



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2023 – 09:44 AM EDT

PDB ID : 2OBX
Title : Lumazine synthase RibH2 from Mesorhizobium loti (Gene mll7281, Swiss-Prot entry Q986N2) complexed with inhibitor 5-Nitro-6-(D-Ribitylamino)-2,4(1H, 3H) Pyrimidinedione
Authors : Klinke, S.; Zylberman, V.; Bonomi, H.R.; Haase, I.; Guimaraes, B.G.; Braden, B.C.; Bacher, A.; Fischer, M.; Goldbaum, F.A.
Deposited on : 2006-12-20
Resolution : 2.53 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 ⓘ 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	:	2.35
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)	:	2.35

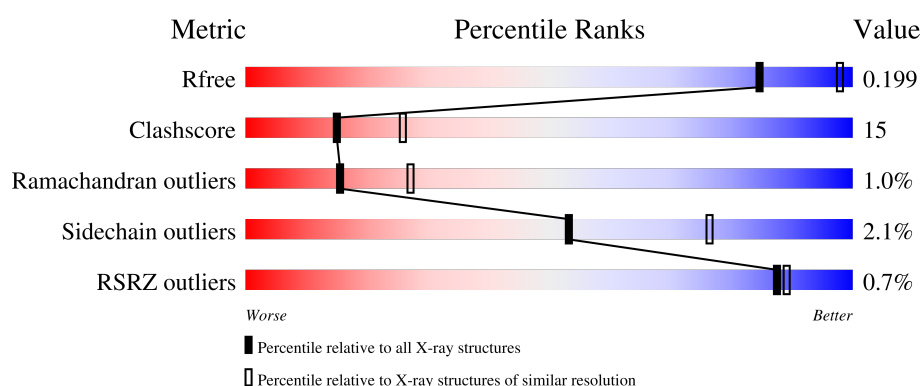
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	157	
1	B	157	
1	C	157	
1	D	157	
1	E	157	

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Mol	Chain	Length	Quality of chain
1	F	157	
1	G	157	
1	H	157	
1	I	157	
1	J	157	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	1001	-	-	X	X
2	PO4	B	1002	-	-	X	-
2	PO4	C	1003	-	-	X	-
2	PO4	E	1004	-	-	X	X
2	PO4	F	1005	-	-	X	X
2	PO4	G	1006	-	-	X	X
2	PO4	I	1007	-	-	X	X
2	PO4	J	1008	-	-	X	X
3	INI	A	201	-	X	-	-
3	INI	B	202	-	X	-	-
3	INI	C	203	-	X	-	-
3	INI	D	204	-	X	-	-
3	INI	E	205	-	X	-	-
3	INI	F	206	-	X	-	-
3	INI	G	207	-	X	-	-
3	INI	H	208	-	X	-	-
3	INI	I	209	-	X	-	-
3	INI	J	210	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11693 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 6,7-dimethyl-8-ribityllumazine synthase 1.

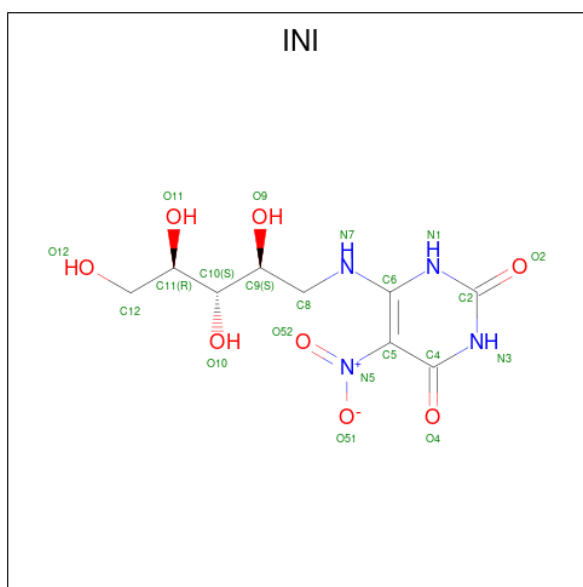
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1145	730	202	208	5			
1	B	147	Total	C	N	O	S	0	0	0
			1124	716	199	204	5			
1	C	147	Total	C	N	O	S	0	0	0
			1116	711	198	202	5			
1	D	146	Total	C	N	O	S	0	0	0
			1118	711	197	205	5			
1	E	146	Total	C	N	O	S	0	0	0
			1111	707	196	203	5			
1	F	148	Total	C	N	O	S	0	0	0
			1130	719	200	206	5			
1	G	148	Total	C	N	O	S	0	0	0
			1126	716	199	206	5			
1	H	147	Total	C	N	O	S	0	0	0
			1125	715	201	204	5			
1	I	146	Total	C	N	O	S	0	0	0
			1112	710	198	199	5			
1	J	146	Total	C	N	O	S	0	0	0
			1112	708	194	205	5			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 5-NITRO-6-RIBITYL-AMINO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: INI) (formula: C₉H₁₄N₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	9	4	8		
3	B	1	Total	C	N	O	0	0
			21	9	4	8		
3	C	1	Total	C	N	O	0	0
			21	9	4	8		
3	D	1	Total	C	N	O	0	0
			21	9	4	8		
3	E	1	Total	C	N	O	0	0
			21	9	4	8		
3	F	1	Total	C	N	O	0	0
			21	9	4	8		
3	G	1	Total	C	N	O	0	0
			21	9	4	8		
3	H	1	Total	C	N	O	0	0
			21	9	4	8		
3	I	1	Total	C	N	O	0	0
			21	9	4	8		
3	J	1	Total	C	N	O	0	0
			21	9	4	8		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	23	Total	O	0	0
			23	23		

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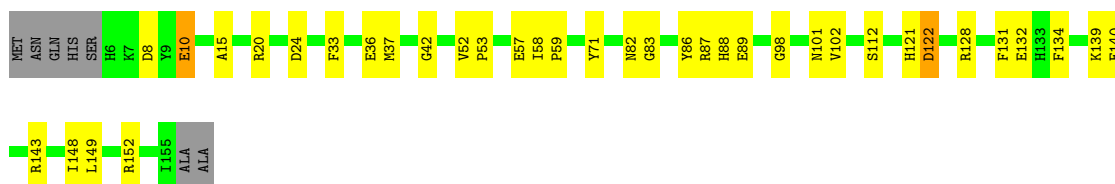
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	22	Total 22	O 22	0	0
4	D	21	Total 21	O 21	0	0
4	E	27	Total 27	O 27	0	0
4	F	20	Total 20	O 20	0	0
4	G	24	Total 24	O 24	0	0
4	H	24	Total 24	O 24	0	0
4	I	16	Total 16	O 16	0	0
4	J	26	Total 26	O 26	0	0

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: 6,7-dimethyl-8-ribityllumazine synthase 1

Chain A: 



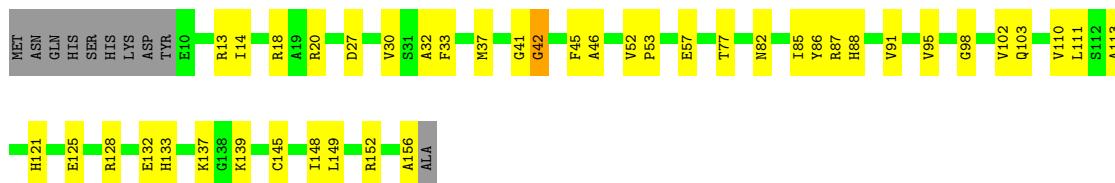
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase 1

Chain B: 



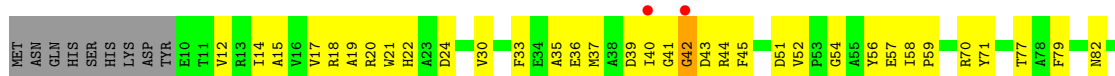
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase 1

Chain C: 



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase 1

Chain D: 

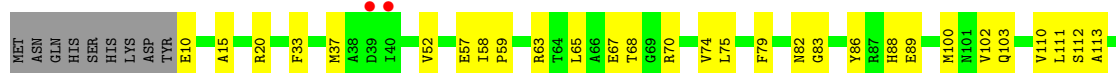




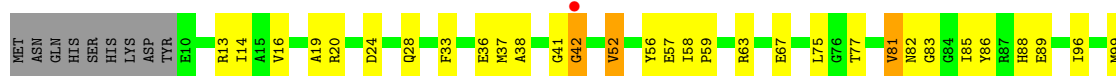
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase 1



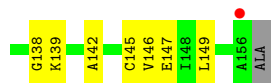
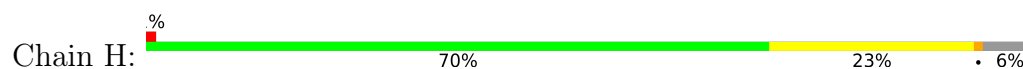
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase 1



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase 1



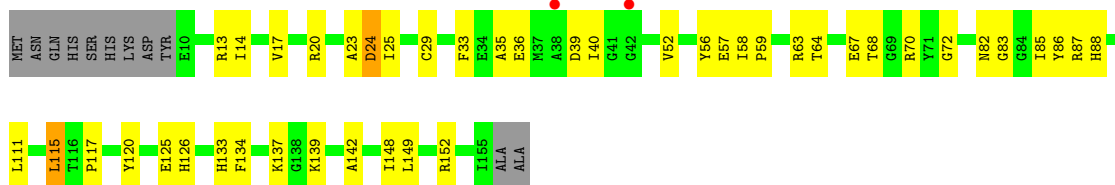
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase 1



