



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:55 AM UTC

PDB ID : 7MMS / pdb_00007mms
Title : Crystal Structure of the Class Ie Ribonucleotide Reductase Beta-NrdI complex from *Aerococcus urinae* in Semiquinone Form with Cu(I) bound
Authors : Palowitch, G.M.; Boal, A.K.
Deposited on : 2021-04-30
Resolution : 1.91 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:

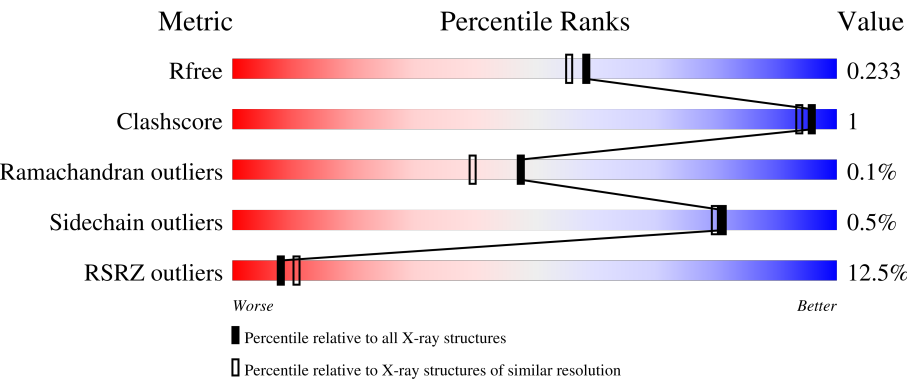
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	342	5% 89%8%
1	B	342	6% 88%8%
1	C	342	4% 87%10%
1	D	342	7% 91%6%
2	E	147	18% 89%10%

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Mol	Chain	Length	Quality of chain
2	F	147	9% 87% • 10%
2	G	147	22% 86% • 12%
2	H	147	50% 76% 7% • 16%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15231 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 Ribonucleoside-diphosphate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	3	0
			2580	1663	417	494	6			
1	B	313	Total	C	N	O	S	0	1	0
			2566	1656	415	489	6			
1	C	309	Total	C	N	O	S	0	4	0
			2554	1648	414	486	6			
1	D	320	Total	C	N	O	S	0	2	0
			2615	1685	425	499	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	SER	-	expression tag	UNP F2I8X9
A	-3	ASN	-	expression tag	UNP F2I8X9
A	-2	ILE	-	expression tag	UNP F2I8X9
A	-1	LEU	-	expression tag	UNP F2I8X9
A	0	GLU	-	expression tag	UNP F2I8X9
B	-4	SER	-	expression tag	UNP F2I8X9
B	-3	ASN	-	expression tag	UNP F2I8X9
B	-2	ILE	-	expression tag	UNP F2I8X9
B	-1	LEU	-	expression tag	UNP F2I8X9
B	0	GLU	-	expression tag	UNP F2I8X9
C	-4	SER	-	expression tag	UNP F2I8X9
C	-3	ASN	-	expression tag	UNP F2I8X9
C	-2	ILE	-	expression tag	UNP F2I8X9
C	-1	LEU	-	expression tag	UNP F2I8X9
C	0	GLU	-	expression tag	UNP F2I8X9
D	-4	SER	-	expression tag	UNP F2I8X9
D	-3	ASN	-	expression tag	UNP F2I8X9
D	-2	ILE	-	expression tag	UNP F2I8X9
D	-1	LEU	-	expression tag	UNP F2I8X9
D	0	GLU	-	expression tag	UNP F2I8X9

- Molecule 2 is a protein called Protein NrdI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	133	Total	C	N	O	S	0	0	0
			1057	674	177	205	1			
2	G	129	Total	C	N	O	S	0	0	0
			1030	658	172	199	1			
2	F	133	Total	C	N	O	S	0	0	0
			1059	676	177	205	1			
2	H	123	Total	C	N	O	S	0	0	0
			981	626	162	192	1			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	SER	-	expression tag	UNP A0A178HGH7
E	-3	ASN	-	expression tag	UNP A0A178HGH7
E	-2	ILE	-	expression tag	UNP A0A178HGH7
E	-1	LEU	-	expression tag	UNP A0A178HGH7
E	0	GLU	-	expression tag	UNP A0A178HGH7
G	-4	SER	-	expression tag	UNP A0A178HGH7
G	-3	ASN	-	expression tag	UNP A0A178HGH7
G	-2	ILE	-	expression tag	UNP A0A178HGH7
G	-1	LEU	-	expression tag	UNP A0A178HGH7
G	0	GLU	-	expression tag	UNP A0A178HGH7
F	-4	SER	-	expression tag	UNP A0A178HGH7
F	-3	ASN	-	expression tag	UNP A0A178HGH7
F	-2	ILE	-	expression tag	UNP A0A178HGH7
F	-1	LEU	-	expression tag	UNP A0A178HGH7
F	0	GLU	-	expression tag	UNP A0A178HGH7
H	-4	SER	-	expression tag	UNP A0A178HGH7
H	-3	ASN	-	expression tag	UNP A0A178HGH7
H	-2	ILE	-	expression tag	UNP A0A178HGH7
H	-1	LEU	-	expression tag	UNP A0A178HGH7
H	0	GLU	-	expression tag	UNP A0A178HGH7

- Molecule 3 is COPPER (I) ION (CCD ID: CU1) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

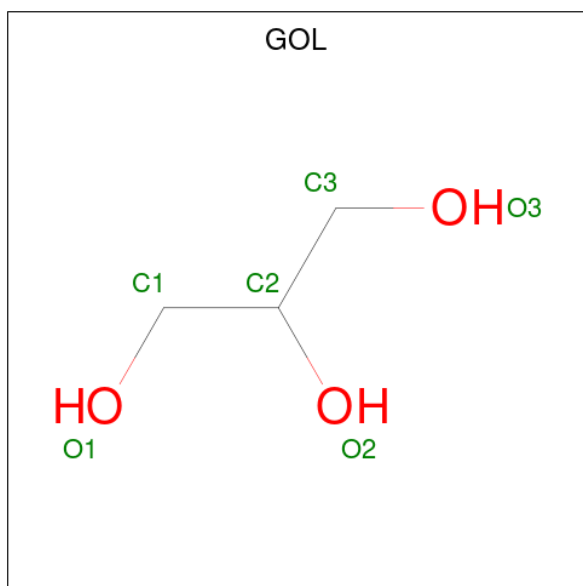
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cu	0	0
			1	1		
3	B	1	Total	Cu	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Cu	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

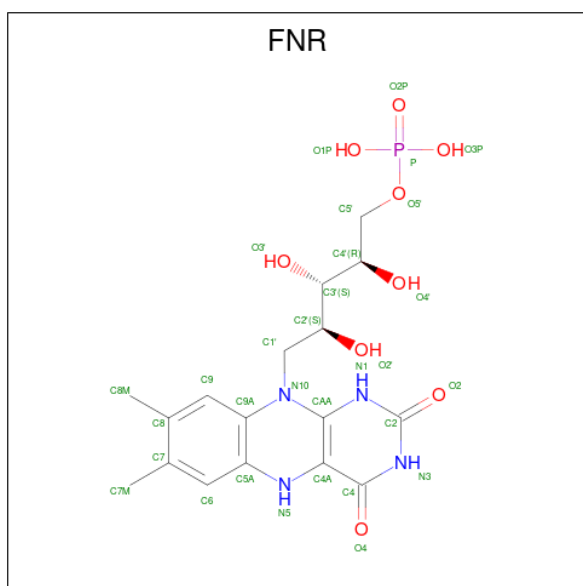


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0

- Molecule 6 is 1-DEOXY-1-(7,8-DIMETHYL-2,4-DIOXO-3,4-DIHYDRO-2H-BENZO[G]PTERIDIN-1-ID-10(5H)-YL)-5-O-PHOSPHONATO-D-RIBITOL (CCD ID: FNR) (formula: $C_{17}H_{23}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O P 31 17 4 9 1	0	0
6	G	1	Total C N O P 31 17 4 9 1	0	0
6	F	1	Total C N O P 31 17 4 9 1	0	0
6	H	1	Total C N O P 31 17 4 9 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	128	Total O 128 128	0	0
7	B	116	Total O 116 116	0	0

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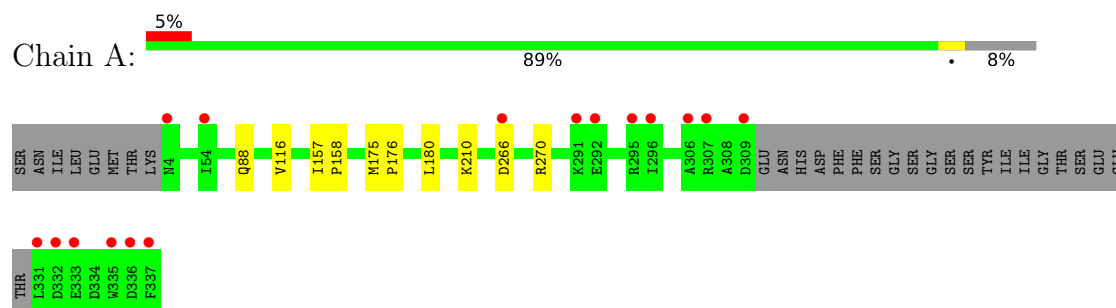
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	135	Total 135	O 135	0	0
7	D	131	Total 131	O 131	0	0
7	E	23	Total 23	O 23	0	0
7	G	21	Total 21	O 21	0	0
7	F	35	Total 35	O 35	0	0
7	H	15	Total 15	O 15	0	0

