

wwPDB X-ray Structure Validation Summary Report (i)

Sep 30, 2024 – 02:18 PM JST

PDB ID : 8J4X

Title: Structure of Mycobacterium tuberculosis NrdF2:NrdIcomplex (oxidised) de-

termined at 3 angstrom resolution

Authors: Yadav, L.R.; Mande, S.C.

Deposited on : 2023-04-21

Resolution : 3.04 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 3.0

buster-report : 1.1.7 (2018)

Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)

CCP4 : 9.0.003 (Gargrove)

Density-Fitness : 1.0.11

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

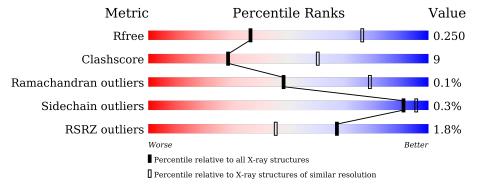
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.04 Å.

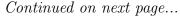
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \textbf{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},\ {\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	164625	3418 (3.08-3.00)
Clashscore	180529	3811 (3.08-3.00)
Ramachandran outliers	177936	3656 (3.08-3.00)
Sidechain outliers	177891	3658 (3.08-3.00)
RSRZ outliers	164620	3430 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	324	71%	17%	12%				
1	В	324	71%	16%	13%				
1	С	324	67%	20%	13%				
1	D	324	71%	17%	12%				
1	Е	324	75%	12%	13%				
1	F	324	69%	19%	12%				





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Mol	Chain	Length							
2	G	150	5% 62%	26%	12%				
2	I	150	69%	21%	• 9%				



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16030 atoms, of which 6 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 Ribonucleoside-diphosphate reductase subunit beta nrdF2.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	A	284	Total	С	N	О	S	7	0	0
1	A	204	2304	1475	378	444	7	1	U	U
1	В	282	Total	С	N	О	S	4	0	0
1	Ъ	202	2286	1464	373	442	7	4	0	
1	С	283	Total	С	N	О	S	6	0	0
1		200	2299	1471	377	444	7	0		
1	D	285	Total	С	N	О	S	16	0	0
1	ט	200	2312	1479	379	447	7	10	0	
1	Е	282	Total	С	N	О	S	74	0	0
1	Ľ	202	2286	1464	373	442	7	14	U	
1	F	286	Total	С	N	О	S	12	0	0
1	I'	200	2320	1485	380	448	7	12	U	U

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	VAL	-	expression tag	UNP P9WH71
В	1	VAL	-	expression tag	UNP P9WH71
С	1	VAL	-	expression tag	UNP P9WH71
D	1	VAL	-	expression tag	UNP P9WH71
Е	1	VAL	-	expression tag	UNP P9WH71
F	1	VAL	-	expression tag	UNP P9WH71

• Molecule 2 is a protein called Protein NrdI.

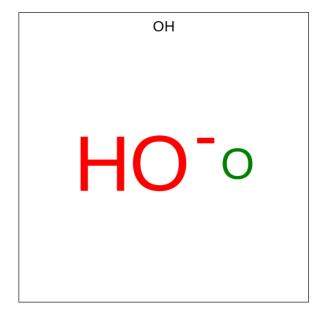
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	G	132	Total	С		0	S	39	0	0
			1029	656	181	189	3			
2	т	I 137	Total	С	N	O	S	34	0	0
	1	137	1065	677	188	196	4	04	U	U

• Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mn 2 2	0	0
3	В	2	Total Mn 2 2	0	0
3	С	2	Total Mn 2 2	0	0
3	D	2	Total Mn 2 2	0	0
3	E	2	Total Mn 2 2	0	0
3	F	2	Total Mn 2 2	0	0

• Molecule 4 is HYDROXIDE ION (three-letter code: OH) (formula: HO) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total H O 2 1 1	0	0
4	В	1	Total H O 2 1 1	0	0
4	С	1	Total H O 2 1 1	0	0
4	D	1	Total H O 2 1 1	0	0
4	E	1	Total H O 2 1 1	0	0

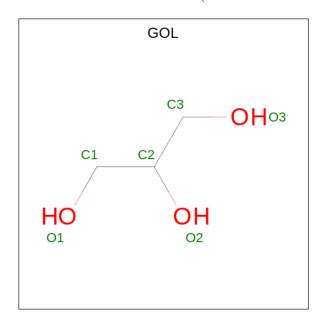
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total 2	H 1	O 1	0	0

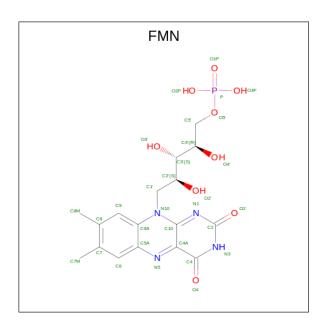
• Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	С	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0

• Molecule 6 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	Atoms					ZeroOcc	AltConf	
6	6 G	C	1	Total	С	N	О	Р	0	0
0		1	31	17	4	9	1	U		
6	т	1	Total	С	N	О	Р	0	0	
0	1	1	31	17	4	9	1	U	U	

• Molecule 7 is water.

