



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:39 PM UTC

PDB ID : 8P2J / pdb_00008p2j
Title : Imine Reductase from *Ajellomyces dermatitidis* in space group C21
Authors : Sharma, M.; Grogan, G.
Deposited on : 2023-05-16
Resolution : 1.73 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

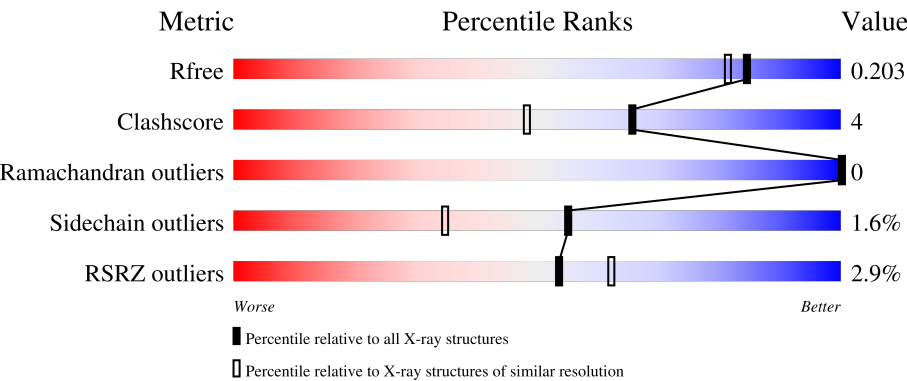
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.73 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	294	2% 91% 6% ..
1	B	294	4% 88% 9% ..
1	C	294	2% 92% 7%
1	D	294	2% 87% 10% .
1	E	294	3% 88% 11% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	294	2% 89% 9%
1	G	294	4% 90% 9%
1	H	294	4% 85% 9%
1	I	294	2% 94%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21304 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 Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	1	0
			2088	1333	352	392	11			
1	B	288	Total	C	N	O	S	0	0	0
			2080	1328	354	386	12			
1	C	293	Total	C	N	O	S	0	1	0
			2136	1362	361	400	13			
1	D	288	Total	C	N	O	S	0	2	0
			2094	1339	353	390	12			
1	E	293	Total	C	N	O	S	0	1	0
			2127	1357	361	398	11			
1	F	288	Total	C	N	O	S	0	1	0
			2098	1337	353	396	12			
1	G	293	Total	C	N	O	S	0	1	0
			2135	1361	361	401	12			
1	H	281	Total	C	N	O	S	0	2	0
			2062	1317	348	387	10			
1	I	288	Total	C	N	O	S	0	0	0
			2099	1336	356	395	12			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP A0A179UH34
A	-4	PHE	-	expression tag	UNP A0A179UH34
A	-3	GLN	-	expression tag	UNP A0A179UH34
A	-2	GLY	-	expression tag	UNP A0A179UH34
A	-1	PRO	-	expression tag	UNP A0A179UH34
A	0	ALA	-	expression tag	UNP A0A179UH34
A	140	GLU	ALA	engineered mutation	UNP A0A179UH34
B	-5	LEU	-	expression tag	UNP A0A179UH34
B	-4	PHE	-	expression tag	UNP A0A179UH34
B	-3	GLN	-	expression tag	UNP A0A179UH34
B	-2	GLY	-	expression tag	UNP A0A179UH34

