Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 04:40 PM JST

PDB ID	:	5V56
Title	:	2.9A XFEL structure of the multi-domain human smoothened receptor (with E194M mutation) in complex with TC114
Authors	:	Zhang, X.; Zhao, F.; Wu, Y.; Yang, J.; Han, G.W.; Zhao, S.; Ishchenko, A.; Ye, L.; Lin, X.; Ding, K.; Dharmarajan, V.; Griffin, P.R.; Gati, C.; Nelson, G.; Hunter, M.S.; Hanson, M.A.; Cherezov, V.; Stevens, R.C.; Tan, W.; Tao, H.; Xu, F.
Deposited on	:	2017-03-13
Resolution	:	2.90 Å(reported)

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

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

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

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

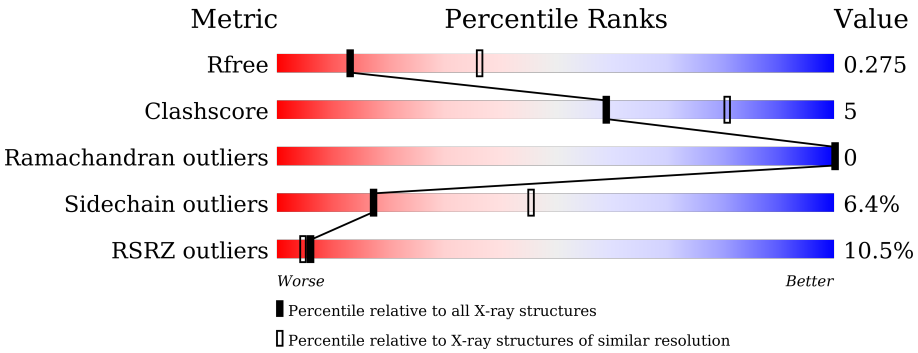
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	653	11% 82% 14%
1	B	653	9% 84% 12%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9901 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 Smoothened homolog,Flavodoxin,Smoothened homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	632	Total	C	N	O	S	0	0	0
			4869	3126	811	896	36			
1	B	634	Total	C	N	O	S	0	0	0
			4878	3128	818	896	36			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	MET	GLU	engineered mutation	UNP Q99835
A	1002	ALA	PRO	engineered mutation	UNP P00323
A	1098	TRP	TYR	engineered mutation	UNP P00323
A	559	HIS	-	expression tag	UNP Q99835
A	560	HIS	-	expression tag	UNP Q99835
A	561	HIS	-	expression tag	UNP Q99835
A	562	HIS	-	expression tag	UNP Q99835
A	563	HIS	-	expression tag	UNP Q99835
A	564	HIS	-	expression tag	UNP Q99835
A	565	HIS	-	expression tag	UNP Q99835
A	566	HIS	-	expression tag	UNP Q99835
A	567	HIS	-	expression tag	UNP Q99835
A	568	HIS	-	expression tag	UNP Q99835
B	194	MET	GLU	engineered mutation	UNP Q99835
B	1002	ALA	PRO	engineered mutation	UNP P00323
B	1098	TRP	TYR	engineered mutation	UNP P00323
B	559	HIS	-	expression tag	UNP Q99835
B	560	HIS	-	expression tag	UNP Q99835
B	561	HIS	-	expression tag	UNP Q99835
B	562	HIS	-	expression tag	UNP Q99835
B	563	HIS	-	expression tag	UNP Q99835
B	564	HIS	-	expression tag	UNP Q99835
B	565	HIS	-	expression tag	UNP Q99835
B	566	HIS	-	expression tag	UNP Q99835
B	567	HIS	-	expression tag	UNP Q99835

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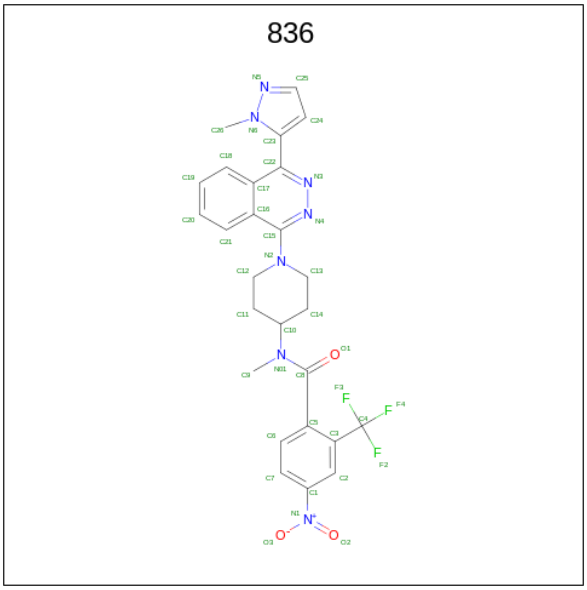
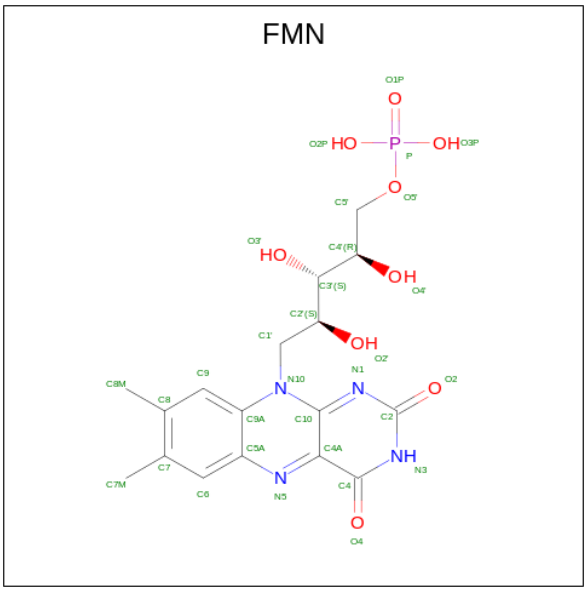
Chain	Residue	Modelled	Actual	Comment	Reference
B	568	HIS	-	expression tag	UNP Q99835

- Molecule 2 is N-methyl-N-[1-[4-(2-methylpyrazol-3-yl)phthalazin-1-yl]piperidin-4-yl]-4-nitro-2-(trifluoromethyl)benzamide (three-letter code: 836) (formula: $C_{26}H_{24}F_3N_7O_3$).



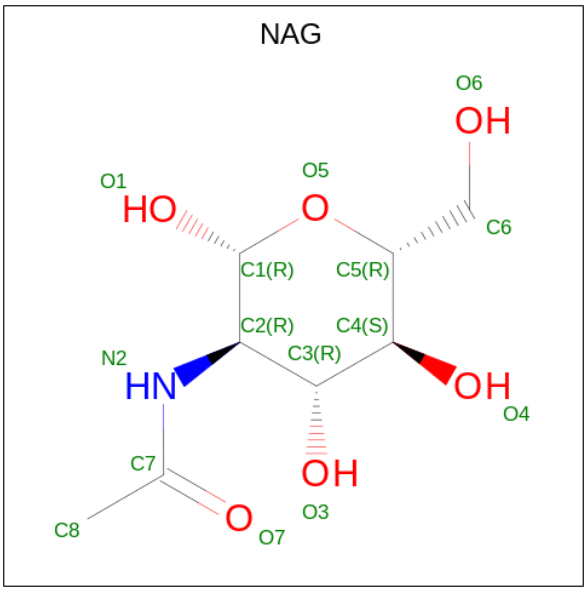
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	B	1	Total	C	F	N	O	0	0
			39	26	3	7	3		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



