



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 06:11 PM UTC

PDB ID : 5V57 / pdb_00005v57
Title : 3.0A SYN structure of the multi-domain human smoothened receptor 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 : 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 ⓘ 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	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12
Ideal geometry (proteins)	: Engh & Huber (2001)

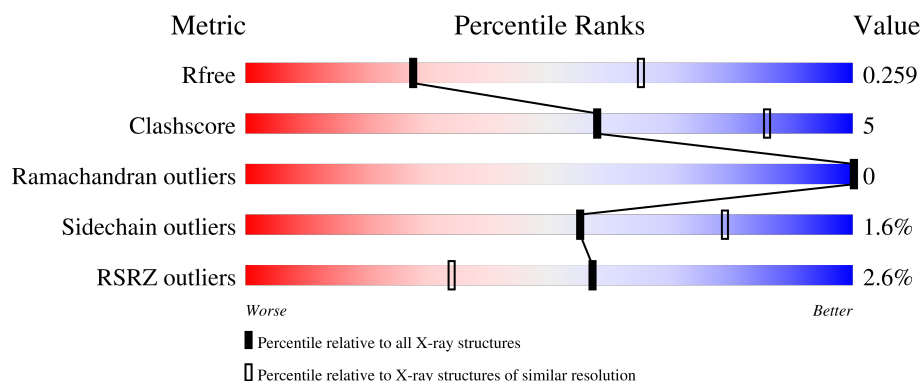
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. 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	648	3% 88% 10% .
1	B	648	2% 86% 12% ..

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10101 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.

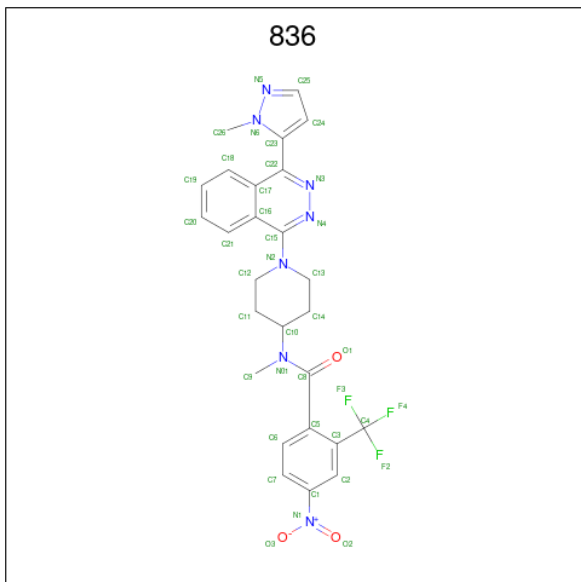
- Molecule 1 is a protein called Smoothened homolog, Flavodoxin, Smoothened homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	645	Total	C	N	O	S	0	0	0
			4981	3194	841	911	35			
1	B	641	Total	C	N	O	S	0	0	0
			4968	3185	834	914	35			

There are 24 discrepancies between the modelled and reference sequences:

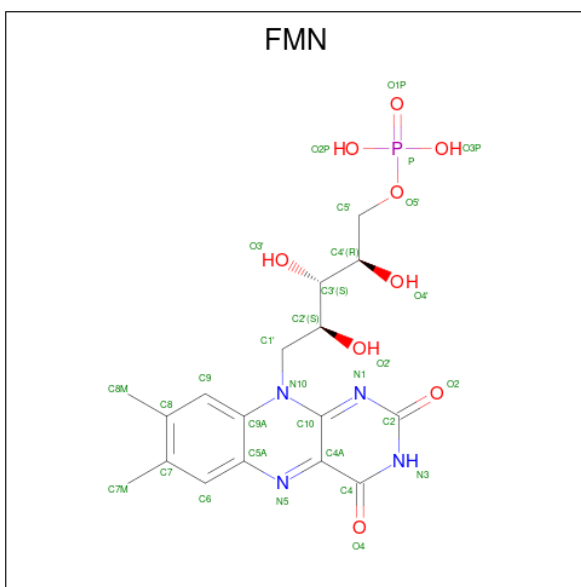
Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	ALA	PRO	engineered mutation	UNP P00323
A	1098	TRP	TYR	engineered mutation	UNP P00323
A	559	HIS	-	expression tag	UNP Q99835
A	560	HIS	-	expression tag	UNP Q99835
A	561	HIS	-	expression tag	UNP Q99835
A	562	HIS	-	expression tag	UNP Q99835
A	563	HIS	-	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	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
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 (CCD ID: 836) (formula: $C_{26}H_{24}F_3N_7O_3$).



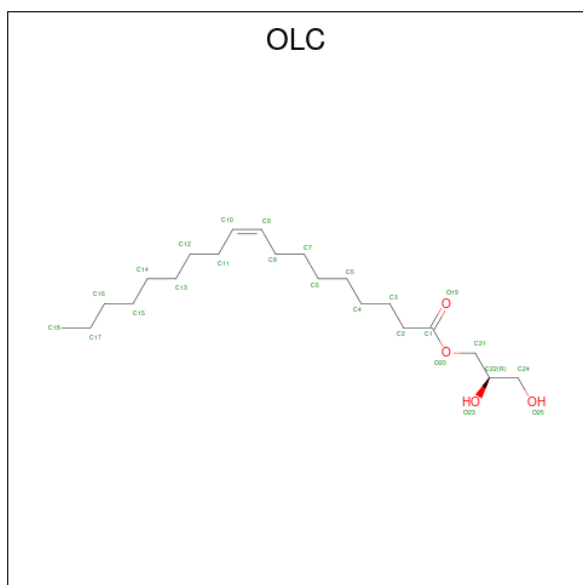
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			39	26	3	7	3		
2	B	1	Total	C	F	N	O	0	0
			39	26	3	7	3		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: 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 (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).