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	PRO	-	expression tag	UNP A0A179UH34
B	0	ALA	-	expression tag	UNP A0A179UH34
B	140	GLU	ALA	engineered mutation	UNP A0A179UH34
C	-5	LEU	-	expression tag	UNP A0A179UH34
C	-4	PHE	-	expression tag	UNP A0A179UH34
C	-3	GLN	-	expression tag	UNP A0A179UH34
C	-2	GLY	-	expression tag	UNP A0A179UH34
C	-1	PRO	-	expression tag	UNP A0A179UH34
C	0	ALA	-	expression tag	UNP A0A179UH34
C	140	GLU	ALA	engineered mutation	UNP A0A179UH34
D	-5	LEU	-	expression tag	UNP A0A179UH34
D	-4	PHE	-	expression tag	UNP A0A179UH34
D	-3	GLN	-	expression tag	UNP A0A179UH34
D	-2	GLY	-	expression tag	UNP A0A179UH34
D	-1	PRO	-	expression tag	UNP A0A179UH34
D	0	ALA	-	expression tag	UNP A0A179UH34
D	140	GLU	ALA	engineered mutation	UNP A0A179UH34
E	-5	LEU	-	expression tag	UNP A0A179UH34
E	-4	PHE	-	expression tag	UNP A0A179UH34
E	-3	GLN	-	expression tag	UNP A0A179UH34
E	-2	GLY	-	expression tag	UNP A0A179UH34
E	-1	PRO	-	expression tag	UNP A0A179UH34
E	0	ALA	-	expression tag	UNP A0A179UH34
E	140	GLU	ALA	engineered mutation	UNP A0A179UH34
F	-5	LEU	-	expression tag	UNP A0A179UH34
F	-4	PHE	-	expression tag	UNP A0A179UH34
F	-3	GLN	-	expression tag	UNP A0A179UH34
F	-2	GLY	-	expression tag	UNP A0A179UH34
F	-1	PRO	-	expression tag	UNP A0A179UH34
F	0	ALA	-	expression tag	UNP A0A179UH34
F	140	GLU	ALA	engineered mutation	UNP A0A179UH34
G	-5	LEU	-	expression tag	UNP A0A179UH34
G	-4	PHE	-	expression tag	UNP A0A179UH34
G	-3	GLN	-	expression tag	UNP A0A179UH34
G	-2	GLY	-	expression tag	UNP A0A179UH34
G	-1	PRO	-	expression tag	UNP A0A179UH34
G	0	ALA	-	expression tag	UNP A0A179UH34
G	140	GLU	ALA	engineered mutation	UNP A0A179UH34
H	-5	LEU	-	expression tag	UNP A0A179UH34
H	-4	PHE	-	expression tag	UNP A0A179UH34
H	-3	GLN	-	expression tag	UNP A0A179UH34
H	-2	GLY	-	expression tag	UNP A0A179UH34

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	PRO	-	expression tag	UNP A0A179UH34
H	0	ALA	-	expression tag	UNP A0A179UH34
H	140	GLU	ALA	engineered mutation	UNP A0A179UH34
I	-5	LEU	-	expression tag	UNP A0A179UH34
I	-4	PHE	-	expression tag	UNP A0A179UH34
I	-3	GLN	-	expression tag	UNP A0A179UH34
I	-2	GLY	-	expression tag	UNP A0A179UH34
I	-1	PRO	-	expression tag	UNP A0A179UH34
I	0	ALA	-	expression tag	UNP A0A179UH34
I	140	GLU	ALA	engineered mutation	UNP A0A179UH34

- # NDP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	E	1	Total 48	C 21	N 7	O 17	P 3	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	G	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	H	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	I	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total 234	O 234	0	0
3	B	201	Total 201	O 201	0	0
3	C	264	Total 264	O 264	0	0
3	D	250	Total 250	O 250	0	0
3	E	204	Total 204	O 204	0	0
3	F	192	Total 192	O 192	0	0
3	G	189	Total 189	O 189	0	0
3	H	179	Total 179	O 179	0	0
3	I	240	Total 240	O 240	0	0