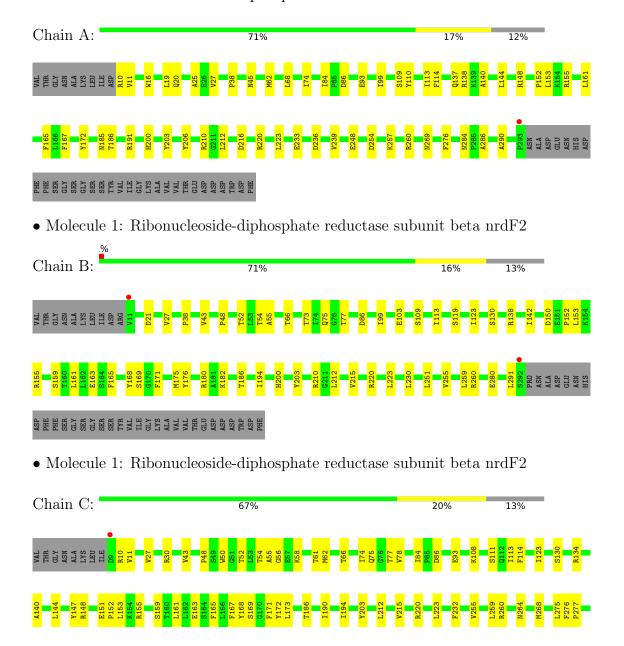
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total O 7 7	0	0
7	В	4	Total O 4 4	0	0
7	С	4	Total O 4 4	0	0
7	D	7	Total O 7 7	0	0
7	Е	2	Total O 2 2	0	0
7	F	5	Total O 5 5	0	0
7	G	1	Total O 1 1	0	0
7	I	1	Total O 1 1	0	0



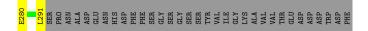
3 Residue-property plots (i)

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

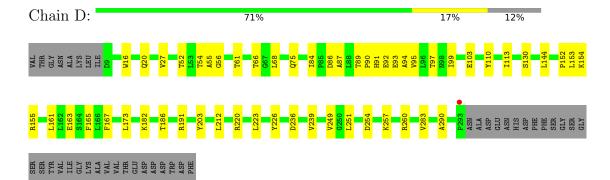
• Molecule 1: Ribonucleoside-diphosphate reductase subunit beta nrdF2



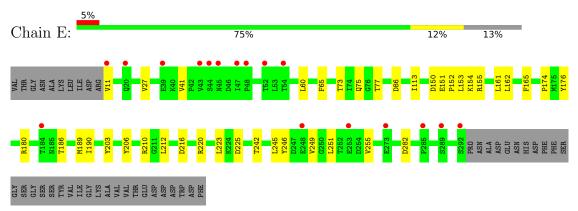




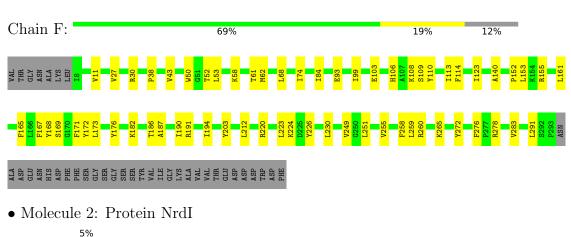
• Molecule 1: Ribonucleoside-diphosphate reductase subunit beta nrdF2

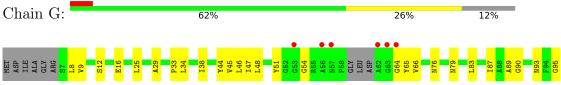


• Molecule 1: Ribonucleoside-diphosphate reductase subunit beta nrdF2

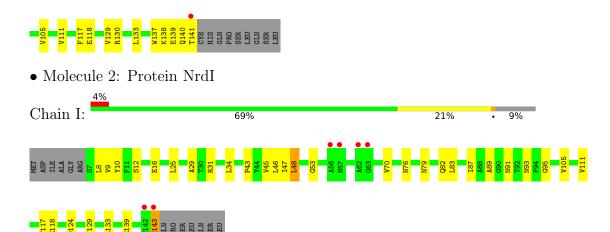


• Molecule 1: Ribonucleoside-diphosphate reductase subunit beta nrdF2











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants	160.50Å 160.50Å 312.08Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.27 - 3.04	Depositor
resolution (A)	48.27 - 3.04	EDS
% Data completeness	99.9 (48.27-3.04)	Depositor
(in resolution range)	99.9 (48.27-3.04)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.99 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.254	Depositor
it, it free	0.215 , 0.250	DCC
R_{free} test set	3972 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.2	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34,61.4	EDS
L-test for twinning ²	$< L >=0.45, < L^2>=0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16030	wwPDB-VP
Average B, all atoms $(Å^2)$	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 46.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1319e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: MN, GOL, OH, FMN

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.25	0/2356	0.45	0/3202	
1	В	0.25	0/2337	0.44	0/3176	
1	С	0.25	0/2350	0.45	0/3193	
1	D	0.25	0/2364	0.45	0/3213	
1	Е	0.24	0/2337	0.42	0/3176	
1	F	0.25	0/2372	0.45	0/3224	
2	G	0.25	0/1053	0.50	0/1429	
2	I	0.25	0/1091	0.49	0/1482	
All	All	0.25	0/16260	0.45	0/22095	

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)	H(added)	Clashes	Symm-Clashes
1	A	2304	0	2251	38	0
1	В	2286	0	2231	34	0
1	С	2299	0	2243	45	0
1	D	2312	0	2255	41	0
1	E	2286	0	2231	30	0

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Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	H(added)	Clashes	Symm-Clashes
1	F	2320	0	2266	47	0
2	G	1029	0	1005	26	0
2	I	1065	0	1036	26	0
3	A	2	0	0	0	0
3	В	2	0	0	0	0
3	С	2	0	0	0	0
3	D	2	0	0	0	0
3	Ε	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	1	0	1	0
4	В	1	1	0	0	0
4	С	1	1	0	0	0
4	D	1	1	0	1	0
4	Ε	1	1	0	0	0
4	F	1	1	0	0	0
5	С	6	0	8	0	0
5	F	6	0	8	0	0
6	G	31	0	19	0	0
6	I	31	0	19	0	0
7	A	7	0	0	0	0
7	В	4	0	0	0	0
7	С	4	0	0	0	0
7	D	7	0	0	1	0
7	Е	2	0	0	0	0
7	F	5	0	0	0	0
7	G	1	0	0	0	0
7	I	1	0	0	0	0
All	All	16024	6	15572	271	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 9.

