:SER:O	1:A:454:VAL:HG23	2.20	0.41
1:A:468:ARG:O	1:A:471:SER:N	2.53	0.41
1:A:968:VAL:HA	1:A:971:ARG:NE	2.35	0.41
1:A:344:LEU:C	1:A:344:LEU:HD13	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:HG12	1:A:443:VAL:O	2.20	0.41
1:A:203:VAL:O	1:A:207:ILE:HG13	2.21	0.41
1:A:403:GLY:HA3	1:A:982:PHE:CD1	2.56	0.41
1:A:12:ALA:HB1	1:A:487:ILE:HG22	2.02	0.41
1:A:108:GLN:HB3	1:A:129:VAL:HG11	2.03	0.41
1:A:864:TYR:CD2	1:A:865:GLN:N	2.89	0.41
1:A:401:ALA:O	1:A:402:ILE:C	2.59	0.41
1:A:892:TYR:OH	1:A:943:ILE:HG23	2.20	0.41
1:A:291:ILE:HG21	1:A:306:ILE:HD11	2.02	0.41
1:A:278:ILE:HD12	1:A:613:ASN:HB3	2.03	0.41
1:A:878:ALA:O	1:A:882:ILE:HG13	2.20	0.41
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.56	0.41
1:A:864:TYR:CD2	1:A:864:TYR:N	2.89	0.41
1:A:531:VAL:HA	1:A:534:ILE:CG1	2.51	0.41
1:A:38:ILE:HG21	1:A:466:ILE:HD11	2.03	0.40
1:A:194:ASN:O	1:A:194:ASN:ND2	2.55	0.40
1:A:931:LEU:O	1:A:935:ILE:HD12	2.21	0.40
1:A:1024:VAL:N	1:A:1027:VAL:HG22	2.36	0.40
1:A:685:ILE:HD11	1:A:819:TYR:HD2	1.86	0.40
1:A:753:ALA:O	1:A:775:SER:OG	2.38	0.40
1:A:254:ASN:O	1:A:256:ASP:N	2.54	0.40
1:A:416:VAL:O	1:A:420:MET:HG3	2.21	0.40
1:A:558:ARG:HD2	1:A:558:ARG:HA	1.96	0.40
1:A:669:PRO:O	1:A:670:ALA:HB3	2.21	0.40
1:A:670:ALA:O	1:A:671:ILE:C	2.60	0.40
1:A:1032:ARG:HH11	1:A:1032:ARG:HG3	1.85	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	1003/1049 (96%)	795 (79%)	134 (13%)	74 (7%)	1 6

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	22	ALA
1	A	34	GLN
1	A	134	SER
1	A	135	SER
1	A	255	GLN
1	A	459	PHE
1	A	472	ILE
1	A	515	TRP
1	A	665	ALA
1	A	670	ALA
1	A	713	LEU
1	A	722	GLU
1	A	794	ALA
1	A	871	ASN
1	A	874	PRO
1	A	889	ALA
1	A	971	ARG
1	A	1017	LEU
1	A	1021	PHE
1	A	1023	PRO
1	A	1025	PHE
1	A	9	PRO
1	A	110	LYS
1	A	152	GLU
1	A	161	ASN
1	A	327	TYR
1	A	340	VAL
1	A	349	ILE
1	A	421	ALA
1	A	424	GLY
1	A	495	THR
1	A	525	HIS
1	A	718	PRO
1	A	723	ASP
1	A	864	TYR
1	A	865	GLN
1	A	875	SER

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Mol	Chain	Res	Type
1	A	954	ASP
1	A	1035	ARG
1	A	74	ASN
1	A	170	SER
1	A	209	ALA
1	A	366	LEU
1	A	405	LEU
1	A	488	LEU
1	A	526	HIS
1	A	671	ILE
1	A	714	THR
1	A	955	LYS
1	A	995	ALA
1	A	1026	PHE
1	A	21	LEU
1	A	538	THR
1	A	638	PRO
1	A	677	ALA
1	A	837	THR
1	A	956	GLU
1	A	894	SER
1	A	905	VAL
1	A	940	LYS
1	A	1034	SER
1	A	372	VAL
1	A	491	ALA
1	A	571	VAL
1	A	893	GLU
1	A	1016	VAL
1	A	1027	VAL
1	A	626	ILE
1	A	943	ILE
1	A	991	ILE
1	A	411	VAL
1	A	672	VAL
1	A	514	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	823/854 (96%)	608 (74%)	215 (26%)	0 1