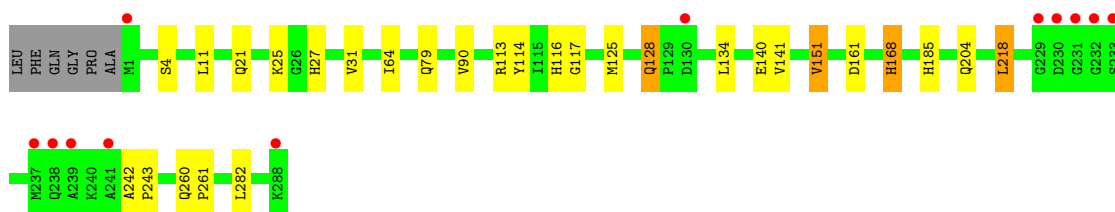
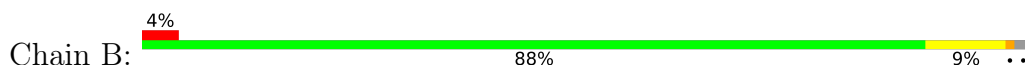
3 Residue-property plots [i](#)

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.

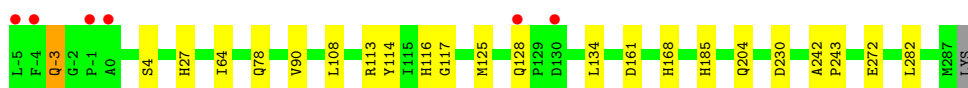
- Molecule 1: Oxidoreductase



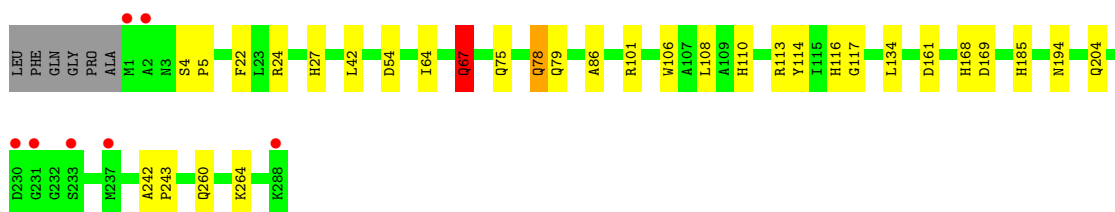
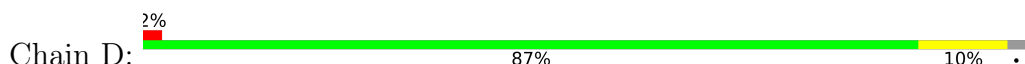
- Molecule 1: Oxidoreductase



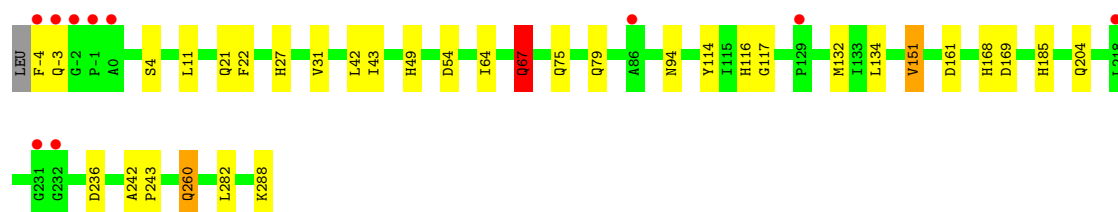
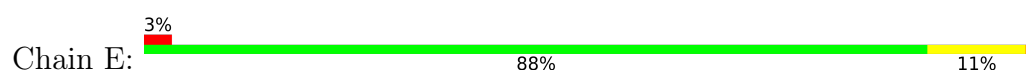
- Molecule 1: Oxidoreductase



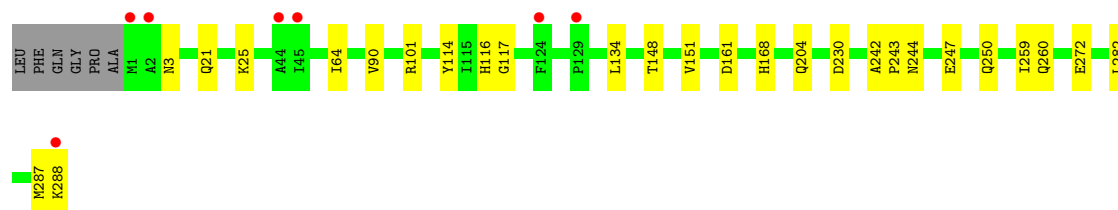
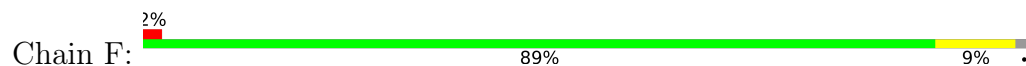
- Molecule 1: Oxidoreductase