The worst 5 of 271 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} & ext{Interatomic} \ & ext{distance} \ & ext{(Å)} \end{aligned}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:B:153:LEU:HB3	1:B:223:LEU:HD21	1.49	0.94
2:I:83:LEU:HG	2:I:111:VAL:HG11	1.60	0.83
1:E:153:LEU:HB3	1:E:223:LEU:HD21	1.61	0.81
2:G:83:LEU:HG	2:G:111:VAL:HG11	1.66	0.77
1:F:52:THR:HG21	1:F:182:LYS:HZ1	1.51	0.75



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	ntiles
1	A	282/324~(87%)	277 (98%)	5 (2%)	0	100	100
1	В	280/324 (86%)	275 (98%)	5 (2%)	0	100	100
1	С	281/324 (87%)	276 (98%)	4 (1%)	1 (0%)	30	62
1	D	283/324 (87%)	280 (99%)	3 (1%)	0	100	100
1	E	280/324 (86%)	275 (98%)	5 (2%)	0	100	100
1	F	284/324 (88%)	280 (99%)	4 (1%)	0	100	100
2	G	128/150 (85%)	116 (91%)	11 (9%)	1 (1%)	16	47
2	I	135/150 (90%)	126 (93%)	9 (7%)	0	100	100
All	All	1953/2244 (87%)	1905 (98%)	46 (2%)	2 (0%)	48	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	140	GLN
1	С	151	GLU

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	249/282 (88%)	247 (99%)	2 (1%)	79 89

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Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	В	247/282~(88%)	247 (100%)	0	100	100
1	С	248/282~(88%)	247 (100%)	1 (0%)	89	94
1	D	$250/282\ (89\%)$	250 (100%)	0	100	100
1	E	247/282~(88%)	247 (100%)	0	100	100
1	F	$251/282\ (89\%)$	251 (100%)	0	100	100
2	G	$107/122\ (88\%)$	107 (100%)	0	100	100
2	I	111/122~(91%)	109 (98%)	2 (2%)	54	77
All	All	1710/1936 (88%)	1705 (100%)	5 (0%)	91	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	248	GLU
1	С	134	ARG
2	I	48	LEU
2	I	143	HIS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 12 are monoatomic and 6 are modelled with single atom - leaving 4 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	Tuno	Type Chain Res Lin		Res Link Bond lengths			ths	Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
6	FMN	G	201	-	33,33,33	1.08	2 (6%)	48,50,50	1.20	7 (14%)	
6	FMN	I	201	-	33,33,33	1.09	2 (6%)	48,50,50	1.24	8 (16%)	
5	GOL	F	1301	-	5,5,5	1.01	0	5,5,5	0.90	0	
5	GOL	С	1303	-	5,5,5	1.03	0	5,5,5	0.89	0	

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
6	FMN	G	201	-	-	1/18/18/18	0/3/3/3
6	FMN	I	201	-	-	0/18/18/18	0/3/3/3
5	GOL	F	1301	-	-	0/4/4/4	-
5	GOL	С	1303	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$Ideal(\AA)$
6	G	201	FMN	C4A-N5	4.00	1.38	1.30
6	I	201	FMN	C4A-N5	3.99	1.38	1.30
6	I	201	FMN	C10-N1	2.56	1.38	1.33
6	G	201	FMN	C10-N1	2.50	1.38	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
6	I	201	FMN	C4-N3-C2	-3.10	119.92	125.64
6	G	201	FMN	C4-N3-C2	-2.97	120.15	125.64
6	I	201	FMN	C4A-C4-N3	2.73	120.11	113.19
6	I	201	FMN	O4-C4-C4A	-2.62	119.64	126.60
6	G	201	FMN	C4A-C4-N3	2.58	119.74	113.19

There are no chirality outliers.



All (1) torsion outliers are listed below:

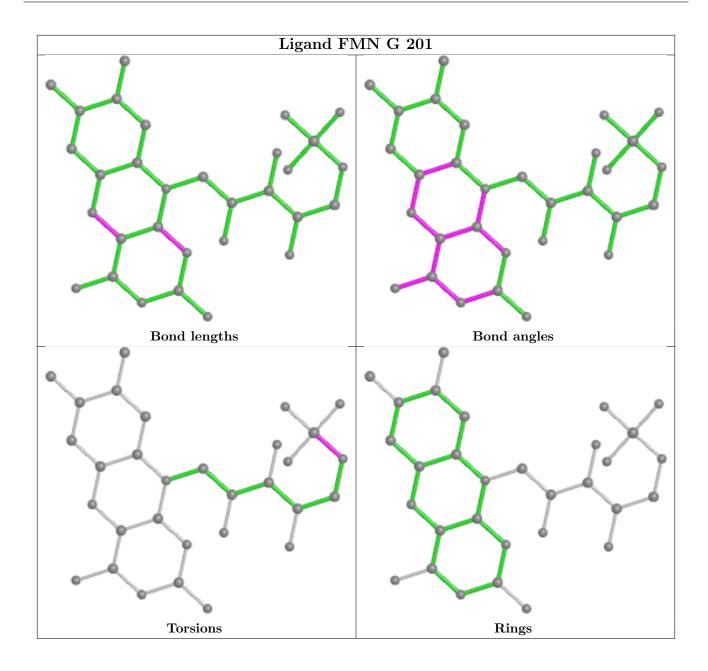
Mol	Chain	Res	Type	Atoms
6	G	201	FMN	C5'-O5'-P-O1P

There are no ring outliers.

