



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 02:57 AM EDT

PDB ID : 1ZIS  
Title : Recombinant Lumazine synthase (hexagonal form)  
Authors : Lopez-Jaramillo, F.J.  
Deposited on : 2005-04-27  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

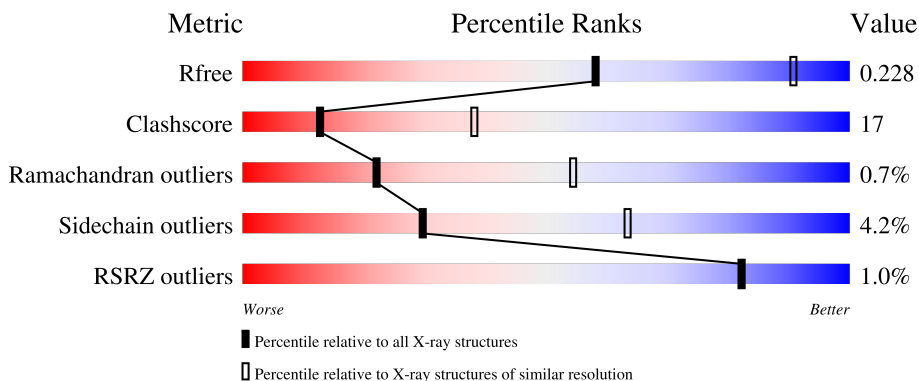
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	154	 71% 25% .
1	B	154	 72% 24% .
1	C	154	 72% 23% 5%
1	D	154	 72% 23% 5%
1	E	154	 70% 27% .

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Mol	Chain	Length	Quality of chain	
1	F	154		•
1	G	154		•
1	H	154		•
1	I	154		•
1	J	154		•

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
3	INI	A	200	-	X	-	-
3	INI	B	201	-	X	-	-
3	INI	C	202	-	X	-	-
3	INI	D	203	-	X	-	-
3	INI	E	204	-	X	-	-
3	INI	F	205	-	X	-	-
3	INI	G	206	-	X	-	-
3	INI	H	207	-	X	-	-
3	INI	I	208	-	X	-	-
3	INI	J	209	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11700 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.

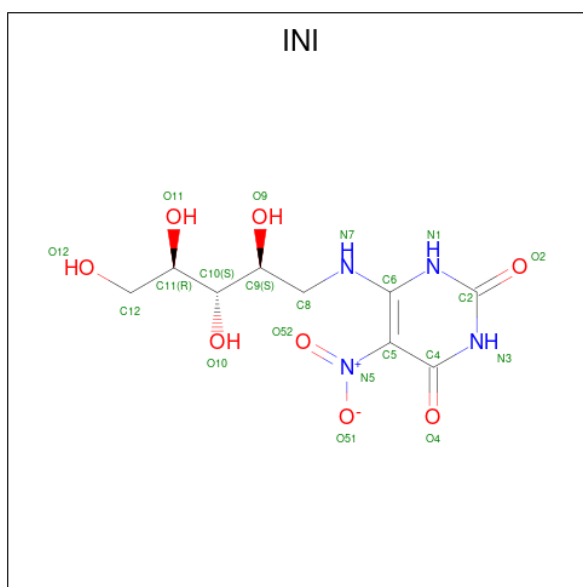
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	154	1144	721	196	222	5	0	0	0
1	B	154	1144	721	196	222	5	0	0	0
1	C	154	1144	721	196	222	5	0	0	0
1	D	154	1144	721	196	222	5	0	0	0
1	E	154	1144	721	196	222	5	0	0	0
1	F	154	1144	721	196	222	5	0	0	0
1	G	154	1144	721	196	222	5	0	0	0
1	H	154	1144	721	196	222	5	0	0	0
1	I	154	1144	721	196	222	5	0	0	0
1	J	154	1144	721	196	222	5	0	0	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is 5-NITRO-6-RIBITYL-AMINO-2,4(1H,3H)-PYRIMIDINEDIONE (three-letter code: INI) (formula: C<sub>9</sub>H<sub>14</sub>N<sub>4</sub>O<sub>8</sub>).

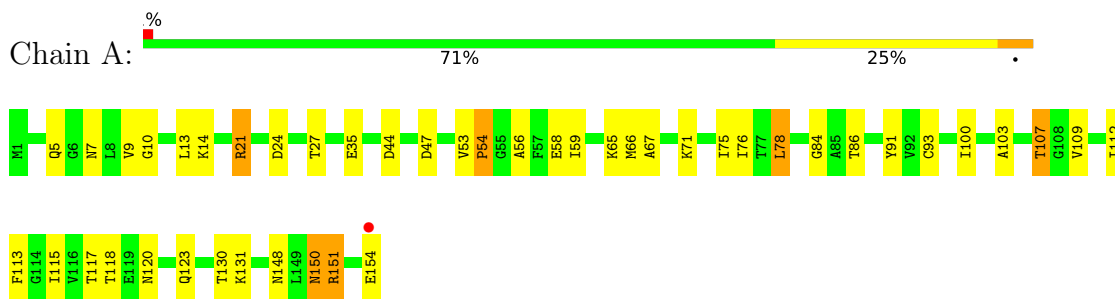


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	21	9	4	8	0	0
3	B	1	21	9	4	8	0	0
3	C	1	21	9	4	8	0	0
3	D	1	21	9	4	8	0	0
3	E	1	21	9	4	8	0	0
3	F	1	21	9	4	8	0	0
3	G	1	21	9	4	8	0	0
3	H	1	21	9	4	8	0	0
3	I	1	21	9	4	8	0	0
3	J	1	21	9	4	8	0	0

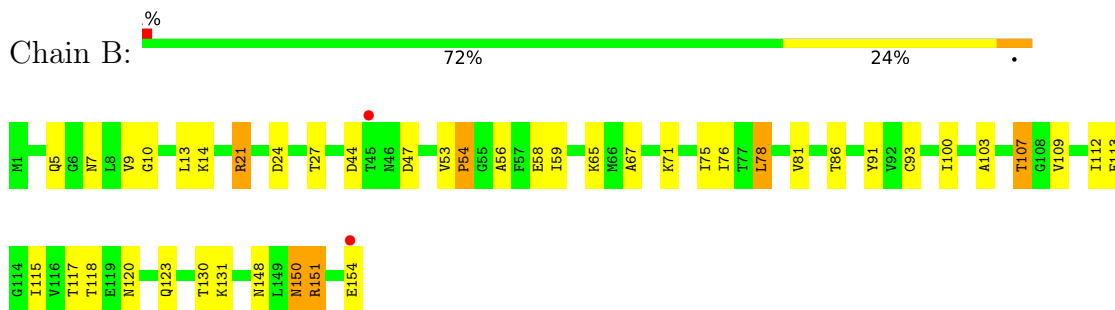
### 3 Residue-property plots [i](#)

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.

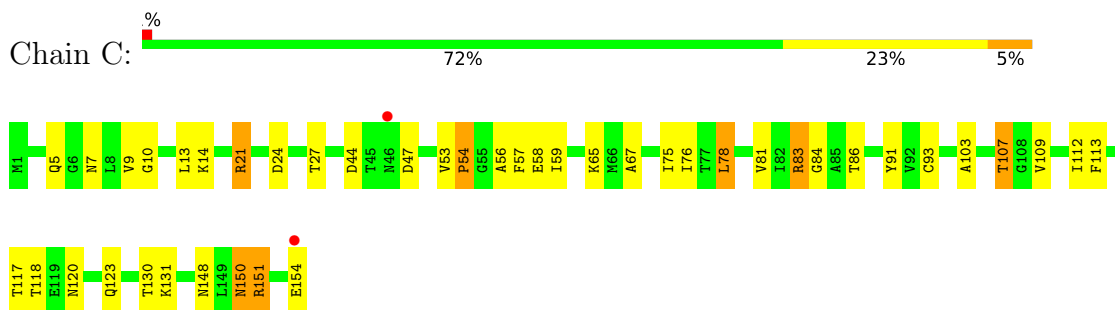
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



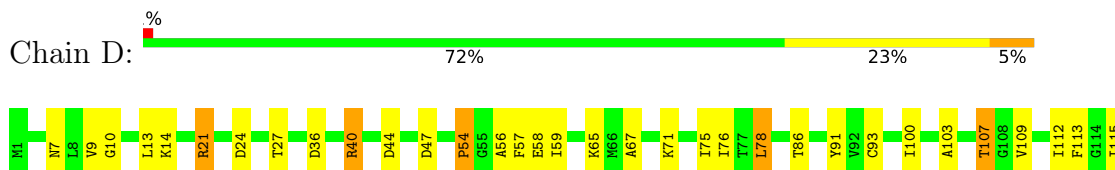
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



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

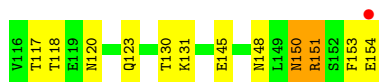
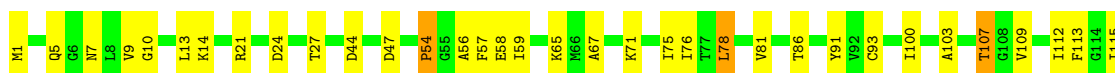


- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase

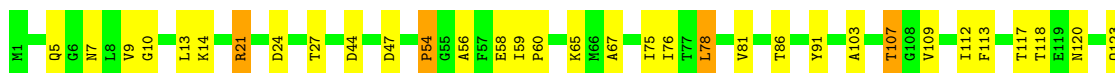
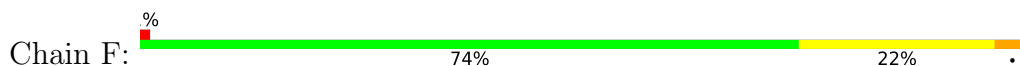




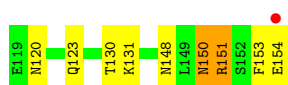
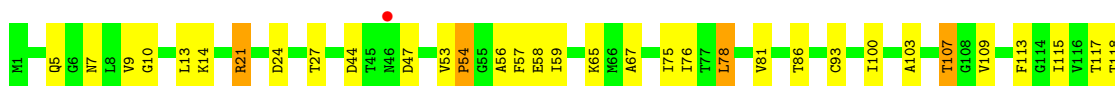
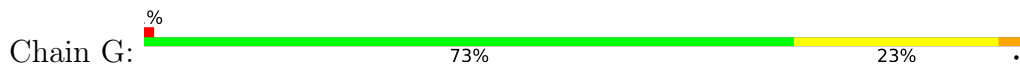
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



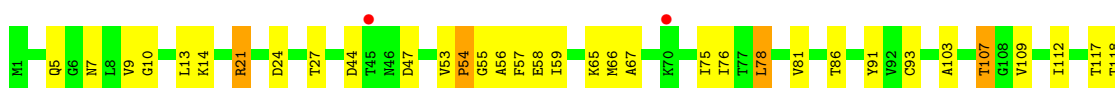
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase



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



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



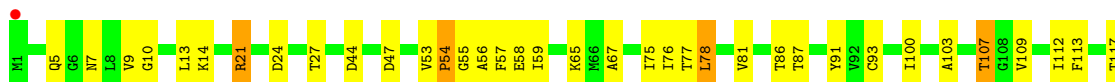
- Molecule 1: 6,7-dimethyl-8-ribityllumazine synthase







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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.69Å 153.69Å 296.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.90 19.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	88.4 (10.00-2.90) 88.2 (19.60-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.87 (at 2.88Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.206 , 0.240 0.194 , 0.228	Depositor DCC
$R_{free}$ test set	4016 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11700	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.43	0/1159	0.76	4/1569 (0.3%)
1	B	0.43	0/1159	0.99	5/1569 (0.3%)
1	C	0.44	0/1159	1.17	7/1569 (0.4%)
1	D	0.46	0/1159	1.35	8/1569 (0.5%)
1	E	0.48	0/1159	1.00	5/1569 (0.3%)
1	F	0.45	0/1159	1.19	6/1569 (0.4%)
1	G	0.42	0/1159	0.76	4/1569 (0.3%)
1	H	0.42	0/1159	0.74	4/1569 (0.3%)
1	I	0.43	0/1159	0.76	4/1569 (0.3%)
1	J	0.44	0/1159	1.00	5/1569 (0.3%)
All	All	0.44	0/11590	0.99	52/15690 (0.3%)

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	40	ARG	NE-CZ-NH1	-25.26	107.67	120.30
1	C	83	ARG	NE-CZ-NH1	-24.14	108.23	120.30
1	D	40	ARG	NE-CZ-NH2	23.57	132.09	120.30
1	C	83	ARG	NE-CZ-NH2	23.16	131.88	120.30
1	F	21	ARG	NE-CZ-NH1	-21.16	109.72	120.30
1	B	151	ARG	NE-CZ-NH1	-19.82	110.39	120.30
1	J	151	ARG	NE-CZ-NH1	-19.67	110.47	120.30
1	D	21	ARG	NE-CZ-NH1	-19.66	110.47	120.30
1	F	21	ARG	NE-CZ-NH2	19.39	130.00	120.30
1	E	21	ARG	NE-CZ-NH1	-19.35	110.63	120.30
1	E	21	ARG	NE-CZ-NH2	18.84	129.72	120.30
1	F	151	ARG	NE-CZ-NH1	-18.14	111.23	120.30
1	J	151	ARG	NE-CZ-NH2	18.09	129.35	120.30
1	D	21	ARG	NE-CZ-NH2	17.89	129.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ARG	NE-CZ-NH2	17.79	129.20	120.30
1	F	151	ARG	NE-CZ-NH2	17.50	129.05	120.30
1	D	40	ARG	CD-NE-CZ	10.91	138.88	123.60
1	C	83	ARG	CD-NE-CZ	10.19	137.86	123.60
1	J	21	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	G	21	ARG	NE-CZ-NH2	-9.58	115.51	120.30
1	F	21	ARG	CD-NE-CZ	9.51	136.91	123.60
1	I	21	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	A	21	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	E	21	ARG	CD-NE-CZ	9.36	136.71	123.60
1	C	21	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	D	21	ARG	CD-NE-CZ	9.30	136.62	123.60
1	J	151	ARG	CD-NE-CZ	9.20	136.48	123.60
1	F	151	ARG	CD-NE-CZ	9.05	136.27	123.60
1	A	21	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	151	ARG	CD-NE-CZ	8.96	136.14	123.60
1	I	21	ARG	NE-CZ-NH1	8.95	124.77	120.30
1	J	21	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	D	151	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	D	151	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	C	21	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	21	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	G	21	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	G	151	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	H	151	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	151	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	E	151	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	151	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	H	21	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	21	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	I	151	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	I	151	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	C	151	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	151	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	H	151	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	G	151	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	E	151	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	H	21	ARG	NE-CZ-NH1	7.28	123.94	120.30

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	1144	0	1157	51	0
1	B	1144	0	1157	45	0
1	C	1144	0	1157	46	0
1	D	1144	0	1157	44	0
1	E	1144	0	1157	48	0
1	F	1144	0	1157	44	0
1	G	1144	0	1157	45	0
1	H	1144	0	1157	46	0
1	I	1144	0	1157	48	0
1	J	1144	0	1157	48	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	1	0
3	A	21	0	14	3	0
3	B	21	0	14	3	0
3	C	21	0	14	5	0
3	D	21	0	14	5	0
3	E	21	0	14	5	0
3	F	21	0	14	5	0
3	G	21	0	14	4	0
3	H	21	0	14	4	0
3	I	21	0	14	3	0
3	J	21	0	14	6	0
All	All	11700	0	11710	388	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 17.