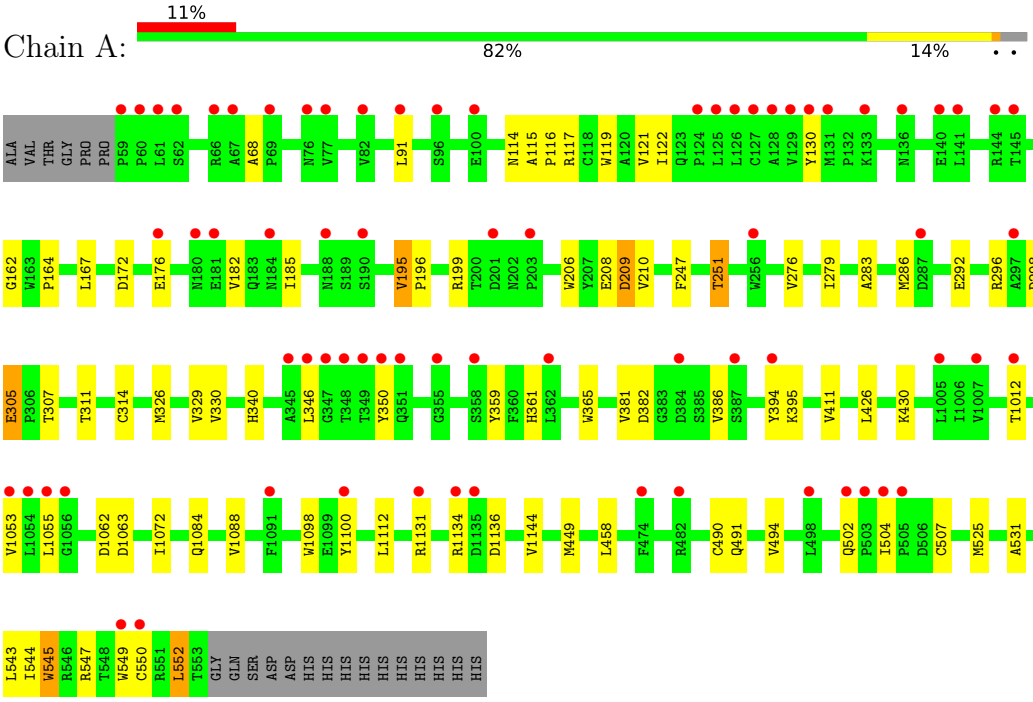
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

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

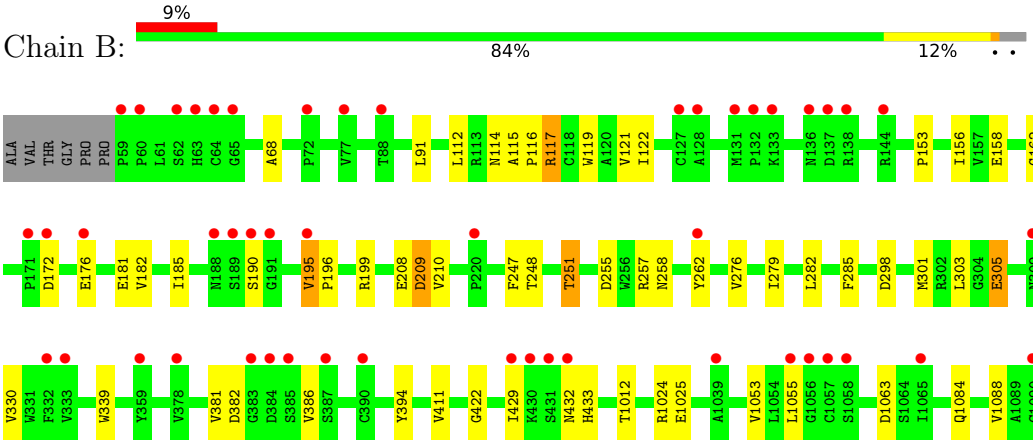
• Molecule 1: Smoothened homolog,Flavodoxin,Smoothened homolog

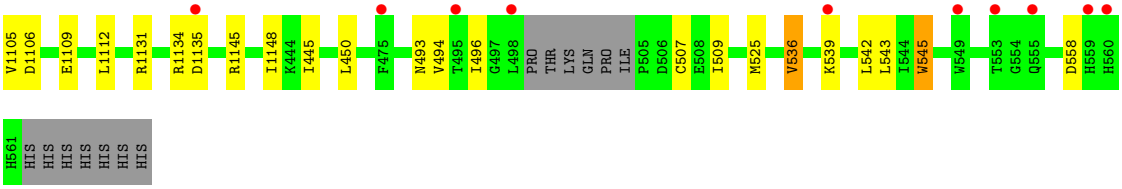
Chain A:



• Molecule 1: Smoothened homolog,Flavodoxin,Smoothened homolog

Chain B:




V1105
D1106
E1109
L1112
R1131
R1134
D1135
R1145
I1148
K444
I445
L450
F475
N493
V494
T495
I496
G497
L498
PRO
THR
LYS
GLN
PRO
ILE
P505
D506
C507
E508
T509
M525
V536
K539
L542
L543
I544
W545
W549
T553
G554
Q555
D558
H559
H560
H561
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	40.59Å 349.54Å 61.76Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	24.90 – 2.90 24.58 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.90-2.90) 100.0 (24.58-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.89Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.218 , 0.239 0.253 , 0.275	Depositor DCC
R_{free} test set	1810 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	82.2	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 73.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9901	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FMN, 836

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	0.46	0/4995	0.62	0/6807
1	B	0.50	0/5004	0.67	2/6815 (0.0%)
All	All	0.48	0/9999	0.64	2/13622 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	433	HIS	N-CA-C	5.46	125.75	111.00
1	B	305	GLU	N-CA-C	-5.14	97.12	111.00

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	4869	0	4661	48	0
1	B	4878	0	4655	42	0
2	A	39	0	0	0	0
2	B	39	0	0	0	0
3	A	31	0	19	1	0
3	B	31	0	19	1	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9901	0	9367	90	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 5.