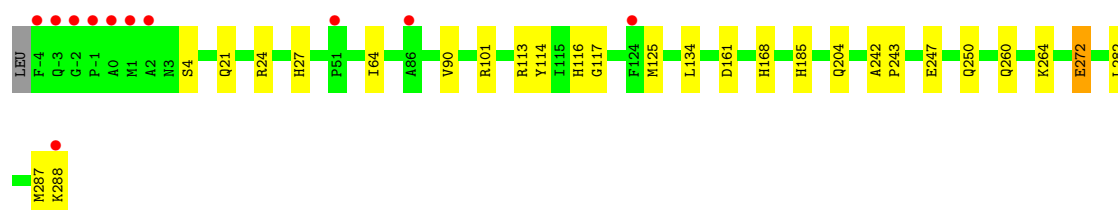
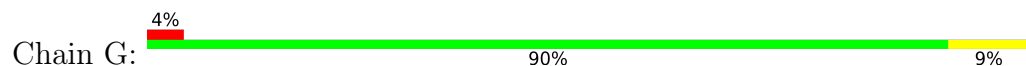
- Molecule 1: Oxidoreductase



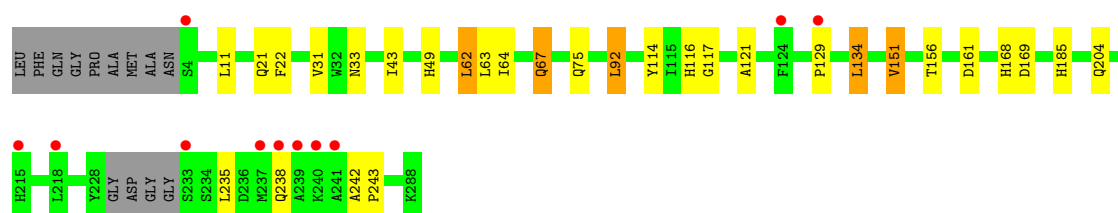
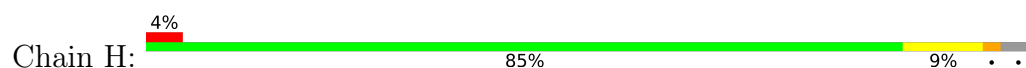
• Molecule 1: Oxidoreductase



• Molecule 1: Oxidoreductase



• Molecule 1: Oxidoreductase



• Molecule 1: Oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.62Å 87.97Å 162.58Å 90.00° 108.45° 90.00°	Depositor
Resolution (Å)	97.16 – 1.73 97.16 – 1.73	Depositor EDS
% Data completeness (in resolution range)	97.8 (97.16-1.73) 97.8 (97.16-1.73)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0405	Depositor
R, R_{free}	0.166 , 0.193 0.178 , 0.203	Depositor DCC
R_{free} test set	13859 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21304	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP

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	0.68	0/2132	0.87	2/2905 (0.1%)
1	B	0.66	0/2121	0.88	3/2892 (0.1%)
1	C	0.68	0/2182	0.90	3/2973 (0.1%)
1	D	0.70	0/2141	0.89	3/2917 (0.1%)
1	E	0.67	0/2173	0.88	3/2962 (0.1%)
1	F	0.65	0/2142	0.88	5/2919 (0.2%)
1	G	0.68	0/2181	0.90	3/2972 (0.1%)
1	H	0.64	0/2108	0.87	2/2874 (0.1%)
1	I	0.66	0/2140	0.89	2/2916 (0.1%)
All	All	0.67	0/19320	0.88	26/26330 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	G	0	1
1	H	0	1
All	All	0	4