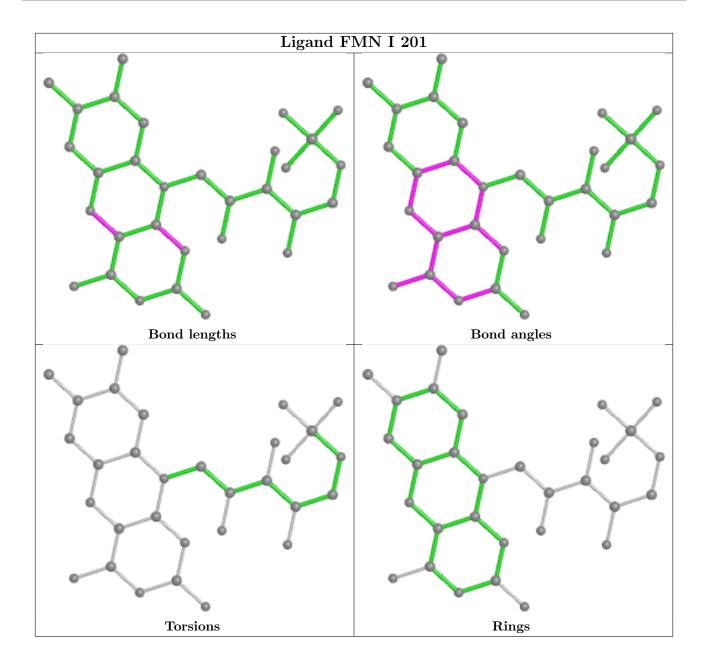
No monomer is involved in short contacts.

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 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></rsrz>	#RSRZ	i>2	$OWAB(Å^2)$	Q<0.9
1	A	284/324 (87%)	-0.53	1 (0%) 89	77	24, 50, 79, 110	2 (0%)
1	В	282/324~(87%)	-0.69	2 (0%) 84	68	23, 46, 76, 94	1 (0%)
1	С	283/324 (87%)	-0.69	1 (0%) 89	77	27, 47, 68, 106	1 (0%)
1	D	285/324 (87%)	-0.68	1 (0%) 89	77	27, 44, 66, 105	4 (1%)
1	E	282/324 (87%)	0.26	17 (6%) 29	16	40, 84, 132, 169	20 (7%)
1	F	286/324 (88%)	-0.78	0 100	100	22, 43, 65, 106	3 (1%)
2	G	132/150 (88%)	0.04	7 (5%) 33	19	31, 75, 107, 127	9 (6%)
2	I	137/150 (91%)	-0.03	6 (4%) 39	23	42, 69, 110, 146	9 (6%)
All	All	1971/2244 (87%)	-0.45	35 (1%) 67	45	22, 52, 104, 169	49 (2%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	292	SER	6.5
1	Е	45	ASN	5.1
1	D	293	PRO	5.0
1	A	293	PRO	4.3
2	I	143	HIS	4.1

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.



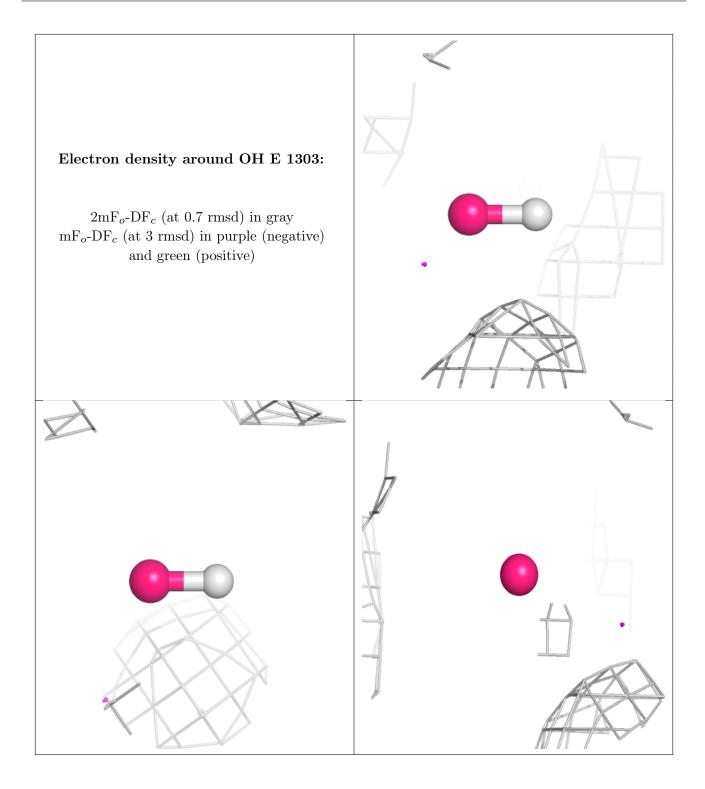
6.4 Ligands (i)

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.