All (90) 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:114:ASN:HB2	1:A:494:VAL:HG12	1.28	1.09
1:A:195:VAL:HG23	1:A:196:PRO:HD3	1.17	1.07
1:A:305:GLU:HB2	1:A:381:VAL:O	1.66	0.94
1:A:130:TYR:CD2	1:A:130:TYR:CZ	2.48	0.92
1:A:115:ALA:HB2	1:A:210:VAL:HG13	1.52	0.90
1:A:195:VAL:CG2	1:A:196:PRO:HD3	2.05	0.85
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.45	0.81
1:A:114:ASN:HB2	1:A:494:VAL:CG1	2.11	0.81
1:B:255:ASP:OD2	1:B:258:ASN:HB2	1.82	0.79
1:A:382:ASP:HB2	1:A:394:TYR:HB2	1.66	0.75
1:B:195:VAL:HG23	1:B:196:PRO:HD3	1.68	0.74
1:A:195:VAL:HG23	1:A:196:PRO:CD	2.09	0.74
1:B:116:PRO:HB3	1:B:190:SER:O	1.88	0.73
1:B:382:ASP:HB2	1:B:394:TYR:HB2	1.71	0.73
1:B:247:PHE:O	1:B:251:THR:HG22	1.92	0.70
1:A:305:GLU:HB3	1:A:381:VAL:HB	1.75	0.68
1:A:1042:GLU:O	1:A:1046:LEU:HD13	1.98	0.64
1:B:115:ALA:HB2	1:B:210:VAL:HG13	1.80	0.63
1:B:251:THR:HB	1:B:545:TRP:CZ3	2.33	0.63
1:B:1055:LEU:HD12	1:B:1112:LEU:HD11	1.81	0.63
1:A:361:HIS:HD2	1:A:365:TRP:HE1	1.45	0.62
1:A:1055:LEU:HD12	1:A:1112:LEU:HD11	1.82	0.61
1:A:305:GLU:CB	1:A:381:VAL:O	2.45	0.59
1:A:117:ARG:HD2	1:A:206:TRP:CZ2	2.36	0.59
1:B:1025:GLU:HG3	1:B:1145:ARG:HH12	1.68	0.58
1:A:164:PRO:HD2	1:A:167:LEU:HB2	1.84	0.58
1:A:292:GLU:OE2	1:A:311:THR:HG21	2.04	0.58
1:A:502:GLN:HB2	1:A:504:ILE:HG12	1.85	0.57
1:B:115:ALA:N	1:B:116:PRO:HD3	2.20	0.56
1:A:283:ALA:O	1:A:286:MET:HG3	2.05	0.56
1:B:164:PRO:HD2	1:B:167:LEU:HB2	1.89	0.55
1:B:276:VAL:HA	1:B:279:ILE:HD12	1.88	0.55
1:B:1012:THR:HB	3:B:1202:FMN:O1P	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:PRO:HG2	1:A:491:GLN:HB3	1.89	0.53
1:A:251:THR:HB	1:A:545:TRP:CZ3	2.43	0.53
1:B:255:ASP:OD2	1:B:258:ASN:CB	2.54	0.53
1:A:302:ARG:HH22	1:A:311:THR:HG23	1.73	0.53
1:B:182:VAL:HA	1:B:185:ILE:HD12	1.91	0.53
1:A:115:ALA:N	1:A:116:PRO:CD	2.73	0.52
1:A:182:VAL:HA	1:A:185:ILE:HD12	1.92	0.52
1:A:494:VAL:HG23	1:A:494:VAL:O	2.09	0.52
1:A:276:VAL:HA	1:A:279:ILE:HD12	1.91	0.52
1:A:114:ASN:CB	1:A:494:VAL:HG12	2.20	0.52
1:A:247:PHE:O	1:A:251:THR:HG22	2.10	0.51
1:A:449:MET:HG3	1:A:449:MET:O	2.11	0.50
1:B:301:MET:HE3	1:B:303:LEU:HD21	1.93	0.50
1:A:296:ARG:HG3	1:A:302:ARG:HG3	1.92	0.50
1:A:305:GLU:HG2	1:A:314:CYS:SG	2.52	0.50
1:B:282:LEU:O	1:B:285:PHE:HD2	1.95	0.50
1:B:117:ARG:HG3	1:B:117:ARG:NH1	2.19	0.49
1:B:1053:VAL:HB	1:B:1088:VAL:HG12	1.93	0.49
1:B:305:GLU:O	1:B:381:VAL:HB	2.12	0.49
1:B:208:GLU:HB3	1:B:209:ASP:H	1.55	0.48
1:B:117:ARG:HA	1:B:117:ARG:HD2	1.76	0.48
1:B:539:LYS:HA	1:B:542:LEU:HD12	1.96	0.47
1:A:303:LEU:HD22	1:A:395:LYS:HG3	1.95	0.47
1:A:1053:VAL:HB	1:A:1088:VAL:HG12	1.96	0.47
1:A:549:TRP:C	1:A:549:TRP:CD1	2.87	0.47
1:B:117:ARG:HH11	1:B:117:ARG:CG	2.22	0.47
1:B:251:THR:HG21	1:B:536:VAL:HG11	1.96	0.47
1:A:121:VAL:HG21	1:A:153:PRO:HG2	1.95	0.46
1:B:121:VAL:HG21	1:B:153:PRO:HG2	1.97	0.46
1:B:68:ALA:HB2	1:B:91:LEU:HD22	1.97	0.46
1:A:541:THR:HA	1:A:544:ILE:HD12	1.98	0.46
1:A:68:ALA:HB2	1:A:91:LEU:HD22	1.98	0.46
1:B:114:ASN:HB2	1:B:494:VAL:HG22	1.98	0.46
1:A:329:VAL:HB	1:A:411:VAL:HG21	1.97	0.46
1:B:114:ASN:ND2	1:B:493:ASN:HB3	2.32	0.44
1:A:247:PHE:CE1	1:A:545:TRP:CZ3	3.06	0.44
1:A:196:PRO:HG2	1:A:491:GLN:CB	2.47	0.44
1:B:1105:VAL:O	1:B:1109:GLU:HG2	2.18	0.44
1:A:326:MET:O	1:A:330:VAL:HG23	2.19	0.43
1:A:158:GLU:HA	1:A:162:GLY:HA2	2.01	0.43
1:B:112:LEU:HD11	1:B:496:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LYS:HA	1:A:542:LEU:HD12	2.01	0.42
1:B:329:VAL:HB	1:B:411:VAL:HG21	2.00	0.42
1:A:208:GLU:HB3	1:A:209:ASP:H	1.46	0.42
1:B:248:THR:HA	1:B:251:THR:HG23	2.01	0.42
1:A:458:LEU:HD23	1:A:531:ALA:HB1	2.00	0.42
1:B:158:GLU:HA	1:B:162:GLY:HA2	2.02	0.42
1:A:552:LEU:HD13	1:A:552:LEU:HA	1.96	0.42
1:B:119:TRP:HA	1:B:122:ILE:HG22	2.03	0.41
1:B:509:ILE:HD12	1:B:509:ILE:O	2.20	0.41
1:A:119:TRP:HA	1:A:122:ILE:HG22	2.03	0.41
1:A:1012:THR:HB	3:A:1202:FMN:O1P	2.20	0.41
1:B:282:LEU:HA	1:B:285:PHE:CE2	2.56	0.41
1:B:156:ILE:CG2	1:B:209:ASP:HB3	2.50	0.41
1:B:326:MET:O	1:B:330:VAL:HG23	2.21	0.41
1:B:339:TRP:CZ3	1:B:422:GLY:HA3	2.56	0.40
1:B:117:ARG:NH1	1:B:117:ARG:CG	2.83	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	630/653 (96%)	598 (95%)	32 (5%)	0	100	100
1	B	630/653 (96%)	601 (95%)	29 (5%)	0	100	100
All	All	1260/1306 (96%)	1199 (95%)	61 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	507/542 (94%)	473 (93%)	34 (7%)	16 43
1	B	506/542 (93%)	475 (94%)	31 (6%)	18 48
All	All	1013/1084 (94%)	948 (94%)	65 (6%)	17 45

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	A	176	GLU
1	A	195	VAL
1	A	199	ARG
1	A	209	ASP
1	A	251	THR
1	A	298	ASP
1	A	305	GLU
1	A	307	THR
1	A	340	HIS
1	A	346	LEU
1	A	350	TYR
1	A	359	TYR
1	A	386	VAL
1	A	426	LEU
1	A	430	LYS
1	A	1062	ASP
1	A	1063	ASP
1	A	1072	ILE
1	A	1084	GLN
1	A	1098	TRP
1	A	1100	TYR
1	A	1131	ARG
1	A	1134	ARG
1	A	1136	ASP
1	A	1144	VAL
1	A	490	CYS