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	67	GLN	CA-C-O	-8.22	113.15	118.33
1	C	161	ASP	CA-CB-CG	7.28	119.88	112.60
1	B	128	GLN	CB-CG-CD	7.24	124.91	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	169	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	161	ASP	CA-CB-CG	7.05	119.66	112.60
1	A	161	ASP	CA-CB-CG	6.89	119.49	112.60
1	E	161	ASP	CA-CB-CG	6.83	119.42	112.60
1	E	67	GLN	CA-C-O	-6.74	114.08	118.33
1	G	161	ASP	CA-CB-CG	6.60	119.20	112.60
1	D	161	ASP	CA-CB-CG	6.58	119.18	112.60
1	F	161	ASP	CA-CB-CG	6.57	119.17	112.60
1	E	169	ASP	CA-CB-CG	6.53	119.13	112.60
1	H	161	ASP	CA-CB-CG	6.49	119.08	112.60
1	I	161	ASP	CA-CB-CG	6.43	119.03	112.60
1	A	215	HIS	CA-CB-CG	6.26	120.06	113.80
1	G	272	GLU	CB-CG-CD	6.04	122.87	112.60
1	D	169	ASP	CA-CB-CG	6.01	118.61	112.60
1	C	272	GLU	CB-CG-CD	5.76	122.39	112.60
1	G	101	ARG	CB-CG-CD	5.62	124.23	111.30
1	F	230	ASP	CA-CB-CG	5.55	118.15	112.60
1	F	272	GLU	CB-CG-CD	5.41	121.80	112.60
1	I	168	HIS	CB-CG-CD2	-5.38	124.20	131.20
1	C	230	ASP	CA-CB-CG	5.25	117.84	112.60
1	F	3	ASN	CA-C-O	-5.19	113.49	119.56
1	F	101	ARG	CB-CG-CD	5.18	123.22	111.30
1	B	168	HIS	CB-CG-CD2	-5.05	124.64	131.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	67	GLN	Mainchain
1	E	67	GLN	Mainchain
1	G	113	ARG	Sidechain
1	H	67	GLN	Mainchain