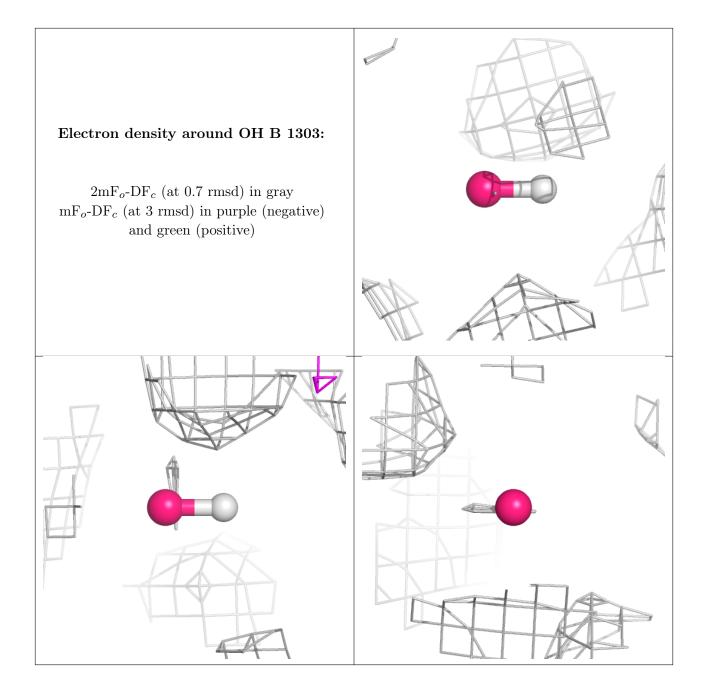
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathring{\mathbf{A}}^2)$	Q<0.9
5	GOL	F	1301	6/6	0.85	0.18	20,49,74,79	0
5	GOL	С	1303	6/6	0.86	0.16	27,52,60,70	0
4	ОН	E	1303	1/1	0.92	0.35	87,87,87,105	0
4	ОН	В	1303	1/1	0.92	0.17	52,52,52,63	0
4	ОН	D	1303	1/1	0.92	0.20	53,53,53,65	0
3	MN	E	1302	1/1	0.93	0.18	120,120,120,120	0
4	ОН	A	1303	1/1	0.94	0.20	50,50,50,60	0
3	MN	D	1301	1/1	0.95	0.12	95,95,95,95	0
3	MN	С	1302	1/1	0.95	0.11	87,87,87,87	0
3	MN	F	1302	1/1	0.95	0.10	83,83,83,83	0
4	ОН	С	1304	1/1	0.97	0.14	40,40,40,49	0
6	FMN	G	201	31/31	0.97	0.07	36,50,61,66	0
3	MN	Ε	1301	1/1	0.98	0.05	95,95,95,95	0
3	MN	A	1302	1/1	0.98	0.11	102,102,102,102	0
4	ОН	F	1304	1/1	0.98	0.19	46,46,46,56	0
6	FMN	I	201	31/31	0.98	0.07	21,46,59,67	0
3	MN	В	1301	1/1	0.99	0.09	86,86,86,86	0
3	MN	F	1303	1/1	0.99	0.02	54,54,54,54	0
3	MN	В	1302	1/1	1.00	0.04	56,56,56,56	0
3	MN	D	1302	1/1	1.00	0.03	56,56,56,56	0
3	MN	С	1301	1/1	1.00	0.03	60,60,60,60	0
3	MN	A	1301	1/1	1.00	0.05	59,59,59,59	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.

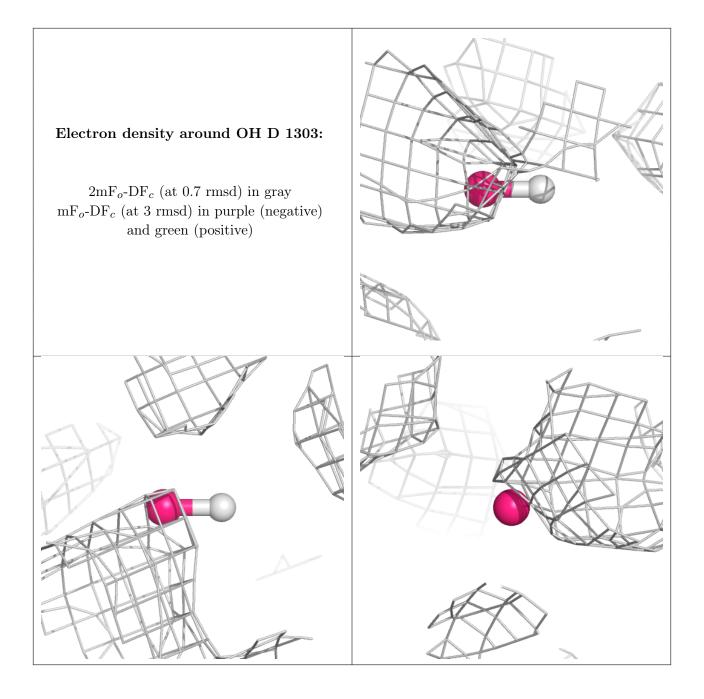




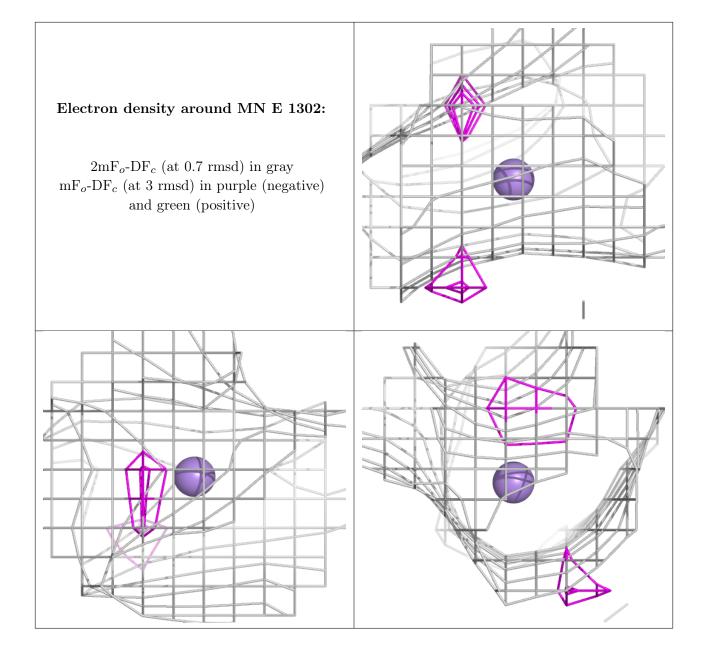














Electron density around OH A 1303: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray $\mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MN D 1301: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