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Mol	Chain	Res	Type
1	A	507	CYS
1	A	525	MET
1	A	543	LEU
1	A	545	TRP
1	A	547	ARG
1	A	550	CYS
1	A	552	LEU
1	B	117	ARG
1	B	172	ASP
1	B	176	GLU
1	B	181	GLU
1	B	195	VAL
1	B	199	ARG
1	B	209	ASP
1	B	251	THR
1	B	257	ARG
1	B	262	TYR
1	B	298	ASP
1	B	386	VAL
1	B	429	ILE
1	B	432	ASN
1	B	1024	ARG
1	B	1063	ASP
1	B	1084	GLN
1	B	1100	TYR
1	B	1106	ASP
1	B	1131	ARG
1	B	1134	ARG
1	B	1135	ASP
1	B	1148	ILE
1	B	445	ILE
1	B	450	LEU
1	B	507	CYS
1	B	525	MET
1	B	536	VAL
1	B	543	LEU
1	B	545	TRP
1	B	558	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	B	114	ASN
1	B	1084	GLN
1	B	555	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

5 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	$\#\|Z\| > 2$
3	FMN	A	1202	-	33,33,33	0.53	0	48,50,50	0.71	1 (2%)
2	836	B	1201	-	41,43,43	3.15	14 (34%)	56,64,64	1.70	13 (23%)
2	836	A	1201	-	41,43,43	3.20	15 (36%)	56,64,64	1.44	7 (12%)
4	NAG	A	1203	1	14,14,15	0.30	0	17,19,21	0.76	1 (5%)
3	FMN	B	1202	-	33,33,33	0.48	0	48,50,50	0.71	1 (2%)

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	FMN	A	1202	-	-	0/18/18/18	0/3/3/3
2	836	B	1201	-	-	3/26/40/40	0/5/5/5
2	836	A	1201	-	-	3/26/40/40	0/5/5/5
4	NAG	A	1203	1	-	0/6/23/26	0/1/1/1
3	FMN	B	1202	-	-	6/18/18/18	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	836	C2-C1	8.78	1.54	1.39
2	A	1201	836	C2-C1	8.63	1.54	1.39
2	A	1201	836	C5-C3	8.58	1.55	1.40
2	A	1201	836	C7-C6	8.13	1.53	1.38
2	B	1201	836	C7-C6	7.73	1.52	1.38
2	B	1201	836	C5-C3	7.68	1.53	1.40
2	B	1201	836	C8-N01	6.58	1.48	1.34
2	A	1201	836	C8-N01	6.40	1.47	1.34
2	A	1201	836	C24-C25	5.89	1.46	1.38
2	B	1201	836	C24-C25	5.49	1.45	1.38
2	B	1201	836	C6-C5	-4.71	1.32	1.39
2	A	1201	836	C6-C5	-4.31	1.33	1.39
2	A	1201	836	C2-C3	-4.26	1.33	1.39
2	B	1201	836	C2-C3	-4.20	1.33	1.39
2	B	1201	836	C25-N5	3.64	1.41	1.34
2	B	1201	836	C24-C23	-3.64	1.34	1.39
2	A	1201	836	C25-N5	3.58	1.41	1.34
2	A	1201	836	C24-C23	-3.55	1.34	1.39
2	B	1201	836	C15-N2	3.47	1.47	1.37
2	B	1201	836	C7-C1	-3.32	1.32	1.38
2	A	1201	836	C15-N2	2.88	1.45	1.37
2	A	1201	836	C10-N01	-2.76	1.43	1.48
2	A	1201	836	O2-N1	-2.70	1.18	1.22
2	B	1201	836	O2-N1	-2.62	1.18	1.22
2	A	1201	836	C7-C1	-2.59	1.34	1.38
2	B	1201	836	C23-C22	2.51	1.54	1.49
2	B	1201	836	C12-N2	-2.49	1.42	1.46
2	A	1201	836	C23-C22	2.28	1.53	1.49
2	A	1201	836	C12-N2	-2.19	1.43	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1201	836	C16-C15-N4	-5.08	118.95	126.80
2	A	1201	836	C12-N2-C13	4.47	121.39	111.52
2	A	1201	836	C16-C15-N4	-4.17	120.36	126.80
2	A	1201	836	C25-C24-C23	3.85	107.90	104.80
2	B	1201	836	C5-C8-N01	3.64	123.46	118.80
2	B	1201	836	F4-C4-C3	-3.57	106.49	112.70
2	B	1201	836	C25-C24-C23	3.43	107.57	104.80
2	B	1201	836	C12-N2-C13	3.06	118.27	111.52
3	A	1202	FMN	P-O5'-C5'	3.04	126.68	118.30
3	B	1202	FMN	P-O5'-C5'	2.88	126.22	118.30
2	B	1201	836	C17-C22-N3	-2.84	119.63	123.00
2	A	1201	836	C23-N6-N5	2.81	114.12	111.96
4	A	1203	NAG	C1-O5-C5	2.81	116.00	112.19
2	B	1201	836	C2-C1-N1	2.79	121.21	118.75
2	B	1201	836	O1-C8-C5	-2.75	114.52	120.06
2	B	1201	836	C4-C3-C5	-2.63	118.33	121.97
2	B	1201	836	C9-N01-C10	2.45	120.70	117.89
2	B	1201	836	C2-C3-C4	2.40	122.40	116.50
2	A	1201	836	C17-C22-N3	-2.30	120.28	123.00
2	B	1201	836	C15-N4-N3	2.28	123.04	118.65
2	B	1201	836	C11-C10-N01	2.19	116.13	111.78
2	A	1201	836	C7-C1-N1	2.19	121.02	119.38
2	A	1201	836	C3-C5-C8	-2.10	119.79	122.83

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	836	C16-C15-N2-C13
2	A	1201	836	N3-C22-C23-C24
2	B	1201	836	C16-C15-N2-C12
2	B	1201	836	N4-C15-N2-C12
2	B	1201	836	N3-C22-C23-C24
3	B	1202	FMN	C5'-O5'-P-O2P
3	B	1202	FMN	C5'-O5'-P-O1P
3	B	1202	FMN	C2'-C3'-C4'-O4'
2	A	1201	836	N4-C15-N2-C13
3	B	1202	FMN	O3'-C3'-C4'-O4'
3	B	1202	FMN	C5'-O5'-P-O3P
3	B	1202	FMN	O2'-C2'-C3'-C4'

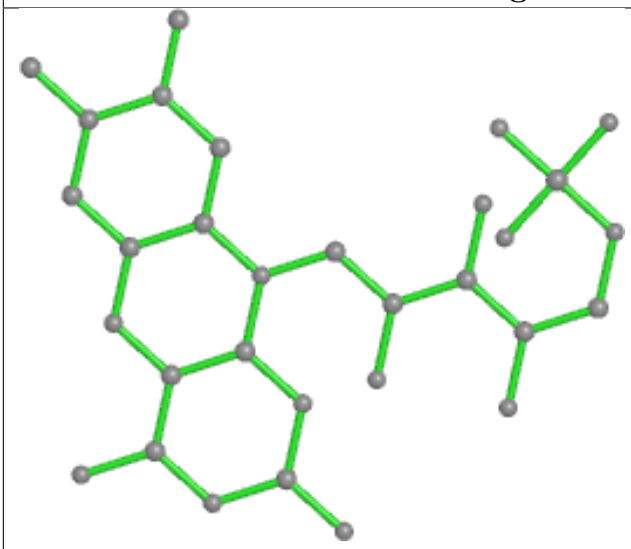
There are no ring outliers.