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	2088	0	2099	12	0
1	B	2080	0	2085	18	0
1	C	2136	0	2143	15	0
1	D	2094	0	2108	26	0
1	E	2127	0	2133	27	0
1	F	2098	0	2106	19	0
1	G	2135	0	2141	17	0
1	H	2062	0	2066	20	0
1	I	2099	0	2108	8	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
2	C	48	0	26	0	0
2	D	48	0	26	1	0
2	E	48	0	26	1	0
2	F	48	0	26	0	0
2	G	48	0	26	0	0
2	H	48	0	26	3	0
2	I	48	0	26	0	0
3	A	234	0	0	4	0
3	B	201	0	0	6	0
3	C	264	0	0	5	0
3	D	250	0	0	10	0
3	E	204	0	0	8	0
3	F	192	0	0	3	1
3	G	189	0	0	7	1
3	H	179	0	0	4	0
3	I	240	0	0	5	0
All	All	21304	0	19223	147	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (147) 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:E:260:GLN:HG3	3:E:548:HOH:O	1.61	0.98
1:G:125:MET:HG2	3:G:402:HOH:O	1.64	0.97
1:F:25:LYS:HG3	1:F:151:VAL:CG2	2.05	0.87
1:A:125:MET:HG2	3:A:401:HOH:O	1.77	0.83
1:F:25:LYS:HG3	1:F:151:VAL:HG21	1.67	0.77
3:E:410:HOH:O	1:F:259:ILE:HG22	1.85	0.75
1:F:25:LYS:HG3	1:F:151:VAL:HG23	1.70	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:GLN:OE1	1:H:168:HIS:HD2	1.75	0.70
1:E:54:ASP:HB2	3:E:454:HOH:O	1.92	0.69
1:D:110:HIS:HE1	3:D:586:HOH:O	1.76	0.68
1:B:140:GLU:HG3	3:B:425:HOH:O	1.92	0.68
1:A:287:MET:O	1:A:288:LYS:HB3	1.94	0.67
1:G:287:MET:O	1:G:288:LYS:CB	2.44	0.66
1:I:225:GLU:OE2	3:I:401:HOH:O	2.13	0.65
1:E:204:GLN:OE1	1:F:168:HIS:HD2	1.79	0.65
1:B:113:ARG:HD2	1:B:141:VAL:HG22	1.78	0.65
1:C:168:HIS:HD2	1:D:204:GLN:OE1	1.80	0.65
1:D:113:ARG:HG3	1:E:-4:PHE:CD1	2.32	0.65
1:A:204:GLN:OE1	1:B:168:HIS:HD2	1.81	0.64
1:A:168:HIS:HD2	1:B:204:GLN:OE1	1.80	0.64
1:E:94:ASN:HD22	1:F:244:ASN:HD22	1.44	0.63
1:B:125:MET:HG3	3:B:539:HOH:O	1.99	0.62
1:E:168:HIS:HE1	3:E:537:HOH:O	1.81	0.62
1:G:168:HIS:HD2	1:H:204:GLN:OE1	1.82	0.61
1:G:21:GLN:NE2	3:G:401:HOH:O	2.25	0.61
1:C:64:ILE:HD13	1:C:90:VAL:HB	1.83	0.60
1:F:21:GLN:HG3	1:F:151:VAL:HG22	1.83	0.60
1:A:215:HIS:CE1	3:A:446:HOH:O	2.53	0.60
1:F:64:ILE:HD13	1:F:90:VAL:HB	1.84	0.60
1:E:94:ASN:ND2	1:F:244:ASN:HD22	1.98	0.60
1:B:21:GLN:HG3	1:B:151:VAL:HG13	1.83	0.60
1:D:260:GLN:HG3	1:D:264:LYS:HE2	1.82	0.60
1:C:113:ARG:HD2	3:C:540:HOH:O	2.01	0.59
1:I:64:ILE:HD13	1:I:90:VAL:HB	1.83	0.59
1:I:288:LYS:HB2	3:I:418:HOH:O	2.02	0.59
1:G:185:HIS:HD2	3:G:456:HOH:O	1.84	0.59
1:C:204:GLN:OE1	1:D:168:HIS:HD2	1.86	0.58
1:D:168:HIS:HE1	3:D:565:HOH:O	1.86	0.58
1:B:64:ILE:HD13	1:B:90:VAL:HB	1.86	0.58
1:F:287:MET:O	1:F:288:LYS:HB2	2.03	0.57
1:D:5:PRO:HG2	3:D:499:HOH:O	2.03	0.57