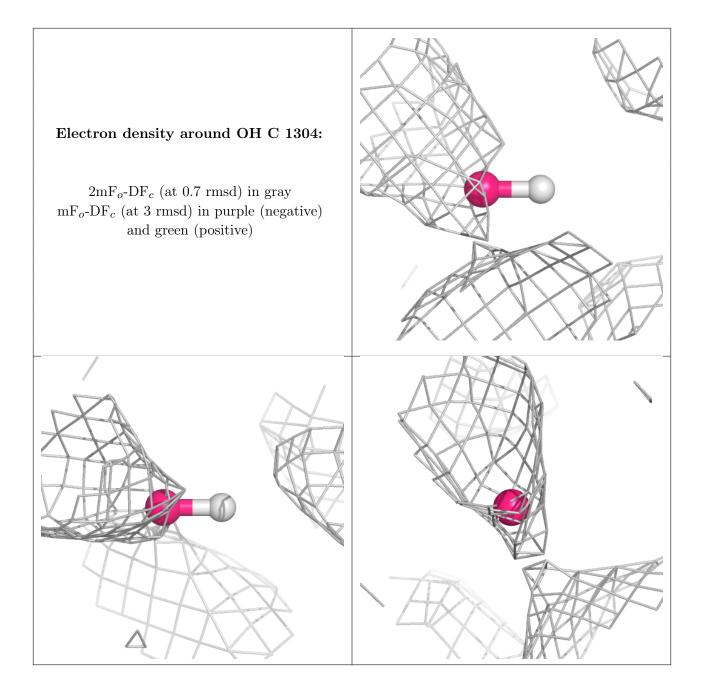


Electron density around MN C 1302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MN F 1302: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)





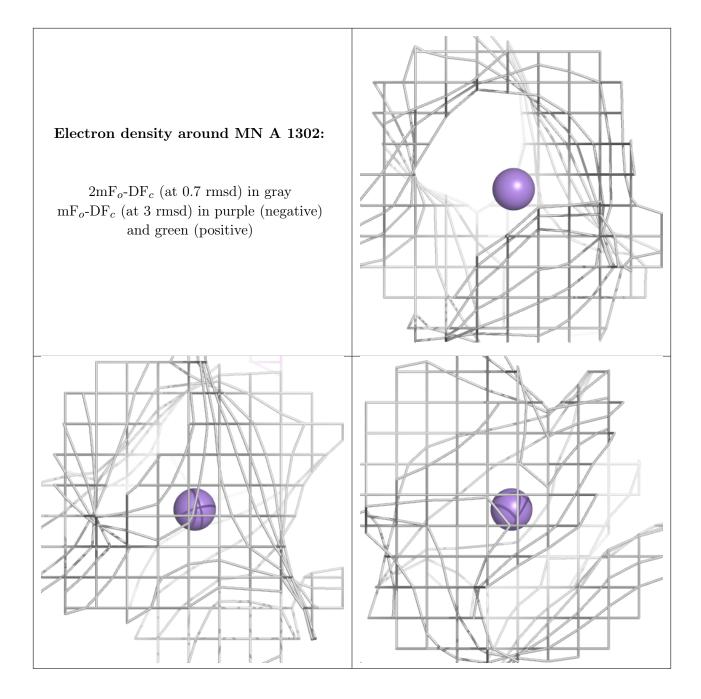


Electron density around FMN G 201: 2mF_o-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

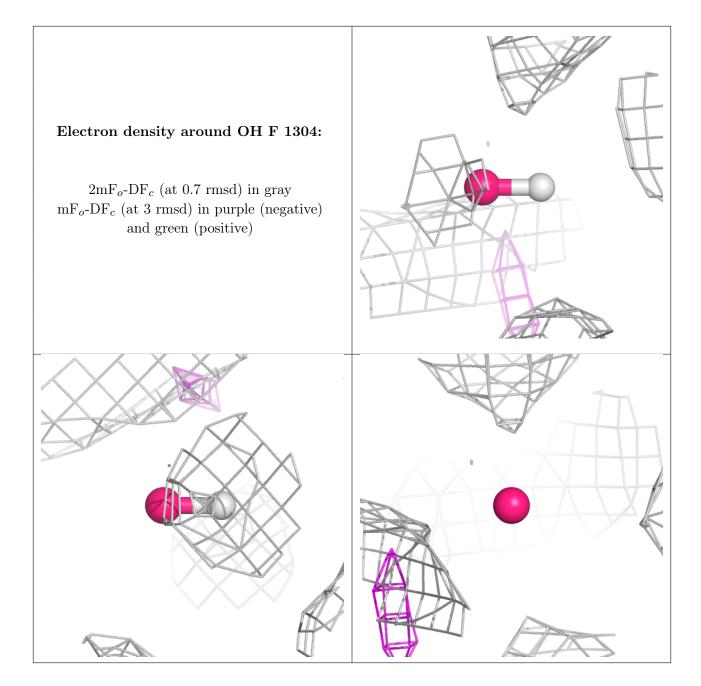


Electron density around MN E 1301: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