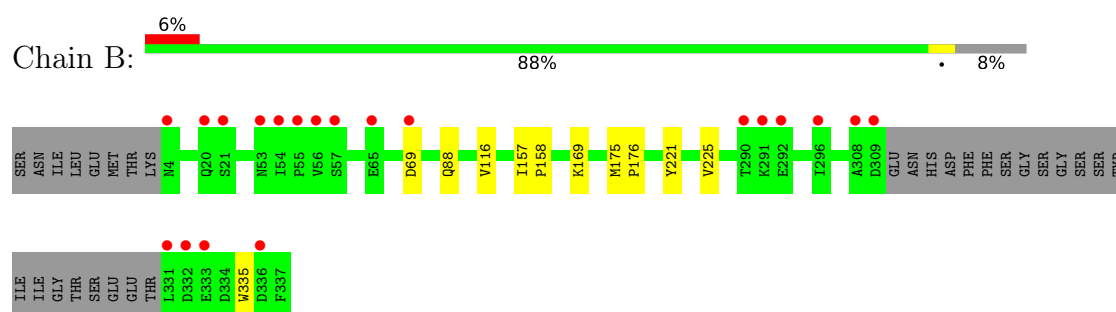
3 Residue-property plots [i](#)

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.

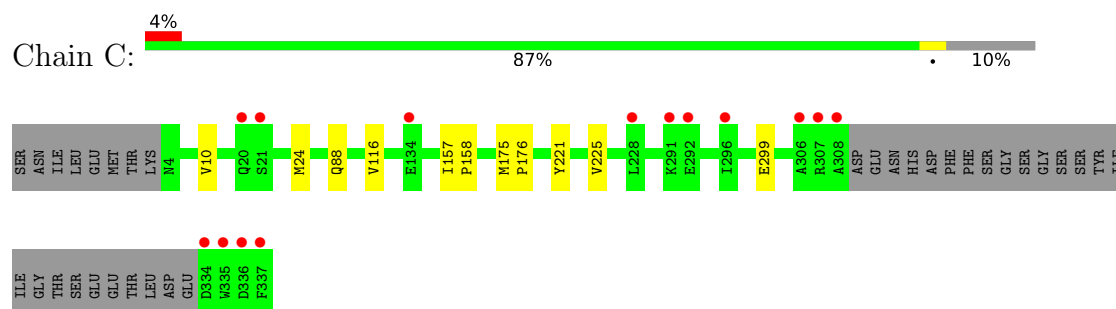
- Molecule 1: Ribonucleoside-diphosphate reductase



- Molecule 1: Ribonucleoside-diphosphate reductase

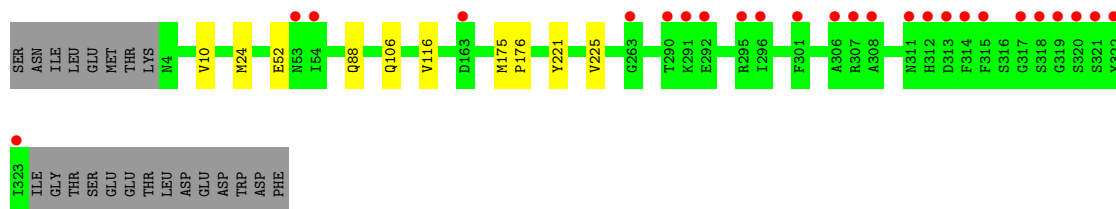


- Molecule 1: Ribonucleoside-diphosphate reductase

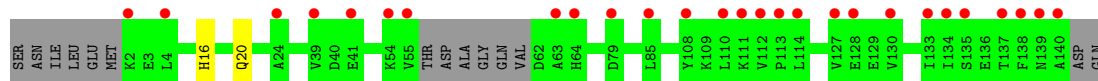


- Molecule 1: Ribonucleoside-diphosphate reductase

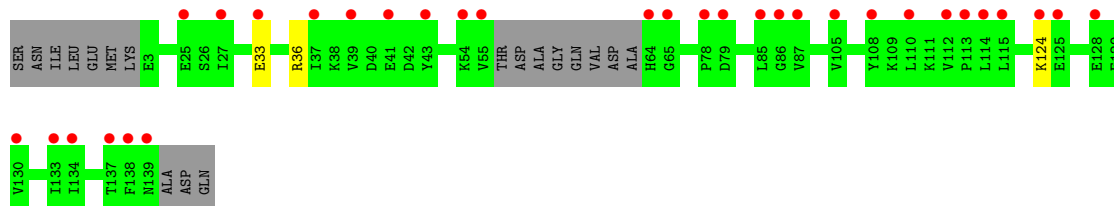
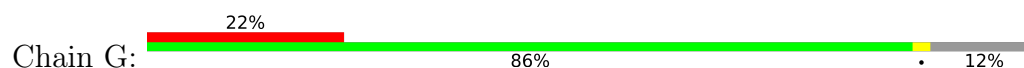




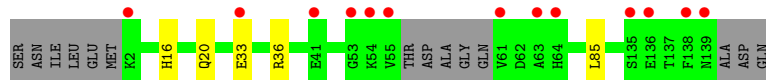
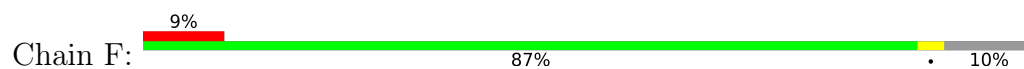
● Molecule 2: Protein NrdI



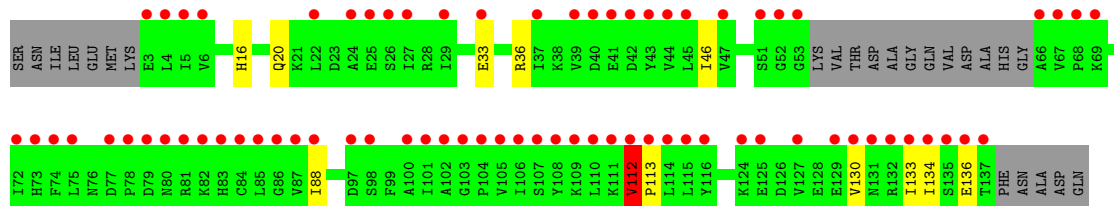
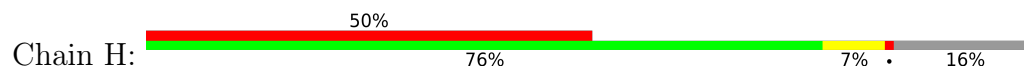
● Molecule 2: Protein NrdI



● Molecule 2: Protein NrdI



● Molecule 2: Protein NrdI



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.35Å 104.79Å 137.41Å 90.00° 100.29° 90.00°	Depositor
Resolution (Å)	49.25 – 1.91 49.25 – 1.91	Depositor EDS
% Data completeness (in resolution range)	96.2 (49.25-1.91) 96.7 (49.25-1.91)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.201 , 0.226 0.208 , 0.233	Depositor DCC
R_{free} test set	8195 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15231	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU1, CA, GOL, FNR

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	0.98	0/2645	1.45	0/3591
1	B	0.98	0/2631	1.45	0/3572
1	C	0.98	0/2619	1.43	0/3555
1	D	0.99	0/2682	1.46	0/3641
2	E	1.01	0/1077	1.39	0/1458
2	F	1.00	0/1079	1.37	0/1461
2	G	1.01	0/1050	1.39	0/1422
2	H	1.03	0/999	1.39	1/1354 (0.1%)
All	All	0.99	0/14782	1.43	1/20054 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	112	VAL	CB-CA-C	5.17	114.40	109.33

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	2580	0	2485	6	0
1	B	2566	0	2478	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2554	0	2466	6	0
1	D	2615	0	2524	6	0
2	E	1057	0	1045	1	0
2	F	1059	0	1049	2	0
2	G	1030	0	1018	1	0
2	H	981	0	971	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	1	0
4	C	6	0	8	0	0
4	D	6	0	8	1	0
4	E	6	0	8	0	0
4	F	12	0	16	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	E	31	0	22	0	0
6	F	31	0	22	0	0
6	G	31	0	22	0	0
6	H	31	0	22	0	0
7	A	128	0	0	0	0
7	B	116	0	0	0	0
7	C	135	0	0	0	0
7	D	131	0	0	0	0
7	E	23	0	0	0	0
7	F	35	0	0	0	0
7	G	21	0	0	0	0
7	H	15	0	0	0	0
All	All	15231	0	14196	33	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 1.