All (388) 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:D:130:THR:HG22	1:D:131:LYS:H	1.23	1.03
1:H:130:THR:HG22	1:H:131:LYS:H	1.23	1.01
1:F:130:THR:HG22	1:F:131:LYS:H	1.24	1.00
1:E:130:THR:HG22	1:E:131:LYS:H	1.23	1.00
1:C:130:THR:HG22	1:C:131:LYS:H	1.26	0.99
1:A:130:THR:HG22	1:A:131:LYS:H	1.24	0.98
1:I:130:THR:HG22	1:I:131:LYS:H	1.25	0.97
1:H:107:THR:HG23	1:H:109:VAL:H	1.28	0.97
1:J:130:THR:HG22	1:J:131:LYS:H	1.28	0.96
1:G:130:THR:HG22	1:G:131:LYS:H	1.29	0.95
1:B:130:THR:HG22	1:B:131:LYS:H	1.29	0.95
1:G:107:THR:HG23	1:G:109:VAL:H	1.35	0.91
1:E:107:THR:HG23	1:E:109:VAL:H	1.35	0.91
1:F:107:THR:HG23	1:F:109:VAL:H	1.36	0.90
1:A:107:THR:HG23	1:A:109:VAL:H	1.32	0.90
1:I:107:THR:HG23	1:I:109:VAL:H	1.37	0.90
1:C:107:THR:HG23	1:C:109:VAL:H	1.36	0.89
1:D:107:THR:HG23	1:D:109:VAL:H	1.36	0.88
1:B:107:THR:HG23	1:B:109:VAL:H	1.37	0.87
1:F:130:THR:HG22	1:F:131:LYS:N	1.90	0.87
1:H:130:THR:HG22	1:H:131:LYS:N	1.87	0.87
1:A:130:THR:HG22	1:A:131:LYS:N	1.91	0.86
1:G:113:PHE:O	3:H:207:INI:H122	1.74	0.85
1:D:150:ASN:HD21	1:E:65:LYS:NZ	1.74	0.85
1:J:107:THR:HG23	1:J:109:VAL:H	1.39	0.85
1:D:130:THR:HG22	1:D:131:LYS:N	1.91	0.85
1:I:130:THR:HG22	1:I:131:LYS:N	1.91	0.85
1:E:130:THR:HG22	1:E:131:LYS:N	1.90	0.84
1:C:130:THR:HG22	1:C:131:LYS:N	1.91	0.84
1:B:130:THR:HG22	1:B:131:LYS:N	1.92	0.84
1:A:150:ASN:HD21	1:B:65:LYS:NZ	1.77	0.83
1:G:130:THR:HG22	1:G:131:LYS:N	1.93	0.82
1:J:130:THR:HG22	1:J:131:LYS:N	1.93	0.82
1:F:65:LYS:NZ	1:J:150:ASN:HD21	1.78	0.81
1:F:5:GLN:HE21	1:G:21:ARG:HH22	1.24	0.81
1:G:150:ASN:HD21	1:H:65:LYS:NZ	1.77	0.81
1:I:5:GLN:HE21	1:J:21:ARG:HH22	1.24	0.81
1:A:21:ARG:HH22	1:E:5:GLN:HE21	1.26	0.80
1:B:5:GLN:HE21	1:C:21:ARG:HH22	1.25	0.80
1:H:5:GLN:HE21	1:I:21:ARG:HH22	1.26	0.80
1:B:150:ASN:HD21	1:C:65:LYS:NZ	1.83	0.77
1:H:107:THR:CG2	1:H:109:VAL:H	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:GLN:NE2	1:G:21:ARG:HH22	1.84	0.75
1:A:21:ARG:HH22	1:E:5:GLN:NE2	1.84	0.75
1:E:107:THR:CG2	1:E:109:VAL:H	1.99	0.74
1:D:107:THR:CG2	1:D:109:VAL:H	2.00	0.74
1:A:5:GLN:HE21	1:B:21:ARG:HH22	1.33	0.74
1:A:107:THR:CG2	1:A:109:VAL:H	2.01	0.74
1:F:107:THR:CG2	1:F:109:VAL:H	2.01	0.73
1:C:107:THR:CG2	1:C:109:VAL:H	2.01	0.73
1:G:107:THR:CG2	1:G:109:VAL:H	2.01	0.73
1:I:130:THR:HG22	1:I:131:LYS:HG2	1.70	0.73
1:G:5:GLN:HE21	1:H:21:ARG:HH22	1.34	0.73
1:F:130:THR:HG22	1:F:131:LYS:HG2	1.71	0.72
1:A:130:THR:HG22	1:A:131:LYS:HG2	1.70	0.72
1:D:130:THR:HG22	1:D:131:LYS:HG2	1.71	0.72
1:H:5:GLN:NE2	1:I:21:ARG:HH22	1.87	0.72
1:H:130:THR:HG22	1:H:131:LYS:HG2	1.70	0.72
1:D:150:ASN:HD21	1:E:65:LYS:HZ3	1.38	0.71
1:H:150:ASN:HD21	1:I:65:LYS:NZ	1.88	0.71
1:E:76:ILE:HG22	1:E:78:LEU:HD13	1.73	0.70
1:I:5:GLN:NE2	1:J:21:ARG:HH22	1.89	0.70
1:B:5:GLN:NE2	1:C:21:ARG:HH22	1.89	0.70
1:I:107:THR:CG2	1:I:109:VAL:H	2.04	0.69
1:G:76:ILE:HG22	1:G:78:LEU:HD13	1.74	0.69
1:B:76:ILE:HG22	1:B:78:LEU:HD13	1.73	0.69
1:C:130:THR:HG22	1:C:131:LYS:HG2	1.74	0.69
1:E:130:THR:HG22	1:E:131:LYS:HG2	1.73	0.69
1:J:130:THR:HG22	1:J:131:LYS:HG2	1.74	0.69
1:I:150:ASN:HD21	1:J:65:LYS:NZ	1.89	0.69
1:J:107:THR:CG2	1:J:109:VAL:H	2.04	0.69
1:H:76:ILE:HG22	1:H:78:LEU:HD13	1.76	0.68
1:B:67:ALA:HB2	1:B:75:ILE:HD12	1.74	0.68
1:I:76:ILE:HG22	1:I:78:LEU:HD13	1.73	0.68
1:B:107:THR:CG2	1:B:109:VAL:H	2.04	0.68
1:J:76:ILE:HG22	1:J:78:LEU:HD13	1.76	0.68
1:C:76:ILE:HG22	1:C:78:LEU:HD13	1.76	0.68
1:F:76:ILE:HG22	1:F:78:LEU:HD13	1.74	0.68
1:I:67:ALA:HB2	1:I:75:ILE:HD12	1.76	0.68
1:A:150:ASN:HD21	1:B:65:LYS:HZ3	1.42	0.67
1:C:67:ALA:HB2	1:C:75:ILE:HD12	1.75	0.67
1:A:67:ALA:HB2	1:A:75:ILE:HD12	1.75	0.67
1:J:67:ALA:HB2	1:J:75:ILE:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:THR:CG2	1:D:131:LYS:H	1.97	0.66
1:G:150:ASN:HD21	1:H:65:LYS:HZ2	1.42	0.66
1:D:76:ILE:HG22	1:D:78:LEU:HD13	1.75	0.66
1:G:130:THR:HG22	1:G:131:LYS:HG2	1.76	0.66
1:H:67:ALA:HB2	1:H:75:ILE:HD12	1.77	0.66
1:A:76:ILE:HG22	1:A:78:LEU:HD13	1.77	0.66
1:C:150:ASN:HD21	1:D:65:LYS:NZ	1.93	0.66
1:G:67:ALA:HB2	1:G:75:ILE:HD12	1.78	0.66
1:B:24:ASP:HA	1:B:27:THR:OG1	1.97	0.65
1:D:67:ALA:HB2	1:D:75:ILE:HD12	1.78	0.65
1:E:67:ALA:HB2	1:E:75:ILE:HD12	1.78	0.65
1:F:24:ASP:HA	1:F:27:THR:OG1	1.96	0.65
1:B:130:THR:HG22	1:B:131:LYS:HG2	1.78	0.65
1:A:24:ASP:HA	1:A:27:THR:OG1	1.97	0.65
1:H:81:VAL:HA	3:H:207:INI:O4	1.97	0.65
1:B:130:THR:CG2	1:B:131:LYS:H	2.00	0.64
1:H:24:ASP:HA	1:H:27:THR:OG1	1.97	0.64
1:E:24:ASP:HA	1:E:27:THR:OG1	1.96	0.64
1:F:65:LYS:HZ2	1:J:150:ASN:HD21	1.44	0.64
1:G:5:GLN:NE2	1:H:21:ARG:HH22	1.96	0.64
1:E:148:ASN:ND2	1:E:151:ARG:NH2	2.45	0.64
1:D:7:ASN:HD21	1:D:9:VAL:HB	1.63	0.64
1:F:81:VAL:HA	3:F:205:INI:O4	1.97	0.64
1:G:7:ASN:HD21	1:G:9:VAL:HB	1.63	0.64
1:F:67:ALA:HB2	1:F:75:ILE:HD12	1.79	0.63
1:H:130:THR:CG2	1:H:131:LYS:H	1.96	0.63
1:C:7:ASN:HD21	1:C:9:VAL:HB	1.62	0.63
1:I:24:ASP:HA	1:I:27:THR:OG1	1.97	0.63
1:A:7:ASN:HD21	1:A:9:VAL:HB	1.63	0.63
1:C:113:PHE:O	3:D:203:INI:H122	1.99	0.63
1:D:107:THR:HG23	1:D:109:VAL:HG23	1.80	0.63
1:A:65:LYS:NZ	1:E:150:ASN:HD21	1.96	0.63
1:J:7:ASN:HD21	1:J:9:VAL:HB	1.62	0.62
1:A:5:GLN:NE2	1:B:21:ARG:HH22	1.96	0.62
1:D:148:ASN:ND2	1:D:151:ARG:NH2	2.47	0.62
1:G:24:ASP:HA	1:G:27:THR:OG1	1.97	0.62
1:C:24:ASP:HA	1:C:27:THR:OG1	1.98	0.62
1:E:7:ASN:HD21	1:E:9:VAL:HB	1.65	0.62
1:B:150:ASN:HD21	1:C:65:LYS:HZ3	1.47	0.62
1:C:81:VAL:HA	3:C:202:INI:O4	1.99	0.62
3:A:200:INI:H122	1:E:113:PHE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:ASP:HA	1:J:27:THR:OG1	1.99	0.62
1:A:148:ASN:ND2	1:A:151:ARG:NH2	2.48	0.62
1:B:7:ASN:HD21	1:B:9:VAL:HB	1.64	0.61
1:I:7:ASN:HD21	1:I:9:VAL:HB	1.64	0.61
1:G:81:VAL:HA	3:G:206:INI:O4	2.00	0.61
1:A:150:ASN:HD21	1:B:65:LYS:HZ2	1.49	0.61
1:D:150:ASN:HD21	1:E:65:LYS:HZ2	1.47	0.61
1:H:7:ASN:HD21	1:H:9:VAL:HB	1.65	0.61
1:E:107:THR:HG23	1:E:109:VAL:HG23	1.83	0.61
1:F:7:ASN:HD21	1:F:9:VAL:HB	1.65	0.61
1:G:148:ASN:ND2	1:G:151:ARG:NH2	2.48	0.61
1:I:148:ASN:ND2	1:I:151:ARG:NH2	2.48	0.61
1:A:117:THR:O	1:B:86:THR:HB	2.01	0.61
1:A:21:ARG:NH2	1:E:5:GLN:HE21	1.98	0.60
1:C:112:ILE:HG23	3:D:203:INI:H121	1.83	0.60
1:D:24:ASP:HA	1:D:27:THR:OG1	2.02	0.60
1:C:148:ASN:ND2	1:C:151:ARG:NH2	2.50	0.59
1:F:5:GLN:HE21	1:G:21:ARG:NH2	1.98	0.59
1:F:65:LYS:HZ3	1:J:150:ASN:HD21	1.49	0.59
1:F:113:PHE:O	3:G:206:INI:H122	2.02	0.59
1:F:150:ASN:HD21	1:G:65:LYS:NZ	2.01	0.59
1:J:148:ASN:ND2	1:J:151:ARG:NH2	2.51	0.58
1:A:10:GLY:HA2	1:A:13:LEU:HD12	1.85	0.58
1:I:81:VAL:HA	3:I:208:INI:O4	2.03	0.58
1:C:130:THR:CG2	1:C:131:LYS:H	1.99	0.58
1:A:86:THR:HB	1:E:117:THR:O	2.03	0.58
3:A:200:INI:H121	1:E:112:ILE:HG23	1.85	0.58
1:C:107:THR:HG23	1:C:109:VAL:HG23	1.86	0.57
1:J:107:THR:HG23	1:J:109:VAL:HG23	1.86	0.57
1:I:117:THR:O	1:J:86:THR:HB	2.04	0.57
1:J:10:GLY:HA2	1:J:13:LEU:HD12	1.86	0.57
1:A:21:ARG:HG3	1:A:53:VAL:O	2.05	0.57
1:A:54:PRO:HD2	1:A:58:GLU:HG2	1.86	0.57
1:G:107:THR:HG23	1:G:109:VAL:HG23	1.87	0.57
1:G:150:ASN:HD21	1:H:65:LYS:HZ3	1.50	0.57
1:G:7:ASN:HD22	1:G:9:VAL:HG23	1.71	0.56
1:I:107:THR:HG23	1:I:109:VAL:HG23	1.87	0.56
1:A:56:ALA:HA	1:A:59:ILE:HG13	1.87	0.56
1:C:83:ARG:HG3	1:C:84:GLY:N	2.20	0.56
1:A:120:ASN:OD1	1:A:123:GLN:HG3	2.06	0.56
1:F:107:THR:HG23	1:F:109:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:ASN:HD21	1:J:65:LYS:HZ3	1.52	0.56
1:J:130:THR:CG2	1:J:131:LYS:H	2.00	0.56
1:D:54:PRO:HD2	1:D:58:GLU:HG2	1.88	0.56
1:H:21:ARG:HG3	1:H:53:VAL:O	2.06	0.56
1:E:10:GLY:HA2	1:E:13:LEU:HD12	1.88	0.55
1:J:118:THR:HB	1:J:123:GLN:HB2	1.88	0.55
1:G:54:PRO:HD2	1:G:58:GLU:HG2	1.88	0.55
1:H:54:PRO:HD2	1:H:58:GLU:HG2	1.88	0.55
1:I:54:PRO:HD2	1:I:58:GLU:HG2	1.89	0.55
1:B:107:THR:HG23	1:B:109:VAL:HG23	1.89	0.55
1:H:107:THR:HG23	1:H:109:VAL:N	2.10	0.55
1:H:148:ASN:ND2	1:H:151:ARG:NH2	2.55	0.55
1:J:7:ASN:ND2	1:J:9:VAL:HB	2.22	0.55
1:B:120:ASN:OD1	1:B:123:GLN:HG3	2.06	0.55
1:D:120:ASN:OD1	1:D:123:GLN:HG3	2.07	0.55
1:C:10:GLY:HA2	1:C:13:LEU:HD12	1.88	0.54
1:D:107:THR:HG23	1:D:109:VAL:N	2.16	0.54
1:J:120:ASN:OD1	1:J:123:GLN:HG3	2.07	0.54
1:A:112:ILE:HG23	3:B:201:INI:H121	1.89	0.54
1:C:21:ARG:HG3	1:C:53:VAL:O	2.07	0.54
1:F:86:THR:HB	1:J:117:THR:O	2.08	0.54
1:B:10:GLY:HA2	1:B:13:LEU:HD12	1.90	0.54
1:B:148:ASN:ND2	1:B:151:ARG:NH2	2.54	0.54
1:B:150:ASN:HD21	1:C:65:LYS:HZ2	1.54	0.54
1:A:118:THR:HB	1:A:123:GLN:HB2	1.88	0.54
1:F:148:ASN:ND2	1:F:151:ARG:NH2	2.56	0.54
1:H:5:GLN:HE21	1:I:21:ARG:NH2	2.02	0.54
1:B:130:THR:CG2	1:B:131:LYS:N	2.62	0.54
1:J:130:THR:CG2	1:J:131:LYS:N	2.63	0.54
1:C:7:ASN:ND2	1:C:9:VAL:HB	2.22	0.54
1:H:150:ASN:HD21	1:I:65:LYS:HZ2	1.54	0.54
1:B:118:THR:HB	1:B:123:GLN:HB2	1.90	0.54
1:D:113:PHE:O	3:E:204:INI:H122	2.08	0.54
1:E:81:VAL:HA	3:E:204:INI:O4	2.06	0.54
1:A:107:THR:HG23	1:A:109:VAL:HG23	1.89	0.54
1:E:118:THR:HB	1:E:123:GLN:HB2	1.88	0.54
1:A:7:ASN:ND2	1:A:9:VAL:HB	2.23	0.54
1:C:120:ASN:OD1	1:C:123:GLN:HG3	2.08	0.54
1:I:112:ILE:HG23	3:J:209:INI:H121	1.89	0.54
1:E:7:ASN:ND2	1:E:9:VAL:HB	2.23	0.53
1:H:107:THR:HG23	1:H:109:VAL:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:HB	1:C:123:GLN:HB2	1.89	0.53
1:E:103:ALA:O	1:E:107:THR:HB	2.07	0.53
1:G:117:THR:O	1:H:86:THR:HB	2.08	0.53
1:G:118:THR:HB	1:G:123:GLN:HB2	1.89	0.53
1:J:81:VAL:HA	3:J:209:INI:O4	2.08	0.53
1:C:130:THR:CG2	1:C:131:LYS:N	2.61	0.53
1:F:56:ALA:HA	1:F:59:ILE:HG13	1.90	0.53
1:H:56:ALA:HA	1:H:59:ILE:HG13	1.91	0.53
1:I:120:ASN:OD1	1:I:123:GLN:HG3	2.08	0.53
1:F:10:GLY:HA2	1:F:13:LEU:HD12	1.90	0.53
1:H:117:THR:O	1:I:86:THR:HB	2.09	0.53
1:C:54:PRO:HD2	1:C:58:GLU:HG2	1.91	0.53
1:H:7:ASN:ND2	1:H:9:VAL:HB	2.24	0.53
1:F:112:ILE:HG23	3:G:206:INI:H121	1.90	0.53
1:B:7:ASN:ND2	1:B:9:VAL:HB	2.24	0.53
1:B:54:PRO:HD2	1:B:58:GLU:HG2	1.91	0.53
1:C:5:GLN:HE21	1:D:21:ARG:HH22	1.57	0.53
1:H:120:ASN:OD1	1:H:123:GLN:HG3	2.09	0.53
1:D:118:THR:HB	1:D:123:GLN:HB2	1.92	0.52
3:F:205:INI:H121	1:J:112:ILE:HG23	1.90	0.52
1:G:21:ARG:HG3	1:G:53:VAL:O	2.09	0.52
1:H:150:ASN:HD21	1:I:65:LYS:HZ3	1.57	0.52
1:I:7:ASN:HD22	1:I:9:VAL:HG23	1.74	0.52
1:B:21:ARG:HG3	1:B:53:VAL:O	2.09	0.52
1:F:54:PRO:HD2	1:F:58:GLU:HG2	1.91	0.52
1:G:10:GLY:HA2	1:G:13:LEU:HD12	1.92	0.52
1:H:10:GLY:HA2	1:H:13:LEU:HD12	1.90	0.52
1:G:56:ALA:HA	1:G:59:ILE:HG13	1.91	0.52
1:I:10:GLY:HA2	1:I:13:LEU:HD12	1.92	0.52
1:H:118:THR:HB	1:H:123:GLN:HB2	1.91	0.52
1:J:56:ALA:HA	1:J:59:ILE:HG13	1.91	0.52
1:J:21:ARG:HG3	1:J:53:VAL:O	2.10	0.52
1:B:7:ASN:HD22	1:B:9:VAL:HG23	1.75	0.52
1:I:118:THR:HB	1:I:123:GLN:HB2	1.91	0.52
1:J:54:PRO:HD2	1:J:58:GLU:HG2	1.90	0.52
1:F:118:THR:HB	1:F:123:GLN:HB2	1.91	0.51
1:C:107:THR:HG23	1:C:109:VAL:N	2.16	0.51
1:D:7:ASN:ND2	1:D:9:VAL:HB	2.25	0.51
1:F:7:ASN:HD22	1:F:9:VAL:HG23	1.74	0.51
1:A:93:CYS:HB3	1:B:91:TYR:CZ	2.45	0.51
1:D:56:ALA:HA	1:D:59:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:CYS:HB3	1:H:91:TYR:CZ	2.45	0.51
1:G:7:ASN:ND2	1:G:9:VAL:HB	2.24	0.51
1:J:103:ALA:O	1:J:107:THR:HB	2.11	0.51
1:A:7:ASN:HD22	1:A:9:VAL:HG23	1.76	0.51
1:F:7:ASN:ND2	1:F:9:VAL:HB	2.25	0.51
1:B:113:PHE:O	3:C:202:INI:H122	2.10	0.51
1:D:7:ASN:HD22	1:D:9:VAL:HG23	1.74	0.51
1:E:7:ASN:HD22	1:E:9:VAL:HG23	1.76	0.51
1:E:54:PRO:HD2	1:E:58:GLU:HG2	1.93	0.51
1:E:56:ALA:HA	1:E:59:ILE:HG13	1.92	0.51
1:I:56:ALA:HA	1:I:59:ILE:HG13	1.93	0.51
1:A:21:ARG:HD2	1:E:145:GLU:OE2	2.11	0.51
1:D:10:GLY:HA2	1:D:13:LEU:HD12	1.93	0.51
1:I:7:ASN:ND2	1:I:9:VAL:HB	2.25	0.51
1:B:117:THR:O	1:C:86:THR:HB	2.11	0.50
1:G:120:ASN:OD1	1:G:123:GLN:HG3	2.11	0.50
1:J:7:ASN:HD22	1:J:9:VAL:HG23	1.76	0.50
1:C:150:ASN:HD21	1:D:65:LYS:HZ3	1.57	0.50
1:G:107:THR:HG23	1:G:109:VAL:N	2.16	0.50
1:A:130:THR:CG2	1:A:131:LYS:H	1.97	0.50
1:C:103:ALA:O	1:C:107:THR:HB	2.11	0.50
1:E:107:THR:HG23	1:E:109:VAL:N	2.15	0.50
1:B:56:ALA:HA	1:B:59:ILE:HG13	1.92	0.50
1:D:130:THR:CG2	1:D:131:LYS:N	2.62	0.50
1:F:130:THR:CG2	1:F:131:LYS:H	1.97	0.50
1:G:130:THR:CG2	1:G:131:LYS:H	2.01	0.50
1:I:93:CYS:HB3	1:J:91:TYR:CZ	2.47	0.50
1:A:107:THR:HG23	1:A:109:VAL:N	2.14	0.49
1:C:117:THR:O	1:D:86:THR:HB	2.11	0.49
1:I:107:THR:HG23	1:I:109:VAL:N	2.17	0.49
1:C:67:ALA:HB1	1:C:107:THR:HG21	1.94	0.49
1:I:150:ASN:HD21	1:J:65:LYS:HZ2	1.59	0.49
1:I:103:ALA:O	1:I:107:THR:HB	2.12	0.49
1:G:103:ALA:O	1:G:107:THR:HB	2.13	0.49
1:B:67:ALA:HB1	1:B:107:THR:HG21	1.95	0.49
1:A:84:GLY:HA3	2:A:501:PO4:O1	2.12	0.48
1:D:67:ALA:HB1	1:D:107:THR:HG21	1.95	0.48
3:A:200:INI:H121	1:E:112:ILE:CG2	2.43	0.48
1:C:7:ASN:HD22	1:C:9:VAL:HG23	1.79	0.48
1:I:58:GLU:OE1	3:I:208:INI:H10	2.14	0.48
1:B:103:ALA:O	1:B:107:THR:HB	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:ARG:HG3	1:I:53:VAL:O	2.13	0.48
1:A:35:GLU:HB2	1:E:1:MET:SD	2.54	0.48
1:C:44:ASP:HB3	1:C:47:ASP:OD2	2.14	0.48
1:C:56:ALA:HA	1:C:59:ILE:HG13	1.94	0.48
1:J:67:ALA:HB1	1:J:107:THR:HG21	1.93	0.48
1:D:103:ALA:O	1:D:107:THR:HB	2.13	0.47
1:J:86:THR:HG23	2:J:509:PO4:O1	2.14	0.47
1:F:120:ASN:OD1	1:F:123:GLN:HG3	2.13	0.47
1:F:67:ALA:HB1	1:F:107:THR:HG21	1.95	0.47
1:H:7:ASN:HD22	1:H:9:VAL:HG23	1.79	0.47
1:F:91:TYR:CZ	1:J:93:CYS:HB3	2.50	0.47
1:I:67:ALA:HB1	1:I:107:THR:HG21	1.96	0.47
1:H:57:PHE:HB2	3:H:207:INI:H9	1.97	0.47
1:D:36:ASP:OD2	1:D:40:ARG:HD3	2.14	0.46
1:F:21:ARG:HH22	1:J:5:GLN:HE21	1.62	0.46
1:G:67:ALA:HB1	1:G:107:THR:HG21	1.95	0.46
1:B:107:THR:HG23	1:B:109:VAL:N	2.18	0.46
1:F:103:ALA:O	1:F:107:THR:HB	2.14	0.46
1:J:58:GLU:OE1	3:J:209:INI:H10	2.15	0.46
1:A:65:LYS:HZ2	1:E:150:ASN:HD21	1.62	0.46
1:F:58:GLU:OE1	3:F:205:INI:H10	2.16	0.46
1:G:150:ASN:ND2	1:H:65:LYS:HZ2	2.11	0.46
1:A:103:ALA:O	1:A:107:THR:HB	2.16	0.46
1:H:44:ASP:HB3	1:H:47:ASP:OD2	2.16	0.46
1:A:66:MET:HG2	1:E:153:PHE:CE1	2.51	0.46
1:E:120:ASN:OD1	1:E:123:GLN:HG3	2.15	0.46
1:D:117:THR:O	1:E:86:THR:HB	2.15	0.45
1:F:150:ASN:HD21	1:G:65:LYS:HZ3	1.63	0.45
1:I:5:GLN:HE21	1:J:21:ARG:NH2	2.04	0.45
1:B:44:ASP:HB3	1:B:47:ASP:OD2	2.16	0.45
1:G:100:ILE:HD11	1:G:115:ILE:HD11	1.98	0.45
1:A:35:GLU:OE2	1:E:1:MET:HG3	2.17	0.45
1:D:44:ASP:HB3	1:D:47:ASP:OD2	2.16	0.45
1:F:65:LYS:HZ2	1:J:150:ASN:ND2	2.13	0.45
1:F:117:THR:O	1:G:86:THR:HB	2.17	0.45
1:C:150:ASN:HD21	1:D:65:LYS:HZ2	1.62	0.45
1:J:77:THR:OG1	1:J:100:ILE:HD13	2.17	0.45
1:D:57:PHE:HB2	3:D:203:INI:H9	1.99	0.44
1:C:93:CYS:HB3	1:D:91:TYR:CZ	2.52	0.44
1:A:65:LYS:HZ3	1:E:150:ASN:HD21	1.63	0.44
1:A:67:ALA:HB1	1:A:107:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ILE:HG23	3:C:202:INI:H121	1.99	0.44
1:H:103:ALA:O	1:H:107:THR:HB	2.17	0.44
1:A:71:LYS:HG2	1:A:71:LYS:O	2.18	0.44
1:A:91:TYR:CZ	1:E:93:CYS:HB3	2.52	0.44
1:E:44:ASP:HB3	1:E:47:ASP:OD2	2.18	0.44
1:H:130:THR:CG2	1:H:131:LYS:N	2.58	0.44
1:J:87:THR:HG1	1:J:91:TYR:HE2	1.62	0.44
1:A:44:ASP:HB3	1:A:47:ASP:OD2	2.18	0.43
1:C:112:ILE:CG2	3:D:203:INI:H121	2.48	0.43
1:D:112:ILE:HG23	3:E:204:INI:H121	2.00	0.43
1:I:44:ASP:HB3	1:I:47:ASP:OD2	2.17	0.43
1:F:44:ASP:HB3	1:F:47:ASP:OD2	2.18	0.43
1:D:71:LYS:O	1:D:71:LYS:HG2	2.18	0.43
1:D:107:THR:HG23	1:D:109:VAL:CG2	2.48	0.43
1:E:67:ALA:HB1	1:E:107:THR:HG21	1.99	0.43
1:H:55:GLY:HA3	3:H:207:INI:O9	2.19	0.43
1:D:21:ARG:O	1:D:24:ASP:HB3	2.19	0.43
1:G:44:ASP:HB3	1:G:47:ASP:OD2	2.18	0.43
1:J:44:ASP:HB3	1:J:47:ASP:OD2	2.19	0.43
1:E:58:GLU:OE1	3:E:204:INI:H10	2.19	0.43
1:H:67:ALA:HB1	1:H:107:THR:HG21	2.00	0.42
1:F:21:ARG:O	1:F:24:ASP:HB3	2.19	0.42
1:C:58:GLU:OE1	3:C:202:INI:H10	2.19	0.42
1:J:55:GLY:HA3	3:J:209:INI:O9	2.19	0.42
1:D:100:ILE:HD11	1:D:115:ILE:HD11	2.01	0.42
1:I:71:LYS:O	1:I:71:LYS:HG2	2.20	0.42
1:I:113:PHE:O	3:J:209:INI:H122	2.19	0.42
1:B:93:CYS:HB3	1:C:91:TYR:CZ	2.55	0.42
1:H:112:ILE:HG23	3:I:208:INI:O12	2.20	0.42
1:J:57:PHE:HB2	3:J:209:INI:H9	2.01	0.41
1:E:71:LYS:O	1:E:71:LYS:HG2	2.20	0.41
1:A:66:MET:HG2	1:E:153:PHE:HE1	1.84	0.41
1:F:145:GLU:OE2	1:G:21:ARG:HD2	2.20	0.41
3:F:205:INI:H122	1:J:113:PHE:O	2.20	0.41
1:G:57:PHE:HB2	3:G:206:INI:H9	2.01	0.41
1:A:21:ARG:O	1:A:24:ASP:HB3	2.20	0.41
1:A:100:ILE:HD11	1:A:115:ILE:HD11	2.01	0.41
1:A:113:PHE:O	3:B:201:INI:H122	2.21	0.41
1:C:21:ARG:O	1:C:24:ASP:HB3	2.19	0.41
1:D:93:CYS:HB3	1:E:91:TYR:CZ	2.55	0.41
1:E:100:ILE:HD11	1:E:115:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:VAL:HG22	3:F:205:INI:N3	2.35	0.41
1:B:71:LYS:O	1:B:71:LYS:HG2	2.20	0.41
1:F:107:THR:HG23	1:F:109:VAL:N	2.16	0.41
1:G:21:ARG:O	1:G:24:ASP:HB3	2.21	0.41
1:C:57:PHE:HB2	3:C:202:INI:H9	2.01	0.41
1:I:31:LEU:HA	1:I:78:LEU:HD23	2.03	0.41
1:D:58:GLU:OE1	3:D:203:INI:H10	2.21	0.41
1:E:57:PHE:HB2	3:E:204:INI:H9	2.02	0.40
1:G:153:PHE:CE1	1:H:66:MET:HG2	2.55	0.40
1:H:93:CYS:HB3	1:I:91:TYR:CZ	2.56	0.40
1:I:5:GLN:HB3	1:I:6:GLY:H	1.75	0.40
1:A:130:THR:CG2	1:A:131:LYS:N	2.61	0.40
1:B:81:VAL:HA	3:B:201:INI:O4	2.21	0.40
1:B:100:ILE:HD11	1:B:115:ILE:HD11	2.02	0.40
1:I:100:ILE:HD11	1:I:115:ILE:HD11	2.02	0.40
1:B:21:ARG:O	1:B:24:ASP:HB3	2.22	0.40
1:I:21:ARG:O	1:I:24:ASP:HB3	2.21	0.40
1:F:59:ILE:HB	1:F:60:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
1	B	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
1	C	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
1	D	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
1	E	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
1	F	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
1	H	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
1	I	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
1	J	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
All	All	1520/1540 (99%)	1451 (96%)	59 (4%)	10 (1%)	22	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	PRO
1	H	54	PRO
1	B	54	PRO
1	E	54	PRO
1	C	54	PRO
1	F	54	PRO
1	G	54	PRO
1	I	54	PRO
1	J	54	PRO
1	D	54	PRO