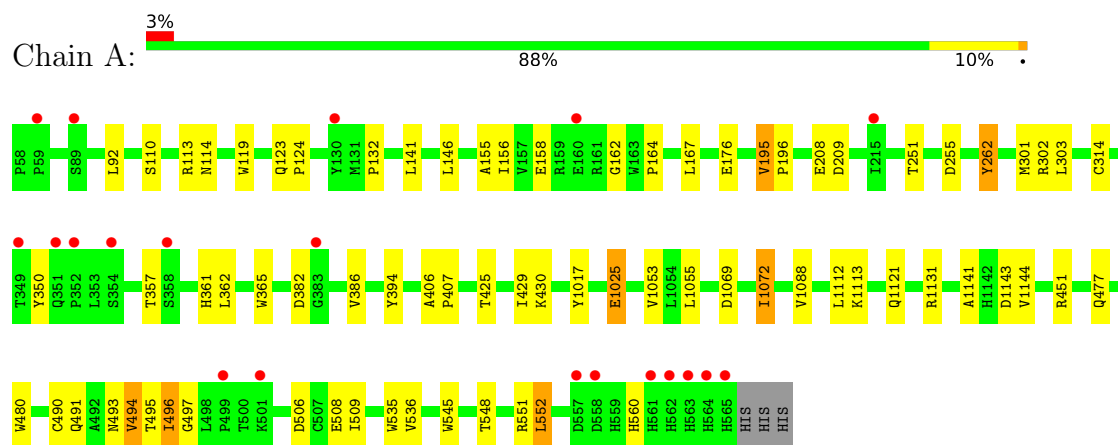


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	8	4		

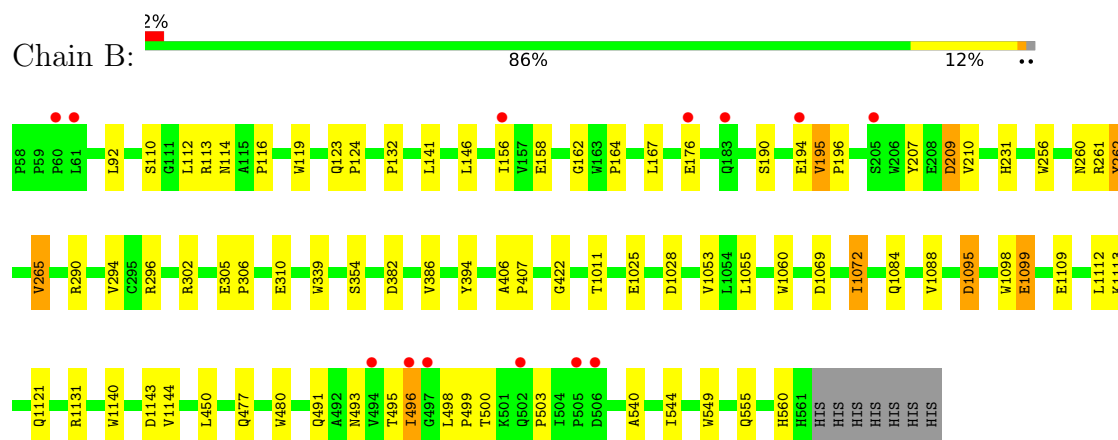
3 Residue-property plots

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



- Molecule 1: Smoothened homolog,Flavodoxin,Smoothened homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.08Å 356.36Å 59.09Å 90.00° 102.79° 90.00°	Depositor
Resolution (Å)	48.38 – 3.00 48.38 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (48.38-3.00) 91.9 (48.38-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.203 , 0.240 0.223 , 0.259	Depositor DCC
R_{free} test set	1502 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10101	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: FMN, 836, OLC

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	0.88	2/5113 (0.0%)	1.25	12/6968 (0.2%)
1	B	0.88	3/5100 (0.1%)	1.24	14/6949 (0.2%)
All	All	0.88	5/10213 (0.0%)	1.25	26/13917 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1072	ILE	CA-CB	7.32	1.57	1.54
1	A	1072	ILE	CA-CB	6.28	1.57	1.54
1	B	195	VAL	CA-C	6.04	1.59	1.52
1	A	195	VAL	CA-C	5.79	1.58	1.52
1	B	265	VAL	CA-C	5.24	1.59	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	ILE	N-CA-C	8.36	119.17	110.72
1	A	497	GLY	N-CA-C	7.89	122.20	112.73
1	A	552	LEU	N-CA-C	-7.34	104.84	114.31
1	A	208	GLU	CA-C-N	6.50	129.28	120.38
1	A	208	GLU	C-N-CA	6.50	129.28	120.38
1	B	354	SER	N-CA-C	6.33	118.71	111.11
1	B	495	THR	N-CA-C	6.28	118.87	111.02
1	B	1099	GLU	CB-CG-CD	6.00	122.81	112.60
1	A	1072	ILE	N-CA-CB	5.69	114.33	110.52
1	A	506	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	496	ILE	N-CA-C	5.58	116.31	110.62
1	A	255	ASP	CA-C-N	5.50	127.92	120.38
1	A	255	ASP	C-N-CA	5.50	127.92	120.38
1	B	1095	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ALA	CA-C-N	5.23	127.91	120.53
1	A	155	ALA	C-N-CA	5.23	127.91	120.53
1	A	1025	GLU	CB-CG-CD	5.17	121.39	112.60
1	B	1072	ILE	N-CA-CB	5.15	113.97	110.52
1	B	1028	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	450	LEU	CA-C-N	5.09	127.10	120.28
1	B	450	LEU	C-N-CA	5.09	127.10	120.28
1	B	1025	GLU	CB-CG-CD	5.07	121.22	112.60
1	B	499	PRO	CA-C-N	5.04	131.16	121.54
1	B	499	PRO	C-N-CA	5.04	131.16	121.54
1	B	194	GLU	CA-C-N	5.03	131.43	122.13
1	B	194	GLU	C-N-CA	5.03	131.43	122.13

There are no chirality outliers.

There are no planarity outliers.