2 monomers are involved in 2 short contacts:

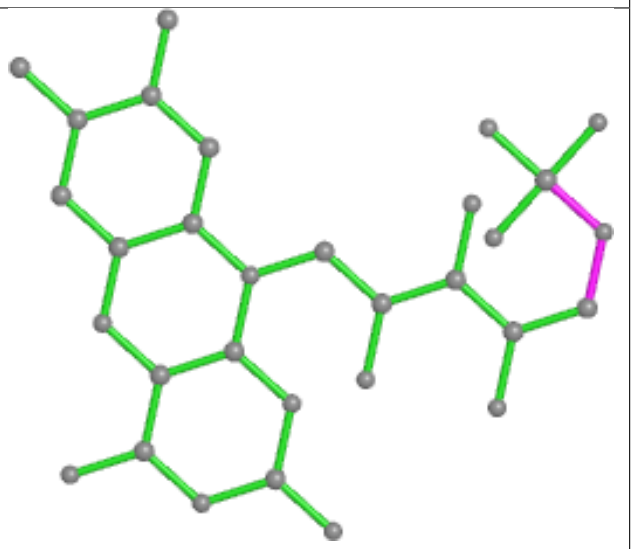
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	FMN	1	0
3	B	1202	FMN	1	0

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.

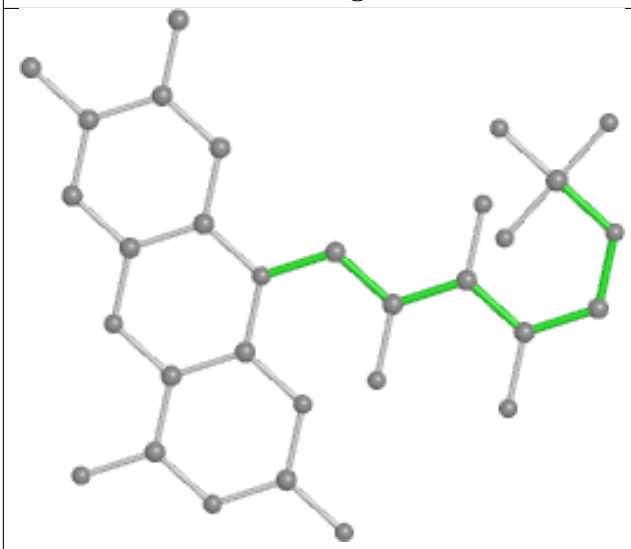
Ligand FMN A 1202



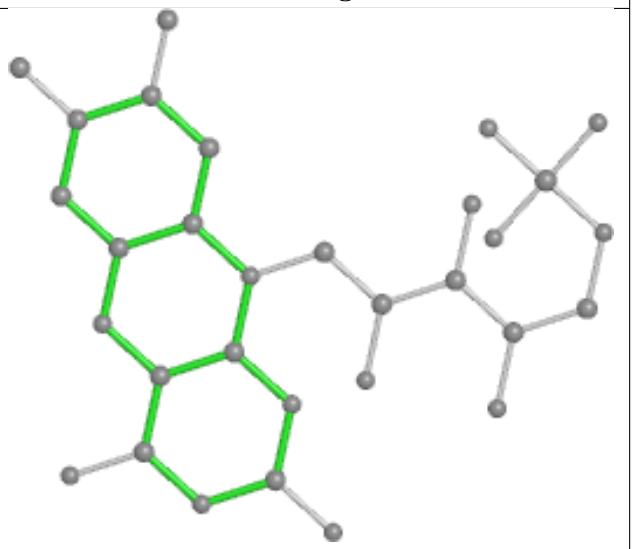
Bond lengths



Bond angles

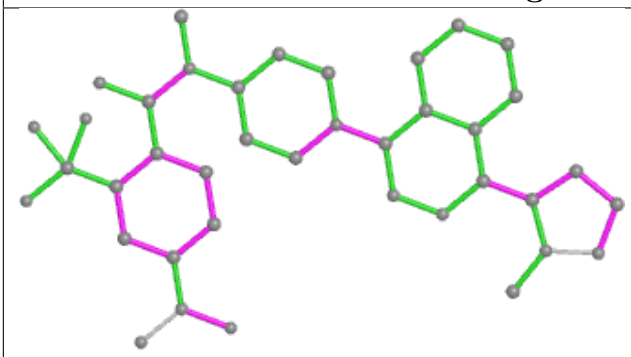


Torsions

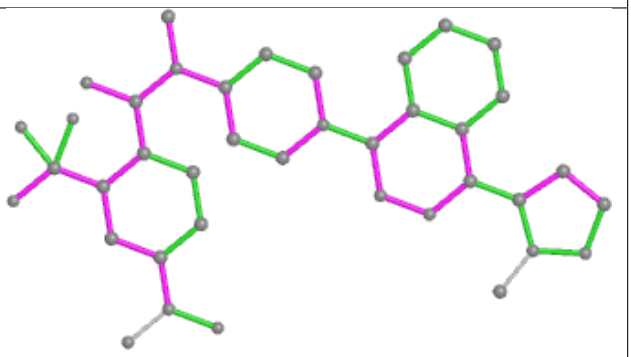


Rings

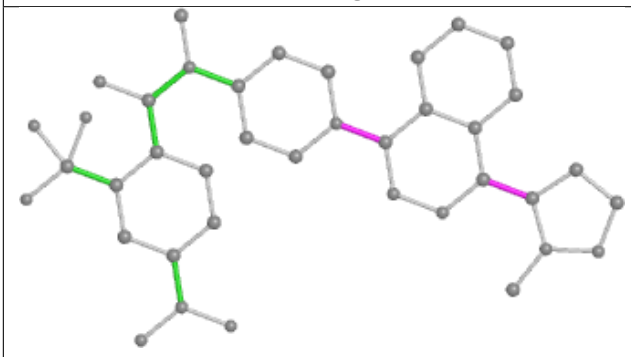
Ligand 836 B 1201



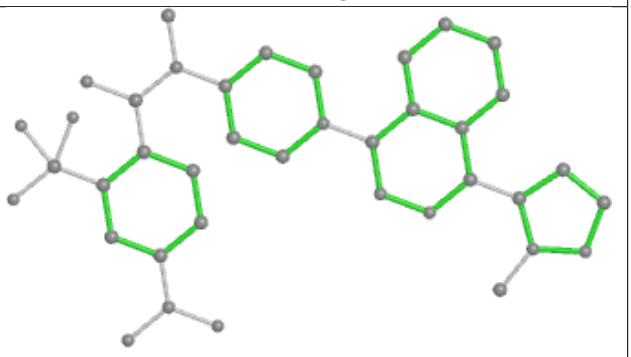
Bond lengths



Bond angles

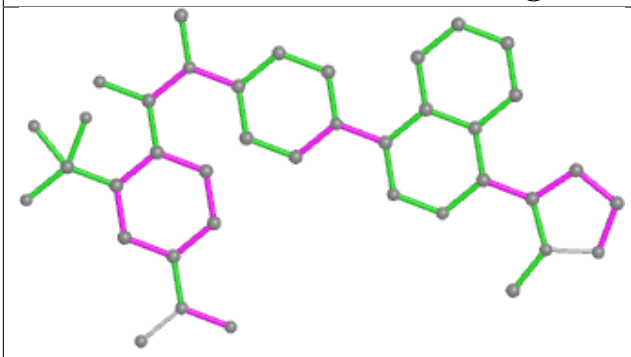


Torsions

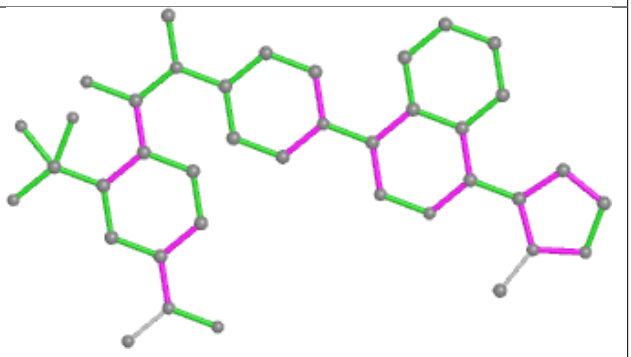


Rings

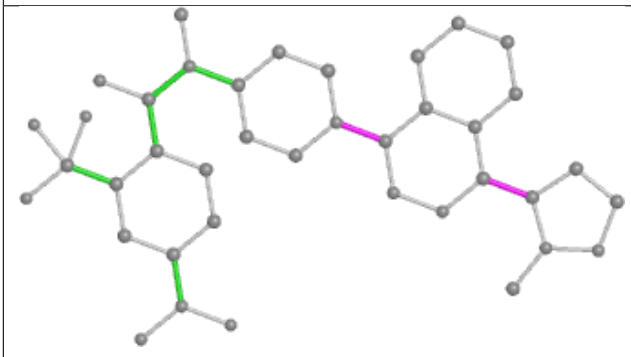
Ligand 836 A 1201



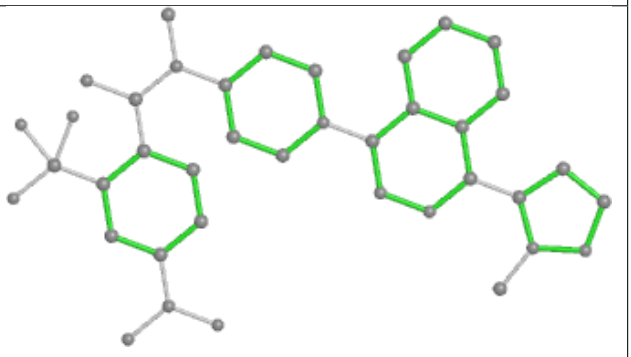
Bond lengths



Bond angles

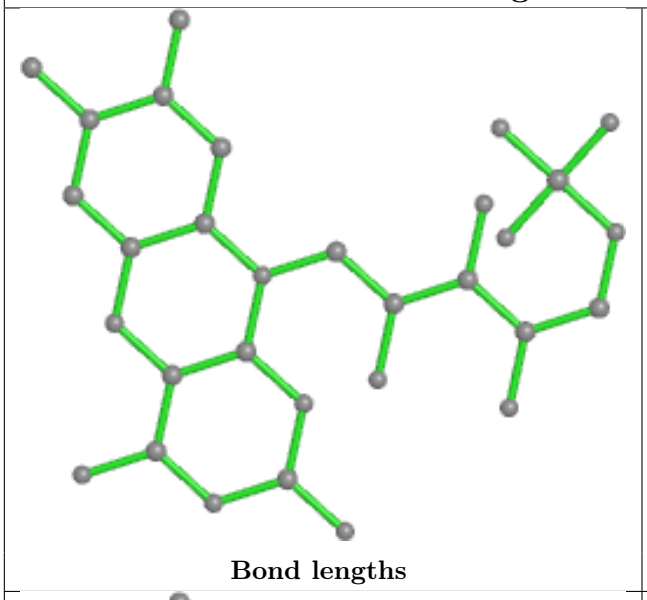


Torsions

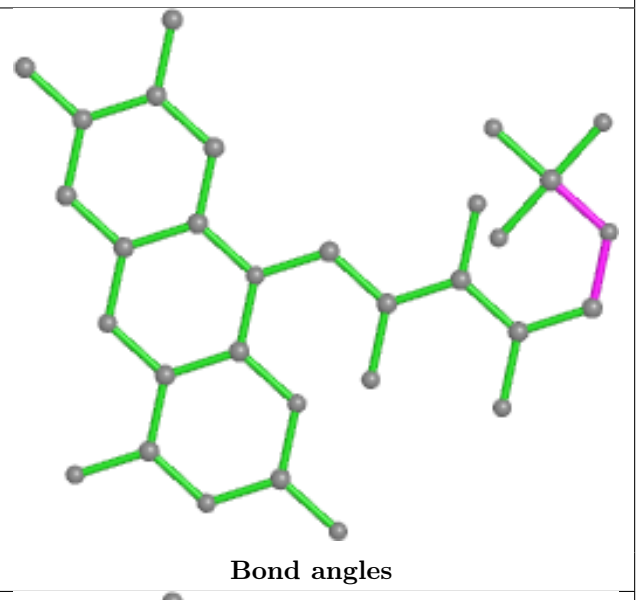


Rings

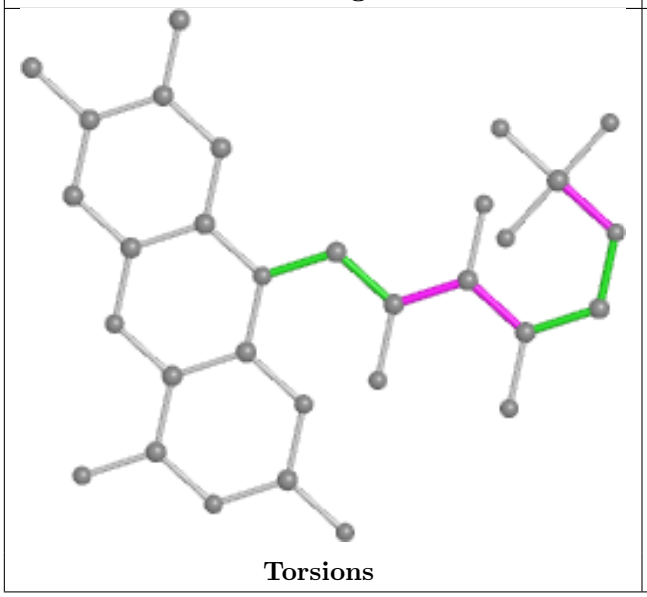
Ligand FMN B 1202



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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	632/653 (96%)	0.52	72 (11%) 5 3	69, 112, 184, 214	0
1	B	634/653 (97%)	0.34	61 (9%) 8 6	61, 107, 172, 195	0
All	All	1266/1306 (96%)	0.43	133 (10%) 6 5	61, 111, 181, 214	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	PRO	12.3
1	A	350	TYR	9.4
1	A	503	PRO	8.2
1	A	60	PRO	8.2