### 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	118/118 (100%)	113 (96%)	5 (4%)	30	63
1	B	118/118 (100%)	113 (96%)	5 (4%)	30	63
1	C	118/118 (100%)	113 (96%)	5 (4%)	30	63
1	D	118/118 (100%)	113 (96%)	5 (4%)	30	63
1	E	118/118 (100%)	113 (96%)	5 (4%)	30	63
1	F	118/118 (100%)	113 (96%)	5 (4%)	30	63
1	G	118/118 (100%)	113 (96%)	5 (4%)	30	63
1	H	118/118 (100%)	113 (96%)	5 (4%)	30	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	118/118 (100%)	113 (96%)	5 (4%)	30	63
1	J	118/118 (100%)	113 (96%)	5 (4%)	30	63
All	All	1180/1180 (100%)	1130 (96%)	50 (4%)	30	63

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	78	LEU
1	A	107	THR
1	A	150	ASN
1	A	154	GLU
1	B	14	LYS
1	B	78	LEU
1	B	107	THR
1	B	150	ASN
1	B	154	GLU
1	C	14	LYS
1	C	78	LEU
1	C	107	THR
1	C	150	ASN
1	C	154	GLU
1	D	14	LYS
1	D	78	LEU
1	D	107	THR
1	D	150	ASN
1	D	154	GLU
1	E	14	LYS
1	E	78	LEU
1	E	107	THR
1	E	150	ASN
1	E	154	GLU
1	F	14	LYS
1	F	78	LEU
1	F	107	THR
1	F	150	ASN
1	F	154	GLU
1	G	14	LYS
1	G	78	LEU
1	G	107	THR
1	G	150	ASN

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Mol	Chain	Res	Type
1	G	154	GLU
1	H	14	LYS
1	H	78	LEU
1	H	107	THR
1	H	150	ASN
1	H	154	GLU
1	I	14	LYS
1	I	78	LEU
1	I	107	THR
1	I	150	ASN
1	I	154	GLU
1	J	14	LYS
1	J	78	LEU
1	J	107	THR
1	J	150	ASN
1	J	154	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	7	ASN
1	A	105	ASN
1	A	148	ASN
1	A	150	ASN
1	B	5	GLN
1	B	7	ASN
1	B	105	ASN
1	B	148	ASN
1	B	150	ASN
1	C	5	GLN
1	C	7	ASN
1	C	105	ASN
1	C	148	ASN
1	C	150	ASN
1	D	5	GLN
1	D	7	ASN
1	D	105	ASN
1	D	148	ASN
1	D	150	ASN
1	E	5	GLN
1	E	7	ASN

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Mol	Chain	Res	Type
1	E	105	ASN
1	E	148	ASN
1	E	150	ASN
1	F	5	GLN
1	F	7	ASN
1	F	105	ASN
1	F	148	ASN
1	F	150	ASN
1	G	5	GLN
1	G	7	ASN
1	G	105	ASN
1	G	148	ASN
1	G	150	ASN
1	H	5	GLN
1	H	7	ASN
1	H	105	ASN
1	H	148	ASN
1	H	150	ASN
1	I	5	GLN
1	I	7	ASN
1	I	105	ASN
1	I	148	ASN
1	I	150	ASN
1	J	5	GLN
1	J	7	ASN
1	J	105	ASN
1	J	148	ASN
1	J	150	ASN

