

Full wwPDB X-ray Structure Validation Report (i)

Jun 21, 2021 – 01:08 PM BST

PDB ID : 7OB0

Title : Structure of RsLOV d2 variant

Authors: Moeglich, A.; Krafft, T.G.A.; Weyand, M.

Deposited on : 2021-04-20

Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp

with specific help available everywhere you see the (i) symbol.

The 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) : 1.13

EDS : 2.20 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

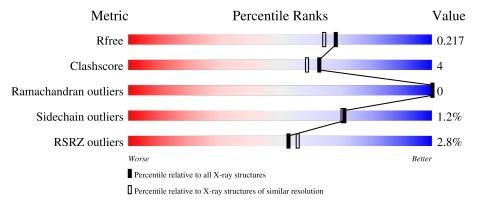
Validation Pipeline (wwPDB-VP) : 2.20

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 1.90 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	176	91%	9% •
1	В	176	94%	5% •
1	С	176	95%	5%
1	D	176	84%	16% •



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6208 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 LOV protein.

Mol	Chain	Residues	${f Atoms}$					ZeroOcc	AltConf	Trace
1	Λ	175	Total	С	N	О	S	0	0	0
1	A	173	1401	876	259	260	6	0	0	
1	В	176	Total	С	N	О	S	0	5	0
1	Б	170	1382	864	262	250	6	U	J	0
1	\sim	176	Total	С	N	О	S	0	3	0
1		170	1352	849	246	251	6	0	3	U
1	D	176	Total	С	N	О	S	0	0	0
1	ש	170	1389	872	256	256	5		0	U

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	LEU	VAL	variant	UNP M1E1F8
A	48	ASP	GLY	engineered mutation	UNP M1E1F8
A	49	GLU	GLN	engineered mutation	UNP M1E1F8
A	77	GLU	LEU	engineered mutation	UNP M1E1F8
A	90	LYS	ALA	engineered mutation	UNP M1E1F8
A	92	GLY	ASP	engineered mutation	UNP M1E1F8
A	157	GLN	SER	engineered mutation	UNP M1E1F8
В	32	LEU	VAL	variant	UNP M1E1F8
В	48	ASP	GLY	engineered mutation	UNP M1E1F8
В	49	GLU	GLN	engineered mutation	UNP M1E1F8
В	77	GLU	LEU	engineered mutation	UNP M1E1F8
В	90	LYS	ALA	engineered mutation	UNP M1E1F8
В	92	GLY	ASP	engineered mutation	UNP M1E1F8
В	157	GLN	SER	engineered mutation	UNP M1E1F8
С	32	LEU	VAL	variant	UNP M1E1F8
С	48	ASP	GLY	engineered mutation	UNP M1E1F8
С	49	GLU	GLN	engineered mutation	UNP M1E1F8
С	77	GLU	LEU	engineered mutation	UNP M1E1F8
С	90	LYS	ALA	engineered mutation	UNP M1E1F8
С	92	GLY	ASP	engineered mutation	UNP M1E1F8
С	157	GLN	SER	engineered mutation	UNP M1E1F8



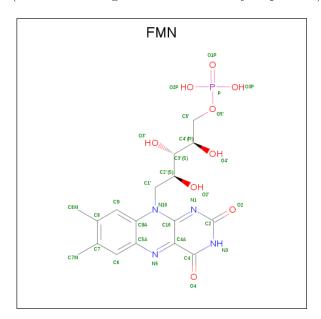
Continued	t_{mom}	marcata care	maaa
-	110111	DIEUIUUS	Duue
0 0 10001000000	J . \circ \circ	r	r

Chain	Residue	Modelled	Actual	Comment	Reference
D	32	LEU	VAL	variant	UNP M1E1F8
D	48	ASP	GLY	engineered mutation	UNP M1E1F8
D	49	GLU	GLN	engineered mutation	UNP M1E1F8
D	77	GLU	LEU	engineered mutation	
D	90	LYS	ALA	engineered mutation	UNP M1E1F8
D	92	GLY	ASP	engineered mutation	UNP M1E1F8
D	157	GLN	SER	engineered mutation	UNP M1E1F8

• Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	В	1	Total Ca 1 1	0	0

• Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



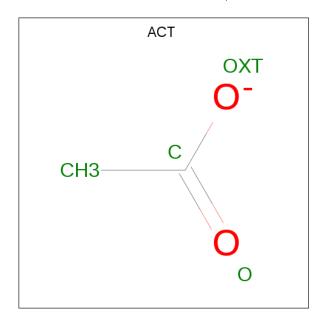
Mol	Chain	Residues		Ato	ms			ZeroOcc	AltConf
3	Δ	1	Total	С	N	О	Р	0	0
3	Λ	1	31	17	4	9	1	U	
2	D	1	Total	С	Ν	О	Р	0	0
)	Ъ	1	31	17	4	9	1		U
2	С	1	Total	С	N	О	Р	0	0
ა			31	17	4	9	1	U	



 $Continued\ from\ previous\ page...$

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf
2	D	1	Total	С	N	О	Р	0	0
3	ש	1	31	17	4	9	1	U	U

• Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	В	1	Total C O 4 2 2	0	0
4	С	1	Total C O 4 2 2	0	0

• Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total Mg	0	0

• Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	В	1	Total Na 1 1	0	0

• Molecule 7 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	157	Total O 157 157	0	1
7	В	145	Total O 145 145	0	1
7	С	132	Total O 132 132	0	1
7	D	109	Total O 110 110	0	2



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: LOV protein

Chain A:

91%
9%
• Molecule 1: LOV protein

Chain B:

94%

5%
• Molecule 1: LOV protein

Chain C:

95%

• Molecule 1: LOV protein

Chain C:

95%

• Molecule 1: LOV protein

Chain C:

95%
• Molecule 1: LOV protein

Chain C:

95%
• Molecule 1: LOV protein



4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	58.06Å 77.17Å 155.00Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	42.93 - 1.90	Depositor	
resolution (A)	42.93 - 1.90	EDS	
% Data completeness	99.6 (42.93-1.90)	Depositor	
(in resolution range)	99.6 (42.93-1.90)	EDS	
R_{merge}	(Not available)	Depositor	
R_{sym}	0.05	Depositor	
$< I/\sigma(I) > 1$	5.34 (at 1.89Å)	Xtriage	
Refinement program	PHENIX 1.19_4092	Depositor	
P. P.	0.176 , 0.218	Depositor	
R, R_{free}	0.175 , 0.217	DCC	
R_{free} test set	2101 reflections (3.78%)	wwPDB-VP	
Wilson B-factor (Å ²)	22.9	Xtriage	
Anisotropy	0.470	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 44.6	EDS	
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.96	EDS	
Total number of atoms	6208	wwPDB-VP	
Average B, all atoms (Å ²)	28.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: MG, NA, FMN, ACT, CA

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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.37	0/1450	0.65	0/1960	
1	В	0.35	0/1422	0.62	0/1919	
1	С	0.36	0/1386	0.60	0/1874	
1	D	0.37	0/1435	0.64	0/1939	
All	All	0.36	0/5693	0.63	0/7692	

There are no bond length outliers.

There are no bond angle outliers.

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1401	0	1378	12	0
1	В	1382	0	1361	6	0
1	С	1352	0	1303	7	0
1	D	1389	0	1357	24	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	31	0	19	0	0
3	В	31	0	19	1	0
3	С	31	0	19	0	0



Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	31	0	19	5	0
4	A	4	0	3	0	0
4	В	4	0	3	0	0
4	С	4	0	3	0	0
5	В	1	0	0	0	0
6	В	1	0	0	0	0
7	A	157	0	0	4	0
7	В	145	0	0	1	0
7	С	132	0	0	3	0
7	D	110	0	0	1	0
All	All	6208	0	5484	48	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 4.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:D:32:LEU:HD21	1:D:35:ALA:HB2	1.63	0.81
1:D:21:THR:HB	1:D:32:LEU:HD11	1.65	0.77
1:A:73[B]:ASP:OD2	1:A:79:ARG:NH2	2.23	0.71
1:C:145[B]:ARG:NH2	7:C:303:HOH:O	2.28	0.67
1:A:163[A]:GLN:NE2	7:A:302:HOH:O	2.30	0.63
1:D:23:VAL:HG21	3:D:201:FMN:HM82	1.84	0.60
1:D:32:LEU:HD13	1:D:55:CYS:SG	2.42	0.59
1:D:45:TYR:HB2	1:D:50[B]:ILE:HD11	1.84	0.59
1:A:9:ILE:HG12	1:A:146[A]:ILE:HG23	1.86	0.57
1:D:47:GLU:HG2	1:D:51:LEU:HD22	1.89	0.55
1:A:172:TRP:O	1:A:175:ARG:HG2	2.07	0.54
1:B:56[A]:ARG:NH2	3:B:204:FMN:O1P	2.40	0.53
1:A:163[A]:GLN:HG2	1:D:127[A]:SER:CB	2.39	0.52
1:C:73:ASP:HB3	7:C:318:HOH:O	2.09	0.51
1:C:107:ARG:CG	1:C:110:ALA:HB3	2.40	0.50
1:D:175:ARG:HG2	1:D:175:ARG:HH11	1.77	0.50
1:A:32:LEU:HD13	1:A:55[A]:CYS:SG	2.52	0.49
1:D:50[B]:ILE:HG23	1:D:57:PHE:CE1	2.47	0.49
1:B:158:ARG:HD3	7:B:358:HOH:O	2.11	0.49
1:D:77:GLU:OE1	1:D:79:ARG:NH2	2.39	0.49
1:A:174:ARG:NH2	7:A:308:HOH:O	2.44	0.48
1:D:50[B]:ILE:HG12	1:D:57:PHE:CZ	2.49	0.48
1:D:112:ASP:OD1	7:D:301:HOH:O	2.20	0.48



Continued from previous page...

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:C:32:LEU:HD13	1:C:55:CYS:SG	2.54	0.47
1:D:23:VAL:CG2	3:D:201:FMN:HM82	2.44	0.47
1:D:72:ARG:NH1	3:D:201:FMN:O3P	2.47	0.46
1:C:107:ARG:HG2	1:C:110:ALA:HB3	1.96	0.46
1:A:159:ARG:O	1:A:163[A]:GLN:HG3	2.16	0.45
1:D:23:VAL:HG12	1:D:32:LEU:HD12	1.98	0.45
1:D:23:VAL:HG13	3:D:201:FMN:HM72	1.97	0.45
1:D:105:GLY:O	1:D:111:PRO:HA	2.17	0.45
1:B:25:MET:HB2	1:B:112:ASP:O	2.17	0.45
1:B:60:ARG:HA	1:B:60:ARG:HD3	1.64	0.44
1:D:91:ASN:OD1	1:D:93[B]:GLU:HG2	2.18	0.44
1:A:21:THR:HB	1:A:32:LEU:HD11	1.99	0.44
1:D:55:CYS:HB2	3:D:201:FMN:O2'	2.17	0.44
1:C:145[A]:ARG:NH2	7:C:314:HOH:O	2.52	0.43
1:D:73:ASP:O	1:D:77:GLU:HG3	2.18	0.43
1:A:156:ASP:OD1	1:A:159:ARG:NH1	2.37	0.42
1:D:107:ARG:HB2	1:D:108:PRO:HD2	2.02	0.42
1:A:102[B]:HIS:CE1	7:A:372:HOH:O	2.73	0.41
1:B:141:GLY:O	1:B:145[A]:ARG:HG2	2.21	0.41
1:A:79:ARG:NE	7:A:305:HOH:O	2.39	0.41
1:D:37:PRO:HB2	1:D:38:PRO:HD3	2.02	0.40
1:C:36:ASN:CG	1:C:38:PRO:HD2	2.42	0.40
1:D:107:ARG:HE	1:D:109:ASP:HB3	1.86	0.40
1:D:88:TYR:CE2	1:D:94:PRO:HB3	2.57	0.40
1:B:133:ALA:HB1	1:B:162:ALA:HB1	2.02	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	Perce	$_{ m ntiles}$
1	A	181/176 (103%)	179 (99%)	2 (1%)	0	100	100



ZY 1' 1	r	•	
Continued	trom	nremons	naae
Continued	$J \cap U \cap U$	preductions	pagc