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	15	ILE
1	A	25	LEU
1	A	27	ILE
1	A	30	LEU
1	A	32	VAL
1	A	38	ILE
1	A	44	THR
1	A	49	TYR
1	A	55	LYS
1	A	58	GLN
1	A	59	ASP
1	A	72	ILE
1	A	80	SER
1	A	82	SER
1	A	87	THR
1	A	102	ILE
1	A	113	LEU
1	A	117	LEU
1	A	122	VAL
1	A	128	SER
1	A	132	SER
1	A	137	LEU
1	A	138	MET
1	A	149	MET
1	A	150	THR
1	A	153	ASP
1	A	155	SER
1	A	162	MET
1	A	164	ASP
1	A	166	ILE
1	A	168	ARG
1	A	169	THR
1	A	177	LEU
1	A	182	TYR

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Mol	Chain	Res	Type
1	A	185	ARG
1	A	193	LEU
1	A	194	ASN
1	A	197	GLN
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	230	LEU
1	A	238	THR
1	A	240	LEU
1	A	243	THR
1	A	253	VAL
1	A	254	ASN
1	A	255	GLN
1	A	263	ARG
1	A	270	LEU
1	A	278	ILE
1	A	280	GLU
1	A	292	LYS
1	A	293	LEU
1	A	300	LEU
1	A	307	ARG
1	A	312	LYS
1	A	313	MET
1	A	321	LEU
1	A	330	THR
1	A	333	VAL
1	A	342	LYS
1	A	343	THR
1	A	345	VAL
1	A	350	LEU
1	A	355	MET
1	A	357	LEU
1	A	359	LEU
1	A	360	GLN
1	A	363	ARG
1	A	366	LEU
1	A	370	ILE
1	A	376	LEU
1	A	379	THR
1	A	404	LEU
1	A	406	VAL

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Mol	Chain	Res	Type
1	A	407	ASP
1	A	408	ASP
1	A	411	VAL
1	A	412	VAL
1	A	417	GLU
1	A	418	ARG
1	A	422	GLU
1	A	423	GLU
1	A	425	LEU
1	A	431	THR
1	A	433	LYS
1	A	435	MET
1	A	439	GLN
1	A	445	ILE
1	A	449	LEU
1	A	452	VAL
1	A	456	MET
1	A	459	PHE
1	A	462	SER
1	A	469	GLN
1	A	471	SER
1	A	472	ILE
1	A	474	ILE
1	A	478	MET
1	A	492	LEU
1	A	497	LEU
1	A	498	LYS
1	A	518	ARG
1	A	519	MET
1	A	526	HIS
1	A	546	LEU
1	A	548	ILE
1	A	557	VAL
1	A	558	ARG
1	A	562	SER
1	A	566	ASP
1	A	569	GLN
1	A	574	THR
1	A	575	MET
1	A	585	GLU
1	A	586	ARG
1	A	596	HIS

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Mol	Chain	Res	Type
1	A	600	THR
1	A	608	SER
1	A	613	ASN
1	A	617	PHE
1	A	622	GLN
1	A	632	LYS
1	A	637	ARG
1	A	640	GLU
1	A	643	LYS
1	A	645	GLU
1	A	650	ARG
1	A	657	GLN
1	A	659	LYS
1	A	662	MET
1	A	667	ASN
1	A	668	LEU
1	A	671	ILE
1	A	672	VAL
1	A	674	LEU
1	A	684	LEU
1	A	685	ILE
1	A	687	GLN
1	A	690	LEU
1	A	692	HIS
1	A	693	GLU
1	A	699	ARG
1	A	708	LYS
1	A	713	LEU
1	A	714	THR
1	A	716	VAL
1	A	730	ASP
1	A	739	LEU
1	A	741	VAL
1	A	748	THR
1	A	757	SER
1	A	763	ILE
1	A	765	ARG
1	A	767	ARG
1	A	775	SER
1	A	782	LEU
1	A	798	MET
1	A	801	PHE

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Mol	Chain	Res	Type
1	A	806	SER
1	A	817	GLU
1	A	818	ARG
1	A	828	LEU
1	A	842	GLU
1	A	844	MET
1	A	846	GLN
1	A	863	SER
1	A	864	TYR
1	A	865	GLN
1	A	866	GLU
1	A	868	LEU
1	A	871	ASN
1	A	872	GLN
1	A	876	LEU
1	A	884	VAL
1	A	895	TRP
1	A	902	MET
1	A	903	LEU
1	A	905	VAL
1	A	910	ILE
1	A	914	LEU
1	A	919	ARG
1	A	923	ASN
1	A	928	GLN
1	A	931	LEU
1	A	933	THR
1	A	934	THR
1	A	940	LYS
1	A	950	LYS
1	A	955	LYS
1	A	961	ILE
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	975	ILE
1	A	976	LEU
1	A	977	MET
1	A	983	ILE
1	A	987	MET
1	A	989	LEU
1	A	991	ILE