1	A	349	THR	8.1
1	B	190	SER	7.3
1	A	127	CYS	6.8
1	A	128	ALA	6.4
1	B	431	SER	6.4
1	A	76	ASN	6.3
1	B	62	SER	6.1
1	B	72	PRO	6.0
1	A	82	VAL	5.5
1	B	63	HIS	5.3
1	A	190	SER	4.9
1	B	384	ASP	4.8
1	A	67	ALA	4.7
1	A	504	ILE	4.6
1	A	130	TYR	4.6
1	A	131	MET	4.6
1	A	136	ASN	4.5
1	B	132	PRO	4.5
1	A	345	ALA	4.3
1	B	195	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	351	GLN	4.2
1	A	347	GLY	4.1
1	A	348	THR	4.1
1	B	176	GLU	4.1
1	A	1056	GLY	4.0
1	B	77	VAL	4.0
1	A	129	VAL	4.0
1	B	136	ASN	4.0
1	B	60	PRO	4.0
1	A	176	GLU	4.0
1	A	355	GLY	3.9
1	A	384	ASP	3.9
1	B	171	PRO	3.9
1	A	1054	LEU	3.9
1	B	559	HIS	3.9
1	B	475	PHE	3.8
1	A	140	GLU	3.8
1	A	287	ASP	3.8
1	B	59	PRO	3.8
1	A	133	LYS	3.8
1	A	201	ASP	3.8
1	A	346	LEU	3.8
1	B	1057	CYS	3.7
1	A	502	GLN	3.7
1	A	124	PRO	3.7
1	A	144	ARG	3.6
1	A	77	VAL	3.6
1	B	188	ASN	3.6
1	A	505	PRO	3.5
1	A	474	PHE	3.5
1	A	362	LEU	3.5
1	B	1065	ILE	3.5
1	B	1100	TYR	3.5
1	B	131	MET	3.5
1	A	180	ASN	3.5
1	A	141	LEU	3.5
1	A	69	PRO	3.4
1	B	560	HIS	3.4
1	B	144	ARG	3.4
1	B	359	TYR	3.3
1	A	126	LEU	3.3
1	A	387	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1055	LEU	3.2
1	A	1053	VAL	3.1
1	B	1135	ASP	3.1
1	B	128	ALA	3.0
1	B	555	GLN	3.0
1	B	430	LYS	2.9
1	A	297	ALA	2.9
1	B	1058	SER	2.9
1	B	127	CYS	2.9
1	A	188	ASN	2.8
1	A	100	GLU	2.8
1	B	390	CYS	2.8
1	B	191	GLY	2.8
1	A	66	ARG	2.7
1	B	220	PRO	2.6
1	B	1091	PHE	2.6
1	B	1039	ALA	2.6
1	A	549	TRP	2.6
1	B	1056	GLY	2.6