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	В	$179/176 \ (102\%)$	178 (99%)	1 (1%)	0	100	100
1	С	177/176 (101%)	173 (98%)	4 (2%)	0	100	100
1	D	182/176 (103%)	181 (100%)	1 (0%)	0	100	100
All	All	719/704 (102%)	711 (99%)	8 (1%)	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	Pe	erce	${f ntiles}$
1	A	141/137 (103%)	140 (99%)	1 (1%)		84	84
1	В	135/137 (98%)	133 (98%)	2 (2%)		65	62
1	С	129/137 (94%)	128 (99%)	1 (1%)		81	82
1	D	135/137 (98%)	133 (98%)	2 (2%)		65	62
All	All	540/548 (98%)	534 (99%)	6 (1%)		71	73

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	PHE
1	В	60	ARG
1	В	114	PHE
1	С	114	PHE
1	D	57	PHE
1	D	114	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN



5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles												
MIOI	туре	Chain	res	rtes	rtes	res	nes	nes	nes	nes	res	nes	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACT	В	205	-	1,3,3	6.29	1 (100%)	0,3,3	0.00	1										
3	FMN	С	201	-	31,33,33	1.34	5 (16%)	40,50,50	1.52	7 (17%)										
3	FMN	В	204	-	31,33,33	1.30	4 (12%)	40,50,50	1.78	9 (22%)										
4	ACT	С	202	-	1,3,3	6.92	1 (100%)	0,3,3	0.00	-										
3	FMN	A	202	-	31,33,33	1.31	6 (19%)	40,50,50	1.82	7 (17%)										
3	FMN	D	201	-	31,33,33	1.40	5 (16%)	40,50,50	1.61	5 (12%)										
4	ACT	A	203	-	1,3,3	7.29	1 (100%)	0,3,3	0.00	-										

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	\mathbf{Res}	Link	Chirals	${f Torsions}$	Rings
3	FMN	С	201	_	-	4/18/18/18	0/3/3/3



$Continued\ from\ previous\ page...$

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMN	В	204	-	-	1/18/18/18	0/3/3/3
3	FMN	D	201	_	-	5/18/18/18	0/3/3/3
3	FMN	A	202	-	-	1/18/18/18	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\text{\AA})$
4	A	203	ACT	СН3-С	7.29	1.58	1.48
4	С	202	ACT	СН3-С	6.92	1.57	1.48
4	В	205	ACT	СН3-С	6.29	1.56	1.48
3	С	201	FMN	C10-N1	3.88	1.38	1.33
3	D	201	FMN	C10-N1	3.87	1.38	1.33
3	В	204	FMN	C10-N1	3.59	1.37	1.33
3	D	201	FMN	C4A-N5	3.22	1.37	1.33
3	D	201	FMN	C4-N3	3.19	1.38	1.33
3	A	202	FMN	C4A-N5	3.18	1.37	1.33
3	A	202	FMN	C4-N3	3.04	1.38	1.33
3	A	202	FMN	C10-N1	2.98	1.37	1.33
3	В	204	FMN	C4-N3	2.97	1.38	1.33
3	С	201	FMN	C4-N3	2.90	1.38	1.33
3	В	204	FMN	C4A-N5	2.78	1.37	1.33
3	С	201	FMN	C1'-N10	2.72	1.51	1.48
3	С	201	FMN	C4A-N5	2.68	1.37	1.33
3	A	202	FMN	C1'-N10	2.29	1.50	1.48
3	В	204	FMN	C5A-N5	2.28	1.39	1.35
3	A	202	FMN	C5A-N5	2.21	1.39	1.35
3	С	201	FMN	C6-C5A	-2.14	1.38	1.41
3	D	201	FMN	C6-C5A	-2.13	1.38	1.41
3	D	201	FMN	C1'-N10	2.08	1.50	1.48
3	A	202	FMN	C6-C5A	-2.02	1.38	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\mathbf{Ideal}(^o)$
3	A	202	FMN	C1'-N10-C9A	6.96	123.77	118.29
3	D	201	FMN	C4-N3-C2	6.49	120.62	115.14
3	В	204	FMN	C4-N3-C2	6.19	120.37	115.14
3	С	201	FMN	C4-N3-C2	5.69	119.95	115.14
3	A	202	FMN	C4-N3-C2	5.21	119.54	115.14
3	В	204	FMN	C1'-N10-C9A	5.19	122.38	118.29
3	D	201	FMN	C5A-C9A-N10	3.81	120.48	117.72
3	С	201	FMN	C1'-N10-C9A	3.37	120.95	118.29



Continued from previous page...