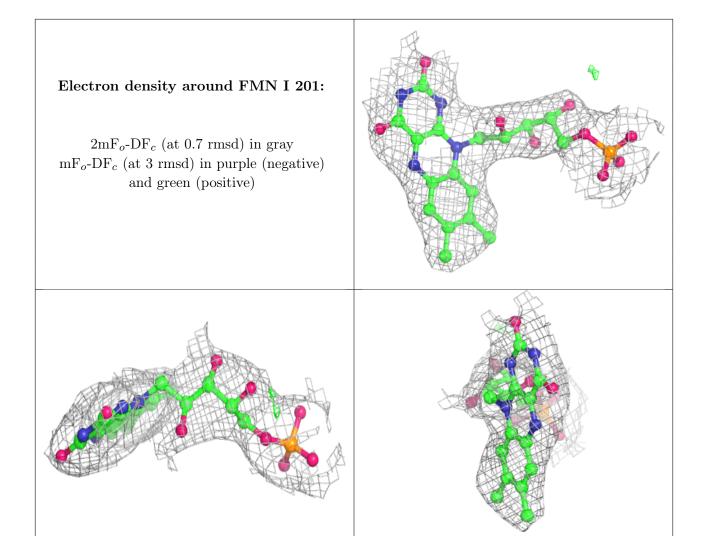




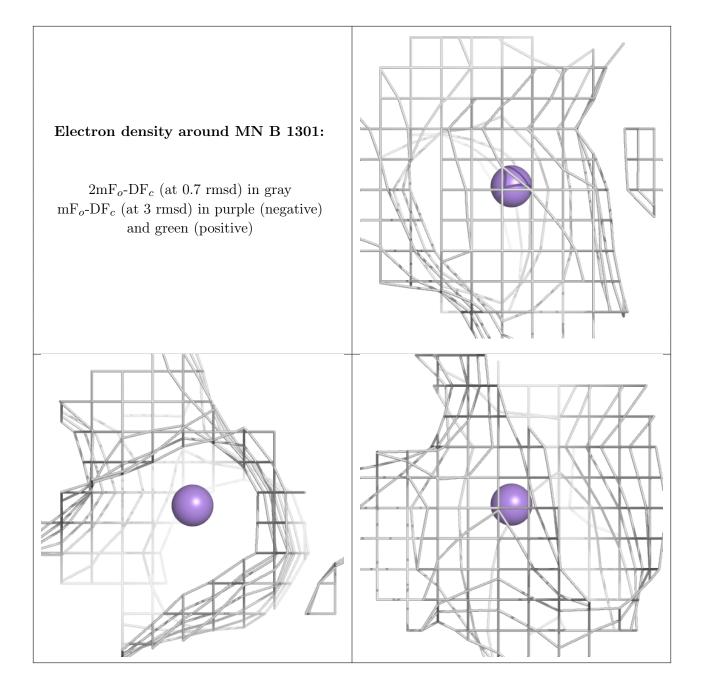




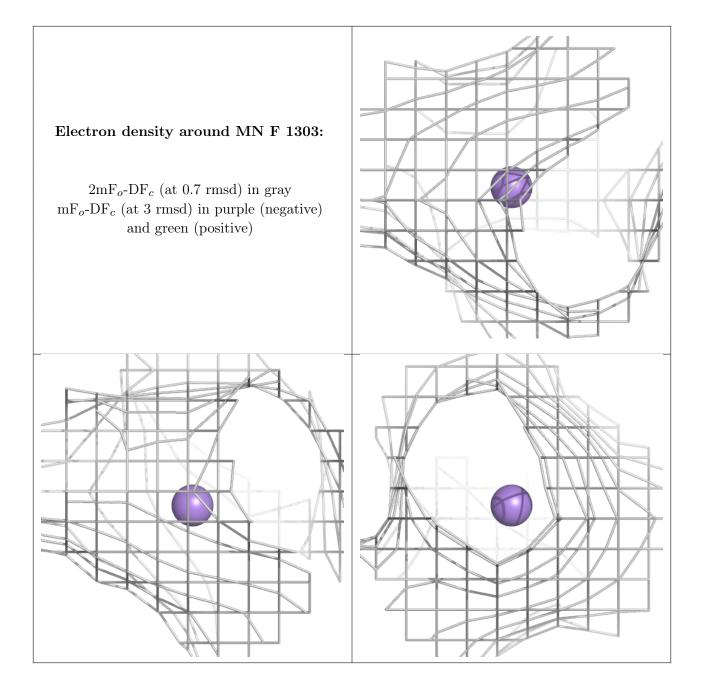




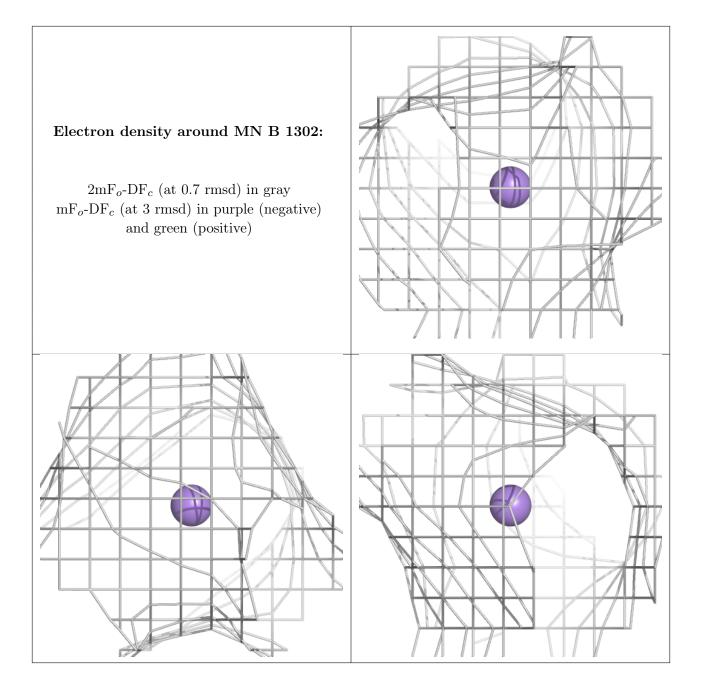