1	B	432	ASN	2.6
1	B	138	ARG	2.6
1	B	549	TRP	2.6
1	A	1005	LEU	2.5
1	A	256	TRP	2.5
1	B	385	SER	2.5
1	B	498	LEU	2.5
1	B	64	CYS	2.5
1	A	1012	THR	2.5
1	A	1131	ARG	2.5
1	B	387	SER	2.5
1	A	1135	ASP	2.4
1	A	203	PRO	2.4
1	A	61	LEU	2.4
1	A	125	LEU	2.4
1	B	189	SER	2.4
1	A	1091	PHE	2.3
1	A	62	SER	2.3
1	B	1090	CYS	2.3
1	B	383	GLY	2.3
1	B	495	THR	2.3
1	B	333	VAL	2.3
1	A	550	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	137	ASP	2.2
1	A	184	ASN	2.2
1	B	65	GLY	2.2
1	B	1055	LEU	2.2
1	A	96	SER	2.2
1	A	145	THR	2.2
1	A	358	SER	2.2
1	B	378	VAL	2.2
1	B	553	THR	2.2
1	A	482	ARG	2.1
1	A	181	GLU	2.1
1	B	429	ILE	2.1
1	B	332	PHE	2.1
1	A	394	TYR	2.1
1	B	133	LYS	2.1
1	B	539	LYS	2.1
1	B	309	ASN	2.1
1	A	1100	TYR	2.1
1	B	172	ASP	2.1
1	B	88	THR	2.0
1	B	262	TYR	2.0
1	A	1007	VAL	2.0
1	A	498	LEU	2.0
1	A	91	LEU	2.0
1	A	1134	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

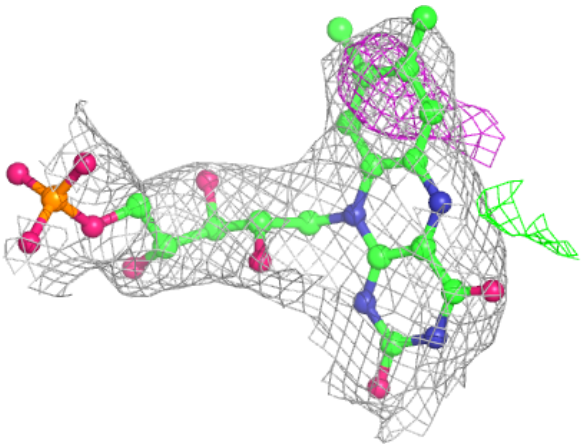
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

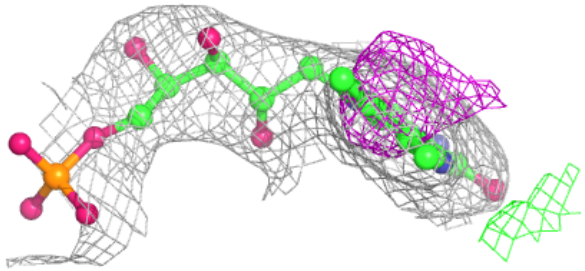
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	1203	14/15	0.73	0.24	172,175,176,176	0
3	FMN	B	1202	31/31	0.91	0.17	41,63,71,74	0
2	836	A	1201	39/39	0.93	0.21	81,93,100,104	0
3	FMN	A	1202	31/31	0.93	0.17	60,72,90,93	0
2	836	B	1201	39/39	0.95	0.22	95,106,112,114	0

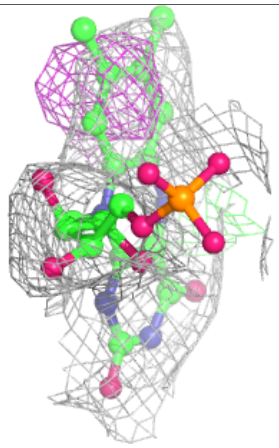
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FMN B 1202:

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

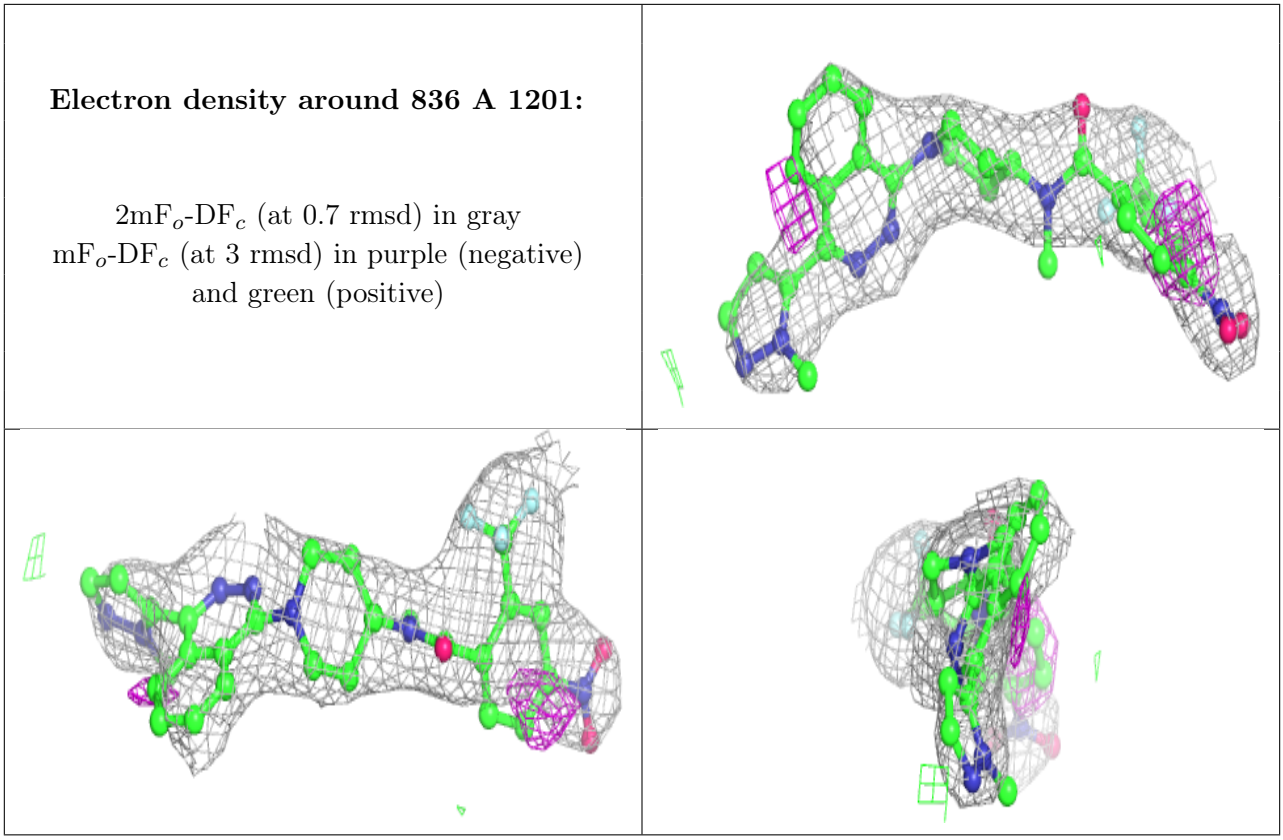






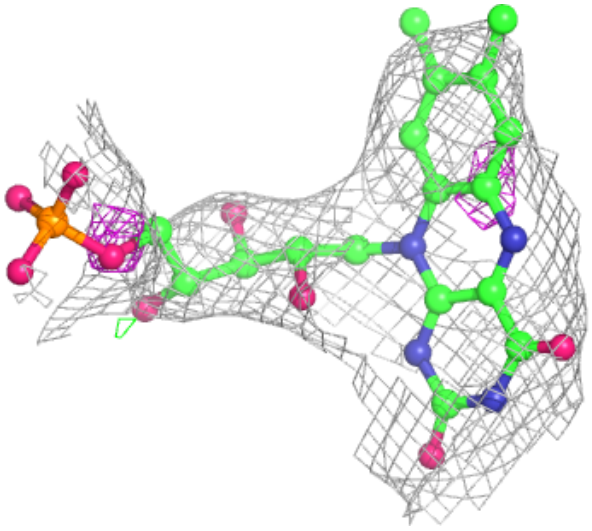
Electron density around 836 A 1201:

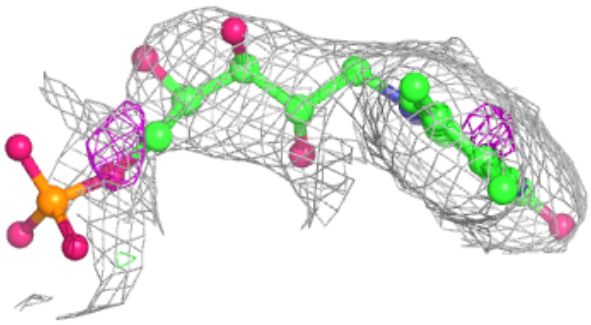
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

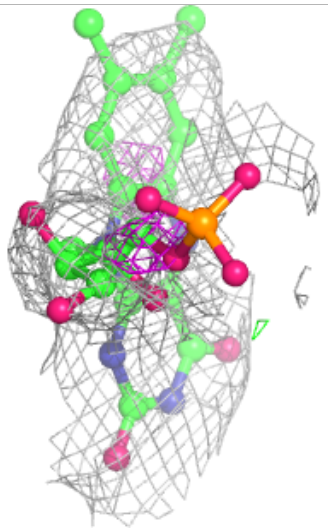


Electron density around FMN A 1202:

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

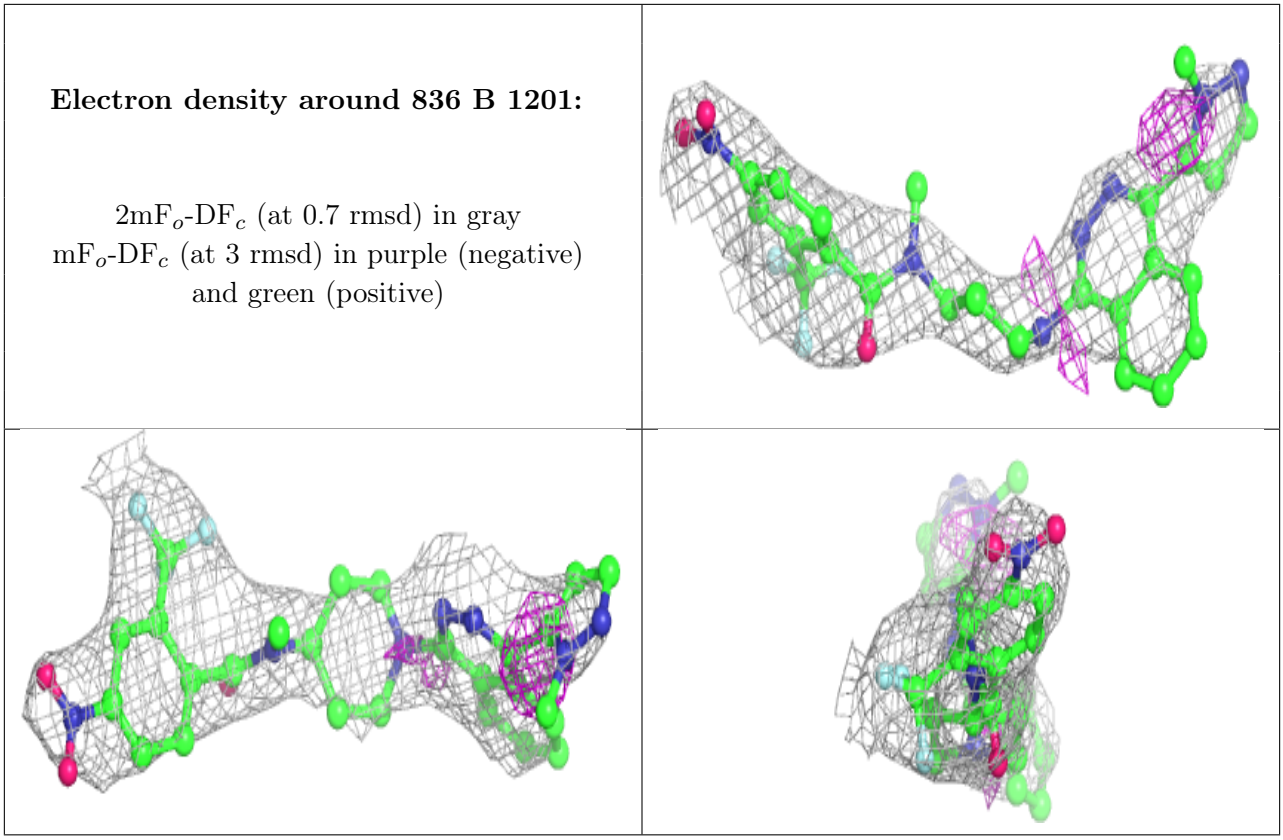






Electron density around 836 B 1201:

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



6.5 Other polymers (i)

There are no such residues in this entry.