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase 1



- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.38Å 122.22Å 94.93Å 90.00° 125.43° 90.00°	Depositor
Resolution (Å)	50.00 – 2.53 38.98 – 2.53	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-2.53) 96.6 (38.98-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.281 0.206 , 0.199	Depositor DCC
R_{free} test set	2345 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.003 for k+l,h+l,-l 0.001 for -k+l,-h-l,-l 0.024 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11693	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: INI, PO4

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	0.39	0/1172	0.62	0/1594
1	B	0.40	0/1150	0.65	0/1563
1	C	0.37	0/1142	0.60	0/1554
1	D	0.39	0/1144	0.61	0/1556
1	E	0.37	0/1137	0.59	0/1548
1	F	0.37	0/1156	0.59	0/1570
1	G	0.39	0/1152	0.62	0/1566
1	H	0.41	0/1151	0.63	0/1565
1	I	0.38	0/1138	0.61	0/1547
1	J	0.39	0/1138	0.62	0/1549
All	All	0.39	0/11480	0.61	0/15612

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 ⓘ

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	1145	0	1096	28	0
1	B	1124	0	1088	39	0
1	C	1116	0	1073	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1118	0	1074	43	0
1	E	1111	0	1061	36	0
1	F	1130	0	1093	34	0
1	G	1126	0	1082	44	0
1	H	1125	0	1086	33	0
1	I	1112	0	1077	29	0
1	J	1112	0	1063	37	0
2	A	5	0	0	3	0
2	B	5	0	0	4	0
2	C	5	0	0	2	0
2	E	5	0	0	3	0
2	F	5	0	0	2	0
2	G	5	0	0	4	0
2	I	5	0	0	2	0
2	J	10	0	0	5	0
3	A	21	0	14	1	0
3	B	21	0	14	2	0
3	C	21	0	14	3	0
3	D	21	0	14	0	0
3	E	21	0	14	1	0
3	F	21	0	14	0	0
3	G	21	0	14	2	0
3	H	21	0	14	3	0
3	I	21	0	14	3	0
3	J	21	0	14	1	0
4	A	16	0	0	0	0
4	B	23	0	0	1	0
4	C	22	0	0	0	0
4	D	21	0	0	1	0
4	E	27	0	0	3	0
4	F	20	0	0	0	0
4	G	24	0	0	1	0
4	H	24	0	0	0	0
4	I	16	0	0	0	0
4	J	26	0	0	0	0
All	All	11693	0	10933	339	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 15.

The worst 5 of 339 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:B:152:ARG:HH11	1:B:152:ARG:HB3	1.17	1.05
1:B:139:LYS:HE2	1:B:143:ARG:NH2	1.84	0.93
1:B:139:LYS:HE2	1:B:143:ARG:HH22	1.33	0.91
1:C:77:THR:HB	1:C:113:ALA:HB3	1.59	0.85
1:B:152:ARG:HB3	1:B:152:ARG:NH1	1.92	0.85

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	148/157 (94%)	143 (97%)	3 (2%)	2 (1%)	11	19
1	B	145/157 (92%)	140 (97%)	3 (2%)	2 (1%)	11	19
1	C	145/157 (92%)	138 (95%)	6 (4%)	1 (1%)	22	37
1	D	144/157 (92%)	134 (93%)	8 (6%)	2 (1%)	11	19
1	E	144/157 (92%)	135 (94%)	6 (4%)	3 (2%)	7	10
1	F	146/157 (93%)	138 (94%)	8 (6%)	0	100	100
1	G	146/157 (93%)	142 (97%)	2 (1%)	2 (1%)	11	19
1	H	145/157 (92%)	140 (97%)	5 (3%)	0	100	100
1	I	144/157 (92%)	135 (94%)	7 (5%)	2 (1%)	11	19
1	J	144/157 (92%)	136 (94%)	8 (6%)	0	100	100
All	All	1451/1570 (92%)	1381 (95%)	56 (4%)	14 (1%)	15	27

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	42	GLY
1	A	42	GLY
1	B	42	GLY

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Mol	Chain	Res	Type
1	C	42	GLY
1	E	122	ASP

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	113/123 (92%)	111 (98%)	2 (2%)	59	80
1	B	112/123 (91%)	108 (96%)	4 (4%)	35	59
1	C	110/123 (89%)	109 (99%)	1 (1%)	78	91
1	D	112/123 (91%)	110 (98%)	2 (2%)	59	80
1	E	110/123 (89%)	107 (97%)	3 (3%)	44	69
1	F	112/123 (91%)	112 (100%)	0	100	100
1	G	111/123 (90%)	107 (96%)	4 (4%)	35	59
1	H	112/123 (91%)	110 (98%)	2 (2%)	59	80
1	I	110/123 (89%)	109 (99%)	1 (1%)	78	91
1	J	111/123 (90%)	107 (96%)	4 (4%)	35	59
All	All	1113/1230 (90%)	1090 (98%)	23 (2%)	53	76

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	115	LEU
1	H	122	ASP
1	H	52	VAL
1	I	134	PHE
1	C	125	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	127	HIS

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Mol	Chain	Res	Type
1	I	121	HIS
1	D	121	HIS
1	E	103	GLN
1	F	121	HIS

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](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	INI	F	206	-	17,21,21	3.78	7 (41%)	21,29,29	4.40	15 (71%)
3	INI	B	202	-	17,21,21	3.50	8 (47%)	21,29,29	4.38	15 (71%)
2	PO4	B	1002	-	4,4,4	1.76	0	6,6,6	0.46	0
2	PO4	E	1004	-	4,4,4	1.69	0	6,6,6	0.43	0
3	INI	E	205	-	17,21,21	3.61	7 (41%)	21,29,29	4.25	16 (76%)
3	INI	J	210	-	17,21,21	3.69	8 (47%)	21,29,29	4.41	16 (76%)
3	INI	G	207	-	17,21,21	3.53	8 (47%)	21,29,29	4.35	15 (71%)
3	INI	I	209	-	17,21,21	3.65	7 (41%)	21,29,29	4.28	15 (71%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	J	1009	-	4,4,4	1.56	0	6,6,6	0.46	0
2	PO4	F	1005	-	4,4,4	1.65	0	6,6,6	0.44	0
2	PO4	C	1003	-	4,4,4	1.72	1 (25%)	6,6,6	0.43	0
3	INI	D	204	-	17,21,21	3.68	7 (41%)	21,29,29	4.41	17 (80%)
3	INI	A	201	-	17,21,21	3.68	7 (41%)	21,29,29	4.32	16 (76%)
3	INI	C	203	-	17,21,21	3.62	9 (52%)	21,29,29	4.44	15 (71%)
3	INI	H	208	-	17,21,21	3.43	8 (47%)	21,29,29	4.35	15 (71%)
2	PO4	G	1006	-	4,4,4	1.78	1 (25%)	6,6,6	0.47	0
2	PO4	A	1001	-	4,4,4	1.65	0	6,6,6	0.43	0
2	PO4	I	1007	-	4,4,4	1.76	1 (25%)	6,6,6	0.42	0
2	PO4	J	1008	-	4,4,4	1.88	2 (50%)	6,6,6	0.43	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
3	INI	I	209	-	-	8/15/19/19	0/1/1/1
3	INI	F	206	-	-	9/15/19/19	0/1/1/1
3	INI	E	205	-	-	8/15/19/19	0/1/1/1
3	INI	J	210	-	-	9/15/19/19	0/1/1/1
3	INI	D	204	-	-	8/15/19/19	0/1/1/1
3	INI	A	201	-	-	9/15/19/19	0/1/1/1
3	INI	C	203	-	-	9/15/19/19	0/1/1/1
3	INI	H	208	-	-	9/15/19/19	0/1/1/1
3	INI	G	207	-	-	9/15/19/19	0/1/1/1
3	INI	B	202	-	-	9/15/19/19	0/1/1/1

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	209	INI	C11-C10	9.74	1.71	1.53
3	F	206	INI	C11-C10	9.68	1.71	1.53
3	G	207	INI	C11-C10	9.59	1.71	1.53
3	C	203	INI	C11-C10	9.50	1.71	1.53
3	A	201	INI	C11-C10	9.47	1.71	1.53

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	203	INI	C2-N3-C4	12.58	125.76	115.14
3	D	204	INI	C2-N3-C4	12.48	125.67	115.14
3	F	206	INI	C2-N3-C4	12.30	125.52	115.14
3	J	210	INI	C2-N3-C4	12.24	125.47	115.14
3	G	207	INI	C2-N3-C4	12.22	125.46	115.14

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	INI	N1-C6-N7-C8
3	A	201	INI	C5-C6-N7-C8
3	A	201	INI	C9-C10-C11-O11
3	A	201	INI	C9-C10-C11-C12
3	A	201	INI	O10-C10-C11-O11