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^o)$
3	D	201	FMN	C4A-C4-N3	-3.12	119.16	123.43
3	В	204	FMN	C4A-C4-N3	-3.10	119.19	123.43
3	A	202	FMN	C4A-C4-N3	-2.99	119.34	123.43
3	В	204	FMN	C4A-N5-C5A	2.92	119.69	116.77
3	С	201	FMN	C4A-C4-N3	-2.83	119.56	123.43
3	С	201	FMN	C5A-C9A-N10	2.82	119.76	117.72
3	В	204	FMN	O5'-C5'-C4'	-2.81	101.87	109.36
3	A	202	FMN	C10-C4A-N5	-2.79	119.33	121.26
3	D	201	FMN	C1'-N10-C9A	2.47	120.23	118.29
3	С	201	FMN	C4A-N5-C5A	2.42	119.19	116.77
3	В	204	FMN	C4'-C3'-C2'	-2.37	108.44	113.36
3	В	204	FMN	C10-C4A-N5	-2.34	119.64	121.26
3	A	202	FMN	C4A-N5-C5A	2.23	119.00	116.77
3	D	201	FMN	C1'-N10-C10	2.22	120.39	118.41
3	С	201	FMN	C9A-N10-C10	-2.18	119.05	121.91
3	A	202	FMN	O2'-C2'-C3'	2.18	114.40	109.10
3	A	202	FMN	C1'-N10-C10	-2.10	116.53	118.41
3	В	204	FMN	O2P-P-O5'	2.10	112.32	106.73
3	С	201	FMN	O3P-P-O5'	2.09	112.29	106.73
3	В	204	FMN	O2'-C2'-C3'	2.08	114.15	109.10

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	201	FMN	C5'-O5'-P-O2P
3	С	201	FMN	C5'-O5'-P-O3P
3	D	201	FMN	C3'-C4'-C5'-O5'
3	D	201	FMN	O4'-C4'-C5'-O5'
3	D	201	FMN	C5'-O5'-P-O1P
3	D	201	FMN	C5'-O5'-P-O2P
3	D	201	FMN	C5'-O5'-P-O3P
3	С	201	FMN	C5'-O5'-P-O1P
3	A	202	FMN	C4'-C5'-O5'-P
3	В	204	FMN	C4'-C5'-O5'-P
3	С	201	FMN	C4'-C5'-O5'-P

There are no ring outliers.

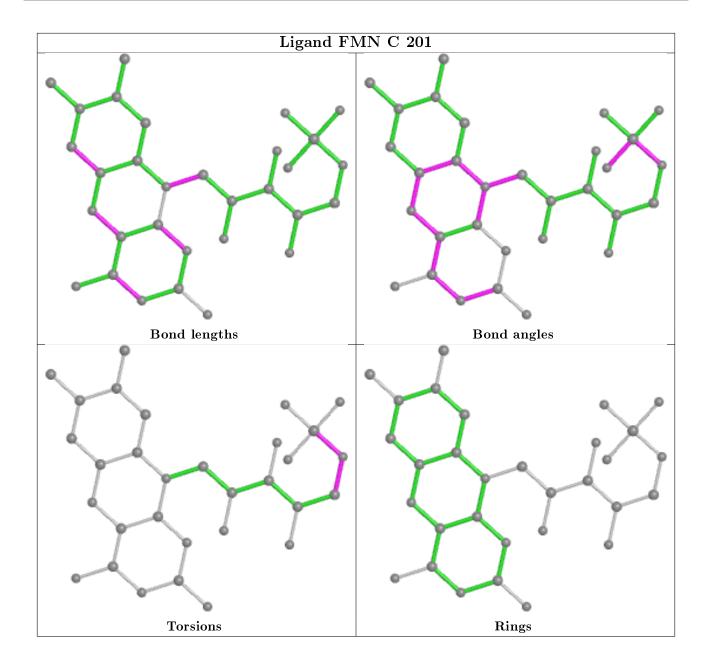
2 monomers are involved in 6 short contacts:



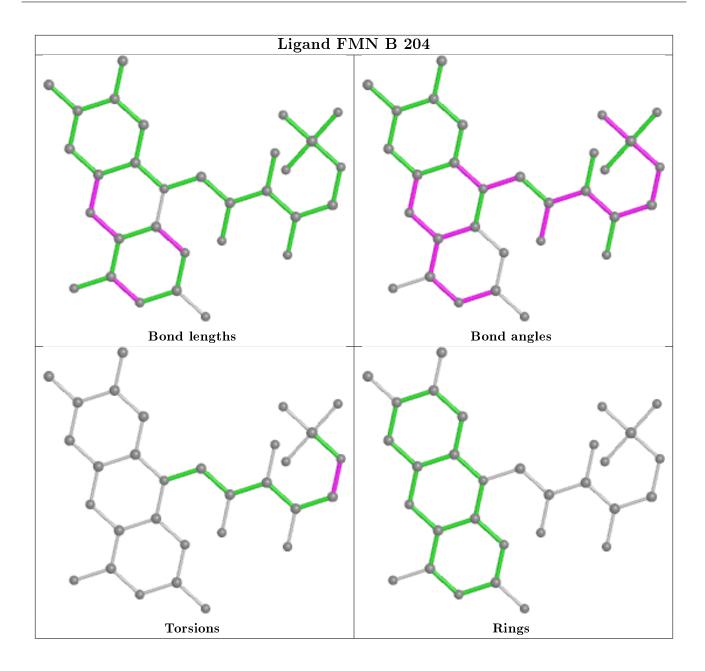
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	204	FMN	1	0
3	D	201	FMN	5	0

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.