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	4981	0	4769	48	0
1	B	4968	0	4769	42	0
2	A	39	0	0	0	0
2	B	39	0	0	0	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0
4	B	12	0	13	0	0
All	All	10101	0	9589	89	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 (89) 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	1.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:VAL:HG23	1:B:196:PRO:HD3	1.62	0.80
1:A:195:VAL:HG23	1:A:196:PRO:HD3	1.68	0.75
1:A:114:ASN:CB	1:A:494:VAL:HG12	2.17	0.73
1:A:156:ILE:HG22	1:A:209:ASP:HB3	1.71	0.72
1:A:251:THR:HG21	1:A:536:VAL:HG21	1.74	0.67
1:A:548:THR:O	1:A:552:LEU:HB2	1.92	0.67
1:A:251:THR:HB	1:A:545:TRP:CH2	2.29	0.66
1:A:251:THR:CG2	1:A:536:VAL:HG21	2.27	0.65
1:A:114:ASN:HB2	1:A:494:VAL:CG1	2.22	0.64
1:A:114:ASN:OD1	1:A:493:ASN:HB3	2.00	0.61
1:B:112:LEU:HD11	1:B:496:ILE:HA	1.82	0.61
1:A:494:VAL:HG23	1:A:494:VAL:O	2.01	0.60
1:B:114:ASN:HB2	1:B:493:ASN:O	2.00	0.60
1:B:210:VAL:HG12	1:B:210:VAL:O	2.01	0.59
1:B:110:SER:O	1:B:113:ARG:HG3	2.03	0.59
1:B:1055:LEU:HD12	1:B:1112:LEU:HD11	1.85	0.58
1:A:110:SER:O	1:A:113:ARG:HG3	2.03	0.58
1:B:1069:ASP:HA	1:B:1072:ILE:HD13	1.86	0.58
1:A:1069:ASP:HA	1:A:1072:ILE:HD13	1.85	0.58
1:A:156:ILE:CG2	1:A:209:ASP:HB3	2.35	0.57
1:B:164:PRO:HD2	1:B:167:LEU:HB2	1.87	0.57
1:B:1053:VAL:HB	1:B:1088:VAL:HG12	1.88	0.56
1:A:164:PRO:HD2	1:A:167:LEU:HB2	1.86	0.56
1:B:195:VAL:CG2	1:B:196:PRO:HD3	2.35	0.56
1:B:256:TRP:O	1:B:260:ASN:HB2	2.06	0.56
1:B:1140:TRP:O	1:B:1144:VAL:HG23	2.08	0.54
1:A:1053:VAL:HB	1:A:1088:VAL:HG12	1.89	0.53
1:B:305:GLU:HG3	1:B:306:PRO:HA	1.90	0.52
1:A:251:THR:HB	1:A:545:TRP:CZ3	2.44	0.52
1:A:1055:LEU:HD12	1:A:1112:LEU:HD11	1.91	0.52
1:A:1017:TYR:CZ	1:A:1131:ARG:HG3	2.44	0.52
1:B:500:THR:HB	1:B:503:PRO:HG3	1.92	0.52
1:B:294:VAL:O	1:B:302:ARG:HG3	2.10	0.51
1:A:195:VAL:CG2	1:A:196:PRO:HD3	2.39	0.51
1:B:207:TYR:CD1	1:B:207:TYR:C	2.88	0.50
1:B:231:HIS:CD2	1:B:290:ARG:NH1	2.79	0.50
1:A:451:ARG:HH12	1:A:535:TRP:HA	1.75	0.50
1:A:361:HIS:HD2	1:A:365:TRP:HE1	1.60	0.50
1:A:495:THR:HG22	1:A:495:THR:O	2.12	0.50
1:A:119:TRP:O	1:A:123:GLN:HG3	2.11	0.50
1:A:1121:GLN:HE22	1:A:1143:ASP:HB3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:TRP:O	1:B:123:GLN:HG3	2.11	0.49
1:B:1121:GLN:HE22	1:B:1143:ASP:HB3	1.77	0.48
1:B:158:GLU:HA	1:B:162:GLY:HA2	1.95	0.48
1:A:195:VAL:HG23	1:A:196:PRO:CD	2.43	0.48
1:A:382:ASP:HB2	1:A:394:TYR:HB2	1.96	0.48
1:A:158:GLU:HA	1:A:162:GLY:HA2	1.94	0.47
1:B:382:ASP:HB2	1:B:394:TYR:HB2	1.96	0.47
1:A:477:GLN:HA	1:A:480:TRP:CE3	2.49	0.47
1:B:477:GLN:HA	1:B:480:TRP:CE3	2.49	0.46
1:B:498:LEU:C	1:B:500:THR:H	2.23	0.46
1:B:156:ILE:HG22	1:B:209:ASP:HB3	1.98	0.46
1:B:1095:ASP:HB3	1:B:1098:TRP:HD1	1.79	0.46
1:A:508:GLU:HG2	1:A:509:ILE:N	2.31	0.46
1:A:406:ALA:HB3	1:A:407:PRO:HD3	1.98	0.46
1:B:302:ARG:HH21	1:B:310:GLU:HB3	1.80	0.46
1:B:195:VAL:HG23	1:B:196:PRO:CD	2.38	0.45
1:B:124:PRO:HB2	1:B:146:LEU:HD11	1.99	0.45
1:A:262:TYR:OH	1:A:357:THR:HA	2.17	0.45
1:B:406:ALA:HB3	1:B:407:PRO:HD3	1.98	0.45
1:B:196:PRO:HD3	1:B:491:GLN:HG2	2.00	0.43
1:B:296:ARG:HG3	1:B:302:ARG:HG2	2.00	0.43
1:A:92:LEU:HD21	1:A:141:LEU:HD23	2.00	0.43
1:B:262:TYR:HA	1:B:265:VAL:HG12	2.00	0.43
1:A:124:PRO:HB2	1:A:146:LEU:HD11	2.01	0.43
1:A:551:ARG:HB3	1:A:560:HIS:HE1	1.83	0.43
1:A:196:PRO:HG2	1:A:491:GLN:CB	2.49	0.43
1:A:114:ASN:CB	1:A:494:VAL:CG1	2.90	0.42
1:B:92:LEU:HD21	1:B:141:LEU:HD23	2.01	0.42
1:A:425:THR:O	1:A:429:ILE:HG12	2.19	0.42
1:A:361:HIS:CD2	1:A:365:TRP:HE1	2.37	0.42
1:B:339:TRP:CZ3	1:B:422:GLY:HA3	2.54	0.42
1:B:116:PRO:HB3	1:B:190:SER:O	2.20	0.42
1:B:1109:GLU:O	1:B:1113:LYS:HB2	2.20	0.42
1:A:493:ASN:HB3	1:A:494:VAL:H	1.58	0.42
1:B:555:GLN:HA	1:B:560:HIS:HB3	2.02	0.42
1:A:1141:ALA:O	1:A:1144:VAL:HG12	2.20	0.42
1:A:301:MET:HE2	1:A:303:LEU:HD21	2.02	0.41
1:A:92:LEU:HD12	1:A:132:PRO:HG3	2.03	0.41
1:A:1088:VAL:HG21	1:A:1112:LEU:HD13	2.03	0.41
1:B:92:LEU:HD12	1:B:132:PRO:HG3	2.03	0.41
1:A:251:THR:HG21	1:A:536:VAL:CG2	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:GLU:HG2	1:A:1141:ALA:HB3	2.02	0.41
1:B:1011:THR:HB	1:B:1060:TRP:CZ2	2.56	0.41
1:A:302:ARG:NE	1:A:314:CYS:HB2	2.36	0.41
1:B:123:GLN:HB2	1:B:124:PRO:HD3	2.03	0.40
1:A:1113:LYS:O	1:B:1131:ARG:HD3	2.21	0.40
1:B:540:ALA:O	1:B:544:ILE:HG12	2.22	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	643/648 (99%)	604 (94%)	39 (6%)	0	100	100
1	B	639/648 (99%)	601 (94%)	38 (6%)	0	100	100
All	All	1282/1296 (99%)	1205 (94%)	77 (6%)	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	518/539 (96%)	509 (98%)	9 (2%)	53	78
1	B	522/539 (97%)	514 (98%)	8 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1040/1078 (96%)	1023 (98%)	17 (2%)	55 79