### 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

20 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	B	201	-	17,21,21	3.13	8 (47%)	21,29,29	4.11	12 (57%)
3	INI	I	208	-	17,21,21	3.02	9 (52%)	21,29,29	4.66	13 (61%)
2	PO4	C	503	-	4,4,4	1.86	2 (50%)	6,6,6	0.44	0
2	PO4	H	508	-	4,4,4	1.06	0	6,6,6	0.45	0
2	PO4	G	506	-	4,4,4	1.62	0	6,6,6	0.39	0
3	INI	A	200	-	17,21,21	3.18	8 (47%)	21,29,29	4.48	14 (66%)
2	PO4	B	502	-	4,4,4	1.68	1 (25%)	6,6,6	0.41	0
3	INI	C	202	-	17,21,21	3.18	9 (52%)	21,29,29	4.47	14 (66%)
3	INI	E	204	-	17,21,21	3.10	8 (47%)	21,29,29	4.42	14 (66%)
2	PO4	F	510	-	4,4,4	1.34	0	6,6,6	0.43	0
2	PO4	J	509	-	4,4,4	1.29	0	6,6,6	0.47	0
3	INI	D	203	-	17,21,21	3.45	8 (47%)	21,29,29	4.35	13 (61%)
2	PO4	I	507	-	4,4,4	1.51	1 (25%)	6,6,6	0.42	0
2	PO4	A	501	-	4,4,4	1.93	1 (25%)	6,6,6	0.46	0
3	INI	G	206	-	17,21,21	3.17	10 (58%)	21,29,29	4.45	13 (61%)
3	INI	H	207	-	17,21,21	3.14	7 (41%)	21,29,29	4.36	13 (61%)
2	PO4	D	505	-	4,4,4	1.86	2 (50%)	6,6,6	0.42	0
2	PO4	D	504	-	4,4,4	1.66	0	6,6,6	0.47	0
3	INI	J	209	-	17,21,21	3.19	8 (47%)	21,29,29	4.32	13 (61%)
3	INI	F	205	-	17,21,21	3.45	9 (52%)	21,29,29	4.33	14 (66%)

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	B	201	-	-	8/15/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	INI	A	200	-	-	9/15/19/19	0/1/1/1
3	INI	E	204	-	-	9/15/19/19	0/1/1/1
3	INI	C	202	-	-	9/15/19/19	0/1/1/1
3	INI	I	208	-	-	9/15/19/19	0/1/1/1
3	INI	G	206	-	-	9/15/19/19	0/1/1/1
3	INI	H	207	-	-	9/15/19/19	0/1/1/1
3	INI	J	209	-	-	9/15/19/19	0/1/1/1
3	INI	D	203	-	-	9/15/19/19	0/1/1/1
3	INI	F	205	-	-	9/15/19/19	0/1/1/1

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	203	INI	C11-C10	8.93	1.70	1.53
3	H	207	INI	C11-C10	7.94	1.68	1.53
3	G	206	INI	C11-C10	7.74	1.68	1.53
3	J	209	INI	C11-C10	7.74	1.68	1.53
3	A	200	INI	C11-C10	7.74	1.68	1.53
3	E	204	INI	C11-C10	7.59	1.67	1.53
3	C	202	INI	C11-C10	7.53	1.67	1.53
3	B	201	INI	C11-C10	7.27	1.67	1.53
3	I	208	INI	C11-C10	7.23	1.67	1.53
3	F	205	INI	C11-C10	7.00	1.66	1.53
3	B	201	INI	C8-C9	6.19	1.60	1.52
3	F	205	INI	C8-C9	5.92	1.60	1.52
3	J	209	INI	C8-C9	5.60	1.60	1.52
3	D	203	INI	C9-C10	5.55	1.63	1.53
3	C	202	INI	C8-C9	5.38	1.59	1.52
3	A	200	INI	C8-C9	5.30	1.59	1.52
3	I	208	INI	C8-C9	5.28	1.59	1.52
3	F	205	INI	C9-C10	5.24	1.63	1.53
3	C	202	INI	C9-C10	5.14	1.63	1.53
3	D	203	INI	C8-C9	4.98	1.59	1.52
3	G	206	INI	C8-C9	4.79	1.59	1.52
3	G	206	INI	C9-C10	4.68	1.62	1.53
3	E	204	INI	C8-C9	4.62	1.58	1.52
3	E	204	INI	C9-C10	4.58	1.62	1.53
3	H	207	INI	C8-C9	4.56	1.58	1.52
3	F	205	INI	C6-N7	4.47	1.41	1.34
3	A	200	INI	C9-C10	4.44	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	205	INI	O52-N5	4.29	1.30	1.22
3	J	209	INI	C9-C10	4.26	1.61	1.53
3	E	204	INI	C6-N7	4.15	1.41	1.34
3	H	207	INI	C6-N7	4.09	1.41	1.34
3	F	205	INI	C12-C11	4.03	1.63	1.52
3	B	201	INI	C6-N7	3.93	1.40	1.34
3	D	203	INI	C6-N7	3.88	1.40	1.34
3	H	207	INI	C12-C11	3.79	1.62	1.52
3	C	202	INI	C6-N7	3.79	1.40	1.34
3	J	209	INI	C6-N7	3.78	1.40	1.34
3	B	201	INI	C12-C11	3.77	1.62	1.52
3	A	200	INI	C6-N7	3.74	1.40	1.34
3	I	208	INI	C9-C10	3.70	1.60	1.53
3	I	208	INI	C12-C11	3.64	1.62	1.52
3	G	206	INI	C6-N7	3.64	1.40	1.34
3	H	207	INI	C6-N1	3.63	1.41	1.34
3	A	200	INI	C4-N3	3.55	1.39	1.33
3	H	207	INI	C9-C10	3.49	1.60	1.53
3	J	209	INI	C12-C11	3.43	1.61	1.52
3	F	205	INI	C6-N1	3.38	1.40	1.34
3	G	206	INI	C4-N3	3.32	1.38	1.33
3	I	208	INI	C6-N7	3.31	1.39	1.34
3	D	203	INI	C12-C11	3.30	1.61	1.52
3	G	206	INI	C12-C11	3.28	1.61	1.52
3	B	201	INI	C9-C10	3.28	1.59	1.53
3	H	207	INI	C4-N3	3.25	1.38	1.33
3	D	203	INI	C6-N1	3.25	1.40	1.34
3	C	202	INI	C6-N1	3.20	1.40	1.34
3	J	209	INI	C4-N3	3.17	1.38	1.33
3	A	200	INI	C12-C11	3.17	1.60	1.52
3	J	209	INI	C6-N1	3.04	1.40	1.34
3	I	208	INI	C6-N1	3.03	1.40	1.34
3	I	208	INI	C8-N7	3.02	1.51	1.45
3	G	206	INI	C6-N1	3.00	1.40	1.34
3	E	204	INI	C6-N1	2.99	1.40	1.34
3	E	204	INI	C4-N3	2.98	1.38	1.33
3	F	205	INI	C8-N7	2.93	1.51	1.45
3	A	200	INI	C6-N1	2.93	1.40	1.34
3	D	203	INI	C4-N3	2.92	1.38	1.33
3	C	202	INI	C4-N3	2.90	1.38	1.33
3	E	204	INI	C12-C11	2.84	1.59	1.52
3	B	201	INI	C6-N1	2.79	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	202	INI	C12-C11	2.73	1.59	1.52
3	F	205	INI	C4-N3	2.62	1.37	1.33
3	D	203	INI	C8-N7	2.54	1.50	1.45
2	A	501	PO4	P-O2	-2.47	1.47	1.54
3	I	208	INI	C4-N3	2.44	1.37	1.33
3	J	209	INI	C8-N7	2.43	1.50	1.45
3	E	204	INI	C8-N7	2.42	1.50	1.45
3	A	200	INI	C8-N7	2.42	1.50	1.45
3	B	201	INI	C4-N3	2.39	1.37	1.33
3	B	201	INI	O52-N5	2.39	1.26	1.22
3	G	206	INI	O52-N5	2.37	1.26	1.22
3	C	202	INI	O52-N5	2.32	1.26	1.22
3	I	208	INI	C5-N5	-2.27	1.41	1.45
2	C	503	PO4	P-O2	-2.24	1.47	1.54
3	C	202	INI	C5-N5	-2.19	1.41	1.45
3	G	206	INI	C5-N5	-2.19	1.41	1.45
2	D	505	PO4	P-O2	-2.14	1.48	1.54
2	D	505	PO4	P-O3	-2.09	1.48	1.54
2	I	507	PO4	P-O2	-2.07	1.48	1.54
2	C	503	PO4	P-O4	-2.04	1.48	1.54
3	G	206	INI	C8-N7	2.04	1.49	1.45
2	B	502	PO4	P-O2	-2.02	1.48	1.54

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	208	INI	C2-N3-C4	12.78	125.93	115.14
3	F	205	INI	C2-N3-C4	12.40	125.61	115.14
3	A	200	INI	C2-N3-C4	11.94	125.22	115.14
3	H	207	INI	C2-N3-C4	11.90	125.19	115.14
3	E	204	INI	C2-N3-C4	11.70	125.02	115.14
3	D	203	INI	C2-N3-C4	11.68	125.00	115.14
3	B	201	INI	C2-N3-C4	11.59	124.93	115.14
3	C	202	INI	C2-N3-C4	11.56	124.90	115.14
3	G	206	INI	C2-N3-C4	11.44	124.80	115.14
3	J	209	INI	C2-N3-C4	11.25	124.64	115.14
3	C	202	INI	C12-C11-C10	7.57	128.83	112.41
3	G	206	INI	C12-C11-C10	7.50	128.68	112.41
3	I	208	INI	C12-C11-C10	7.40	128.47	112.41
3	J	209	INI	C12-C11-C10	7.40	128.46	112.41
3	D	203	INI	C12-C11-C10	7.40	128.45	112.41
3	A	200	INI	C12-C11-C10	7.33	128.30	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	207	INI	C12-C11-C10	7.24	128.10	112.41
3	I	208	INI	C8-N7-C6	-7.19	110.45	123.25
3	E	204	INI	C12-C11-C10	7.01	127.61	112.41
3	G	206	INI	C6-C5-C4	6.89	119.04	114.53
3	B	201	INI	C12-C11-C10	6.86	127.29	112.41
3	I	208	INI	C6-C5-C4	6.65	118.88	114.53
3	C	202	INI	C6-C5-C4	6.49	118.78	114.53
3	F	205	INI	C12-C11-C10	6.47	126.43	112.41
3	J	209	INI	C6-C5-C4	6.43	118.74	114.53
3	E	204	INI	C6-C5-C4	6.32	118.66	114.53
3	A	200	INI	C8-N7-C6	-6.25	112.13	123.25
3	F	205	INI	C8-N7-C6	-6.16	112.29	123.25
3	D	203	INI	C6-C5-C4	6.14	118.55	114.53
3	H	207	INI	C6-C5-C4	6.14	118.55	114.53
3	A	200	INI	C6-C5-C4	5.99	118.45	114.53
3	E	204	INI	C8-N7-C6	-5.99	112.59	123.25
3	C	202	INI	C8-N7-C6	-5.88	112.79	123.25
3	G	206	INI	C8-N7-C6	-5.66	113.17	123.25
3	B	201	INI	C8-N7-C6	-5.62	113.25	123.25
3	J	209	INI	C8-N7-C6	-5.54	113.39	123.25
3	D	203	INI	C8-N7-C6	-5.50	113.46	123.25
3	A	200	INI	C6-N1-C2	5.44	126.26	113.80
3	H	207	INI	C8-N7-C6	-5.43	113.59	123.25
3	F	205	INI	C6-N1-C2	5.33	126.00	113.80
3	E	204	INI	C6-N1-C2	5.28	125.88	113.80
3	F	205	INI	O11-C11-C10	-5.22	96.40	109.10
3	I	208	INI	O11-C11-C10	-5.22	96.41	109.10
3	B	201	INI	C6-N1-C2	5.18	125.65	113.80
3	G	206	INI	C6-N1-C2	5.09	125.45	113.80
3	C	202	INI	C6-N1-C2	5.09	125.44	113.80
3	J	209	INI	C6-N1-C2	5.08	125.43	113.80
3	I	208	INI	C6-N1-C2	5.07	125.41	113.80
3	G	206	INI	O11-C11-C10	-5.05	96.81	109.10
3	H	207	INI	C6-N1-C2	5.01	125.28	113.80
3	B	201	INI	O11-C11-C10	-5.00	96.93	109.10
3	A	200	INI	O11-C11-C10	-5.00	96.94	109.10
3	D	203	INI	C6-N1-C2	4.99	125.22	113.80
3	C	202	INI	O11-C11-C10	-4.96	97.05	109.10
3	A	200	INI	C5-C4-N3	-4.79	116.88	123.43
3	D	203	INI	O11-C11-C10	-4.67	97.73	109.10
3	G	206	INI	C5-C4-N3	-4.64	117.08	123.43
3	C	202	INI	C5-C4-N3	-4.59	117.15	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	209	INI	C5-C4-N3	-4.58	117.17	123.43
3	H	207	INI	O11-C11-C10	-4.55	98.03	109.10
3	J	209	INI	O11-C11-C10	-4.55	98.05	109.10
3	E	204	INI	C5-C4-N3	-4.50	117.28	123.43
3	H	207	INI	C5-C4-N3	-4.50	117.28	123.43
3	I	208	INI	C5-C4-N3	-4.42	117.39	123.43
3	E	204	INI	O11-C11-C10	-4.37	98.48	109.10
3	D	203	INI	C5-C4-N3	-4.11	117.82	123.43
3	F	205	INI	C6-C5-C4	4.07	117.19	114.53
3	F	205	INI	C5-C4-N3	-4.02	117.93	123.43
3	B	201	INI	C5-C4-N3	-3.98	117.99	123.43
3	G	206	INI	C8-C9-C10	3.97	123.51	110.93
3	C	202	INI	O11-C11-C12	-3.94	99.90	109.14
3	E	204	INI	C11-C10-C9	3.93	121.53	113.36
3	B	201	INI	C6-C5-C4	3.93	117.10	114.53
3	D	203	INI	O11-C11-C12	-3.92	99.96	109.14
3	F	205	INI	C8-C9-C10	3.86	123.18	110.93
3	I	208	INI	C4-C5-N5	-3.81	115.07	121.64
3	H	207	INI	C8-C9-C10	3.78	122.93	110.93
3	I	208	INI	O11-C11-C12	-3.76	100.32	109.14
3	H	207	INI	C11-C10-C9	3.76	121.18	113.36
3	J	209	INI	C8-C9-C10	3.76	122.83	110.93
3	C	202	INI	C11-C10-C9	3.75	121.15	113.36
3	E	204	INI	C8-C9-C10	3.73	122.76	110.93
3	A	200	INI	C8-C9-C10	3.71	122.70	110.93
3	D	203	INI	C11-C10-C9	3.60	120.84	113.36
3	G	206	INI	C11-C10-C9	3.60	120.84	113.36
3	J	209	INI	O11-C11-C12	-3.54	100.84	109.14
3	G	206	INI	O11-C11-C12	-3.52	100.89	109.14
3	E	204	INI	O12-C12-C11	-3.47	103.51	111.07
3	D	203	INI	C8-C9-C10	3.46	121.90	110.93
3	C	202	INI	C8-C9-C10	3.46	121.88	110.93
3	J	209	INI	C11-C10-C9	3.45	120.54	113.36
3	E	204	INI	O11-C11-C12	-3.44	101.07	109.14
3	H	207	INI	O11-C11-C12	-3.41	101.15	109.14
3	B	201	INI	C11-C10-C9	3.40	120.43	113.36
3	C	202	INI	O12-C12-C11	-3.39	103.68	111.07
3	F	205	INI	C11-C10-C9	3.35	120.32	113.36
3	G	206	INI	C4-C5-N5	-3.32	115.91	121.64
3	B	201	INI	C8-C9-C10	3.30	121.39	110.93
3	B	201	INI	O11-C11-C12	-3.30	101.41	109.14
3	A	200	INI	C11-C10-C9	3.29	120.20	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	200	INI	O11-C11-C12	-3.29	101.44	109.14
3	C	202	INI	C4-C5-N5	-3.27	116.00	121.64
3	F	205	INI	C4-C5-N5	-3.26	116.02	121.64
3	I	208	INI	C11-C10-C9	3.21	120.04	113.36
3	I	208	INI	O12-C12-C11	-3.19	104.12	111.07
3	F	205	INI	O11-C11-C12	-3.18	101.68	109.14
3	H	207	INI	C4-C5-N5	-3.10	116.29	121.64
3	D	203	INI	O12-C12-C11	-3.05	104.42	111.07
3	I	208	INI	C8-C9-C10	3.02	120.51	110.93
3	E	204	INI	C4-C5-N5	-3.01	116.44	121.64
3	D	203	INI	C4-C5-N5	-2.98	116.49	121.64
3	A	200	INI	C4-C5-N5	-2.97	116.52	121.64
3	J	209	INI	C4-C5-N5	-2.93	116.59	121.64
3	B	201	INI	O12-C12-C11	-2.87	104.81	111.07
3	G	206	INI	O9-C9-C8	-2.84	103.96	109.69
3	H	207	INI	O9-C9-C8	-2.84	103.96	109.69
3	J	209	INI	O9-C9-C8	-2.75	104.14	109.69
3	J	209	INI	O12-C12-C11	-2.73	105.13	111.07
3	A	200	INI	O12-C12-C11	-2.70	105.19	111.07
3	F	205	INI	C5-C6-N7	2.69	126.58	123.37
3	D	203	INI	O9-C9-C8	-2.65	104.33	109.69
3	G	206	INI	O12-C12-C11	-2.64	105.32	111.07
3	A	200	INI	O9-C9-C8	-2.58	104.49	109.69
3	E	204	INI	O9-C9-C8	-2.51	104.63	109.69
3	I	208	INI	O9-C9-C8	-2.49	104.67	109.69
3	C	202	INI	O9-C9-C8	-2.44	104.77	109.69
3	E	204	INI	C5-C6-N7	2.41	126.24	123.37
3	A	200	INI	C5-C6-N7	2.39	126.21	123.37
3	C	202	INI	C5-C6-N7	2.18	125.96	123.37
3	F	205	INI	O9-C9-C8	-2.14	105.38	109.69
3	B	201	INI	C4-C5-N5	-2.05	118.10	121.64
3	F	205	INI	O12-C12-C11	-2.04	106.64	111.07
3	H	207	INI	O9-C9-C10	-2.00	104.23	109.10