All (33) 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:266:ASP:OD2	1:A:270:ARG:NH1	2.13	0.82
2:G:33:GLU:O	2:G:36:ARG:NH1	2.30	0.64
2:H:112:VAL:HG22	2:H:113:PRO:HD2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:33:GLU:O	2:F:36:ARG:NH1	2.31	0.58
1:B:335:TRP:O	4:B:402:GOL:H2	2.08	0.53
1:D:175:MET:HB3	1:D:176:PRO:HD3	1.92	0.51
1:B:88:GLN:HB3	1:B:116:VAL:HG11	1.93	0.51
1:B:221:TYR:CZ	1:B:225:VAL:HG11	2.45	0.50
1:D:106:GLN:NE2	4:D:401:GOL:H32	2.27	0.50
1:A:175:MET:HB3	1:A:176:PRO:CD	2.43	0.49
1:C:88:GLN:HB3	1:C:116:VAL:HG11	1.95	0.49
1:D:88:GLN:HB3	1:D:116:VAL:HG11	1.95	0.47
1:D:221:TYR:CZ	1:D:225:VAL:HG11	2.50	0.46
1:A:88:GLN:HB3	1:A:116:VAL:HG11	1.97	0.46
2:F:16:HIS:O	2:F:20:GLN:HG2	2.16	0.44
2:E:16:HIS:O	2:E:20:GLN:HG2	2.16	0.44
2:H:46:ILE:HA	2:H:88:ILE:O	2.18	0.43
1:A:175:MET:HB3	1:A:176:PRO:HD3	2.00	0.43
1:D:175:MET:HB3	1:D:176:PRO:CD	2.49	0.42
1:B:157:ILE:N	1:B:158:PRO:CD	2.82	0.42
2:H:130:VAL:O	2:H:134:ILE:HG23	2.19	0.42
1:C:175:MET:HB3	1:C:176:PRO:HD3	2.00	0.42
1:B:175:MET:HB3	1:B:176:PRO:HD3	2.01	0.42
1:B:175:MET:HB3	1:B:176:PRO:CD	2.50	0.42
1:C:175:MET:HB3	1:C:176:PRO:CD	2.49	0.42
1:D:10:VAL:O	1:D:24:MET:HA	2.20	0.42
1:C:221:TYR:CZ	1:C:225:VAL:HG11	2.55	0.41
1:A:180:LEU:HD22	1:A:210:LYS:HE3	2.02	0.41
1:A:157:ILE:N	1:A:158:PRO:CD	2.84	0.41
2:H:16:HIS:O	2:H:20:GLN:HG2	2.21	0.41
1:C:10:VAL:O	1:C:24:MET:HA	2.21	0.40
2:H:33:GLU:O	2:H:36:ARG:NH1	2.48	0.40
1:C:157:ILE:N	1:C:158:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	312/342 (91%)	307 (98%)	5 (2%)	0	100	100
1	B	310/342 (91%)	306 (99%)	4 (1%)	0	100	100
1	C	309/342 (90%)	306 (99%)	3 (1%)	0	100	100
1	D	320/342 (94%)	316 (99%)	4 (1%)	0	100	100
2	E	129/147 (88%)	125 (97%)	4 (3%)	0	100	100
2	F	129/147 (88%)	126 (98%)	3 (2%)	0	100	100
2	G	125/147 (85%)	120 (96%)	5 (4%)	0	100	100
2	H	119/147 (81%)	111 (93%)	7 (6%)	1 (1%)	16	6
All	All	1753/1956 (90%)	1717 (98%)	35 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	136	GLU

5.3.2 Protein sidechains ⓘ

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	278/301 (92%)	278 (100%)	0	100	100
1	B	276/301 (92%)	274 (99%)	2 (1%)	76	73
1	C	275/301 (91%)	274 (100%)	1 (0%)	84	83
1	D	282/301 (94%)	281 (100%)	1 (0%)	84	83
2	E	119/131 (91%)	119 (100%)	0	100	100
2	F	120/131 (92%)	119 (99%)	1 (1%)	73	71
2	G	117/131 (89%)	116 (99%)	1 (1%)	70	67
2	H	112/131 (86%)	110 (98%)	2 (2%)	51	39
All	All	1579/1728 (91%)	1571 (100%)	8 (0%)	81	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	69	ASP
1	B	169	LYS
1	C	299	GLU
1	D	52	GLU
2	G	124	LYS
2	F	85	LEU
2	H	112	VAL
2	H	133	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	99	ASN
1	A	111	ASN
1	B	46	GLN
1	B	99	ASN
1	B	111	ASN
1	B	275	ASN
1	B	281	GLN
1	B	282	ASN
1	C	30	ASN
1	C	46	GLN
1	C	99	ASN
1	C	111	ASN
1	C	275	ASN
1	D	30	ASN
1	D	99	ASN
1	D	111	ASN
1	D	281	GLN
2	E	14	ASN
2	E	20	GLN
2	E	117	GLN
2	F	117	GLN

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](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	A	402	-	5,5,5	0.10	0	5,5,5	0.30	0
6	FNR	E	201	-	32,33,33	0.63	0	41,50,50	0.69	1 (2%)
4	GOL	D	401	-	5,5,5	0.10	0	5,5,5	0.28	0
4	GOL	A	403	-	5,5,5	0.10	0	5,5,5	0.30	0
4	GOL	B	402	-	5,5,5	0.09	0	5,5,5	0.30	0
4	GOL	F	501	-	5,5,5	0.09	0	5,5,5	0.28	0
6	FNR	G	201	-	32,33,33	0.64	0	41,50,50	0.72	1 (2%)
6	FNR	F	502	-	32,33,33	0.63	0	41,50,50	0.68	1 (2%)
6	FNR	H	201	-	32,33,33	0.65	0	41,50,50	0.68	0
4	GOL	F	503	-	5,5,5	0.09	0	5,5,5	0.28	0
4	GOL	C	402	-	5,5,5	0.10	0	5,5,5	0.28	0
4	GOL	B	403	-	5,5,5	0.09	0	5,5,5	0.26	0
4	GOL	E	202	-	5,5,5	0.09	0	5,5,5	0.24	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
4	GOL	A	402	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FNR	E	201	-	-	0/18/18/18	0/3/3/3
4	GOL	D	401	-	-	2/4/4/4	-
4	GOL	A	403	-	-	2/4/4/4	-
4	GOL	B	402	-	-	2/4/4/4	-
4	GOL	F	501	-	-	0/4/4/4	-
6	FNR	G	201	-	-	0/18/18/18	0/3/3/3
6	FNR	F	502	-	-	0/18/18/18	0/3/3/3
6	FNR	H	201	-	-	0/18/18/18	0/3/3/3
4	GOL	F	503	-	-	2/4/4/4	-
4	GOL	C	402	-	-	2/4/4/4	-
4	GOL	B	403	-	-	2/4/4/4	-
4	GOL	E	202	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	201	FNR	C4-C4A-N5	2.19	121.96	116.37
6	E	201	FNR	C4-C4A-N5	2.14	121.84	116.37
6	F	502	FNR	C4-C4A-N5	2.07	121.67	116.37

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	GOL	O1-C1-C2-C3
4	A	403	GOL	C1-C2-C3-O3
4	B	402	GOL	C1-C2-C3-O3
4	B	403	GOL	C1-C2-C3-O3
4	B	403	GOL	O2-C2-C3-O3
4	F	503	GOL	O1-C1-C2-C3
4	A	402	GOL	C1-C2-C3-O3
4	C	402	GOL	C1-C2-C3-O3
4	D	401	GOL	O1-C1-C2-C3
4	A	402	GOL	O1-C1-C2-O2
4	A	403	GOL	O2-C2-C3-O3
4	F	503	GOL	O1-C1-C2-O2
4	B	402	GOL	O2-C2-C3-O3
4	C	402	GOL	O2-C2-C3-O3
4	A	402	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	D	401	GOL	O1-C1-C2-O2

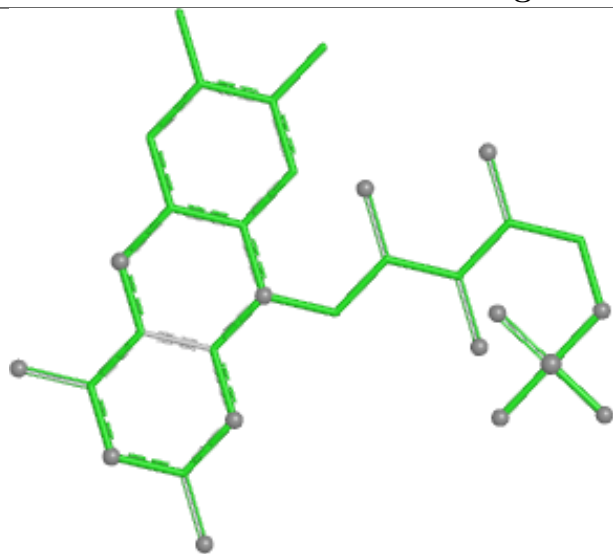
There are no ring outliers.