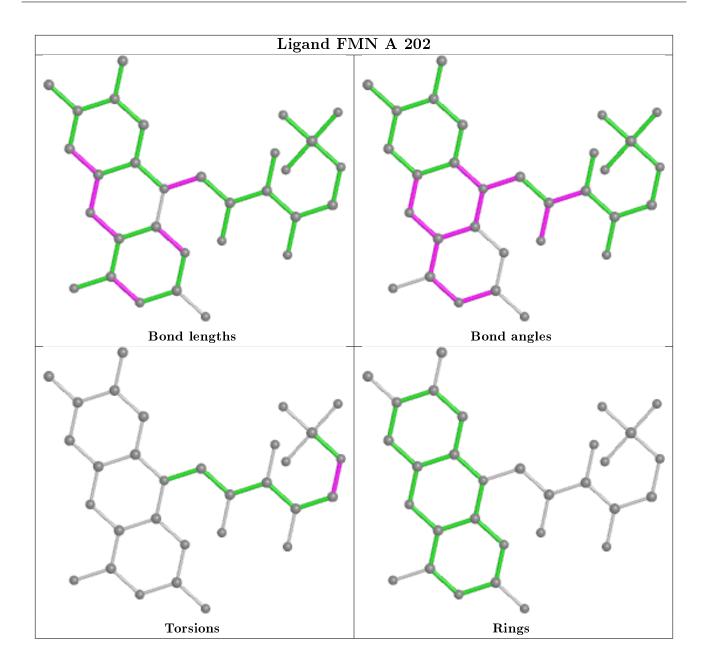




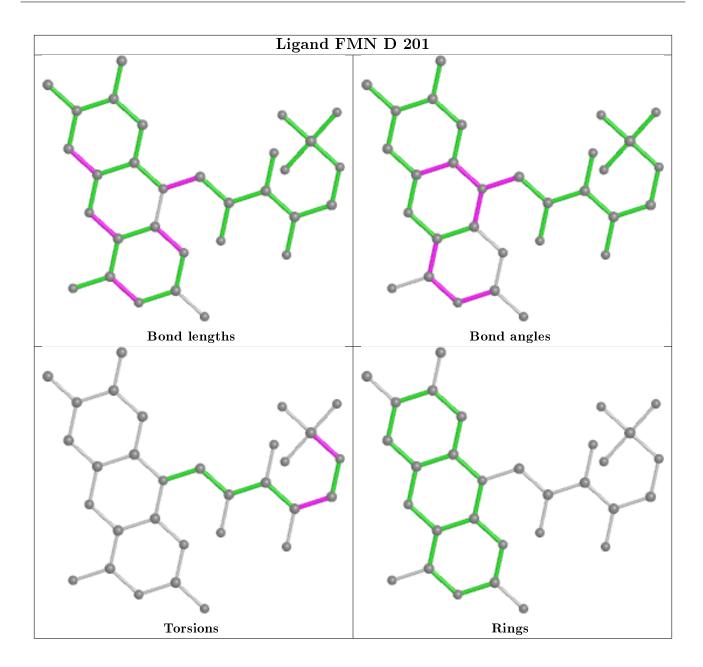












5.7 Other polymers (i)

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)

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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	175/176 (99%)	-0.14	2 (1%) 80 82	11, 22, 42, 63	0
1	В	176/176 (100%)	-0.13	6 (3%) 45 48	11, 24, 49, 81	0
1	С	176/176 (100%)	-0.12	4 (2%) 60 63	11, 26, 49, 83	0
1	D	176/176 (100%)	0.11	8 (4%) 33 36	13, 29, 56, 94	0
All	All	703/704 (99%)	-0.07	20 (2%) 53 56	11, 25, 50, 94	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	GLY	7.2
1	В	176	GLY	6.6
1	В	61	GLY	4.4
1	В	1	MET	4.4
1	С	176	GLY	3.9
1	D	175	ARG	3.8
1	С	61	GLY	3.8
1	D	176	GLY	3.7
1	В	60	ARG	3.3
1	С	62	ASP	2.9
1	D	1	MET	2.8
1	В	53	PHE	2.7
1	D	107	ARG	2.7
1	D	50[A]	ILE	2.5
1	В	175	ARG	2.4
1	D	60	ARG	2.3
1	A	109	ASP	2.3
1	A	175	ARG	2.2
1	D	109	ASP	2.1
1	С	59	GLN	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.

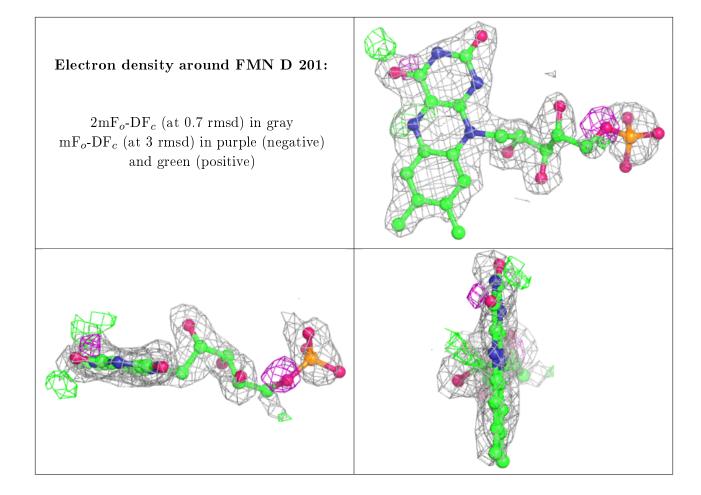
6.4 Ligands (i)

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.