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	200	INI	N1-C6-N7-C8
3	A	200	INI	C5-C6-N7-C8
3	A	200	INI	C9-C10-C11-O11
3	A	200	INI	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
3	A	200	INI	O10-C10-C11-O11
3	B	201	INI	N1-C6-N7-C8
3	B	201	INI	C5-C6-N7-C8
3	B	201	INI	C9-C10-C11-O11
3	B	201	INI	C9-C10-C11-C12
3	B	201	INI	O10-C10-C11-O11
3	C	202	INI	N1-C6-N7-C8
3	C	202	INI	C5-C6-N7-C8
3	C	202	INI	C9-C10-C11-O11
3	C	202	INI	C9-C10-C11-C12
3	C	202	INI	O10-C10-C11-O11
3	D	203	INI	N1-C6-N7-C8
3	D	203	INI	C5-C6-N7-C8
3	D	203	INI	C9-C10-C11-O11
3	D	203	INI	C9-C10-C11-C12
3	D	203	INI	O10-C10-C11-O11
3	D	203	INI	C10-C11-C12-O12
3	E	204	INI	N1-C6-N7-C8
3	E	204	INI	C5-C6-N7-C8
3	E	204	INI	C9-C10-C11-O11
3	E	204	INI	C9-C10-C11-C12
3	E	204	INI	O10-C10-C11-O11
3	F	205	INI	N1-C6-N7-C8
3	F	205	INI	C5-C6-N7-C8
3	F	205	INI	C9-C10-C11-O11
3	F	205	INI	C9-C10-C11-C12
3	F	205	INI	O10-C10-C11-O11
3	G	206	INI	N1-C6-N7-C8
3	G	206	INI	C5-C6-N7-C8
3	G	206	INI	C9-C10-C11-O11
3	G	206	INI	C9-C10-C11-C12
3	G	206	INI	O10-C10-C11-O11
3	H	207	INI	N1-C6-N7-C8
3	H	207	INI	C5-C6-N7-C8
3	H	207	INI	C9-C10-C11-O11
3	H	207	INI	C9-C10-C11-C12
3	H	207	INI	O10-C10-C11-O11
3	I	208	INI	N1-C6-N7-C8
3	I	208	INI	C5-C6-N7-C8
3	I	208	INI	C9-C10-C11-O11
3	I	208	INI	C9-C10-C11-C12
3	I	208	INI	O10-C10-C11-O11

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Mol	Chain	Res	Type	Atoms
3	J	209	INI	N1-C6-N7-C8
3	J	209	INI	C5-C6-N7-C8
3	J	209	INI	C9-C10-C11-O11
3	J	209	INI	C9-C10-C11-C12
3	J	209	INI	O10-C10-C11-O11
3	I	208	INI	O11-C11-C12-O12
3	A	200	INI	C10-C11-C12-O12
3	C	202	INI	C10-C11-C12-O12
3	E	204	INI	C10-C11-C12-O12
3	F	205	INI	C10-C11-C12-O12
3	G	206	INI	C10-C11-C12-O12
3	H	207	INI	C10-C11-C12-O12
3	J	209	INI	C10-C11-C12-O12
3	A	200	INI	O10-C10-C11-C12
3	B	201	INI	O10-C10-C11-C12
3	C	202	INI	O10-C10-C11-C12
3	D	203	INI	O10-C10-C11-C12
3	E	204	INI	O10-C10-C11-C12
3	F	205	INI	O10-C10-C11-C12
3	G	206	INI	O10-C10-C11-C12
3	H	207	INI	O10-C10-C11-C12
3	I	208	INI	O10-C10-C11-C12
3	J	209	INI	O10-C10-C11-C12
3	D	203	INI	O11-C11-C12-O12
3	I	208	INI	C10-C11-C12-O12
3	J	209	INI	O11-C11-C12-O12
3	B	201	INI	N7-C8-C9-C10
3	F	205	INI	N7-C8-C9-C10
3	A	200	INI	O11-C11-C12-O12
3	E	204	INI	O11-C11-C12-O12
3	G	206	INI	O11-C11-C12-O12
3	C	202	INI	O11-C11-C12-O12
3	H	207	INI	O11-C11-C12-O12
3	A	200	INI	N7-C8-C9-C10
3	D	203	INI	N7-C8-C9-C10
3	E	204	INI	N7-C8-C9-C10
3	G	206	INI	N7-C8-C9-C10
3	H	207	INI	N7-C8-C9-C10
3	I	208	INI	N7-C8-C9-C10
3	J	209	INI	N7-C8-C9-C10
3	C	202	INI	N7-C8-C9-C10
3	F	205	INI	O11-C11-C12-O12

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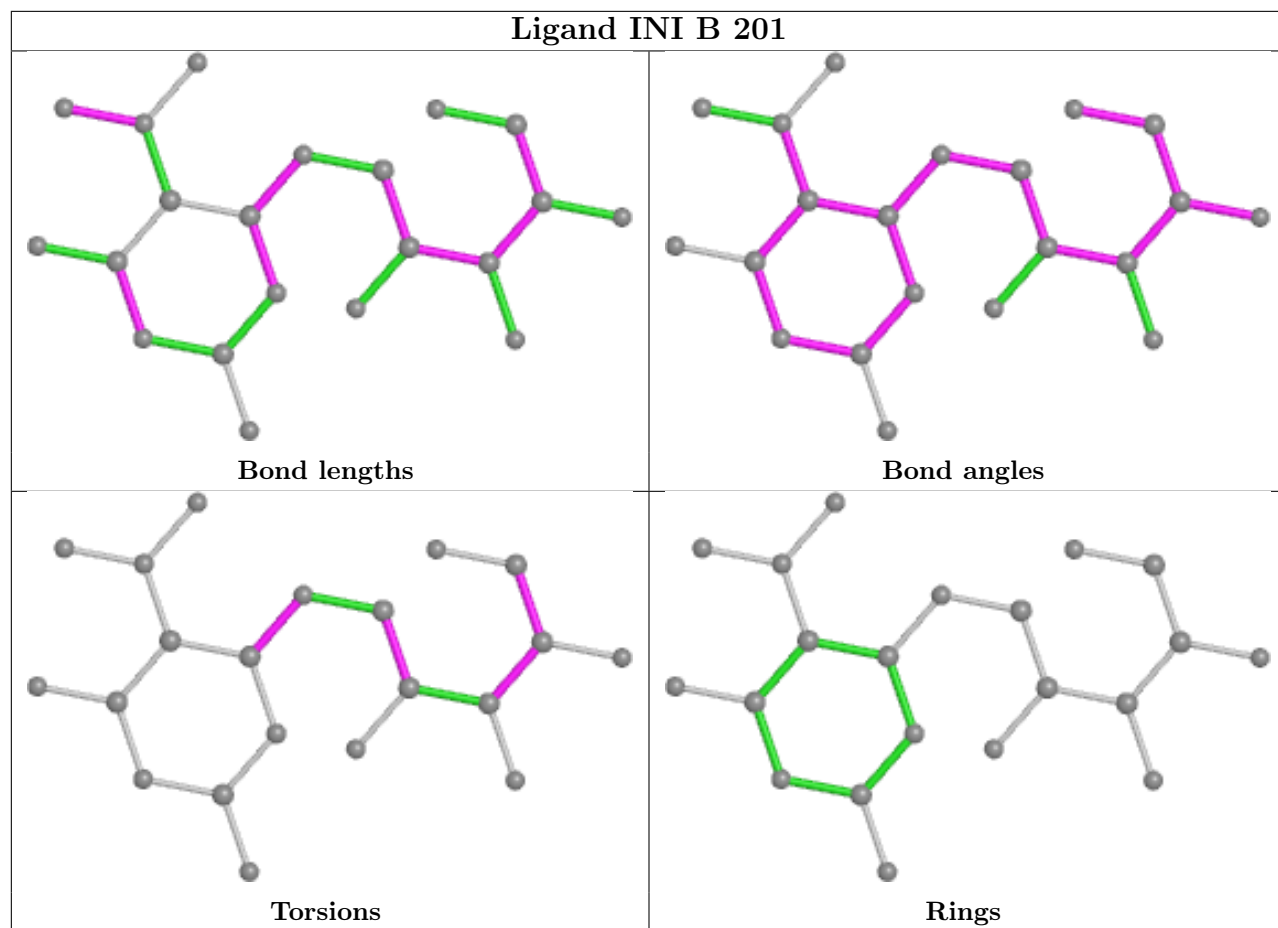
Mol	Chain	Res	Type	Atoms
3	B	201	INI	C10-C11-C12-O12

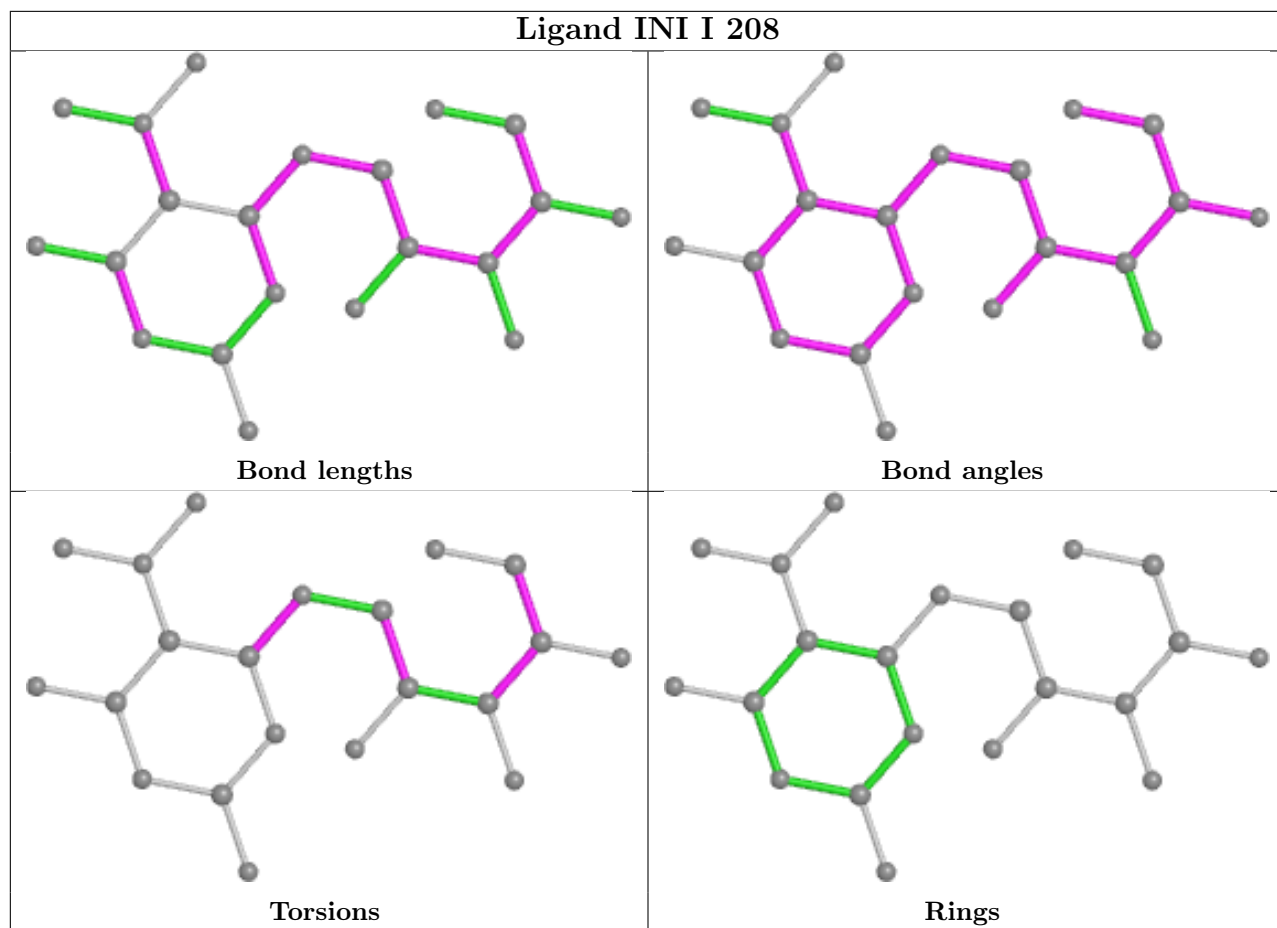
There are no ring outliers.

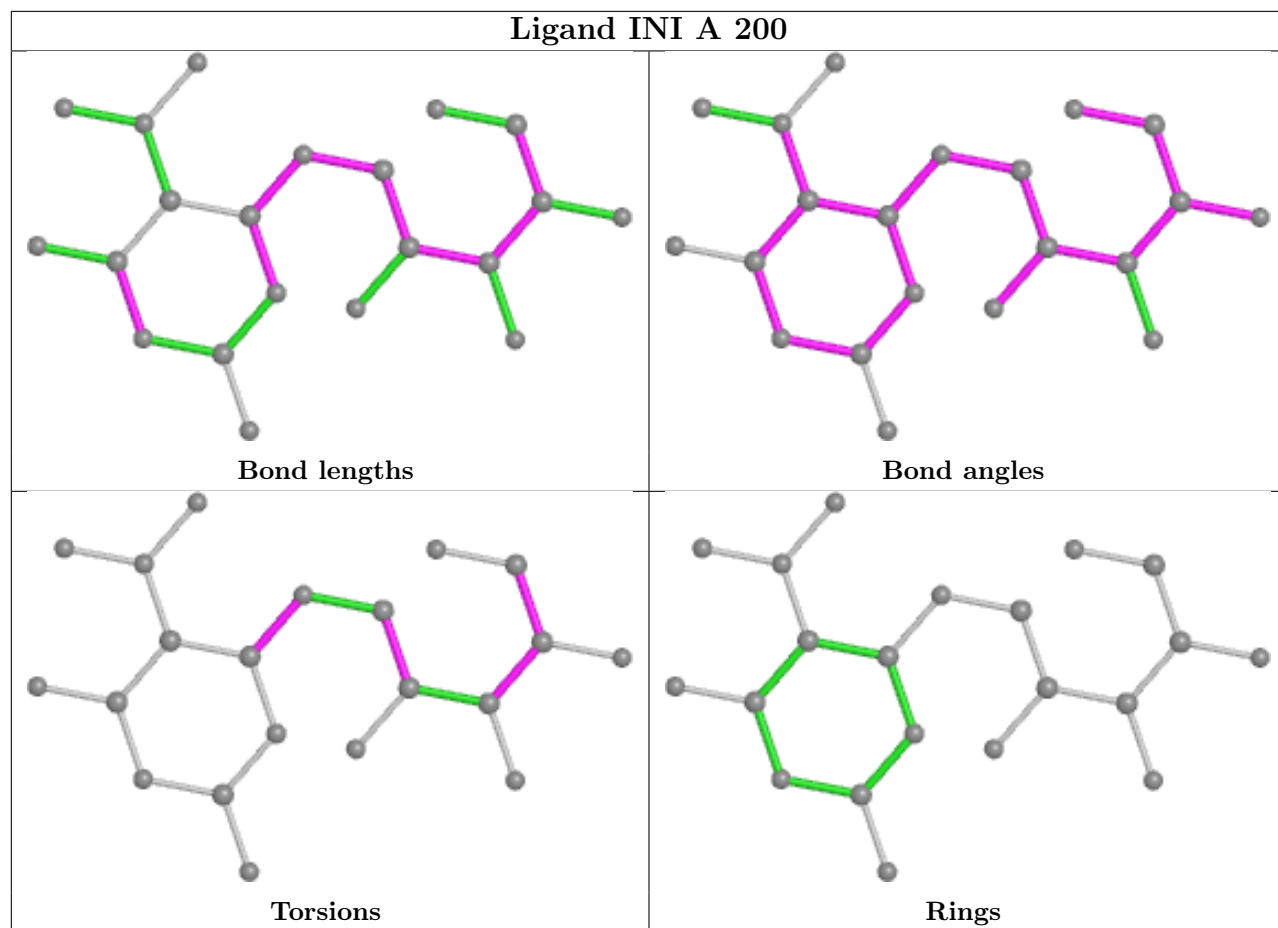
12 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	INI	3	0
3	I	208	INI	3	0
3	A	200	INI	3	0
3	C	202	INI	5	0
3	E	204	INI	5	0
2	J	509	PO4	1	0
3	D	203	INI	5	0
2	A	501	PO4	1	0
3	G	206	INI	4	0
3	H	207	INI	4	0
3	J	209	INI	6	0
3	F	205	INI	5	0