2 monomers are involved in 2 short contacts:

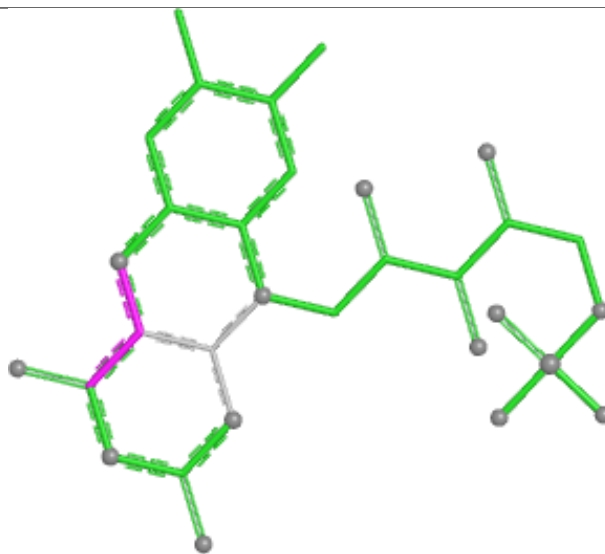
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	401	GOL	1	0
4	B	402	GOL	1	0

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 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.

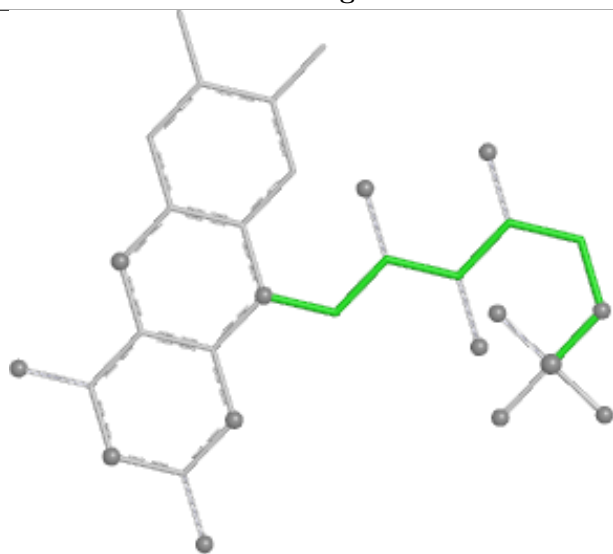
Ligand FNR E 201



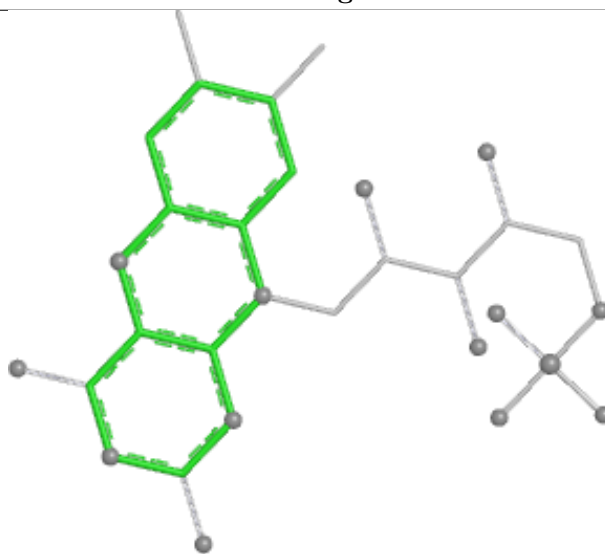
Bond lengths



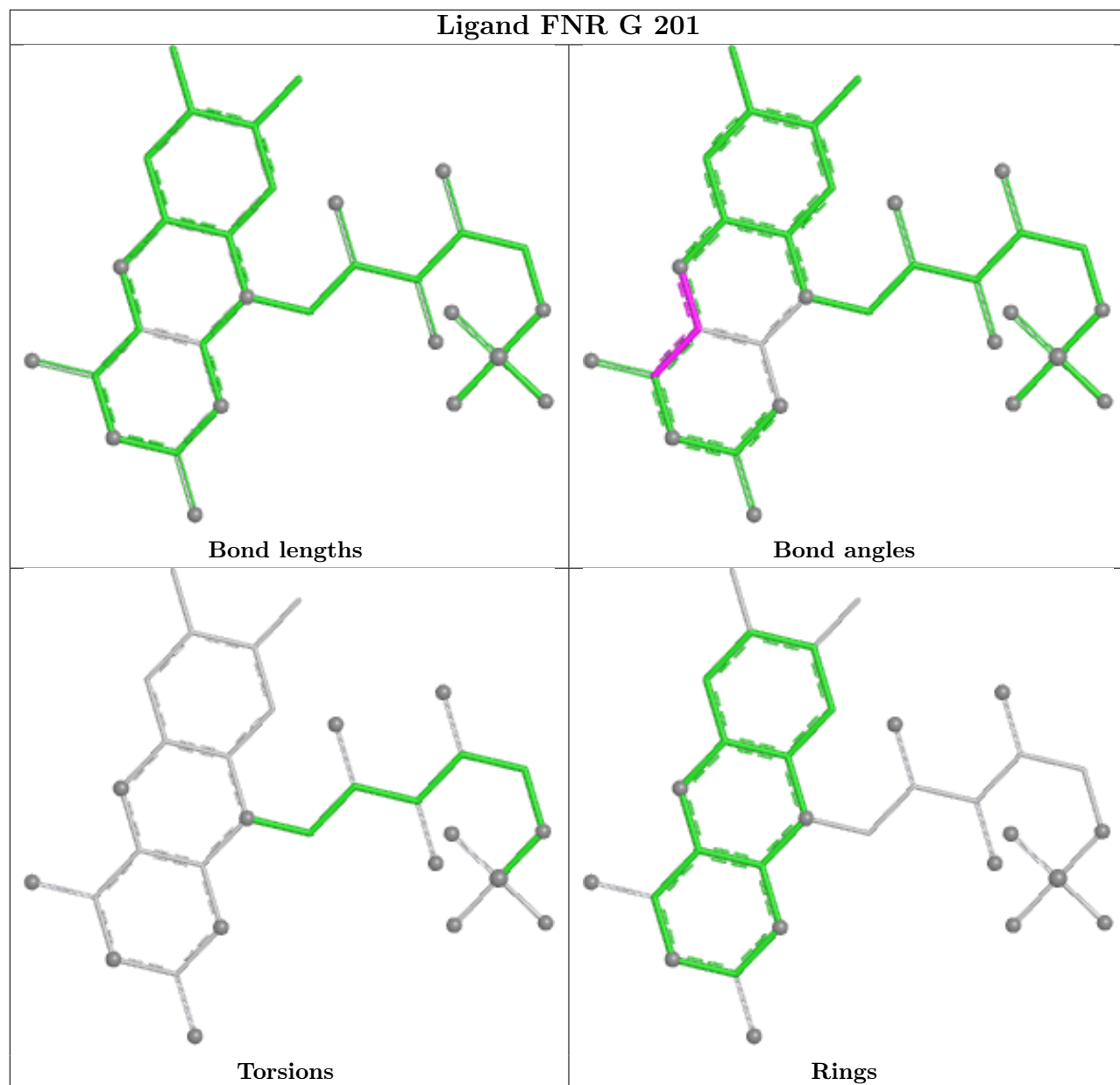
Bond angles



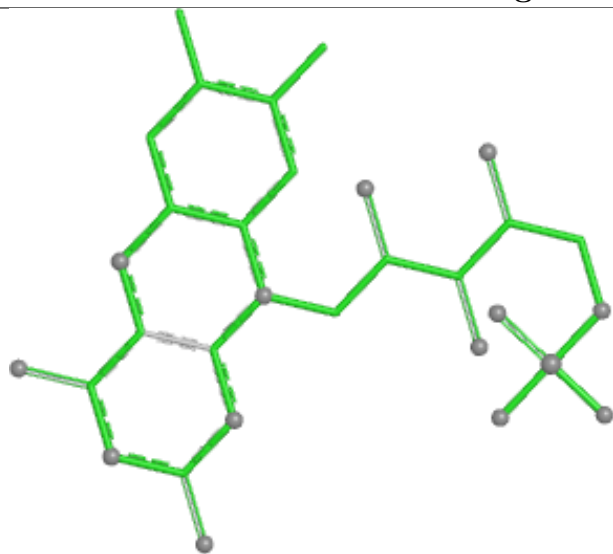
Torsions



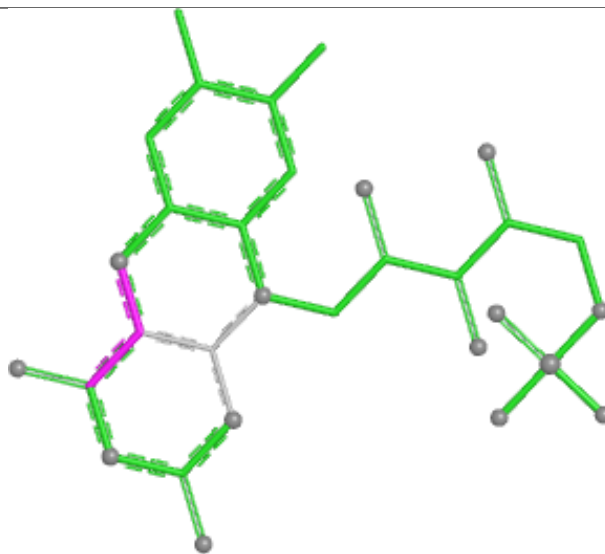
Rings



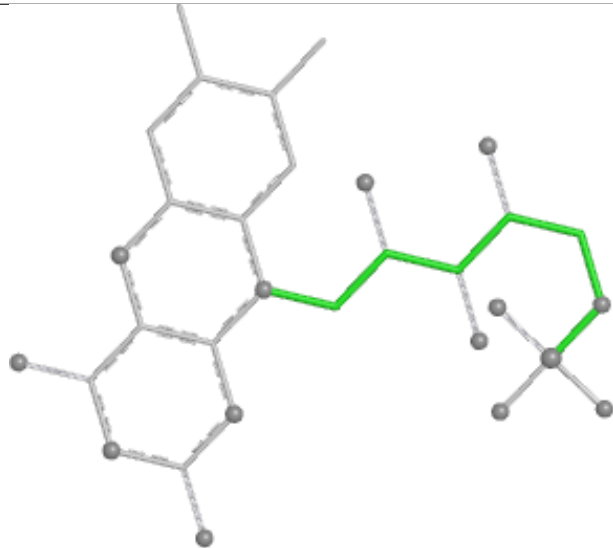
Ligand FNR F 502



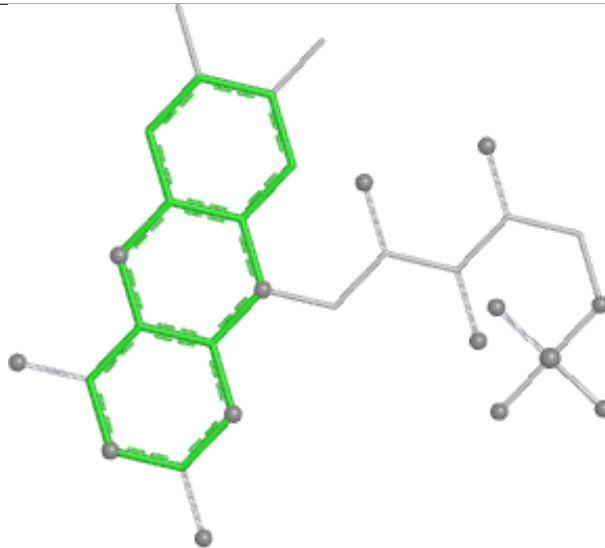
Bond lengths