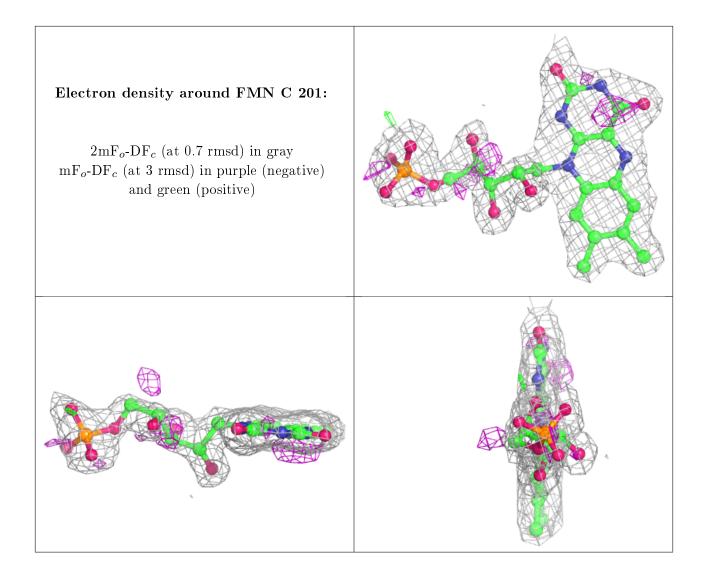
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	ACT	С	202	4/4	0.81	0.34	44,57,59,62	0
3	FMN	D	201	31/31	0.82	0.20	20,34,60,70	31
4	ACT	A	203	4/4	0.84	0.22	36,48,50,57	0
4	ACT	В	205	4/4	0.89	0.16	41,56,58,60	0
3	FMN	С	201	31/31	0.90	0.16	19,29,54,61	0
2	CA	В	202	1/1	0.92	0.08	45,45,45,45	0
3	FMN	A	202	31/31	0.93	0.13	17,23,33,37	0
3	FMN	В	204	31/31	0.94	0.14	17,22,36,38	4
2	CA	A	201	1/1	0.96	0.23	49,49,49,49	0
5	MG	В	201	1/1	0.97	0.08	32,32,32,32	0
6	NA	В	203	1/1	1.00	0.05	19,19,19,19	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.

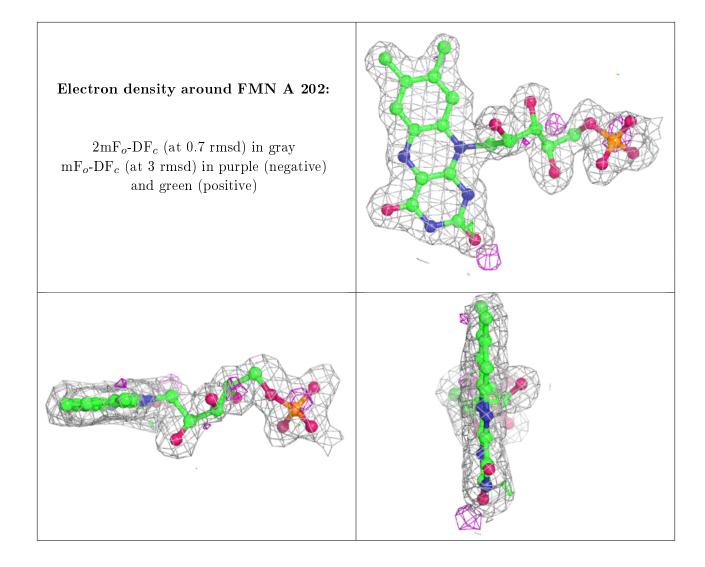




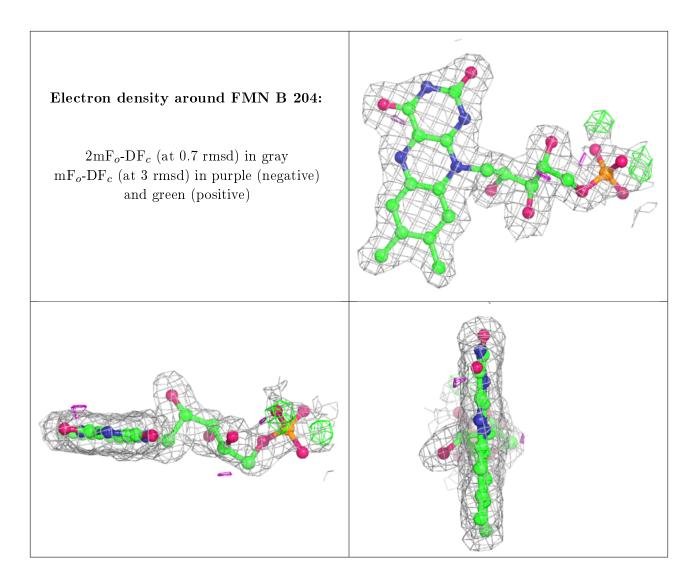












6.5 Other polymers (i)

There are no such residues in this entry.