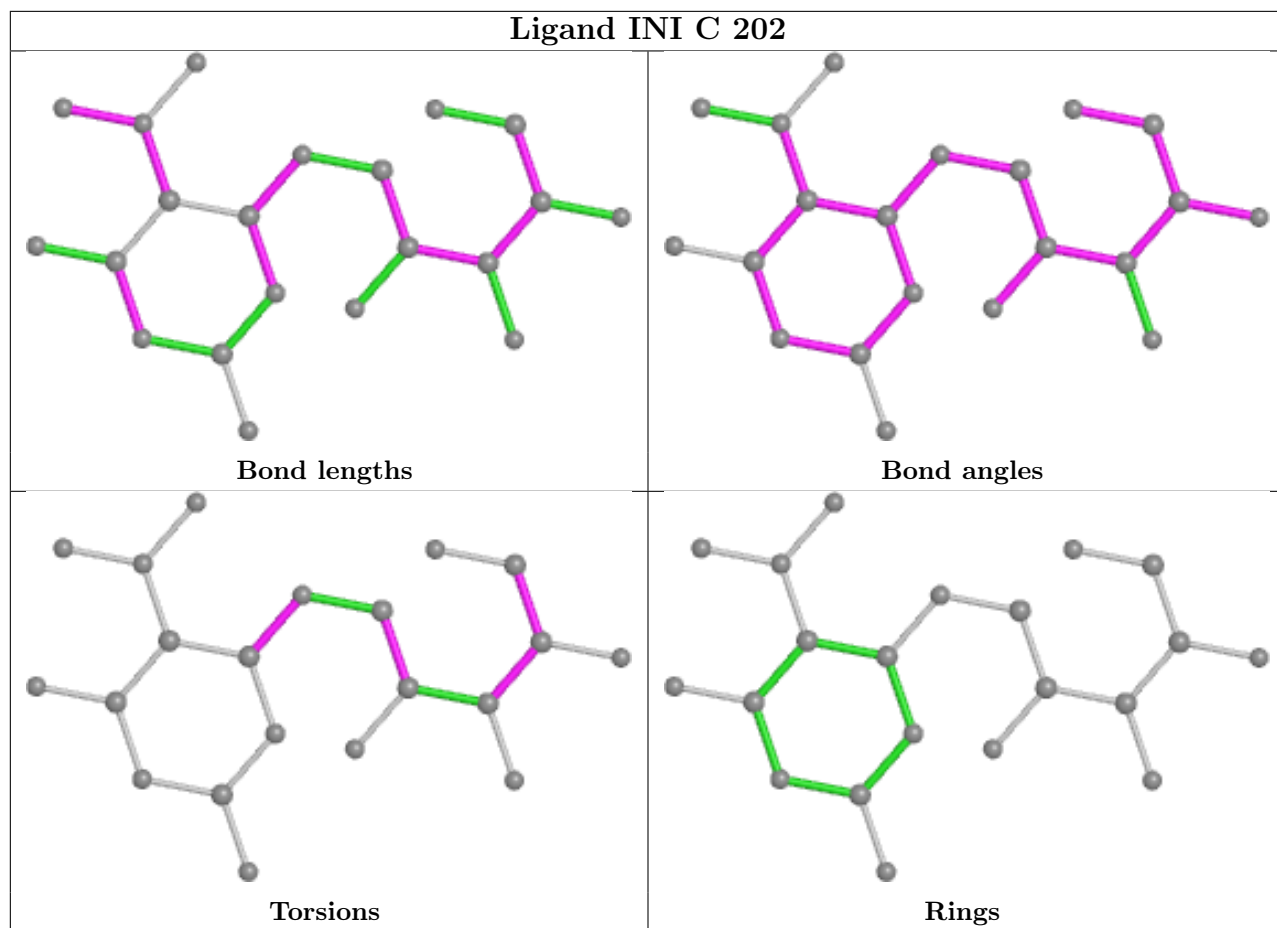
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