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Mol	Chain	Res	Type
1	A	992	SER
1	A	1007	VAL
1	A	1017	LEU
1	A	1020	PHE
1	A	1022	VAL
1	A	1024	VAL
1	A	1027	VAL
1	A	1030	ARG
1	A	1031	ARG
1	A	1032	ARG
1	A	1035	ARG
1	A	1036	LYS

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

Mol	Chain	Res	Type
1	A	68	ASN
1	A	124	GLN
1	A	125	GLN
1	A	181	GLN
1	A	194	ASN
1	A	213	GLN
1	A	218	GLN
1	A	254	ASN
1	A	361	ASN
1	A	415	ASN
1	A	437	GLN
1	A	577	GLN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	709	HIS
1	A	719	ASN
1	A	760	ASN
1	A	830	GLN
1	A	872	GLN
1	A	923	ASN
1	A	1000	GLN
1	A	1001	ASN

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)

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	CPF	A	5002	1	19,27,27	1.23	2 (10%)	20,40,40	1.00	1 (5%)
2	CPF	A	5001	-	19,27,27	1.23	2 (10%)	20,40,40	1.00	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
2	CPF	A	5002	1	-	0/8/22/22	0/4/4/4
2	CPF	A	5001	-	-	0/8/22/22	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	CPF	C2-C3	4.11	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5002	CPF	C2-C3	4.07	1.51	1.47
2	A	5002	CPF	O3-C4	2.55	1.27	1.23
2	A	5001	CPF	O3-C4	2.48	1.27	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5001	CPF	C4-C5-C10	3.11	121.30	118.59
2	A	5002	CPF	C4-C5-C10	3.11	121.30	118.59

There are no chirality outliers.

There are no torsion outliers.

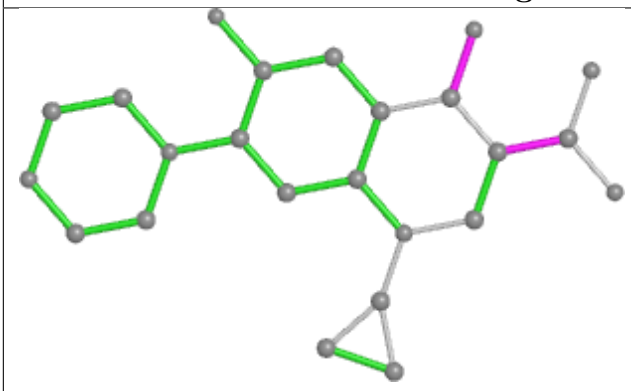
There are no ring outliers.

1 monomer is involved in 10 short contacts:

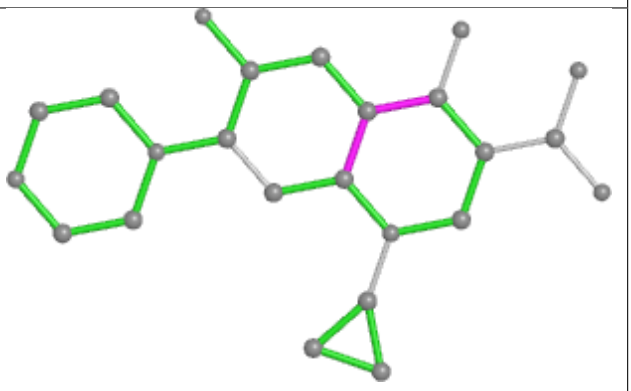
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5002	CPF	10	0

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.