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLU
1	A	262	TYR
1	A	350	TYR
1	A	362	LEU
1	A	386	VAL
1	A	430	LYS
1	A	490	CYS
1	A	494	VAL
1	A	496	ILE
1	B	176	GLU
1	B	209	ASP
1	B	261	ARG
1	B	262	TYR
1	B	386	VAL
1	B	1084	GLN
1	B	1099	GLU
1	B	549	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	ASN
1	A	1014	ASN
1	A	1121	GLN
1	A	470	HIS
1	B	396	ASN
1	B	1084	GLN
1	B	1121	GLN
1	B	470	HIS
1	B	559	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
4	OLC	B	1203	-	11,11,24	1.43	1 (9%)	12,12,25	1.13	1 (8%)
2	836	A	1201	-	42,43,43	3.15	14 (33%)	54,64,64	1.51	9 (16%)
3	FMN	A	1202	-	33,33,33	0.48	0	48,50,50	0.54	0
3	FMN	B	1202	-	33,33,33	0.44	0	48,50,50	0.51	0
2	836	B	1201	-	42,43,43	3.13	15 (35%)	54,64,64	1.49	10 (18%)

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
4	OLC	B	1203	-	-	4/11/11/24	-
2	836	A	1201	-	-	4/28/40/40	0/5/5/5
3	FMN	A	1202	-	-	3/18/18/18	0/3/3/3
3	FMN	B	1202	-	-	3/18/18/18	0/3/3/3
2	836	B	1201	-	-	4/28/40/40	0/5/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	836	C7-C6	9.32	1.53	1.38
2	B	1201	836	C7-C6	9.29	1.53	1.38
2	A	1201	836	C2-C1	9.03	1.54	1.39
2	A	1201	836	C5-C3	8.72	1.54	1.40
2	B	1201	836	C5-C3	8.52	1.54	1.40
2	B	1201	836	C2-C1	8.37	1.53	1.39
2	B	1201	836	C8-N01	6.60	1.47	1.34
2	A	1201	836	C8-N01	6.21	1.46	1.34
2	B	1201	836	C2-C3	-5.05	1.32	1.39
4	B	1203	OLC	O20-C1	4.53	1.46	1.33
2	B	1201	836	C6-C5	-4.52	1.33	1.39
2	A	1201	836	C6-C5	-4.47	1.33	1.39
2	A	1201	836	C2-C3	-4.41	1.33	1.39
2	B	1201	836	C24-C25	3.35	1.45	1.39
2	A	1201	836	C24-C25	3.32	1.45	1.39
2	A	1201	836	C25-N5	3.27	1.41	1.33
2	B	1201	836	C25-N5	3.17	1.41	1.33
2	B	1201	836	C7-C1	-3.15	1.33	1.38
2	A	1201	836	C7-C1	-3.06	1.33	1.38
2	B	1201	836	C24-C23	-2.55	1.34	1.39
2	A	1201	836	O3-N1	-2.53	1.18	1.35
2	B	1201	836	O3-N1	-2.53	1.18	1.35
2	A	1201	836	O2-N1	-2.53	1.18	1.22
2	B	1201	836	O2-N1	-2.50	1.18	1.22
2	A	1201	836	C24-C23	-2.46	1.34	1.39
2	A	1201	836	C12-N2	-2.42	1.42	1.46
2	A	1201	836	C15-N2	2.39	1.47	1.39
2	B	1201	836	C15-N2	2.29	1.46	1.39
2	B	1201	836	C12-N2	-2.25	1.42	1.46
2	B	1201	836	C5-C8	2.07	1.53	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	836	C16-C15-N4	-5.17	118.81	126.80
2	B	1201	836	C16-C15-N4	-4.78	119.41	126.80
2	A	1201	836	C25-N5-N6	-3.54	102.96	104.41
2	B	1201	836	C25-N5-N6	-3.22	103.09	104.41
2	A	1201	836	C24-C25-N5	-2.98	108.16	112.37
2	B	1201	836	C24-C25-N5	-2.92	108.24	112.37
2	B	1201	836	C12-N2-C13	2.92	118.13	111.57
2	A	1201	836	C12-N2-C13	2.79	117.84	111.57
2	B	1201	836	C7-C1-N1	2.67	121.67	119.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	836	C17-C22-N3	-2.65	119.82	122.83
2	A	1201	836	C25-C24-C23	2.63	107.76	104.82
4	B	1203	OLC	O20-C1-C2	2.60	119.76	111.83
2	B	1201	836	C25-C24-C23	2.52	107.64	104.82
2	B	1201	836	C17-C22-N3	-2.47	120.02	122.83
2	B	1201	836	C15-N4-N3	2.21	122.91	118.72
2	A	1201	836	C15-C16-C17	2.21	119.11	116.37
2	A	1201	836	C15-N4-N3	2.20	122.89	118.72
2	B	1201	836	C15-C16-C17	2.17	119.07	116.37
2	A	1201	836	C9-N01-C10	2.08	120.28	117.91
2	B	1201	836	C9-N01-C10	2.01	120.20	117.91

There are no chirality outliers.

All (18) torsion outliers are listed below:

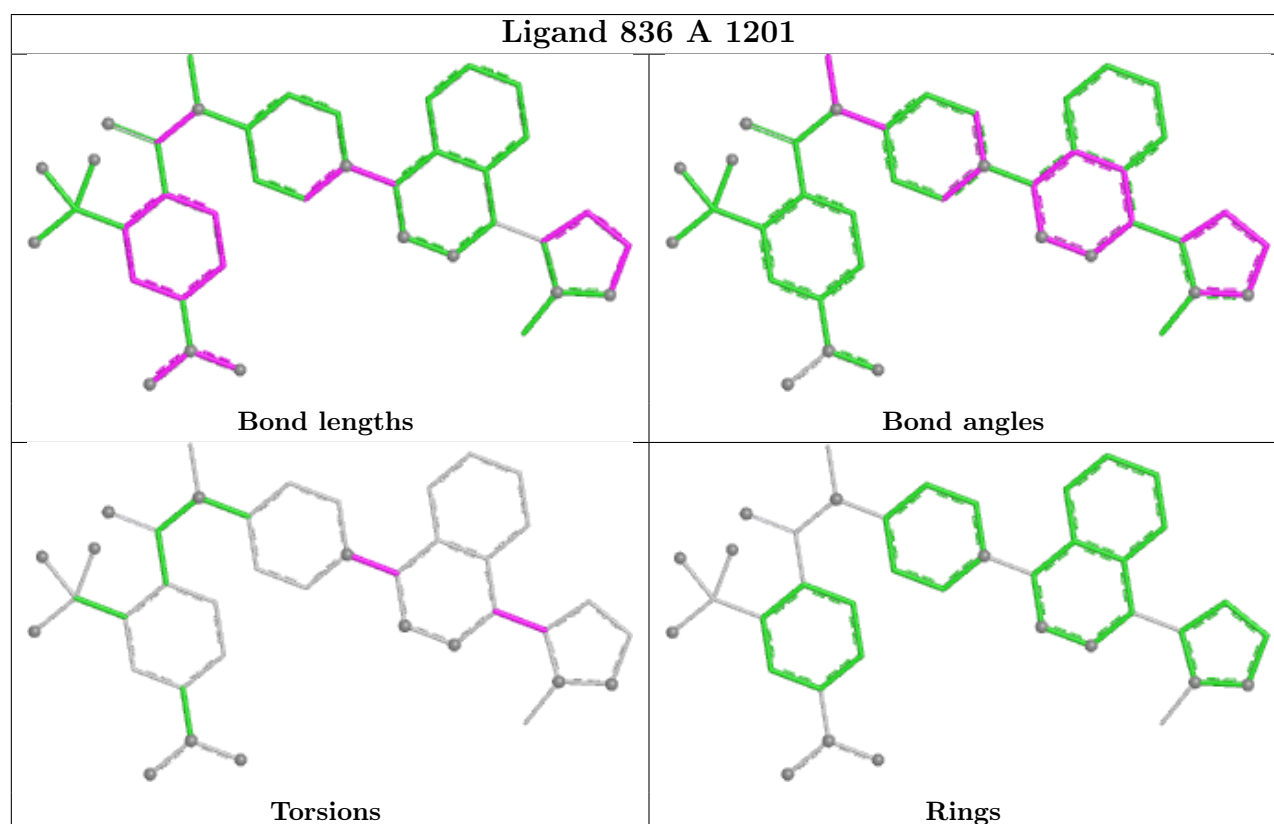
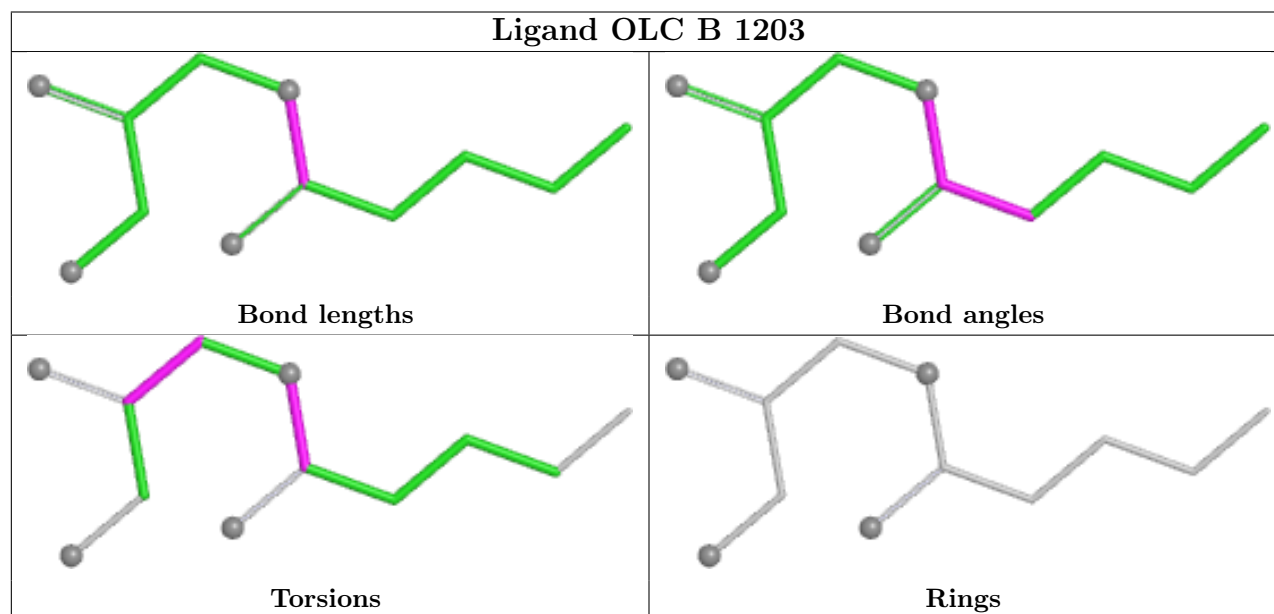
Mol	Chain	Res	Type	Atoms
3	A	1202	FMN	C5'-O5'-P-O2P
3	B	1202	FMN	C5'-O5'-P-O2P
2	B	1201	836	N4-C15-N2-C12
4	B	1203	OLC	C2-C1-O20-C21
4	B	1203	OLC	O19-C1-O20-C21
4	B	1203	OLC	O20-C21-C22-O23
4	B	1203	OLC	O20-C21-C22-C24
2	A	1201	836	N4-C15-N2-C13
3	A	1202	FMN	C5'-O5'-P-O1P
3	B	1202	FMN	C5'-O5'-P-O1P
3	B	1202	FMN	C5'-O5'-P-O3P
2	A	1201	836	N3-C22-C23-N6
2	B	1201	836	N3-C22-C23-N6
2	A	1201	836	N3-C22-C23-C24
2	B	1201	836	N3-C22-C23-C24
3	A	1202	FMN	C5'-O5'-P-O3P
2	A	1201	836	C16-C15-N2-C13
2	B	1201	836	C16-C15-N2-C12

There are no ring outliers.