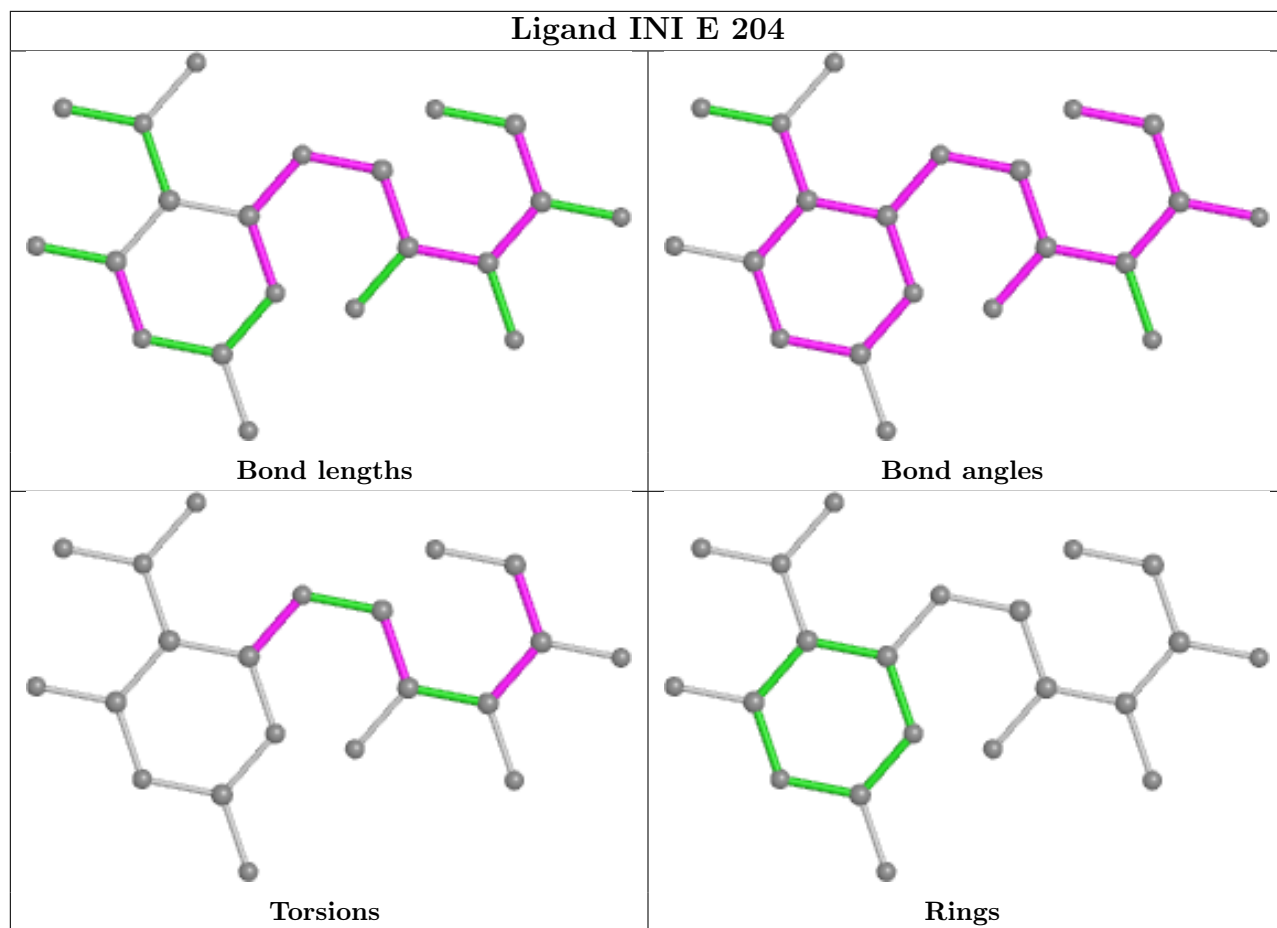


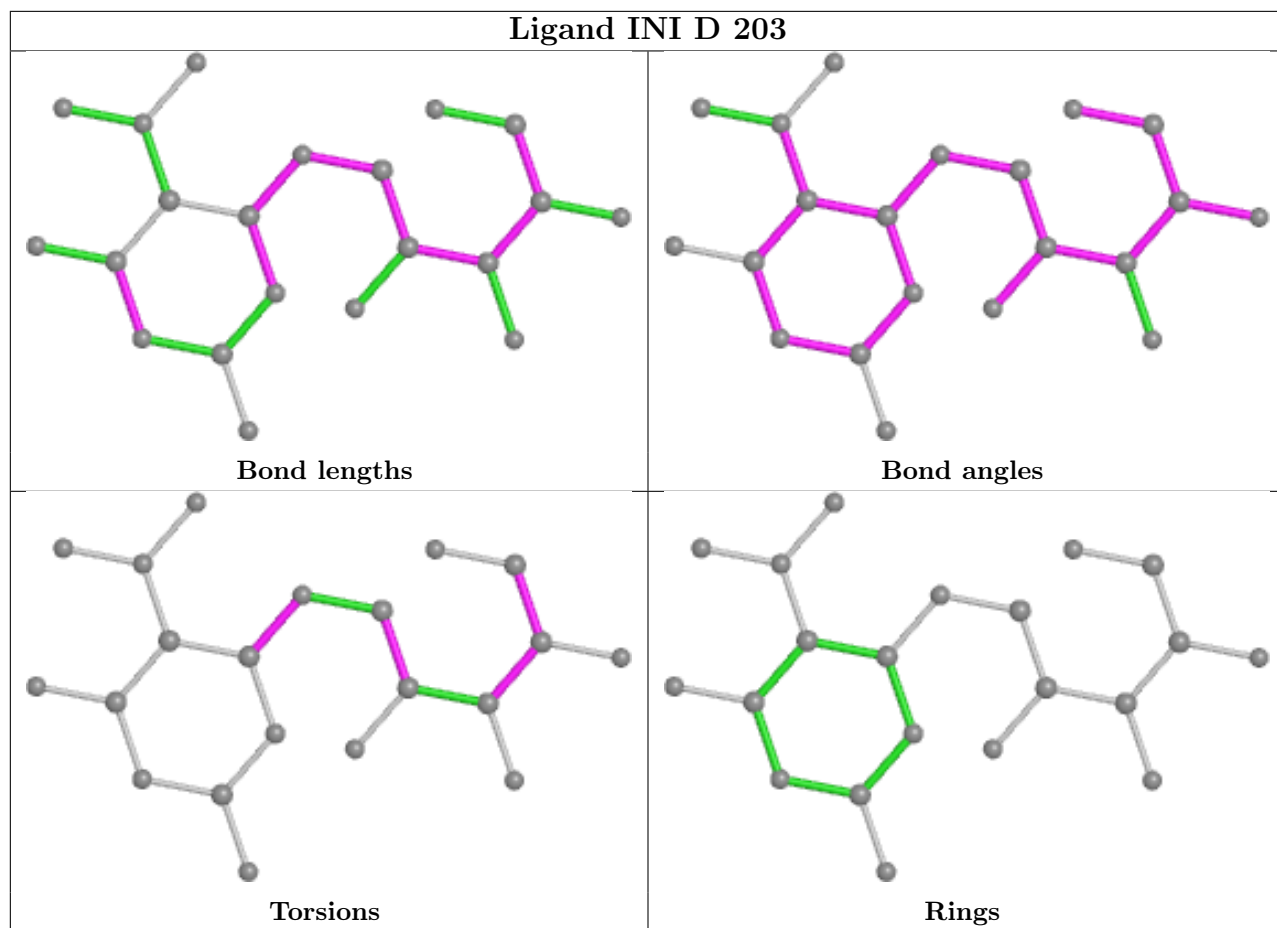


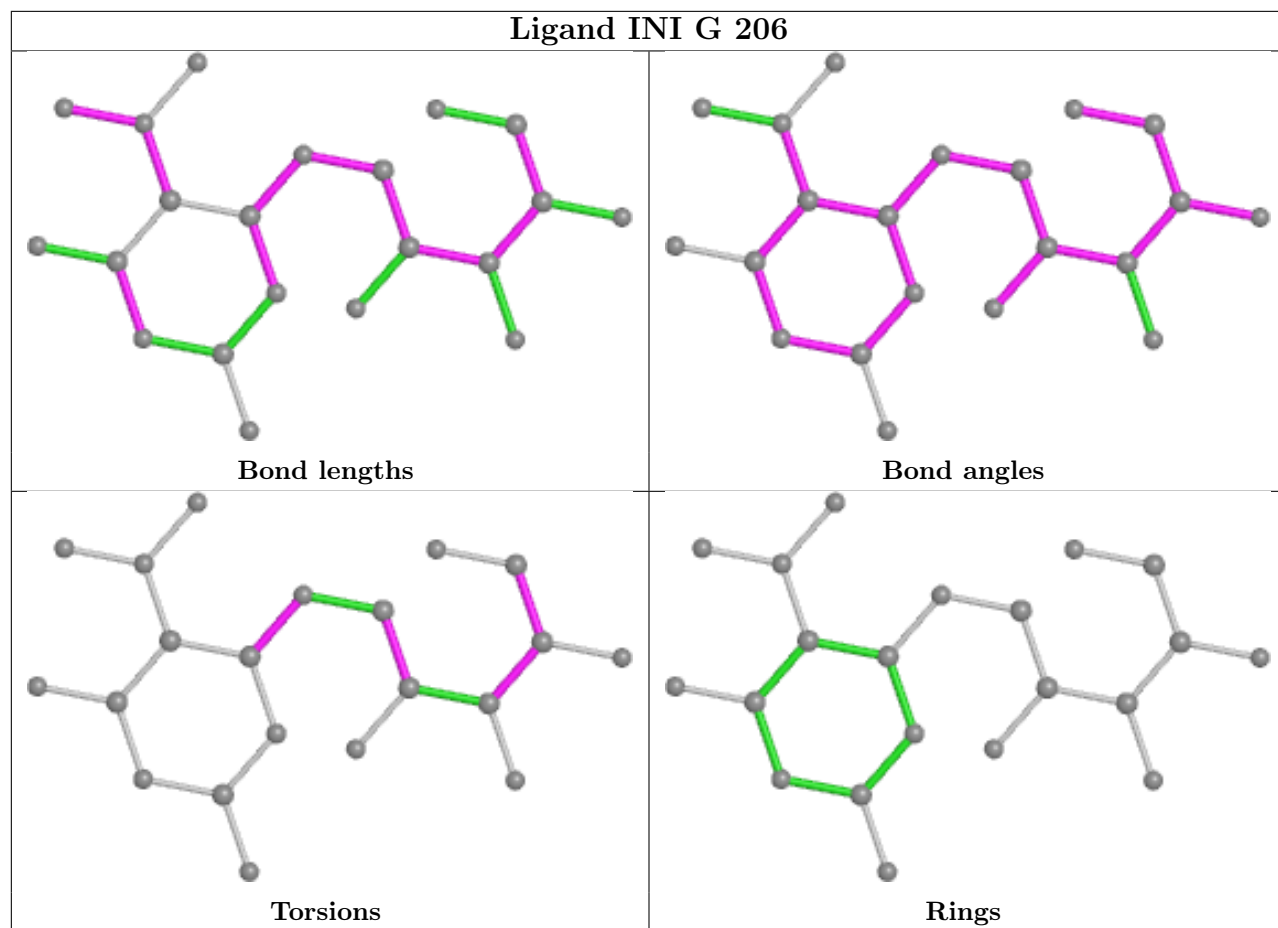


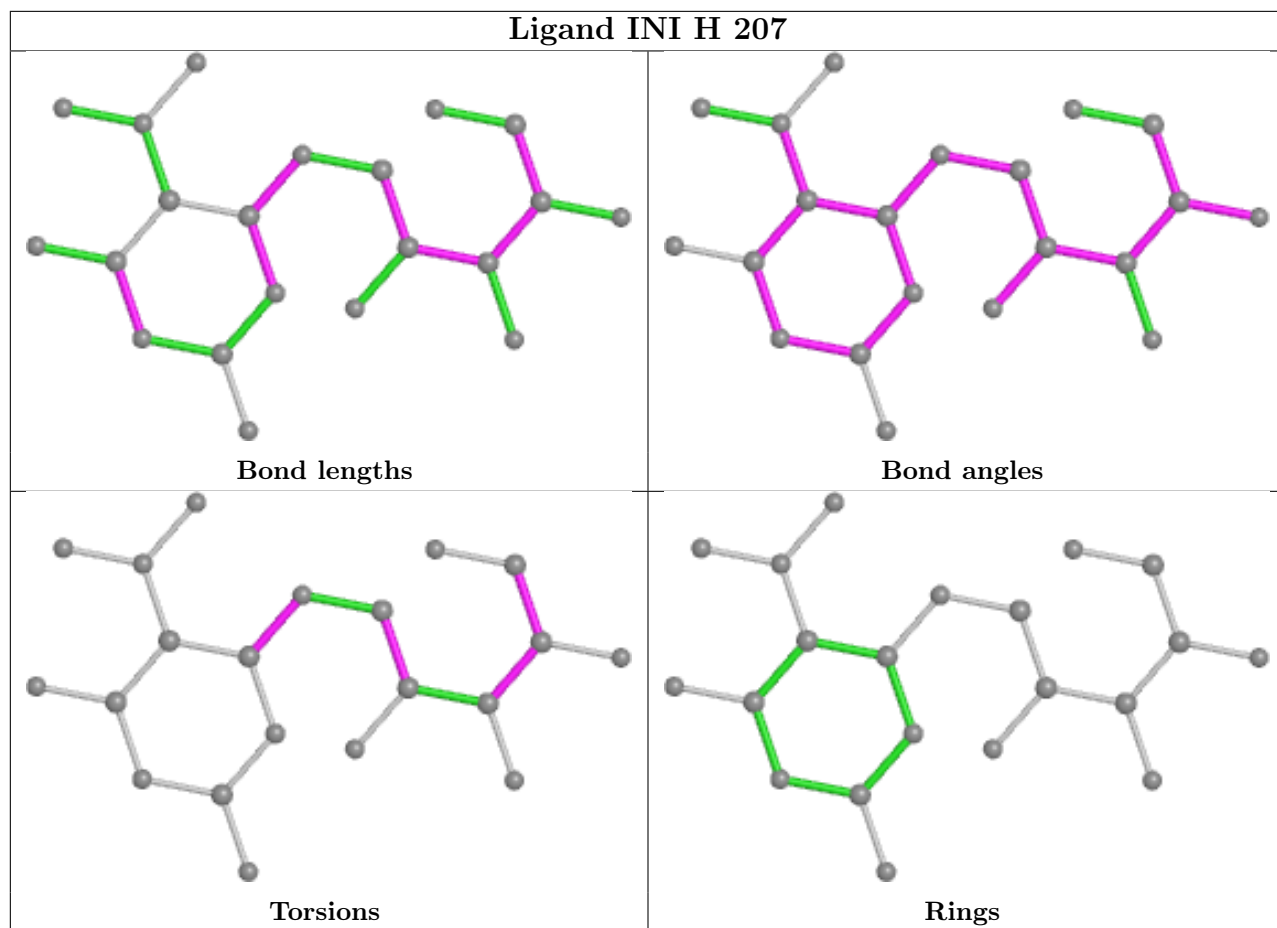


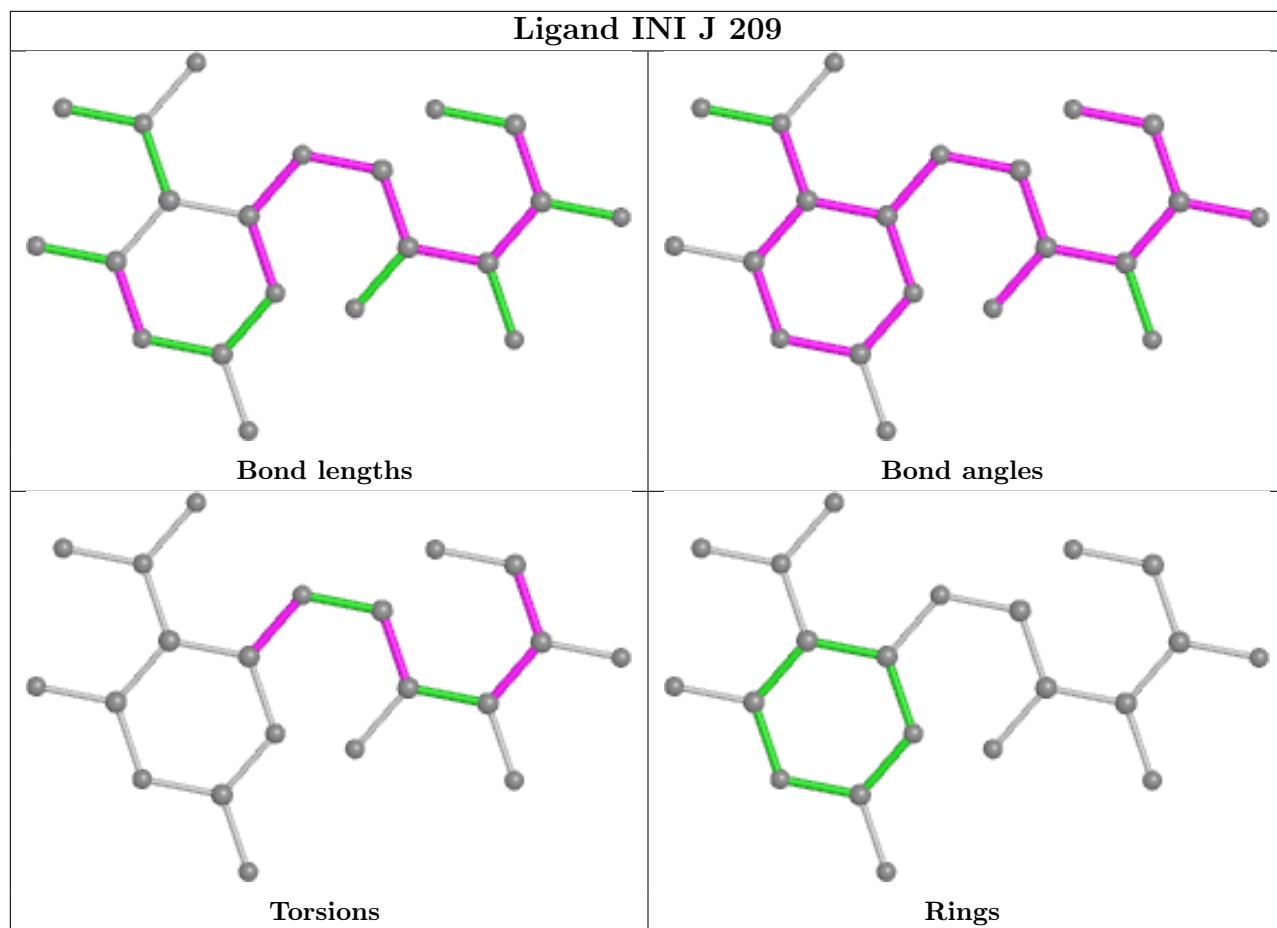


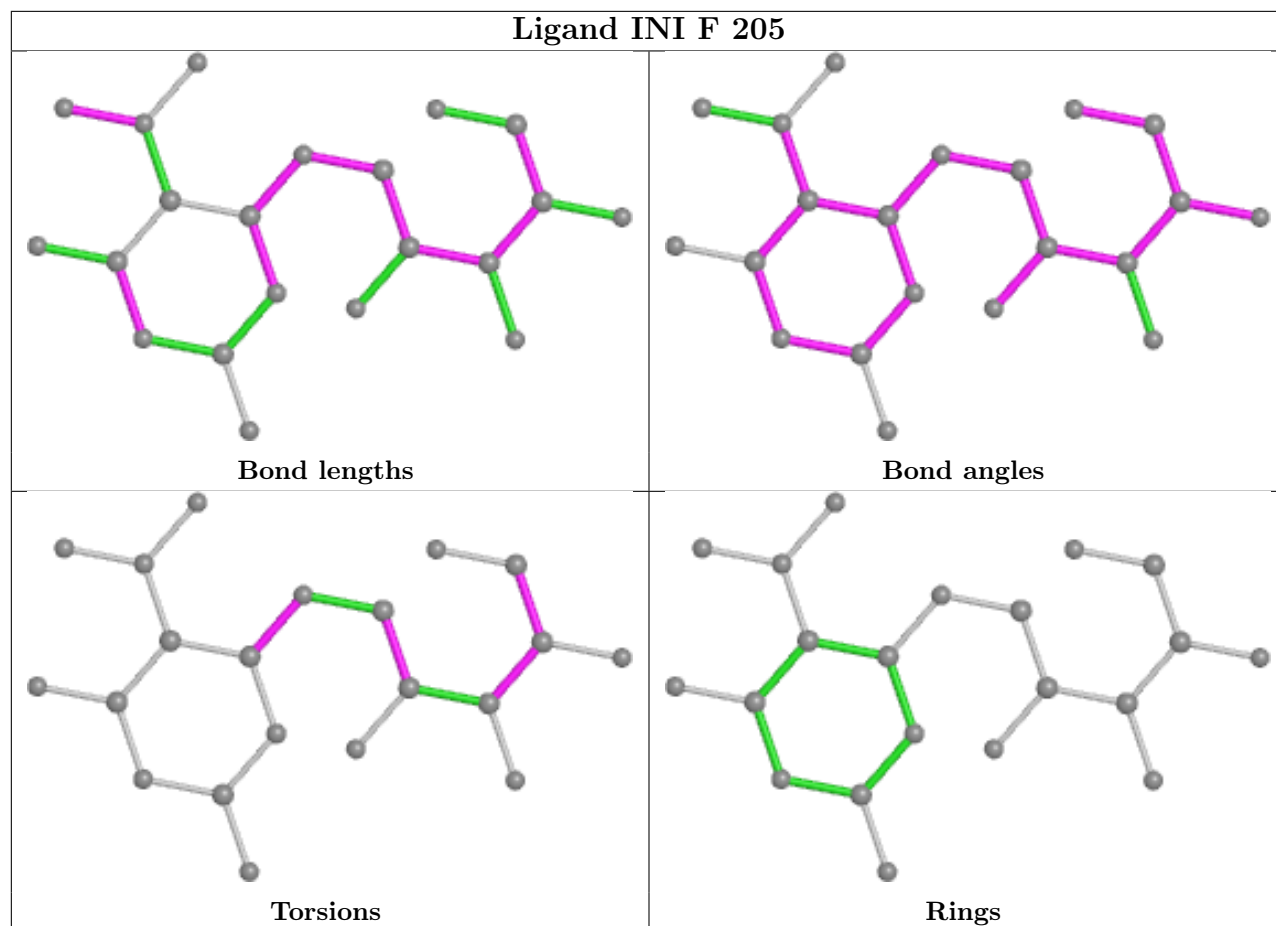












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	154/154 (100%)	-0.44	1 (0%) 89 89	16, 40, 66, 159	0
1	B	154/154 (100%)	-0.29	2 (1%) 77 77	15, 42, 64, 148	0
1	C	154/154 (100%)	-0.32	2 (1%) 77 77	17, 42, 67, 151	0
1	D	154/154 (100%)	-0.41	1 (0%) 89 89	17, 36, 62, 134	0
1	E	154/154 (100%)	-0.54	1 (0%) 89 89	11, 33, 61, 150	0
1	F	154/154 (100%)	-0.33	1 (0%) 89 89	25, 44, 66, 147	0
1	G	154/154 (100%)	-0.36	2 (1%) 77 77	13, 44, 72, 141	0
1	H	154/154 (100%)	-0.31	3 (1%) 66 65	21, 44, 71, 154	0
1	I	154/154 (100%)	-0.31	1 (0%) 89 89	17, 43, 69, 158	0
1	J	154/154 (100%)	-0.32	2 (1%) 77 77	22, 42, 68, 168	0
All	All	1540/1540 (100%)	-0.36	16 (1%) 82 82	11, 41, 68, 168	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	154	GLU	6.4
1	J	154	GLU	5.9
1	C	154	GLU	5.4
1	B	154	GLU	5.0
1	F	154	GLU	4.8
1	D	154	GLU	4.4
1	I	154	GLU	4.3
1	A	154	GLU	4.2
1	G	154	GLU	4.0
1	H	154	GLU	3.7
1	B	45	THR	2.9
1	H	45	THR	2.2
1	H	70	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	46	ASN	2.1
1	G	46	ASN	2.0
1	J	1	MET	2.0

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

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

## 6.3 Carbohydrates [i](#)

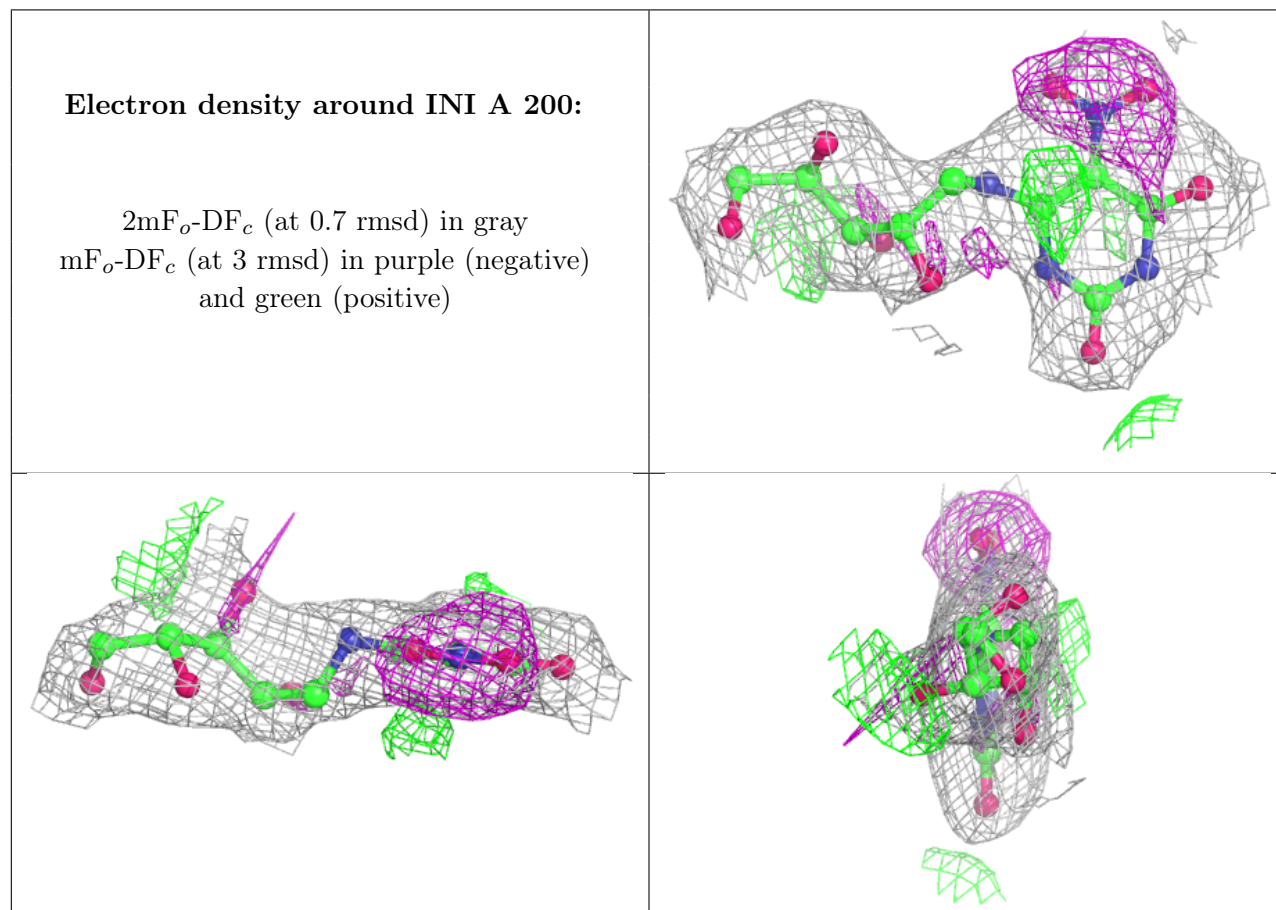
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

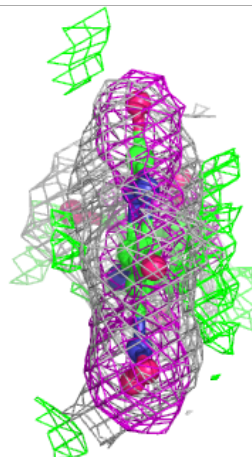
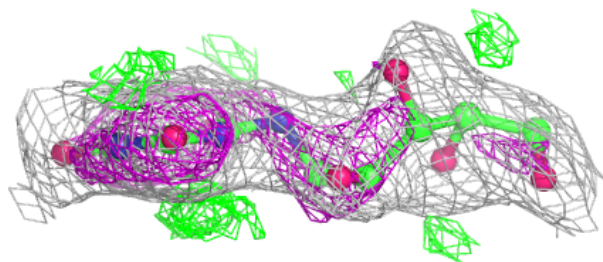
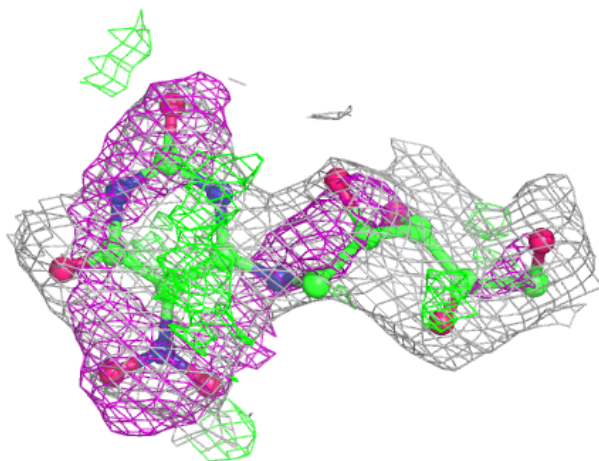
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	INI	A	200	21/21	0.89	0.18	16,16,18,20	0
3	INI	F	205	21/21	0.91	0.23	13,13,14,17	0
3	INI	G	206	21/21	0.91	0.16	16,16,18,20	0
3	INI	D	203	21/21	0.92	0.17	16,16,18,20	0
3	INI	E	204	21/21	0.92	0.19	16,16,18,20	0
3	INI	B	201	21/21	0.92	0.18	13,13,14,17	0
3	INI	C	202	21/21	0.92	0.18	16,16,18,20	0
3	INI	I	208	21/21	0.93	0.19	13,13,14,17	0
3	INI	J	209	21/21	0.93	0.17	16,16,18,20	0
2	PO4	H	508	5/5	0.94	0.19	21,52,57,57	0
3	INI	H	207	21/21	0.94	0.20	16,16,18,20	0
2	PO4	A	501	5/5	0.95	0.14	49,49,49,49	0
2	PO4	C	503	5/5	0.97	0.10	49,49,49,49	0
2	PO4	D	504	5/5	0.97	0.10	49,49,49,49	0
2	PO4	B	502	5/5	0.97	0.11	49,49,49,49	0
2	PO4	I	507	5/5	0.97	0.10	29,53,53,53	0
2	PO4	J	509	5/5	0.97	0.11	29,53,53,53	0
2	PO4	F	510	5/5	0.98	0.14	27,53,53,53	0
2	PO4	G	506	5/5	0.98	0.10	29,53,53,53	0
2	PO4	D	505	5/5	0.98	0.10	49,49,49,49	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.