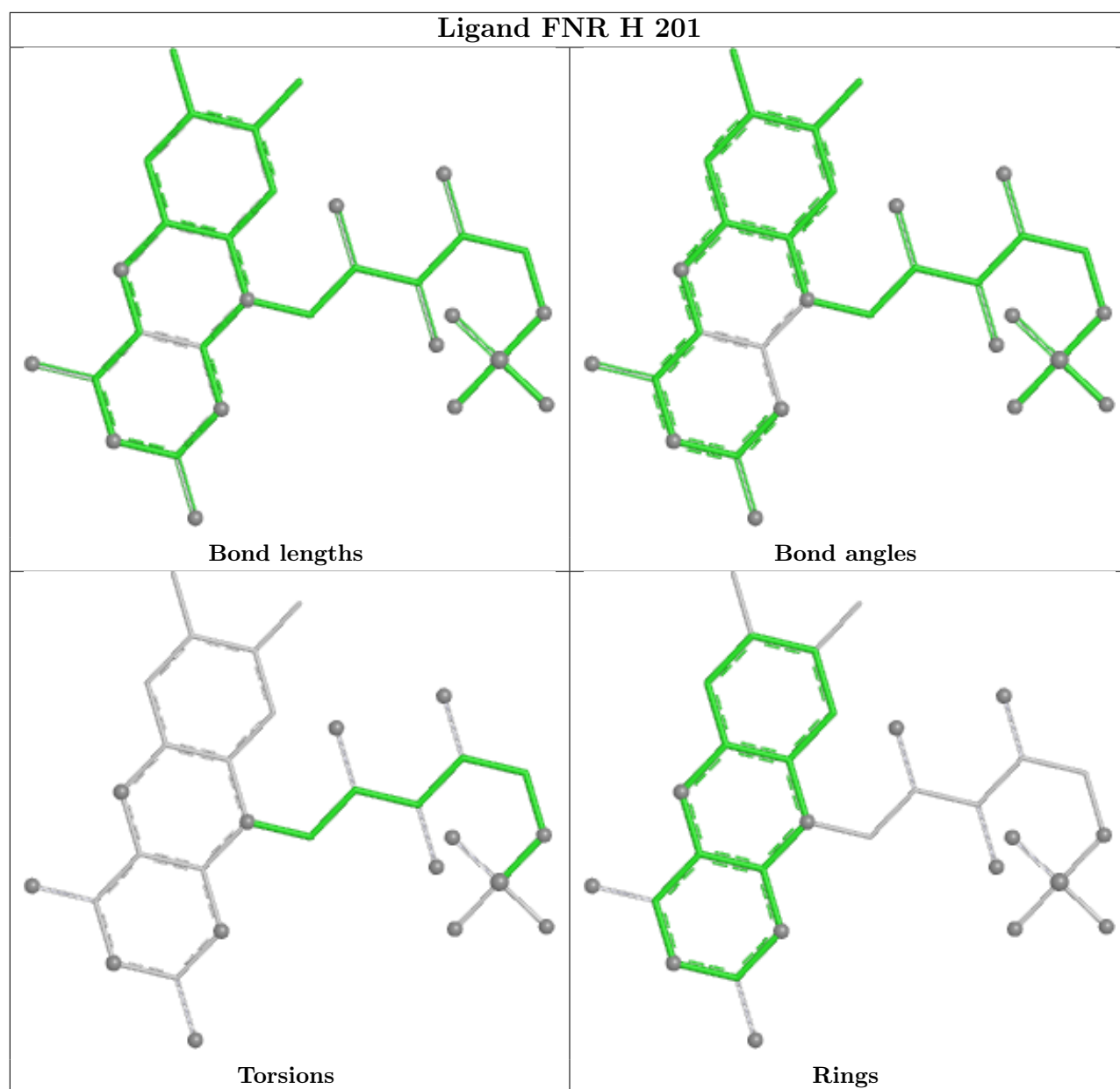
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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(Å²)	Q<0.9
1	A	313/342 (91%)	0.29	16 (5%)	33	37	7, 19, 36, 62	3 (0%)
1	B	313/342 (91%)	0.40	20 (6%)	25	29	8, 20, 39, 57	1 (0%)
1	C	309/342 (90%)	0.21	14 (4%)	38	43	7, 18, 33, 63	4 (1%)
1	D	320/342 (93%)	0.51	25 (7%)	19	22	8, 22, 44, 56	2 (0%)
2	E	133/147 (90%)	1.23	27 (20%)	3	3	16, 29, 48, 68	0
2	F	133/147 (90%)	0.53	13 (9%)	13	16	13, 22, 41, 48	0
2	G	129/147 (87%)	1.33	32 (24%)	2	2	18, 34, 52, 62	0
2	H	123/147 (83%)	2.43	74 (60%)	0	0	20, 41, 59, 65	0
All	All	1773/1956 (90%)	0.65	221 (12%)	8	10	7, 22, 48, 68	10 (0%)