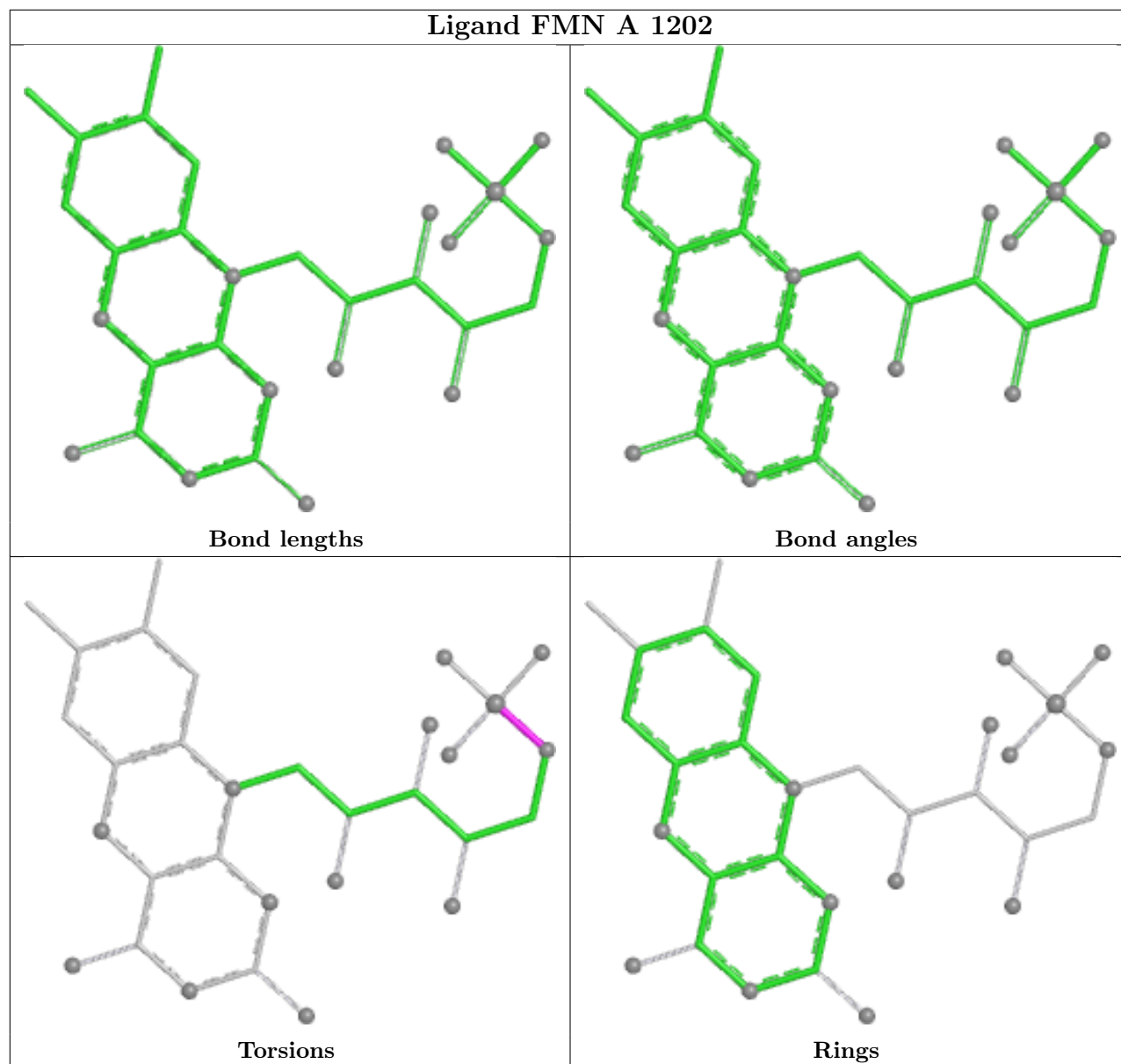
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

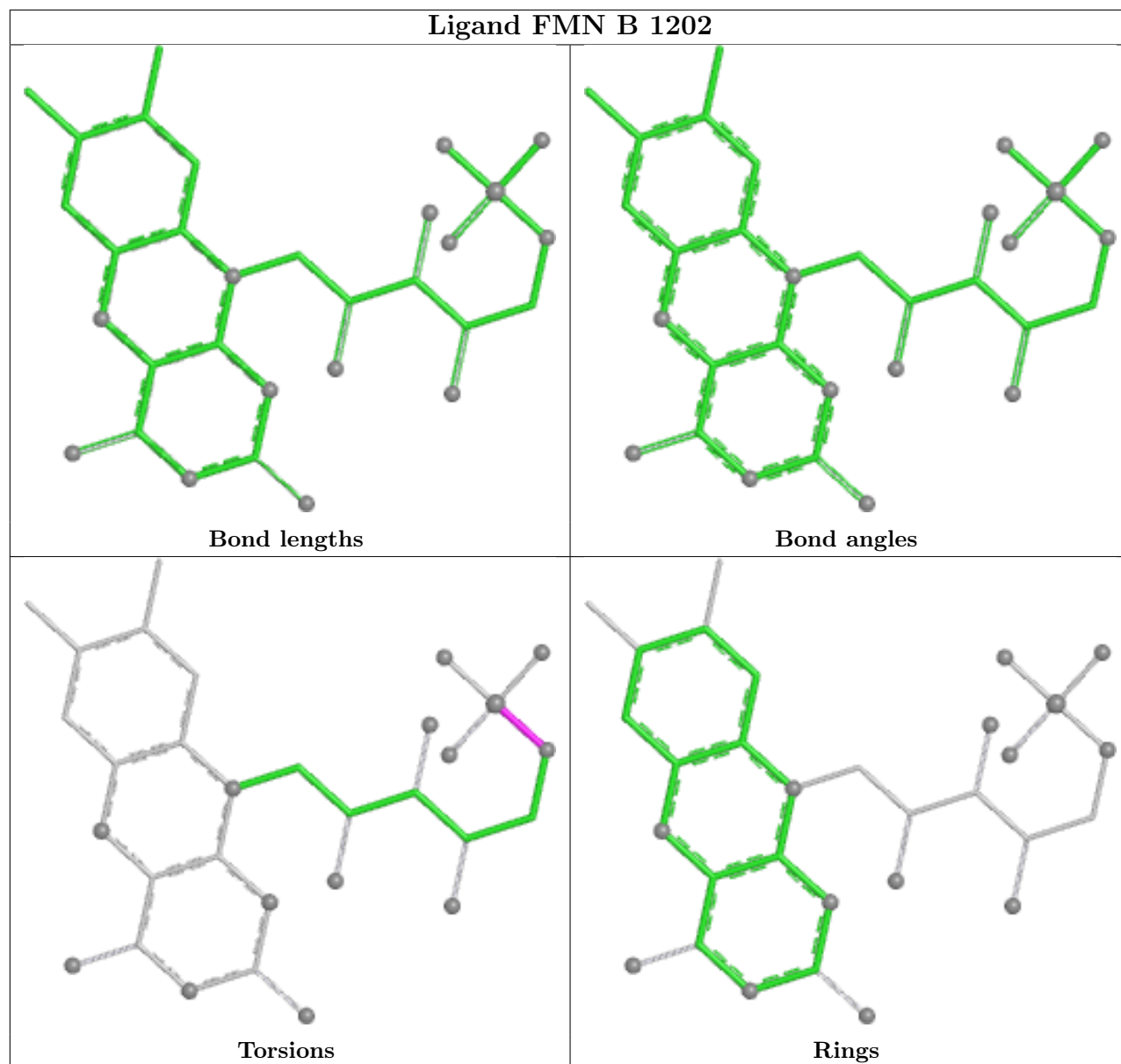
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