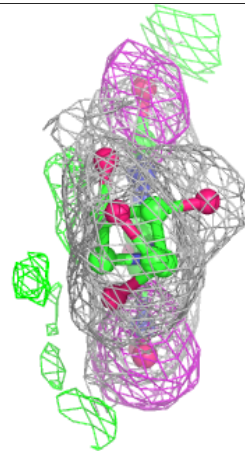
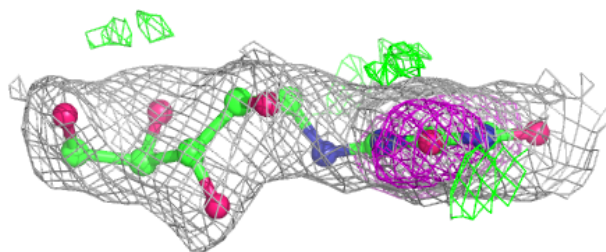
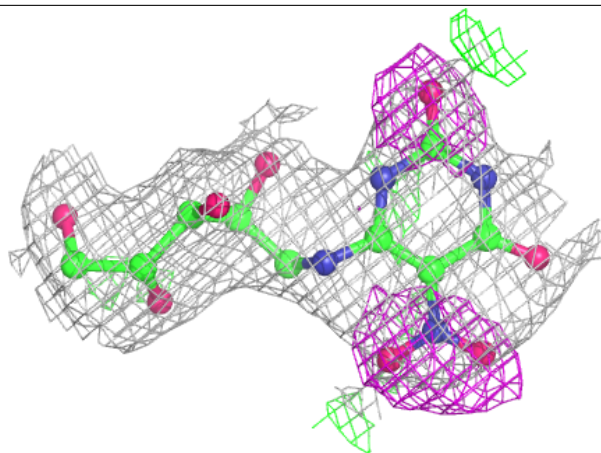
**Electron density around INI F 205:**

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



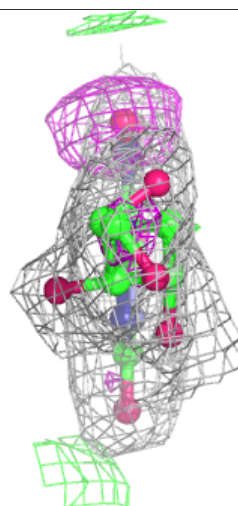
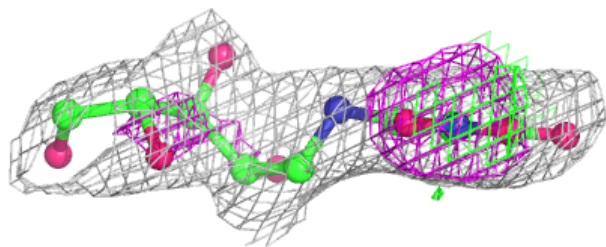
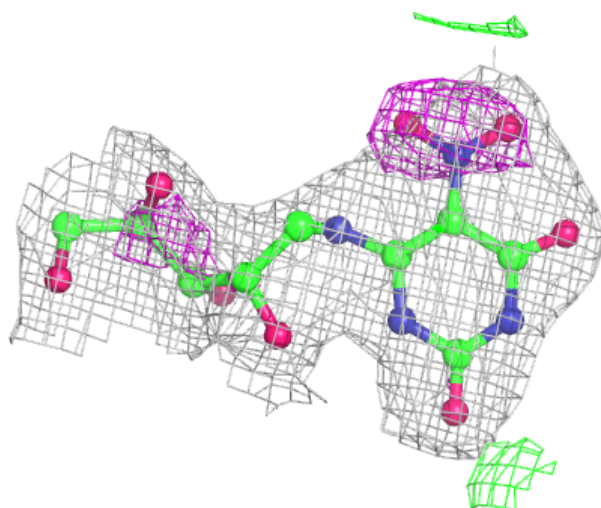
**Electron density around INI G 206:**

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



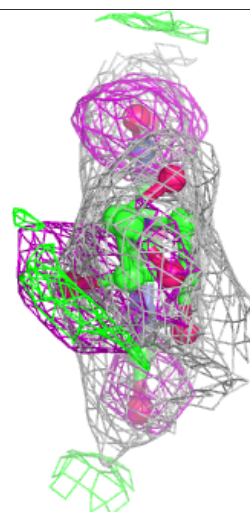
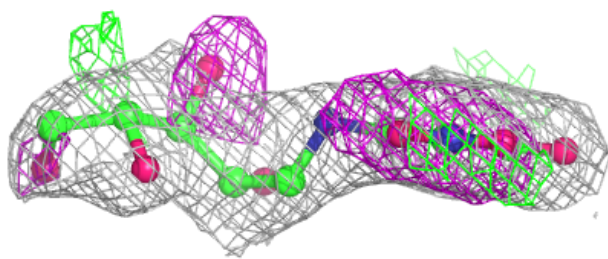
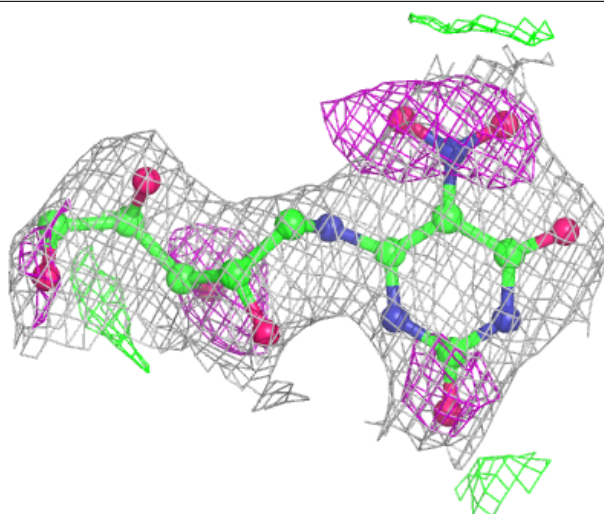
**Electron density around INI D 203:**

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



**Electron density around INI E 204:**

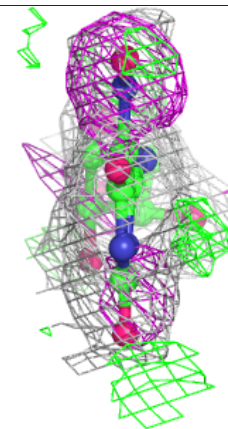
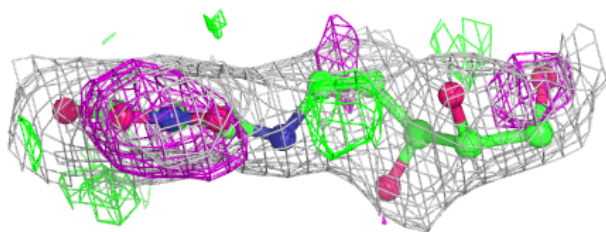
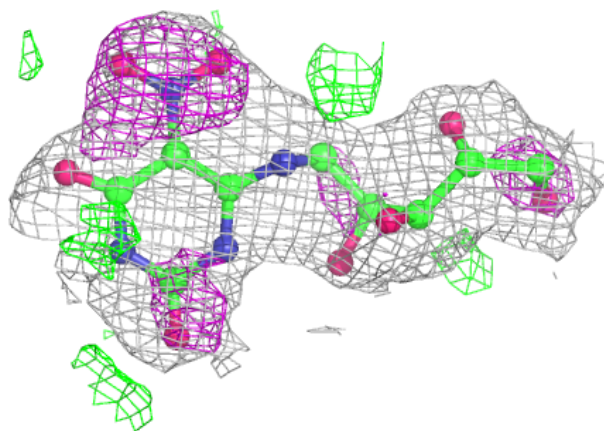
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





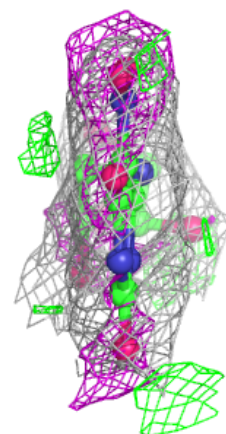
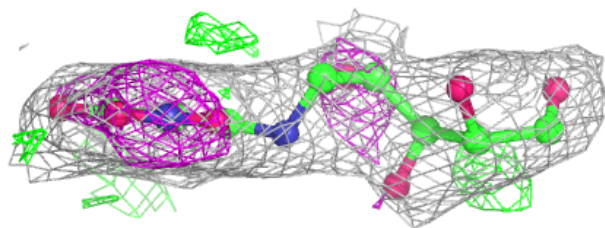
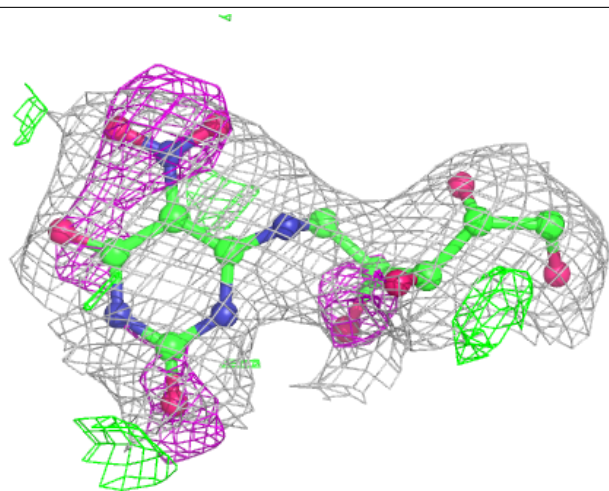
**Electron density around INI B 201:**

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



**Electron density around INI C 202:**

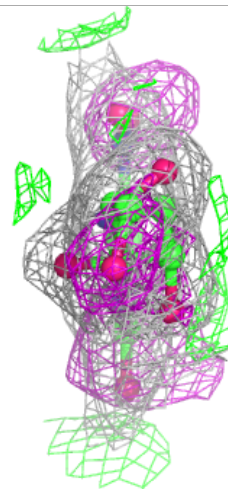
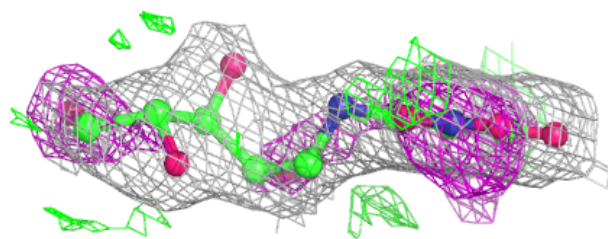
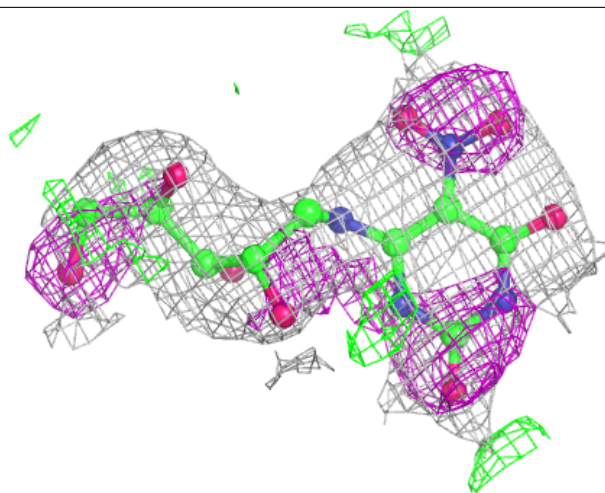
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





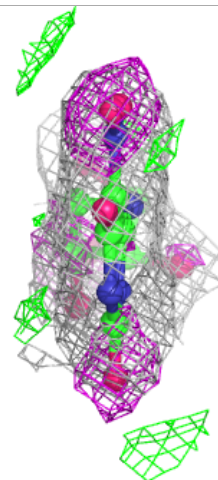
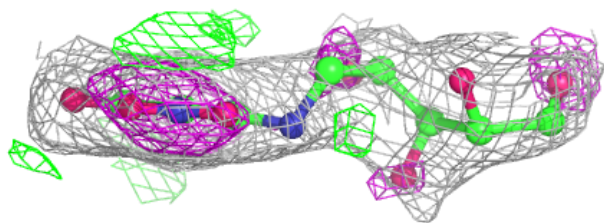
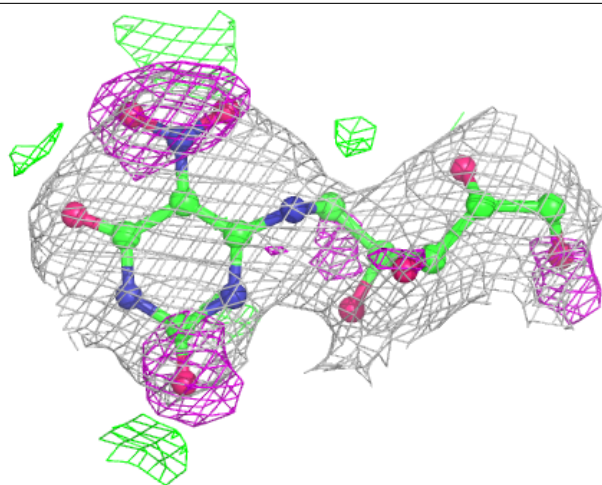
**Electron density around INI I 208:**

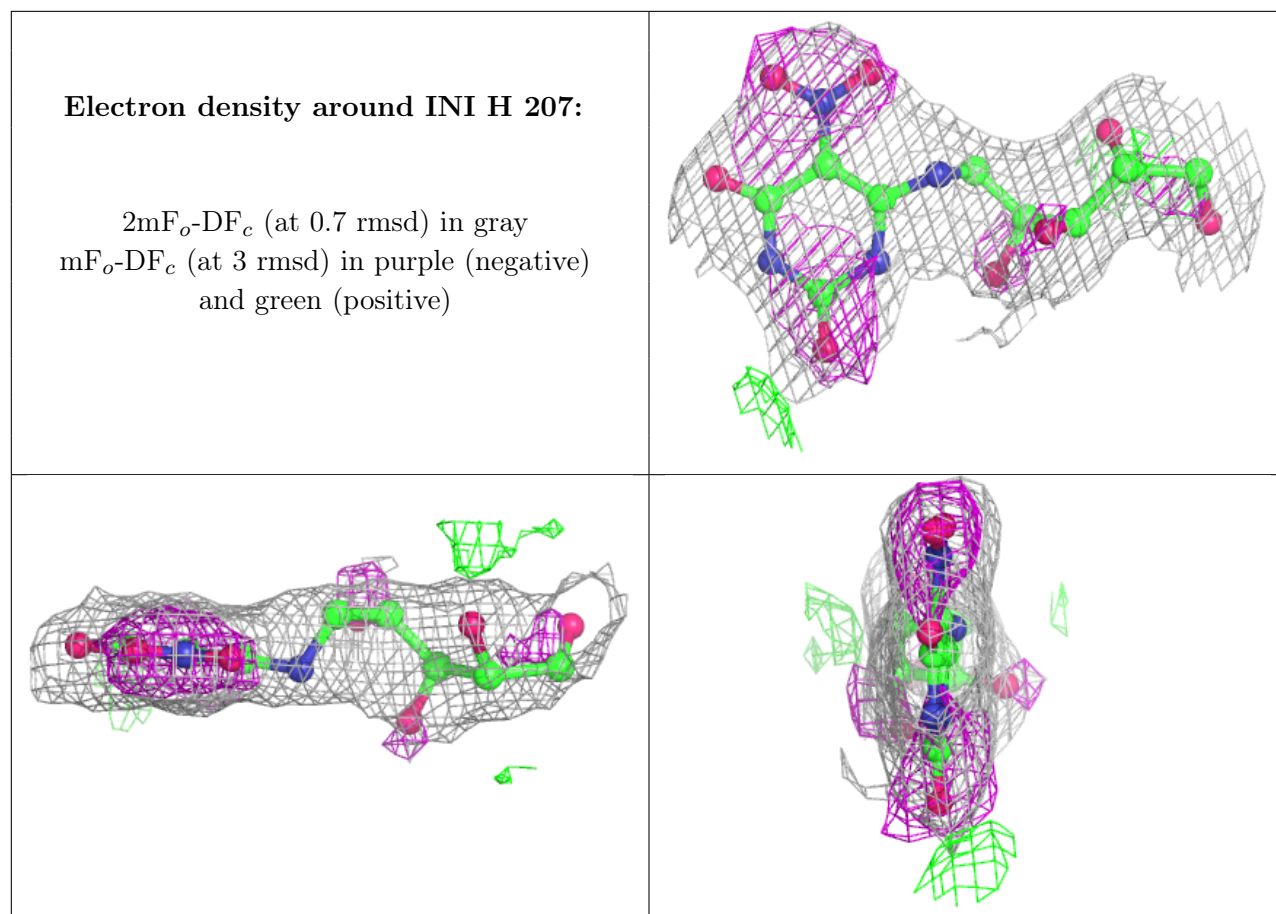
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around INI J 209:**

$2mF_o-DF_c$  (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.