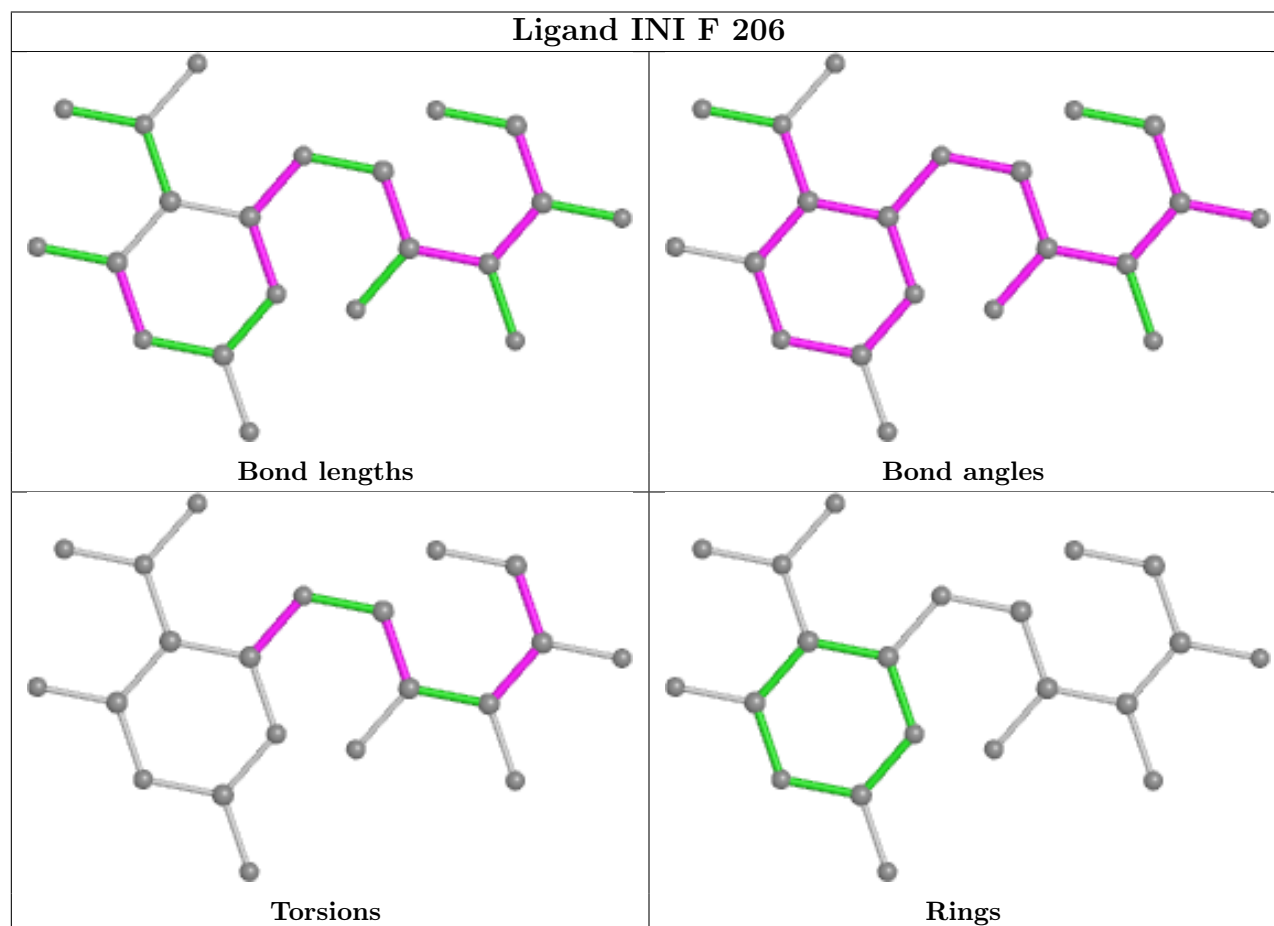
There are no ring outliers.

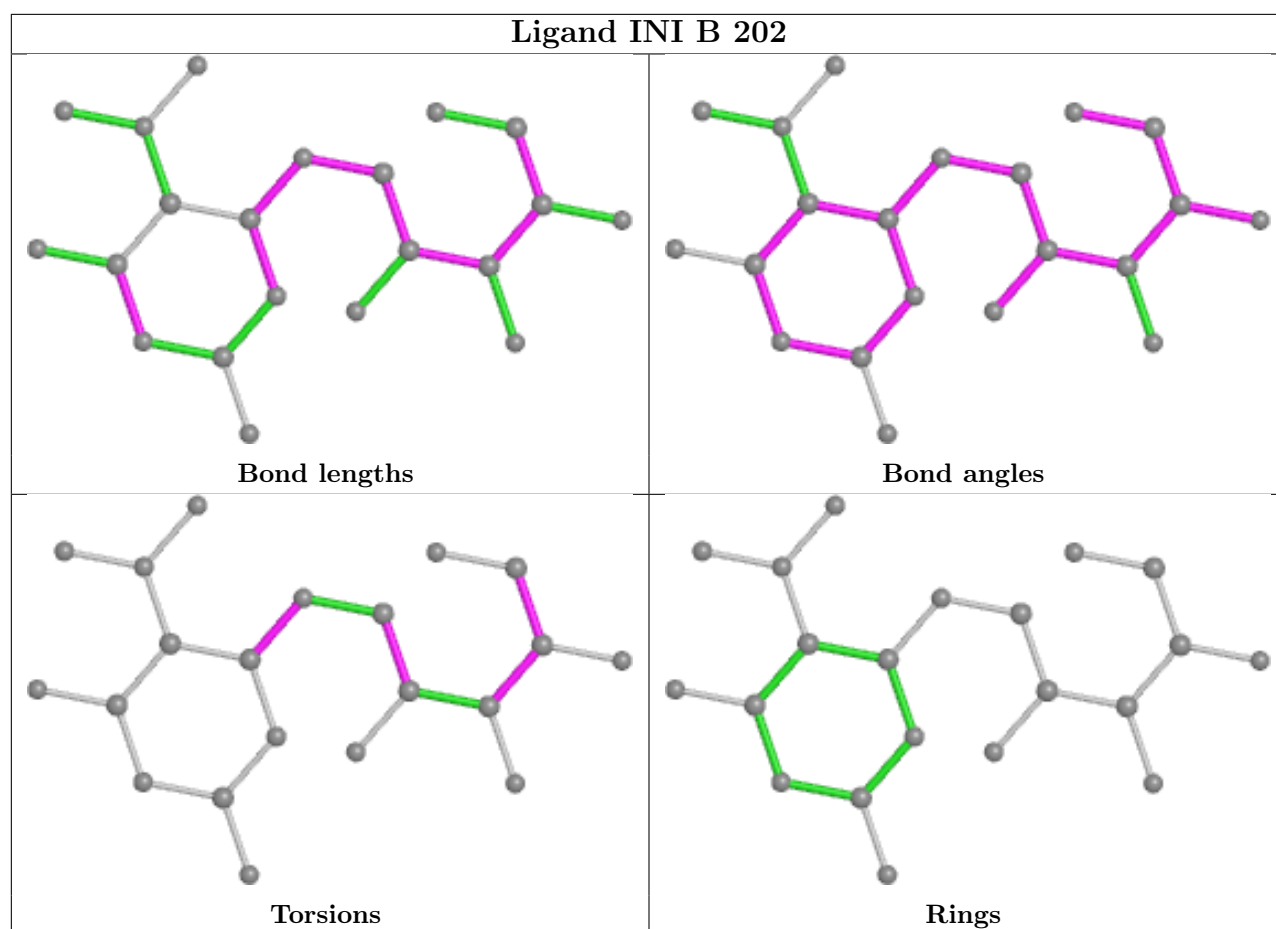
16 monomers are involved in 41 short contacts:

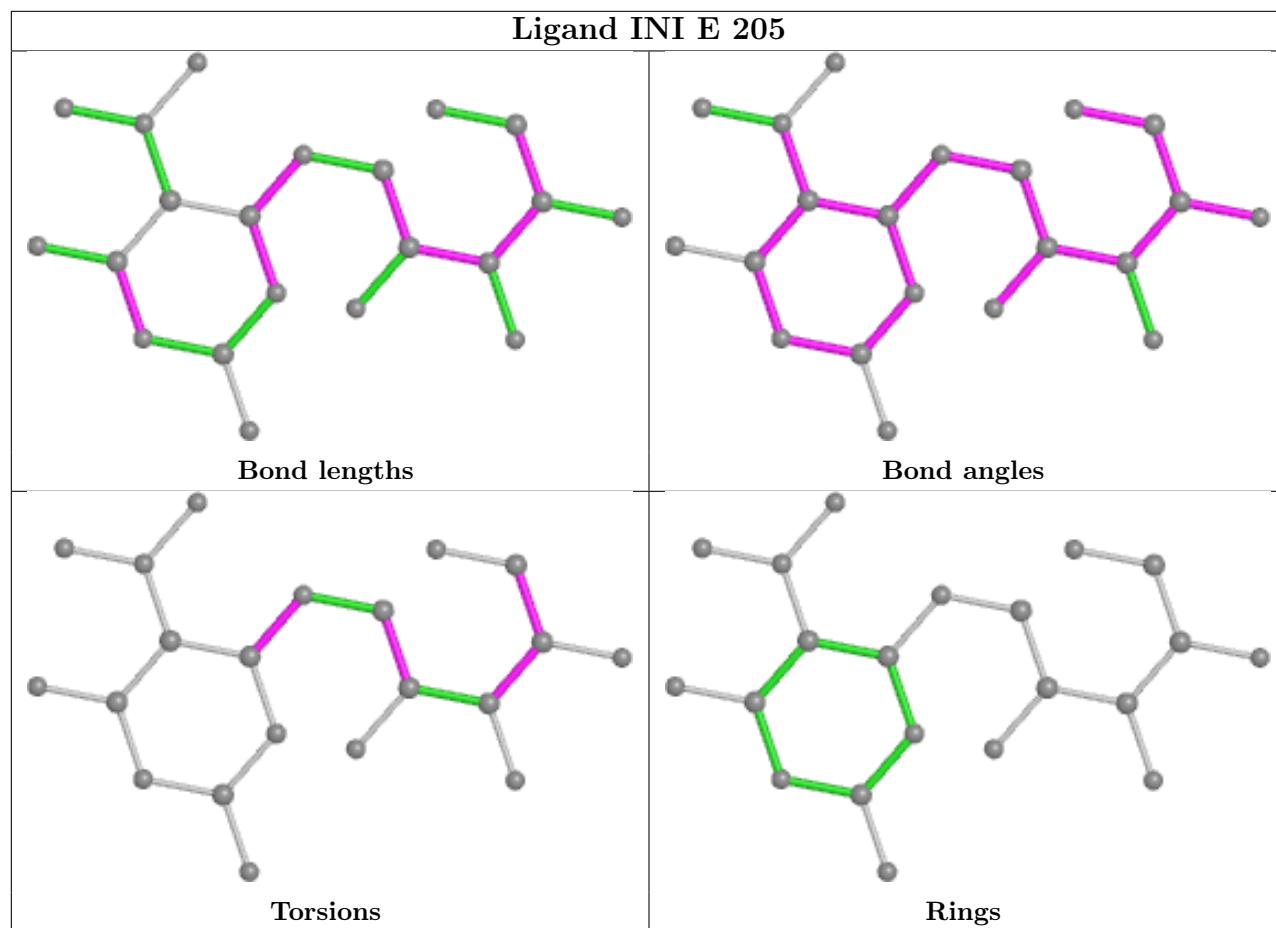
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	INI	2	0
2	B	1002	PO4	4	0
2	E	1004	PO4	3	0
3	E	205	INI	1	0
3	J	210	INI	1	0
3	G	207	INI	2	0
3	I	209	INI	3	0
2	F	1005	PO4	2	0
2	C	1003	PO4	2	0
3	A	201	INI	1	0
3	C	203	INI	3	0
3	H	208	INI	3	0
2	G	1006	PO4	4	0
2	A	1001	PO4	3	0
2	I	1007	PO4	2	0
2	J	1008	PO4	5	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 than 5% of the Mogul distribution of torsion angles is