All (221) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	105	VAL	7.7
2	E	140	ALA	6.6
2	H	106	ILE	6.2
2	H	133	ILE	5.9
2	H	134	ILE	5.8
2	E	55	VAL	5.8
2	H	52	GLY	5.6
2	H	137	THR	5.5
1	D	296	ILE	5.5
2	G	108	TYR	5.4
2	H	103	GLY	5.3
1	D	320	SER	5.3
2	H	108	TYR	5.3
2	G	55	VAL	5.1
2	H	104	PRO	5.0
2	H	101	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	331	LEU	4.9
2	H	87	VAL	4.8
2	H	107	SER	4.7
2	H	110	LEU	4.7
2	H	115	LEU	4.7
2	F	61	VAL	4.6
2	H	112	VAL	4.6
2	H	102	ALA	4.6
2	H	130	VAL	4.5
2	H	109	LYS	4.4
2	H	85	LEU	4.4
2	F	55	VAL	4.4
1	A	331	LEU	4.4
2	H	66	ALA	4.4
2	E	108	TYR	4.3
2	H	113	PRO	4.2
2	G	64	HIS	4.1
2	H	84	CYS	4.1
1	D	323	ILE	4.0
2	H	53	GLY	4.0
2	H	78	PRO	3.9
2	H	39	VAL	3.9
1	C	337	PHE	3.8
1	D	318	SER	3.8
2	F	54	LYS	3.8
2	H	114	LEU	3.6
2	H	124	LYS	3.6
2	E	110	LEU	3.6
2	H	86	GLY	3.5
2	H	72	ILE	3.5
2	G	138	PHE	3.5
2	E	41	GLU	3.5
2	E	128	GLU	3.5
2	H	135	SER	3.5
2	E	138	PHE	3.5
1	A	291	LYS	3.5
2	H	41	GLU	3.4
1	C	335	TRP	3.4
2	G	85	LEU	3.4
2	G	139	ASN	3.3
1	D	315	PHE	3.3
2	H	81	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	85	LEU	3.3
2	H	127	VAL	3.3
1	D	292	GLU	3.2
2	G	54	LYS	3.2
2	H	125	GLU	3.2
1	C	334	ASP	3.2
1	D	322	TYR	3.2
2	E	133	ILE	3.1
1	B	53	ASN	3.1
2	H	74	PHE	3.1
2	G	134	ILE	3.0
2	H	75	LEU	3.0
2	G	39	VAL	3.0
1	A	335	TRP	3.0
2	H	83	HIS	3.0
2	H	40	ASP	3.0
2	H	88	ILE	3.0
2	G	112	VAL	3.0
2	G	41	GLU	3.0
2	F	64	HIS	3.0
2	G	78	PRO	3.0
2	H	100	ALA	3.0
2	G	110	LEU	3.0
2	E	2	LYS	3.0
2	H	69	LYS	3.0
1	D	317	GLY	3.0
1	C	308	ALA	3.0
2	E	39	VAL	2.9
1	A	295	ARG	2.9
2	G	33	GLU	2.9
1	D	306	ALA	2.9
2	H	24	ALA	2.9
1	B	309	ASP	2.9
2	H	116	TYR	2.9
1	A	292	GLU	2.9
2	E	139	ASN	2.9
2	F	63	ALA	2.9
1	B	291	LYS	2.9
1	B	54	ILE	2.9
2	H	3	GLU	2.9
1	B	292	GLU	2.9
1	C	296	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	44	VAL	2.8
1	D	308	ALA	2.8
1	A	336	ASP	2.8
2	H	80	ASN	2.8
1	D	290	THR	2.8
1	B	308	ALA	2.8
1	D	314	PHE	2.8
1	A	54	ILE	2.8
2	F	41	GLU	2.8
2	H	33	GLU	2.8
2	H	45	LEU	2.8
2	E	111	LYS	2.7
1	D	312	HIS	2.7
1	A	266	ASP	2.7
2	E	134	ILE	2.7
1	D	53	ASN	2.7
1	C	291	LYS	2.7
2	E	63	ALA	2.7
1	B	333	GLU	2.7
1	D	291	LYS	2.7
1	A	337	PHE	2.7
2	H	132	ARG	2.7
2	H	79	ASP	2.6
2	G	137	THR	2.6
2	H	131	ASN	2.6
1	B	21	SER	2.6
2	H	51	SER	2.6
2	H	5	ILE	2.6
1	B	69	ASP	2.6
1	B	332	ASP	2.6
1	D	319	GLY	2.6
2	G	130	VAL	2.6
2	H	67	VAL	2.6
2	E	137	THR	2.6
2	F	136	GLU	2.6
2	E	112	VAL	2.6
1	B	55	PRO	2.5
1	D	295	ARG	2.5
2	G	113	PRO	2.5
2	F	33	GLU	2.5
1	A	309	ASP	2.5
1	D	313	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	306	ALA	2.5
1	C	21	SER	2.5
2	H	82	LYS	2.5
2	G	105	VAL	2.5
2	H	43	TYR	2.5
2	E	64	HIS	2.5
2	H	37	ILE	2.5
2	H	129	GLU	2.5
1	D	163	ASP	2.5
2	E	130	VAL	2.5
1	D	263	GLY	2.4
1	B	4	ASN	2.4
2	G	27	ILE	2.4
2	F	139	ASN	2.4
1	D	54	ILE	2.4
1	B	56	VAL	2.4
2	H	73	HIS	2.4
2	G	79	ASP	2.4
2	H	97	ASP	2.4
1	C	307	ARG	2.4
1	D	311	ASN	2.3
2	F	53	GLY	2.3
2	F	2	LYS	2.3
2	E	114	LEU	2.3
1	A	296	ILE	2.3
2	H	6	VAL	2.3
1	C	134	GLU	2.3
2	G	37	ILE	2.3
2	G	65	GLY	2.3
2	E	135	SER	2.3
1	C	20	GLN	2.3
2	E	127	VAL	2.3
2	H	26	SER	2.2
2	H	98	SER	2.2
1	A	4	ASN	2.2
2	G	124	LYS	2.2
2	H	68	PRO	2.2
1	B	290	THR	2.2
2	H	22	LEU	2.2
1	B	57	SER	2.2
2	H	77	ASP	2.2
1	B	20	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	228	LEU	2.2
2	E	4	LEU	2.2
2	G	114	LEU	2.2
1	D	307	ARG	2.2
1	C	292	GLU	2.1
1	D	301	PHE	2.1
2	G	25	GLU	2.1
2	G	128	GLU	2.1
2	G	86	GLY	2.1
2	H	111	LYS	2.1
1	A	333	GLU	2.1
2	F	138	PHE	2.1
2	H	27	ILE	2.1
1	C	336	ASP	2.1
2	E	79	ASP	2.1
2	H	42	ASP	2.1
2	F	135	SER	2.1
1	A	307	ARG	2.1
2	G	87	VAL	2.1
1	B	65	GLU	2.1
1	B	336	ASP	2.1
2	G	43	TYR	2.1
1	D	321	SER	2.1
2	G	125	GLU	2.1
2	E	113	PRO	2.1
2	G	115	LEU	2.1
2	H	4	LEU	2.1
2	E	24	ALA	2.1
1	A	332	ASP	2.1
2	H	25	GLU	2.0
2	H	136	GLU	2.0
1	A	306	ALA	2.0
2	E	54	LYS	2.0
1	B	296	ILE	2.0
2	G	133	ILE	2.0
2	H	29	ILE	2.0
2	H	47	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

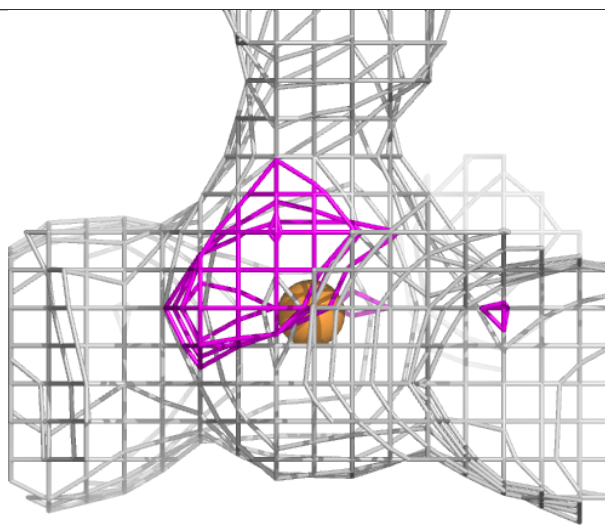
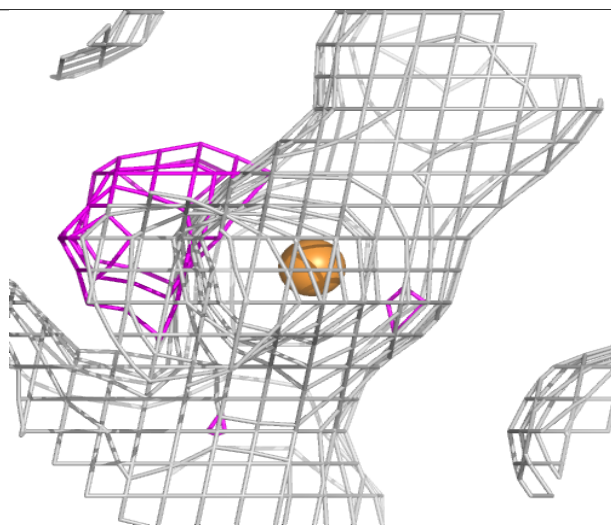
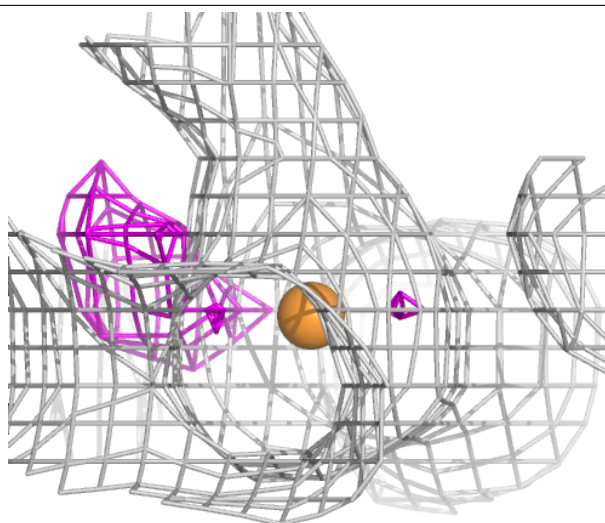
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	GOL	B	402	6/6	0.53	0.29	58,59,60,61	0
4	GOL	D	401	6/6	0.69	0.27	33,36,36,37	6
4	GOL	B	403	6/6	0.77	0.21	41,42,42,43	0
4	GOL	A	402	6/6	0.77	0.16	25,28,29,31	0
4	GOL	F	503	6/6	0.80	0.18	36,38,38,38	0
4	GOL	F	501	6/6	0.82	0.14	44,46,46,47	0
4	GOL	A	403	6/6	0.83	0.22	44,45,46,47	0
4	GOL	C	402	6/6	0.87	0.16	43,45,46,46	0
4	GOL	E	202	6/6	0.91	0.11	29,30,30,30	6
5	CA	B	404	1/1	0.93	0.12	42,42,42,42	0
3	CU1	C	401	1/1	0.95	0.12	41,41,41,41	1
5	CA	C	404	1/1	0.95	0.07	44,44,44,44	0
3	CU1	A	401	1/1	0.96	0.18	36,36,36,36	1
5	CA	A	404	1/1	0.96	0.09	40,40,40,40	0
6	FNR	H	201	31/31	0.96	0.07	17,21,21,22	0
3	CU1	C	403	1/1	0.97	0.07	41,41,41,41	1
6	FNR	E	201	31/31	0.97	0.05	12,15,15,15	0
6	FNR	G	201	31/31	0.97	0.06	15,17,18,19	0
6	FNR	F	502	31/31	0.97	0.05	11,12,12,13	0
3	CU1	B	401	1/1	0.97	0.11	36,36,36,36	1

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.