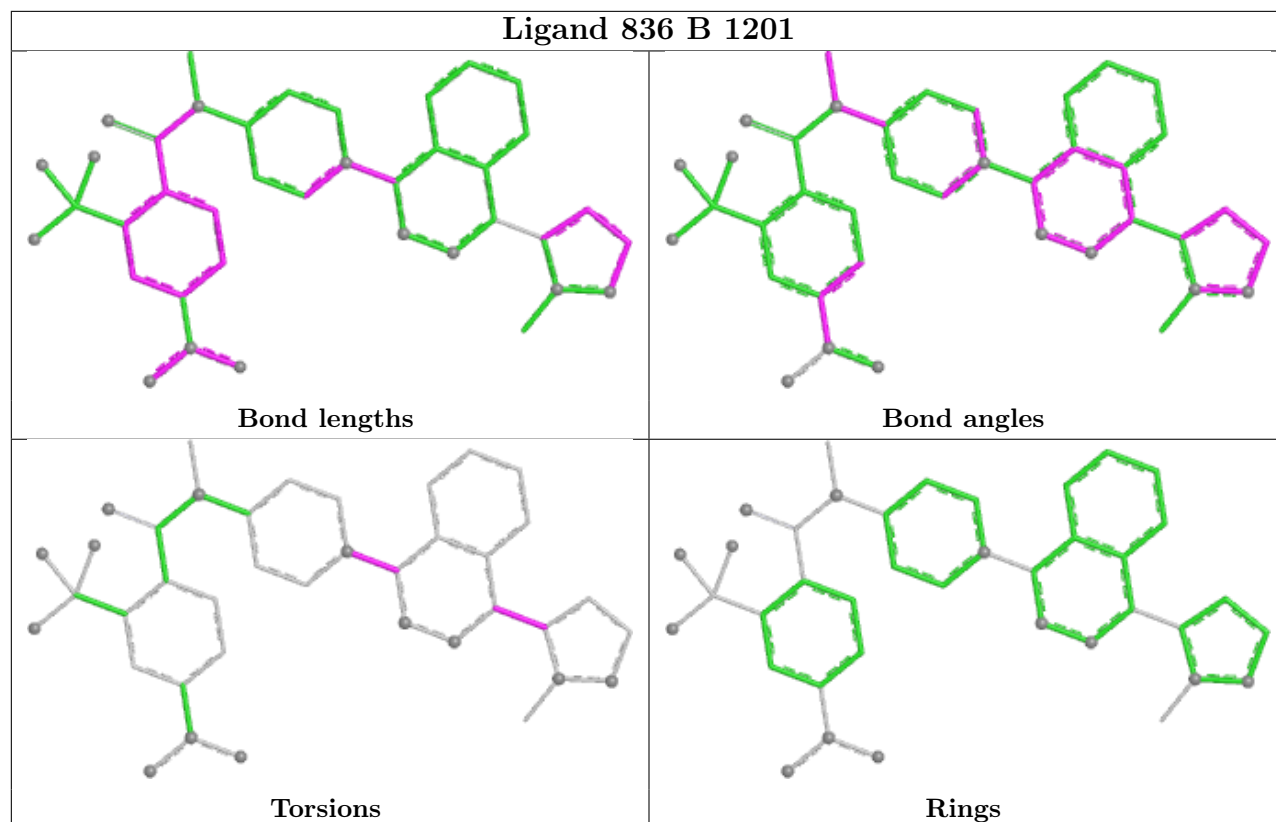


Ligand FMN A 1202



Ligand FMN B 1202





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	645/648 (99%)	0.16	20 (3%)	51 30	41, 77, 147, 174	0
1	B	641/648 (98%)	-0.02	13 (2%)	65 41	40, 70, 142, 175	0
All	All	1286/1296 (99%)	0.07	33 (2%)	57 34	40, 74, 145, 175	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	563	HIS	3.1
1	A	565	HIS	3.1
1	A	351	GLN	3.1
1	B	506	ASP	3.0
1	A	358	SER	2.9
1	B	496	ILE	2.9
1	A	59	PRO	2.8
1	A	354	SER	2.8
1	A	215	ILE	2.8
1	A	352	PRO	2.6
1	A	160	GLU	2.4
1	B	505	PRO	2.4
1	A	557	ASP	2.4
1	A	130	TYR	2.4
1	B	494	VAL	2.4
1	B	183	GLN	2.4
1	B	194	GLU	2.4
1	A	562	HIS	2.3
1	A	89	SER	2.3
1	B	502	GLN	2.2
1	A	564	HIS	2.2
1	B	497	GLY	2.1
1	A	561	HIS	2.1
1	B	60	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	205	SER	2.1
1	A	558	ASP	2.1
1	B	156	ILE	2.1
1	B	176	GLU	2.1
1	A	501	LYS	2.1
1	A	499	PRO	2.1
1	B	61	LEU	2.0
1	A	349	THR	2.0
1	A	383	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

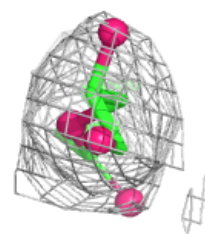
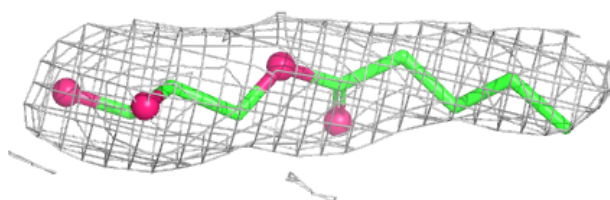
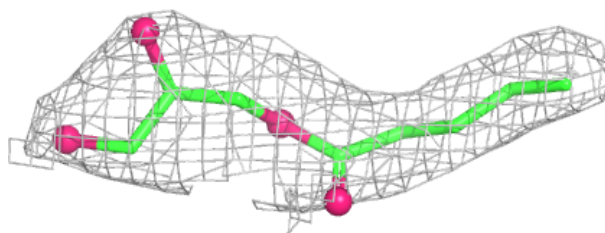
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OLC	B	1203	12/25	0.89	0.14	71,79,84,85	0
2	836	B	1201	39/39	0.93	0.11	66,70,91,94	0
2	836	A	1201	39/39	0.93	0.10	73,79,98,100	0
3	FMN	B	1202	31/31	0.96	0.07	39,45,49,52	0
3	FMN	A	1202	31/31	0.96	0.06	48,50,57,59	0