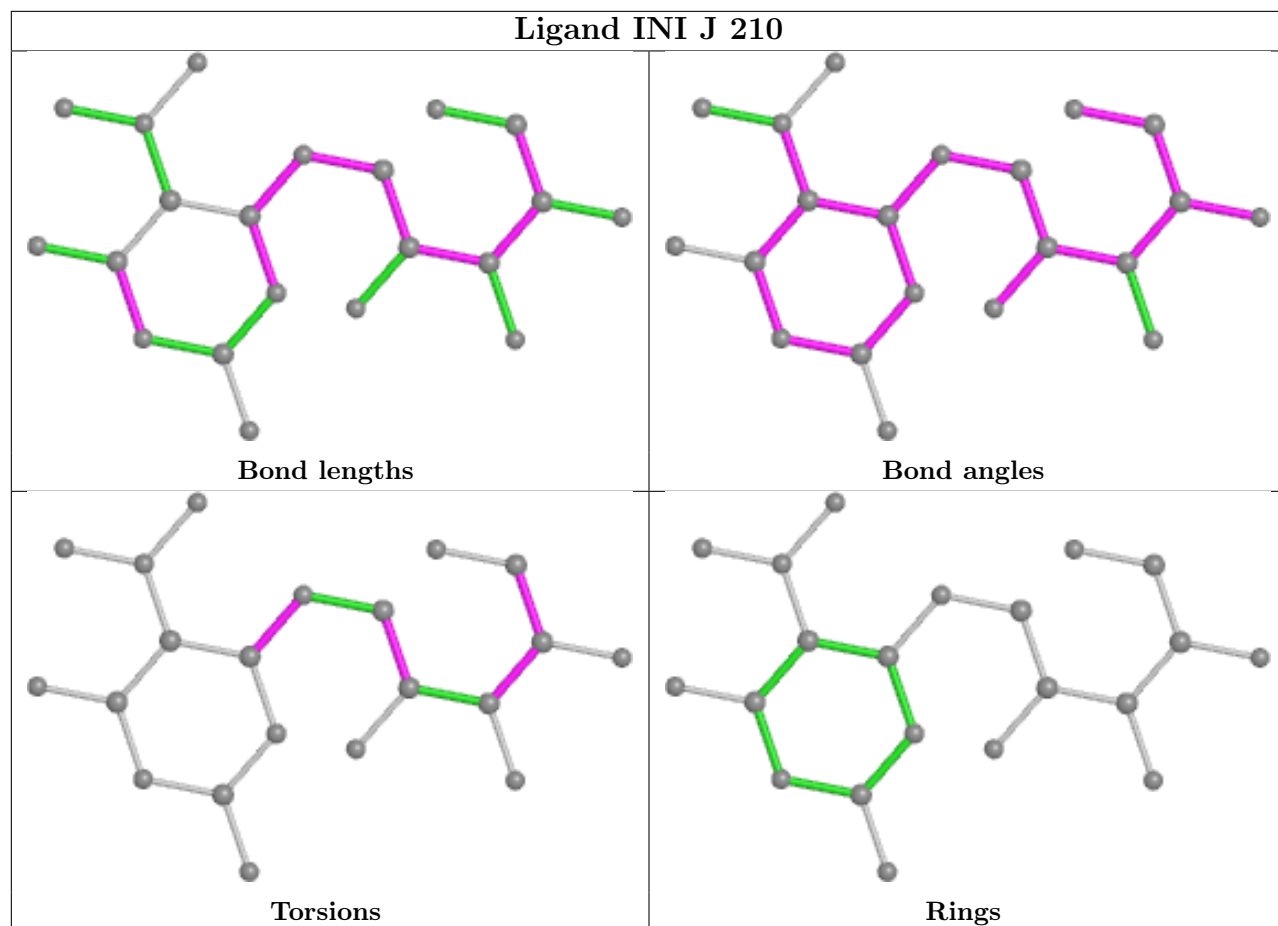
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question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