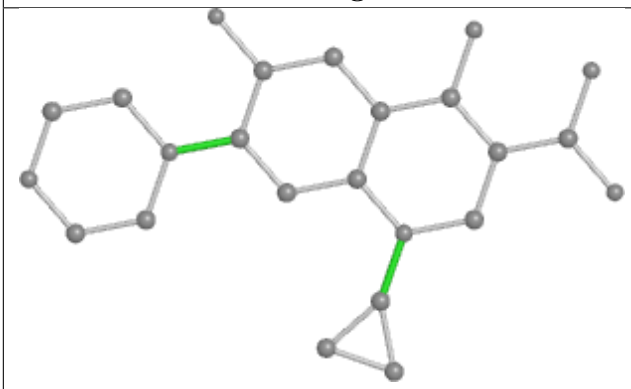
Ligand CPF A 5002



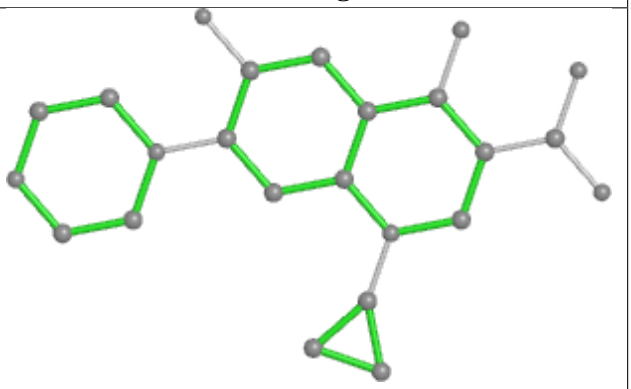
Bond lengths



Bond angles

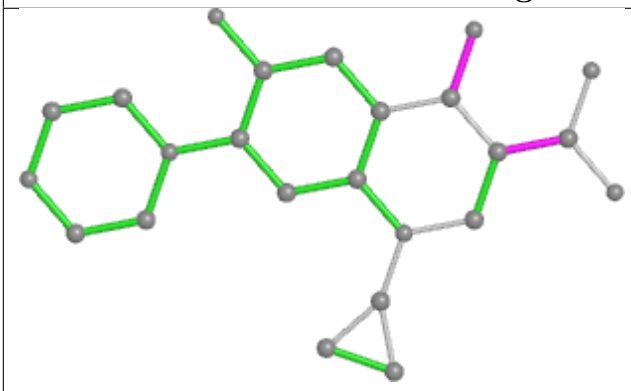


Torsions

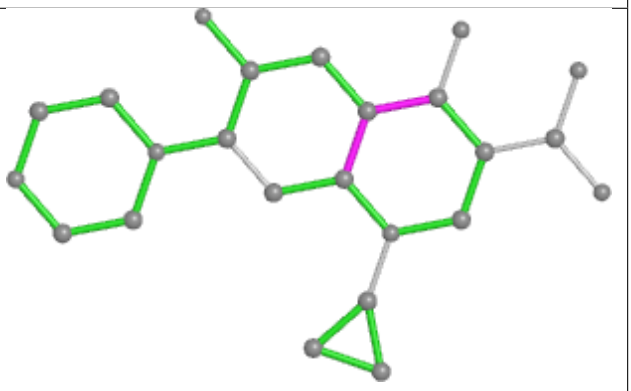


Rings

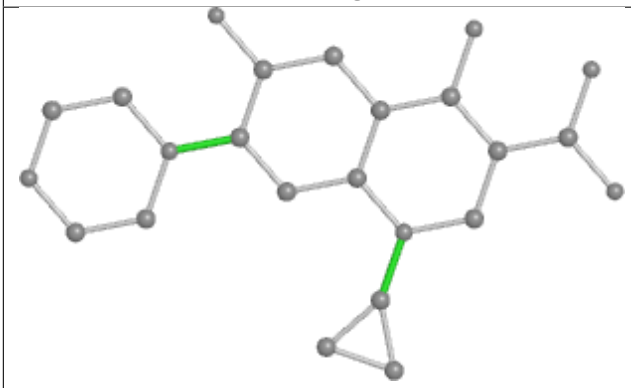
Ligand CPF A 5001



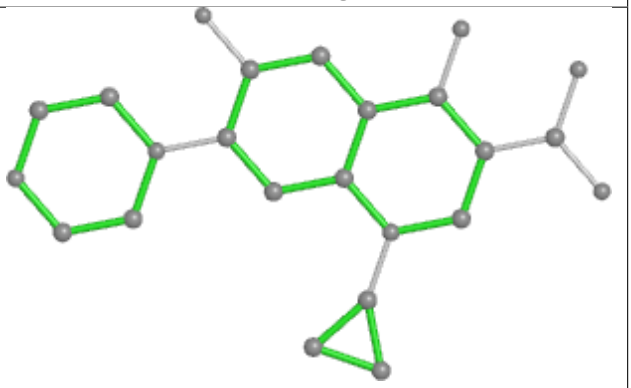
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.