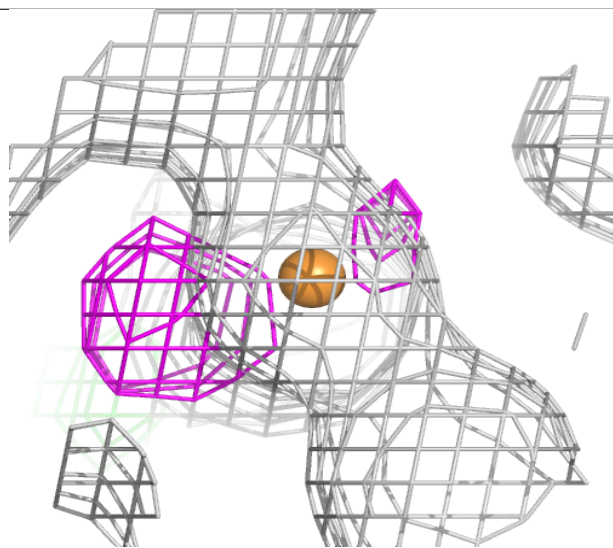
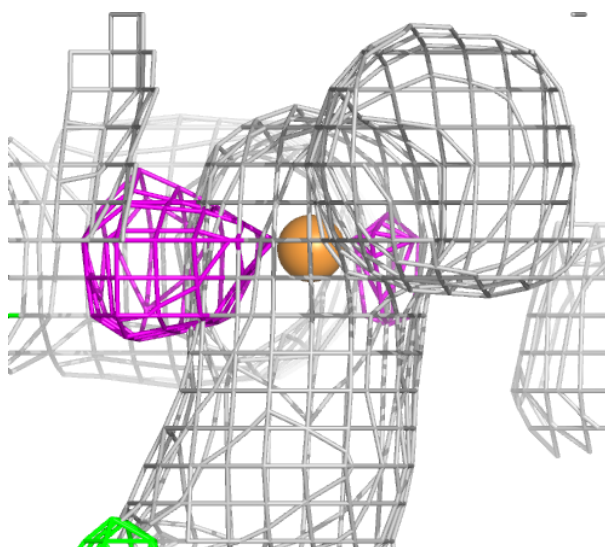
Electron density around CU1 C 401:

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



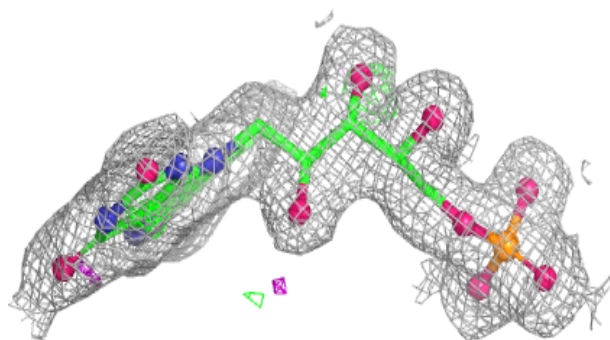
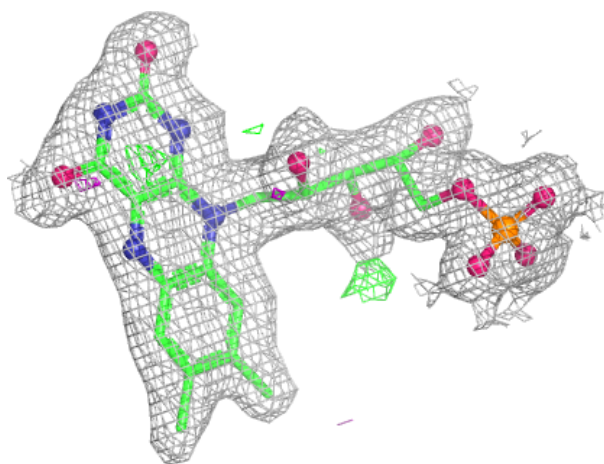
Electron density around CU1 A 401:

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



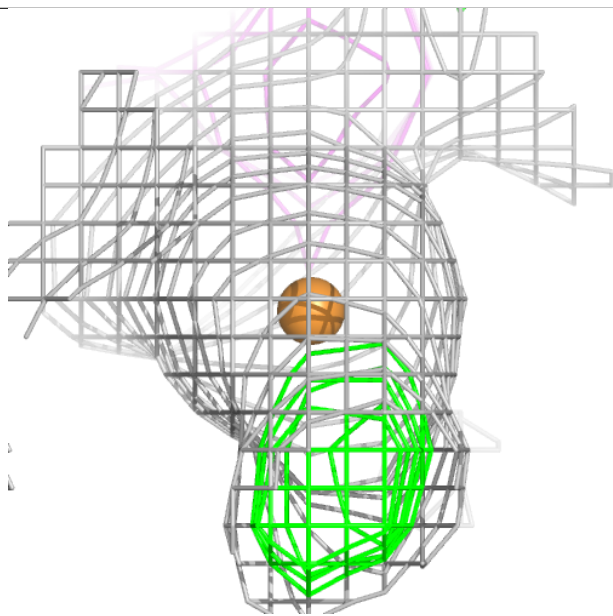
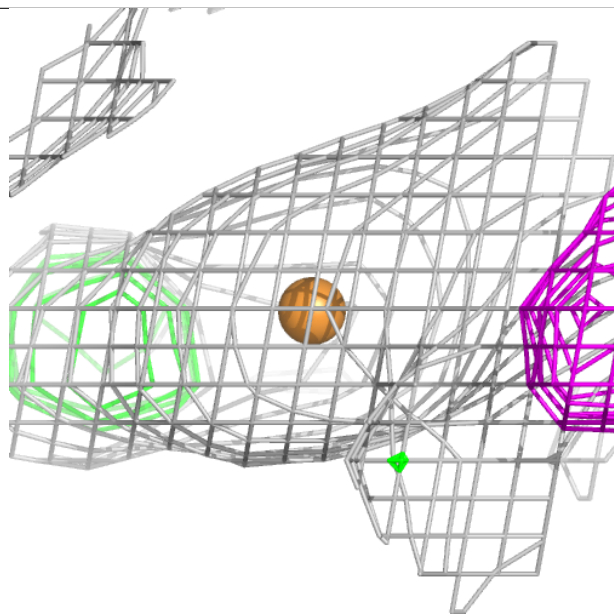
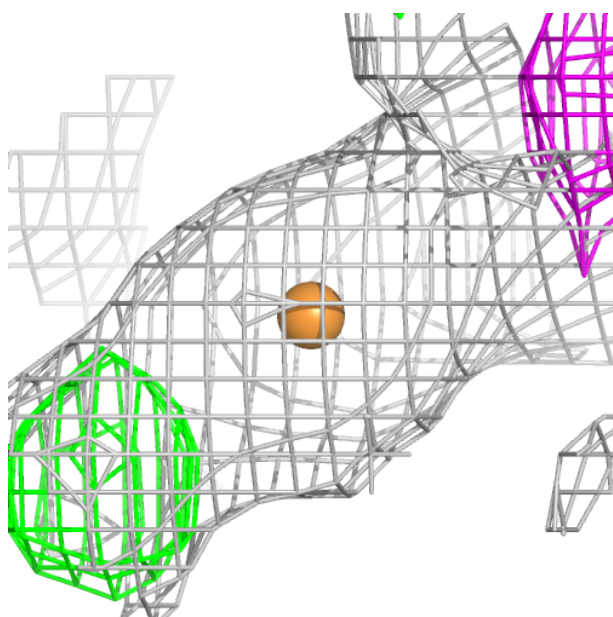
Electron density around FNR H 201:

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



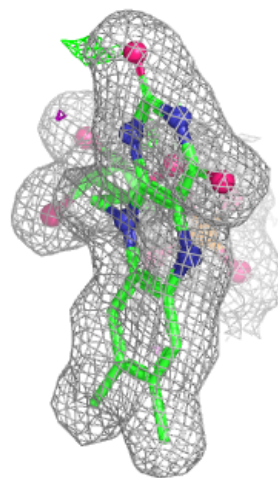
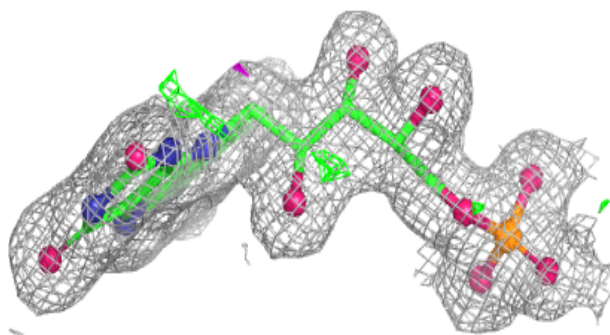
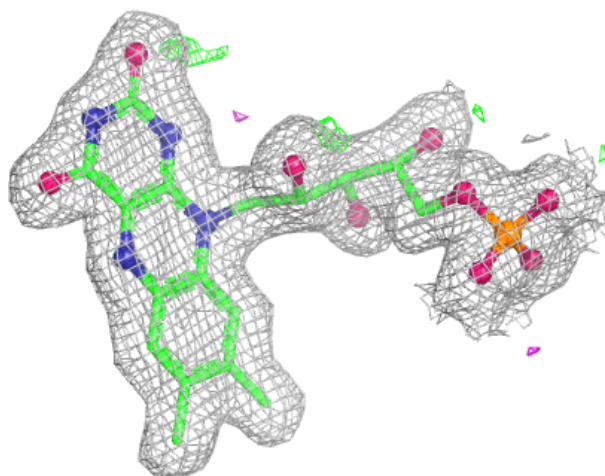
Electron density around CU1 C 403:

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



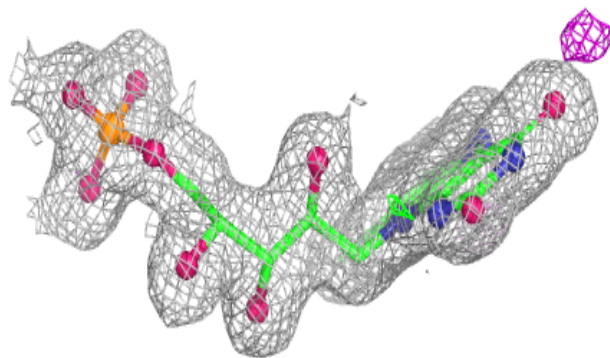
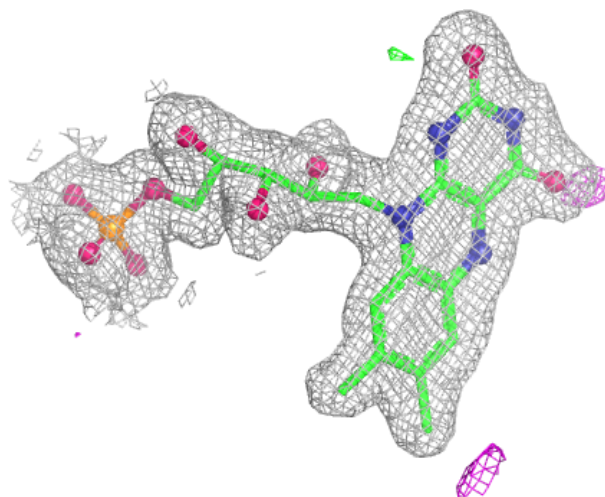
Electron density around FNR E 201:

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



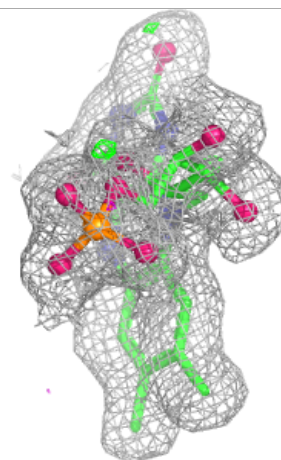
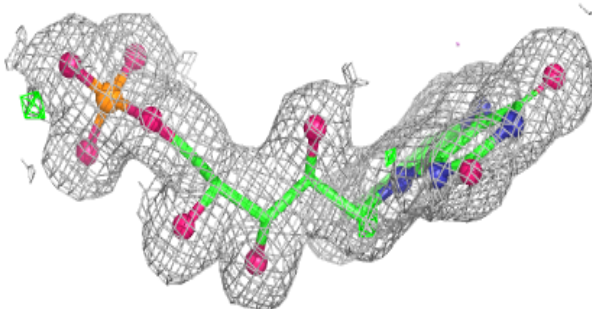
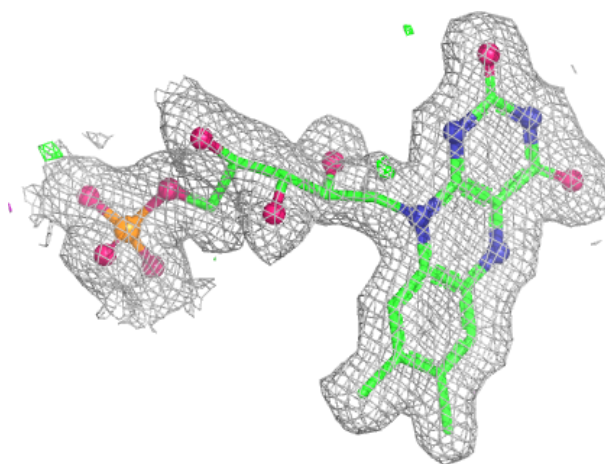
Electron density around FNR G 201:

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



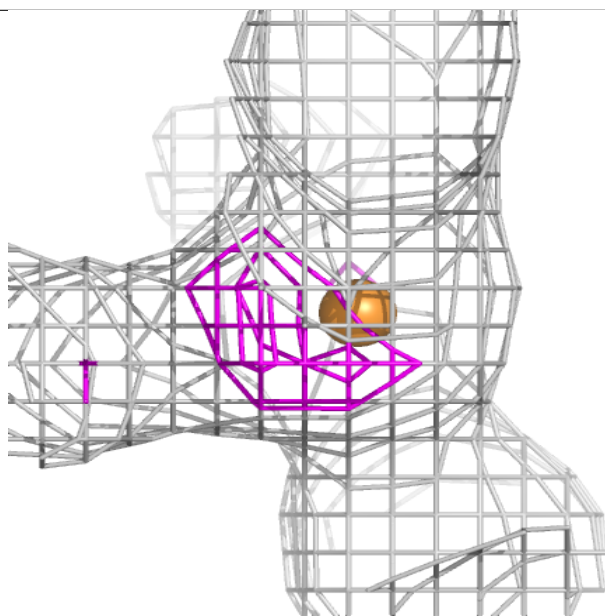
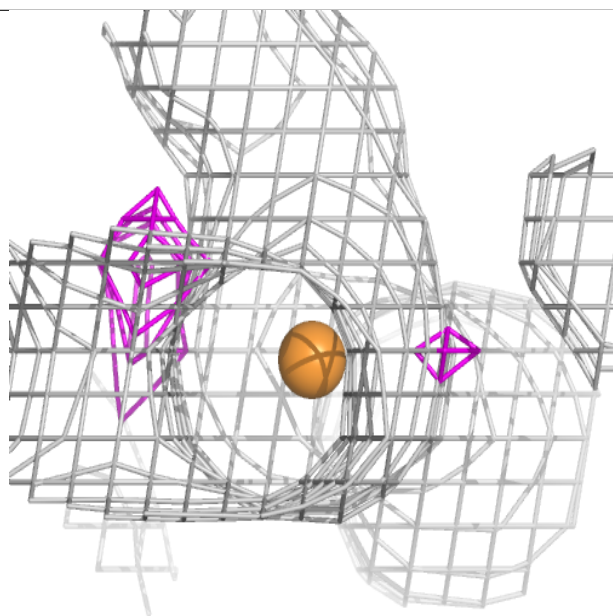
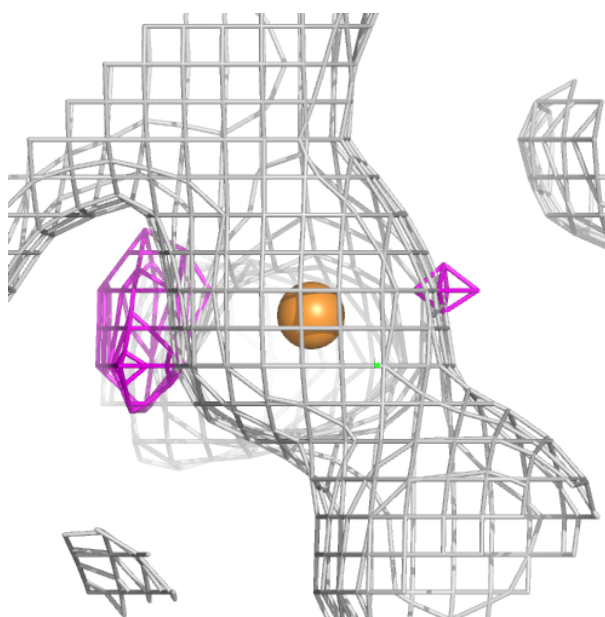
Electron density around FNR F 502:

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



Electron density around CU1 B 401:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.