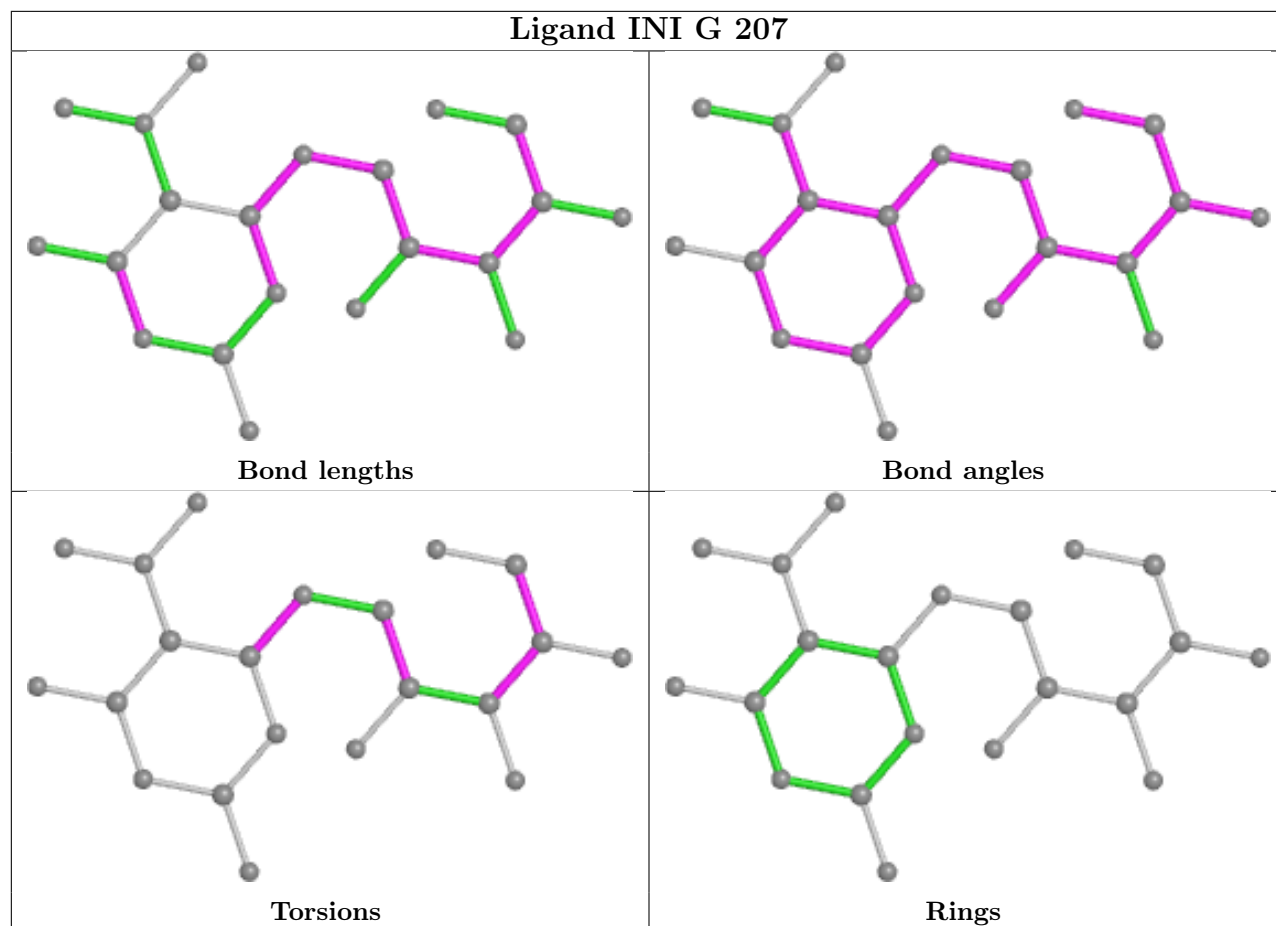


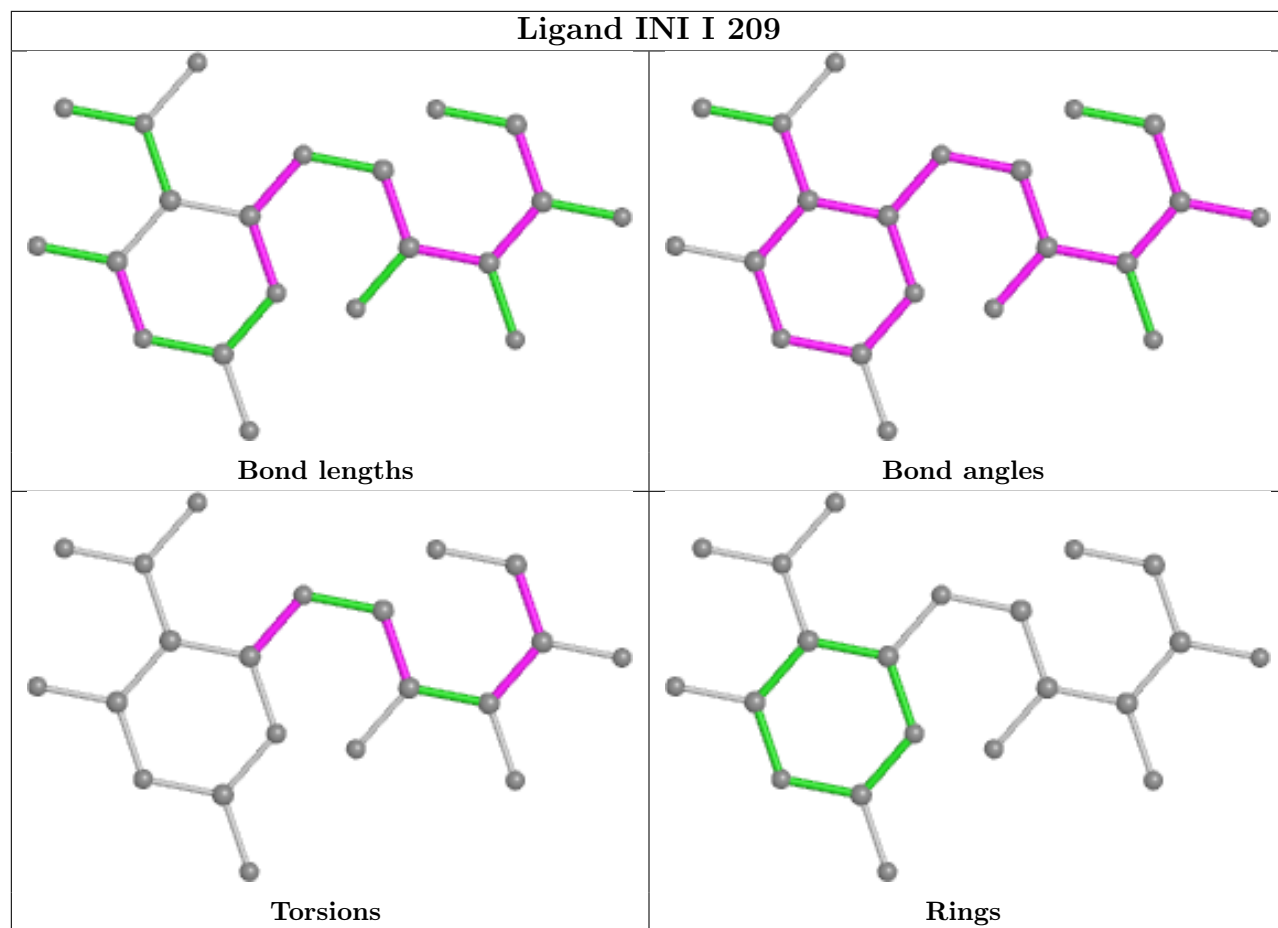


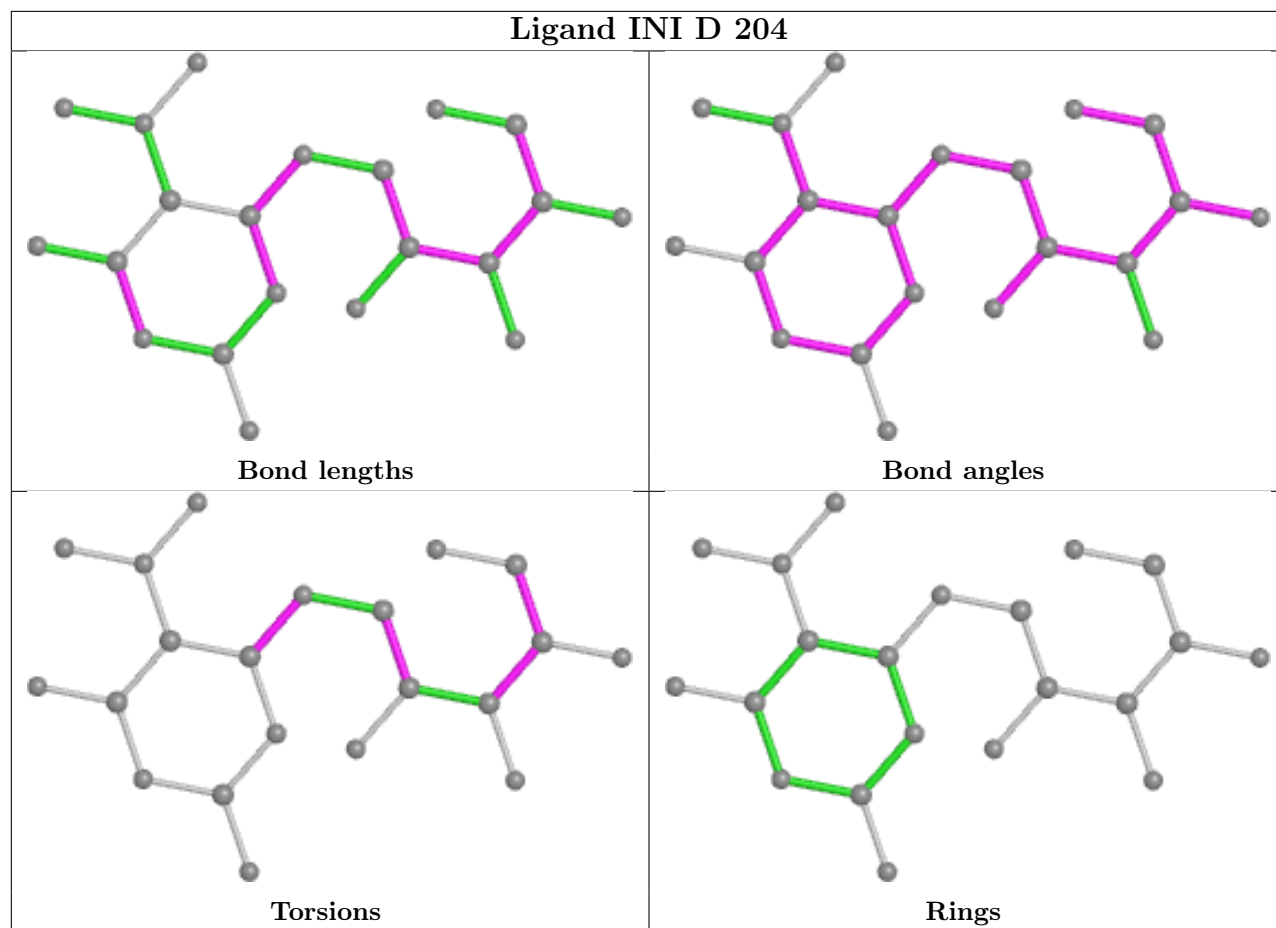


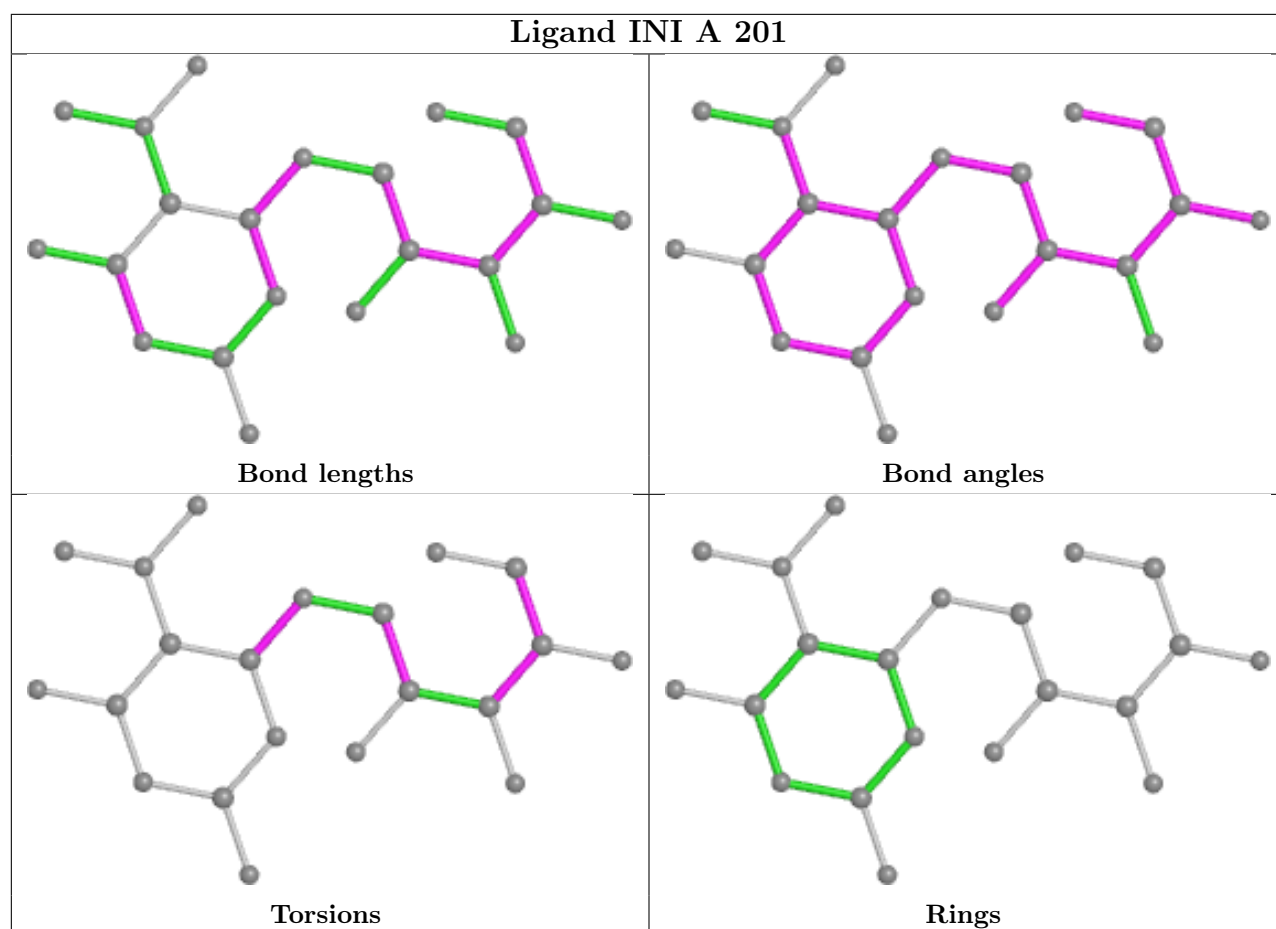
Ligand INI J 210



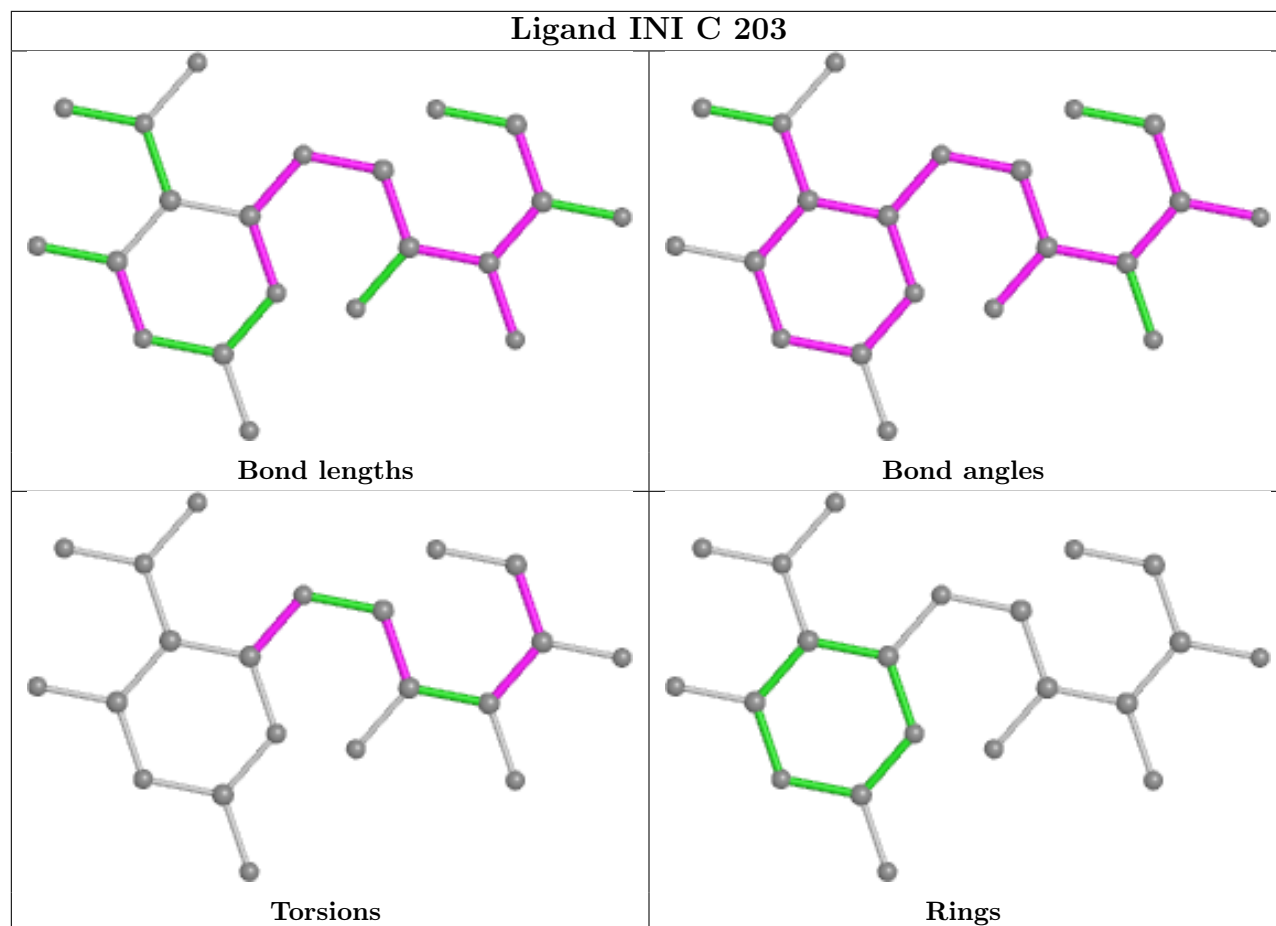


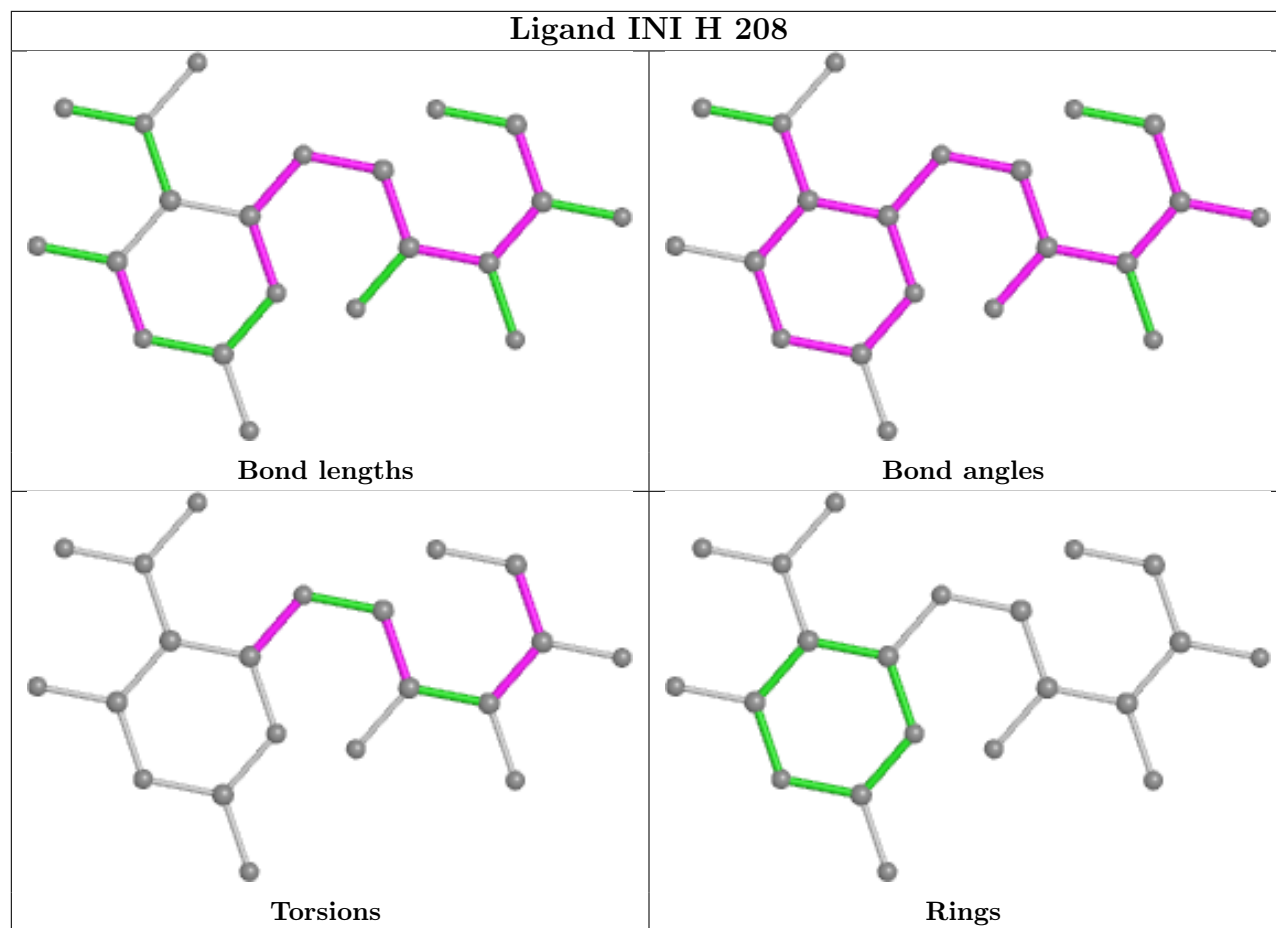






Ligand INI C 203





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	150/157 (95%)	-0.23	0 100 100	12, 24, 39, 56	2 (1%)
1	B	147/157 (93%)	-0.40	0 100 100	11, 21, 39, 48	3 (2%)
1	C	147/157 (93%)	-0.34	0 100 100	12, 24, 43, 51	0
1	D	146/157 (92%)	-0.29	2 (1%) 75 78	12, 23, 41, 53	2 (1%)
1	E	146/157 (92%)	-0.19	1 (0%) 87 89	12, 24, 45, 54	2 (1%)
1	F	148/157 (94%)	-0.26	3 (2%) 65 68	14, 25, 43, 60	1 (0%)
1	G	148/157 (94%)	-0.17	2 (1%) 75 78	14, 27, 47, 59	3 (2%)
1	H	147/157 (93%)	-0.34	1 (0%) 87 89	10, 24, 39, 50	0
1	I	146/157 (92%)	-0.30	0 100 100	14, 25, 48, 59	1 (0%)
1	J	146/157 (92%)	-0.21	2 (1%) 75 78	10, 24, 42, 49	2 (1%)
All	All	1471/1570 (93%)	-0.27	11 (0%) 87 89	10, 24, 44, 60	16 (1%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	42	GLY	5.0
1	H	156	ALA	4.3
1	D	42	GLY	4.1
1	F	40	ILE	3.3
1	F	157	ALA	2.6

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 monosaccharides in this entry.