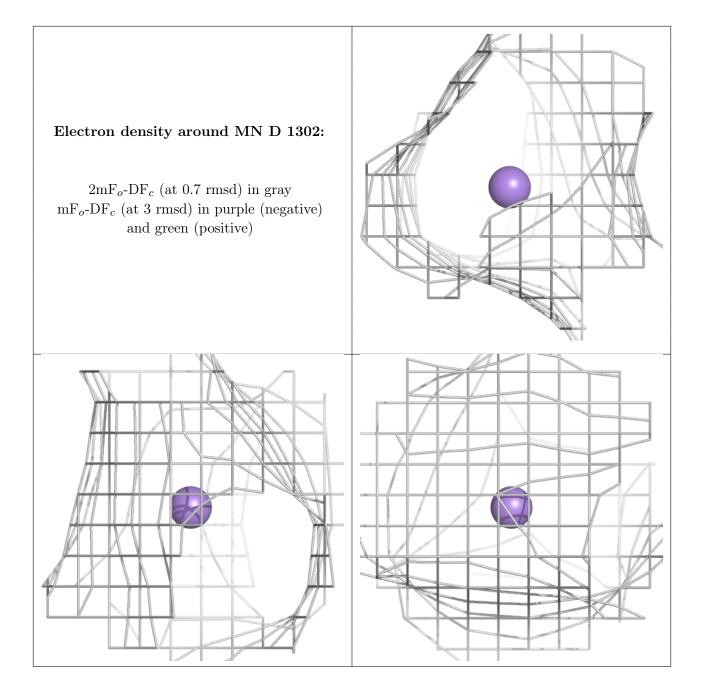




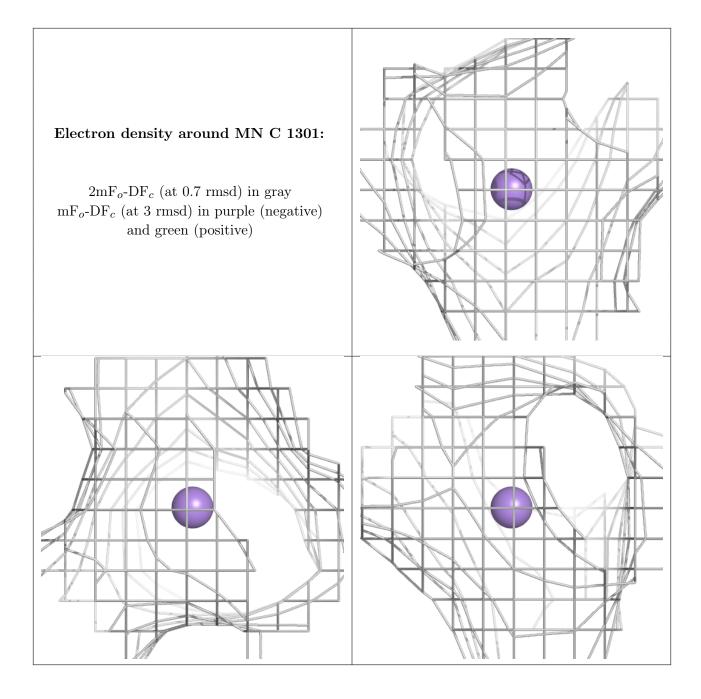




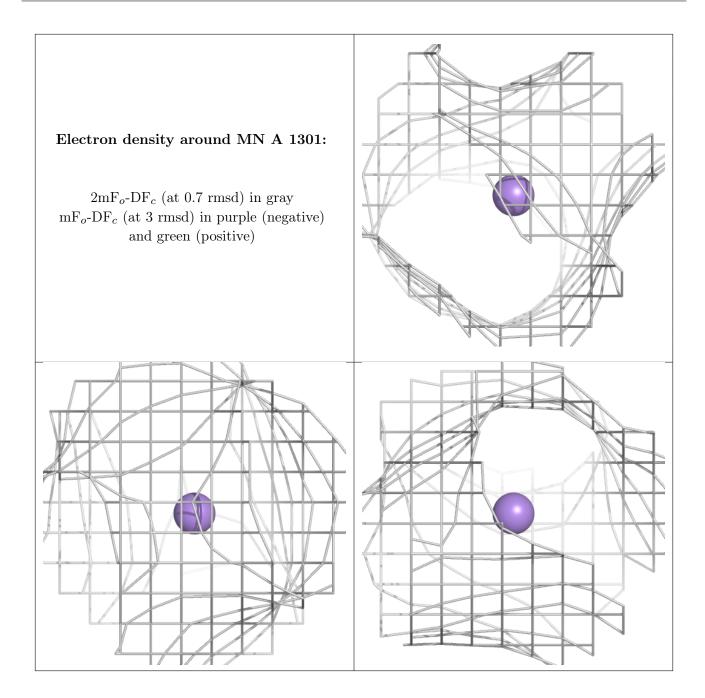












6.5 Other polymers (i)

There are no such residues in this entry.