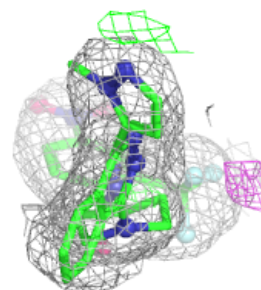
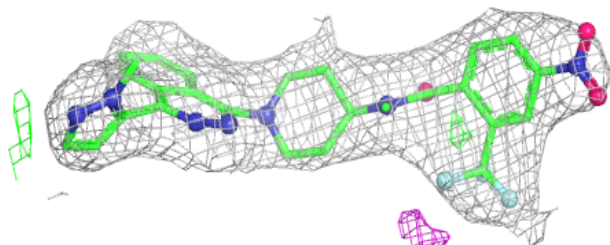
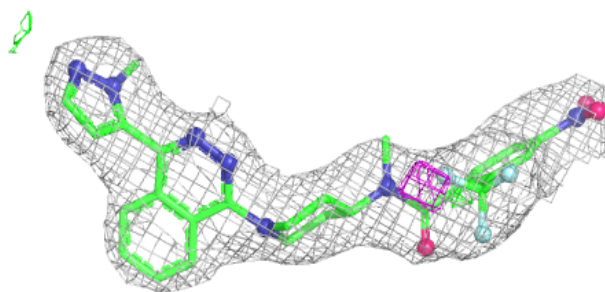
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC B 1203:

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

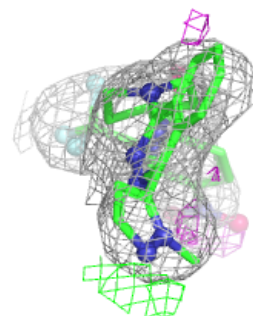
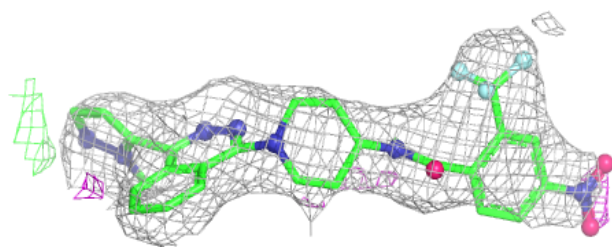
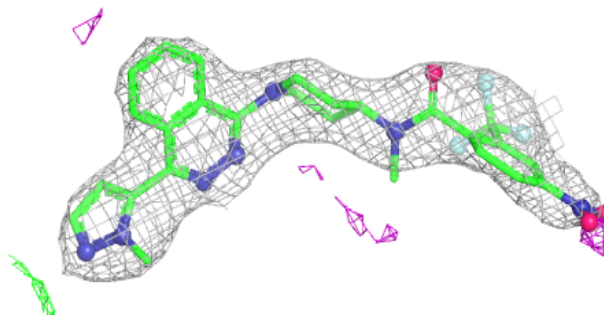
**Electron density around 836 B 1201:**

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

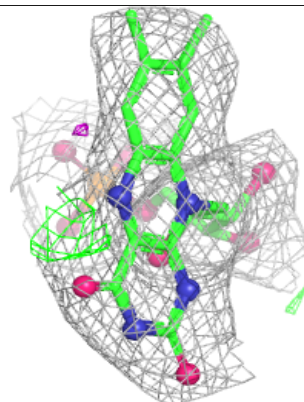
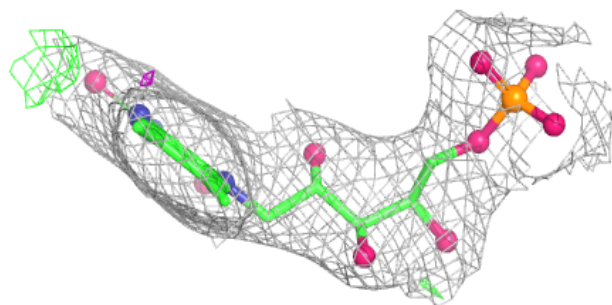
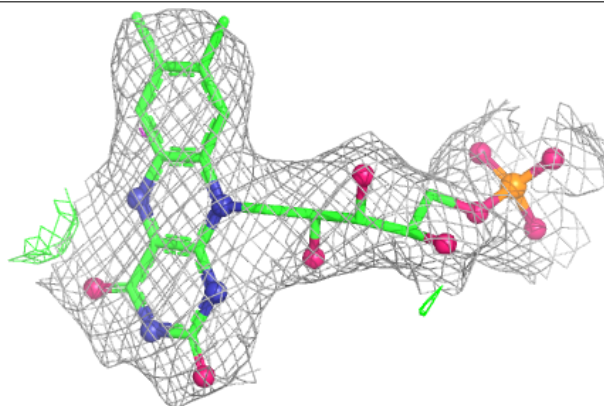


Electron density around 836 A 1201:

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

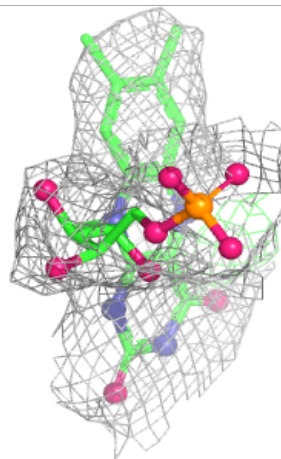
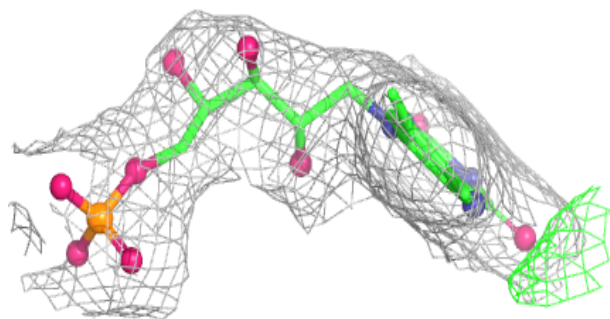
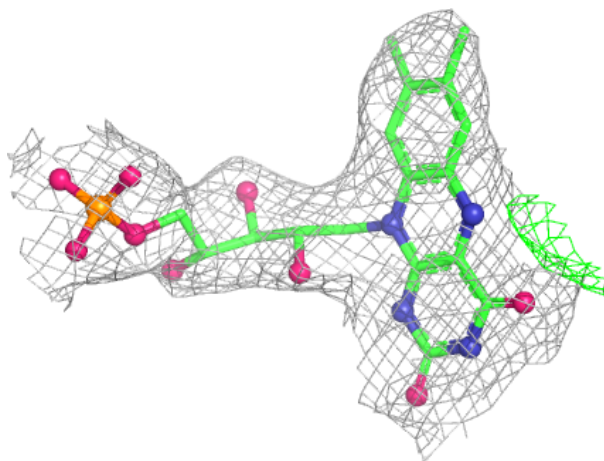
**Electron density around FMN B 1202:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.