6.4 Ligands ⓘ

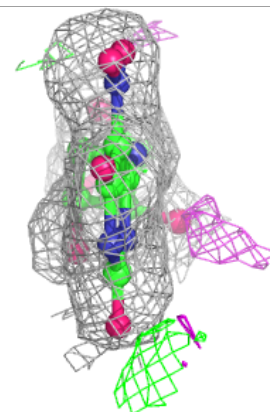
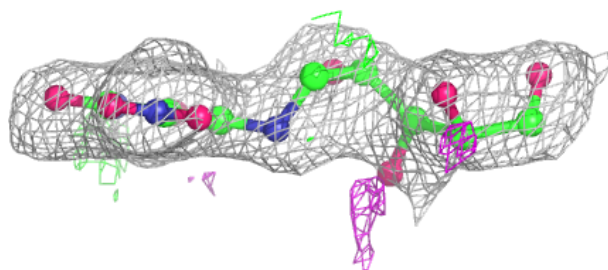
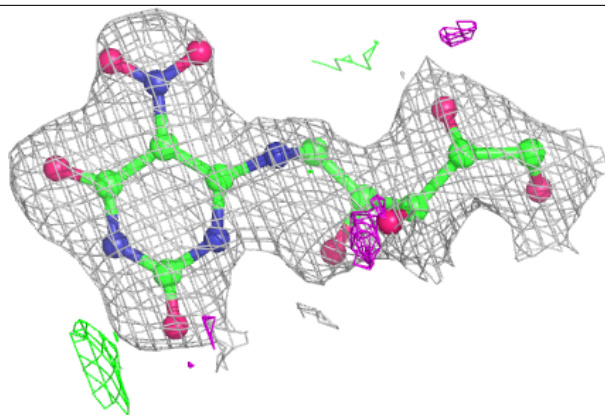
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	A	1001	5/5	0.64	0.59	60,61,62,62	5
2	PO4	J	1008	5/5	0.66	0.49	49,49,49,50	5
2	PO4	F	1005	5/5	0.70	0.56	56,57,57,57	5
2	PO4	E	1004	5/5	0.74	0.44	56,57,58,58	5
2	PO4	G	1006	5/5	0.76	0.53	50,50,51,51	5
2	PO4	I	1007	5/5	0.78	0.56	55,56,56,57	5
2	PO4	C	1003	5/5	0.81	0.41	55,56,56,56	5
2	PO4	B	1002	5/5	0.87	0.75	61,61,61,61	5
3	INI	A	201	21/21	0.88	0.21	24,38,44,47	0
3	INI	B	202	21/21	0.89	0.18	22,30,40,45	0
3	INI	G	207	21/21	0.89	0.19	20,31,40,43	0
3	INI	I	209	21/21	0.89	0.16	14,28,36,39	0
3	INI	E	205	21/21	0.90	0.18	27,30,37,39	0
3	INI	F	206	21/21	0.90	0.19	25,32,42,44	0
3	INI	H	208	21/21	0.91	0.17	17,33,42,45	0
3	INI	C	203	21/21	0.91	0.18	28,34,41,45	0
3	INI	D	204	21/21	0.92	0.17	24,35,44,49	0
3	INI	J	210	21/21	0.92	0.17	30,33,37,40	0
2	PO4	J	1009	5/5	0.94	0.19	43,44,47,50	5

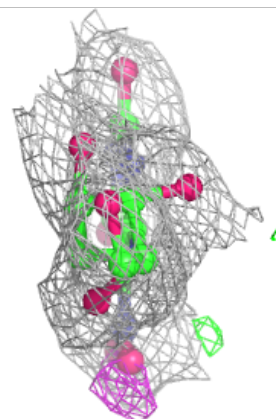
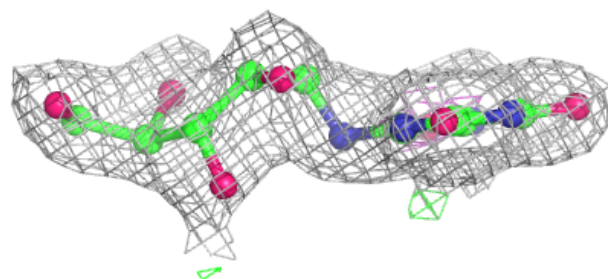
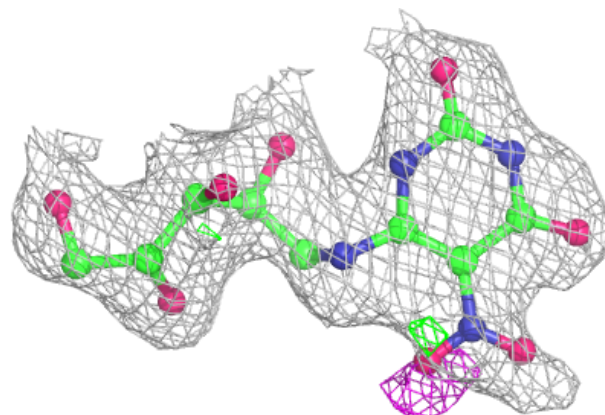
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around INI A 201:

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

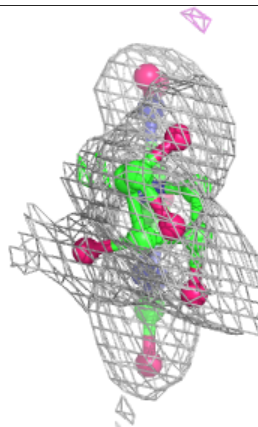
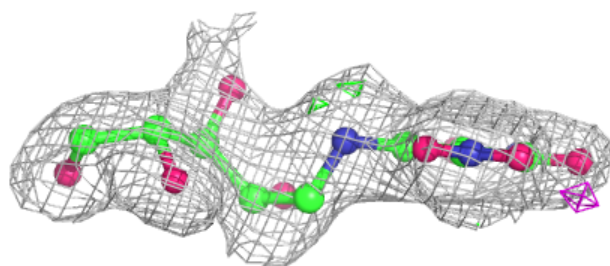
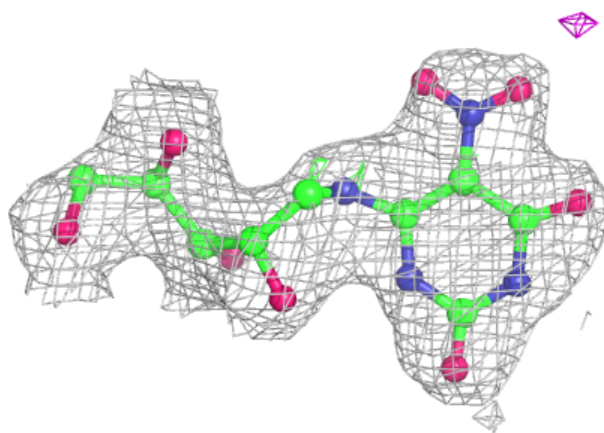
**Electron density around INI B 202:**

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



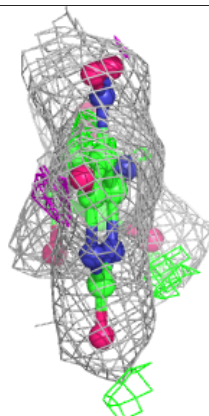
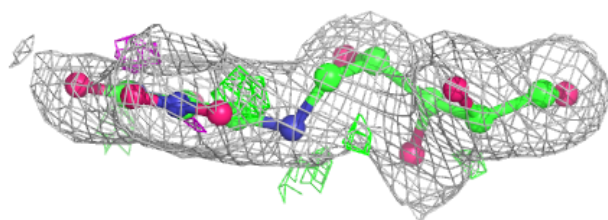
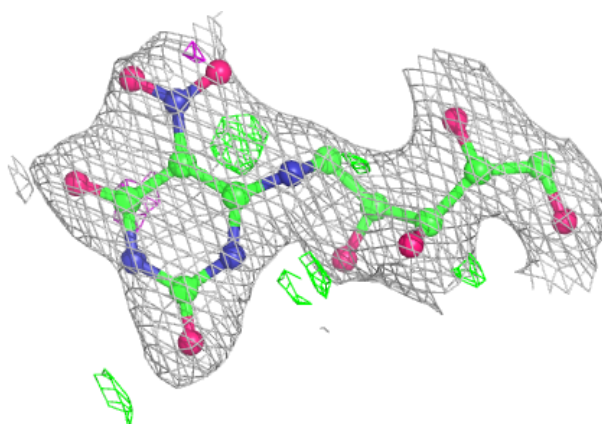
Electron density around INI G 207:

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



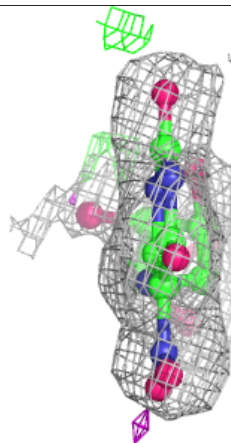
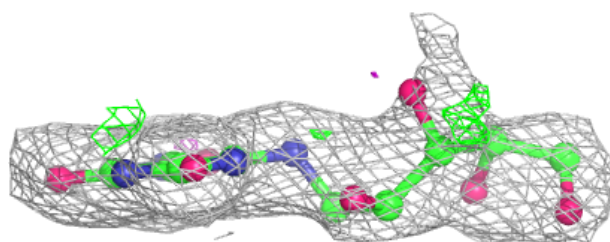
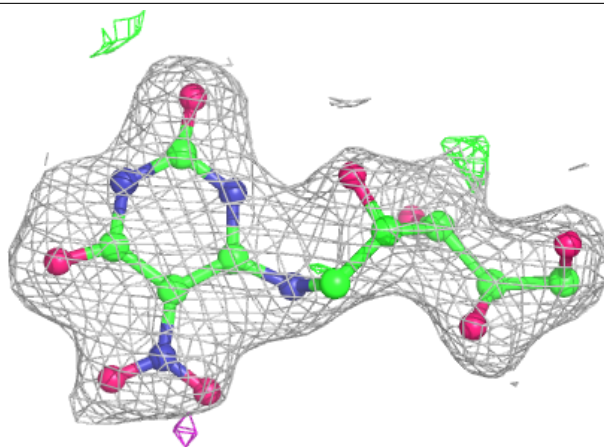
Electron density around INI I 209:

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

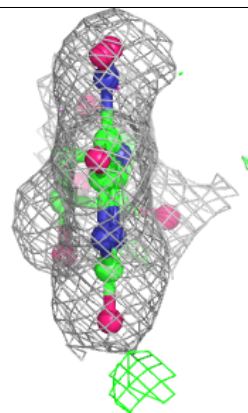
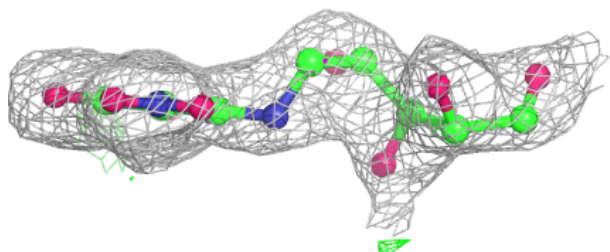
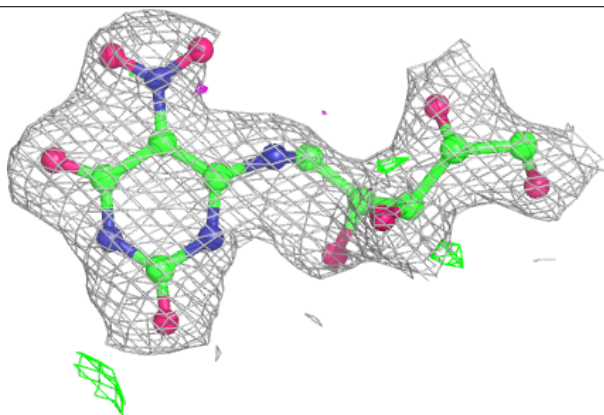


Electron density around INI E 205:

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and green (positive)

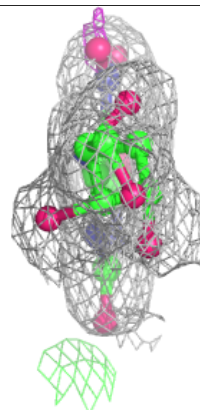
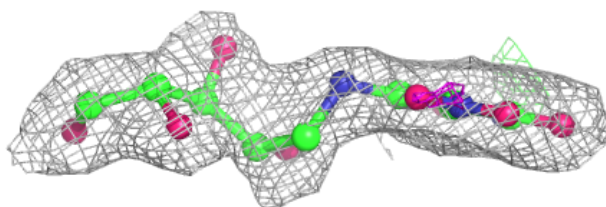
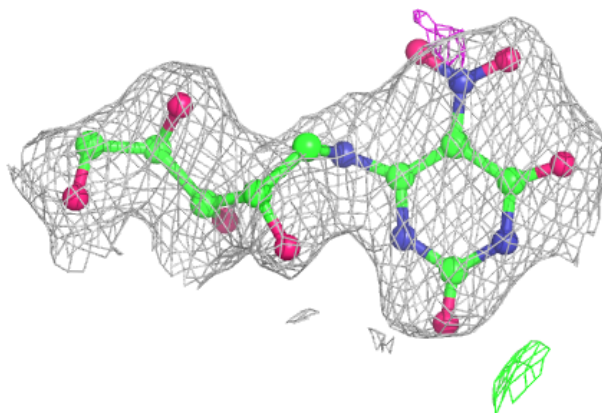
**Electron density around INI F 206:**

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

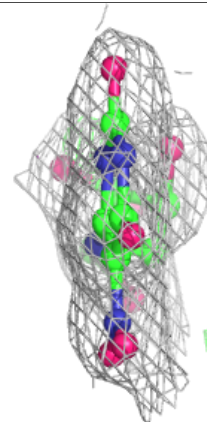
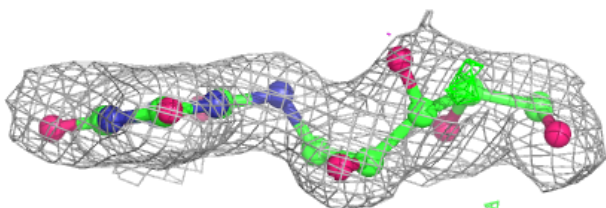
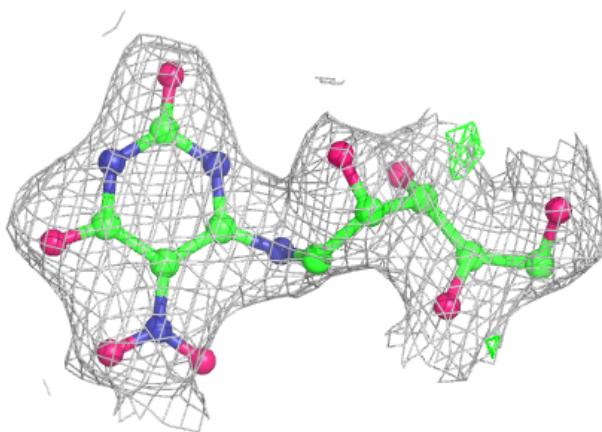


Electron density around INI H 208:

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

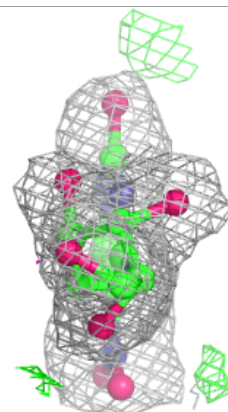
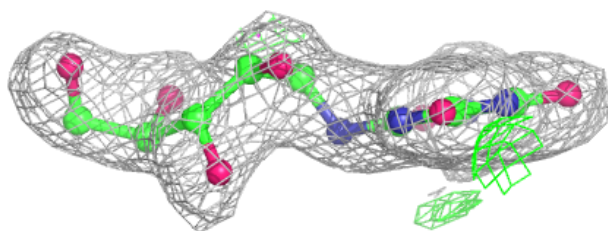
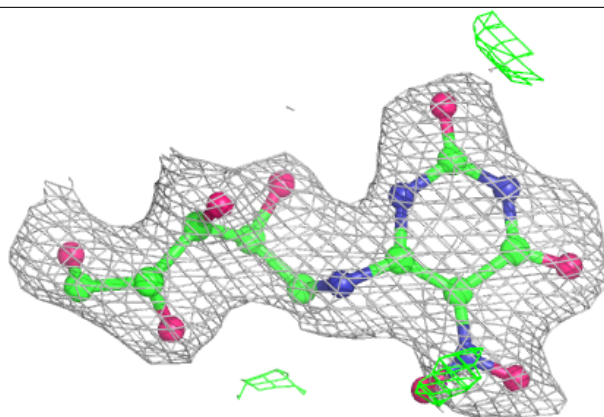
**Electron density around INI C 203:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

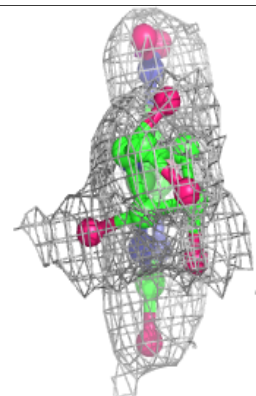
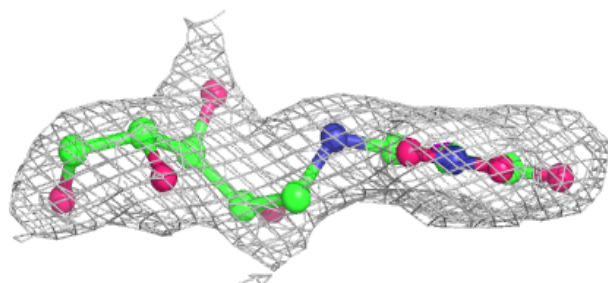
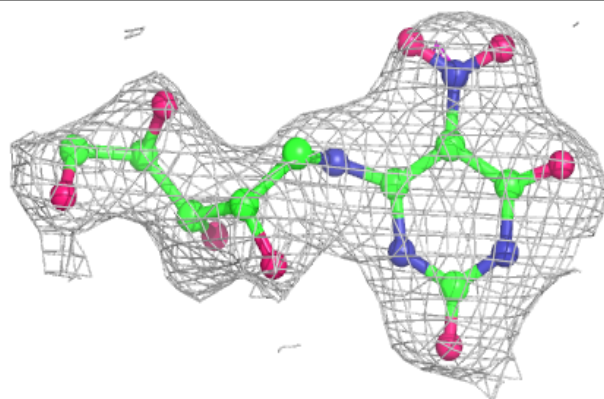


Electron density around INI D 204:

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

**Electron density around INI J 210:**

$2mF_o-DF_c$ (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.