1:G:64:ILE:HD13	1:G:90:VAL:HB	1.87	0.56
1:E:114:TYR:OH	1:E:116:HIS:HD2	1.88	0.56
1:H:114:TYR:OH	1:H:116:HIS:HD2	1.88	0.56
1:B:114:TYR:OH	1:B:116:HIS:HD2	1.89	0.56
1:C:114:TYR:OH	1:C:116:HIS:HD2	1.88	0.55
1:A:114:TYR:OH	1:A:116:HIS:HD2	1.89	0.55
1:F:114:TYR:OH	1:F:116:HIS:HD2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:11:LEU:H	1:H:33:ASN:ND2	2.04	0.55
1:D:114:TYR:OH	1:D:116:HIS:HD2	1.89	0.55
1:A:128:GLN:NE2	3:A:401:HOH:O	2.29	0.55
1:I:114:TYR:OH	1:I:116:HIS:HD2	1.89	0.55
1:B:79:GLN:CG	3:B:434:HOH:O	2.55	0.54
1:C:27:HIS:HE1	3:C:599:HOH:O	1.90	0.54
1:H:168:HIS:HE1	3:H:542:HOH:O	1.90	0.54
1:A:22:PHE:CE2	1:A:64:ILE:HD12	2.42	0.54
1:E:168:HIS:HD2	1:F:204:GLN:OE1	1.91	0.54
1:G:4:SER:O	1:G:27:HIS:HD2	1.91	0.54
1:D:101:ARG:NH1	3:D:402:HOH:O	2.27	0.53
1:H:43:ILE:HD11	1:H:49:HIS:HB2	1.89	0.53
1:B:4:SER:O	1:B:27:HIS:HD2	1.91	0.53
1:D:4:SER:O	1:D:27:HIS:HD2	1.91	0.53
1:H:62:LEU:CD2	1:H:62:LEU:C	2.82	0.53
1:D:86:ALA:HA	1:E:-4:PHE:CE1	2.44	0.53
1:E:236:ASP:O	3:E:401:HOH:O	2.19	0.53
1:A:4:SER:O	1:A:27:HIS:HD2	1.92	0.52
1:E:4:SER:O	1:E:27:HIS:HD2	1.92	0.52
1:D:24:ARG:CG	3:D:545:HOH:O	2.58	0.52
1:C:4:SER:O	1:C:27:HIS:HD2	1.93	0.51
1:G:27:HIS:HE1	3:G:552:HOH:O	1.92	0.51
1:D:22:PHE:CE2	1:D:64:ILE:HD12	2.45	0.51
1:C:125[B]:MET:CE	1:C:128:GLN:OE1	2.58	0.51
1:E:21:GLN:HG3	1:E:151:VAL:HG13	1.92	0.51
1:E:185:HIS:HD2	3:E:475:HOH:O	1.94	0.51
1:E:43:ILE:HD11	1:E:49:HIS:HB2	1.93	0.50
1:H:129:PRO:HA	3:H:454:HOH:O	2.11	0.50
1:E:75:GLN:O	1:E:79:GLN:HG2	2.12	0.50
1:H:21:GLN:HG3	1:H:151:VAL:HG13	1.93	0.50
1:D:106:TRP:O	1:D:110:HIS:HD2	1.95	0.50
1:E:132:MET:SD	3:F:517:HOH:O	2.60	0.50
1:I:21:GLN:NE2	3:I:405:HOH:O	2.35	0.50
1:G:114:TYR:OH	1:G:116:HIS:HD2	1.95	0.49
1:I:168:HIS:HE1	3:I:445:HOH:O	1.94	0.49
1:H:185:HIS:HD2	3:H:451:HOH:O	1.96	0.49
1:E:288:LYS:C	3:E:448:HOH:O	2.55	0.49
1:H:22:PHE:CE2	1:H:64:ILE:HD12	2.48	0.49
1:G:260:GLN:HG3	1:G:264:LYS:HE2	1.93	0.49
1:D:242:ALA:HB3	1:D:243:PRO:HD3	1.95	0.48
1:B:185:HIS:HD2	3:B:477:HOH:O	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ALA:HB2	1:E:-3:GLN:O	2.12	0.48
1:H:92:LEU:HD12	1:H:117:GLY:HA3	1.96	0.48
1:A:168:HIS:HE1	3:A:434:HOH:O	1.96	0.48
1:D:67:GLN:O	2:D:301:NDP:H52N	2.14	0.48
1:H:117:GLY:HA2	1:H:134:LEU:O	2.14	0.47
1:B:168:HIS:HE1	3:B:471:HOH:O	1.96	0.47
1:D:27:HIS:HE1	3:D:580:HOH:O	1.95	0.47
1:D:113:ARG:HG3	1:E:-4:PHE:CE1	2.50	0.47
1:D:117:GLY:HA2	1:D:134:LEU:O	2.15	0.47
1:I:27:HIS:NE2	3:I:404:HOH:O	2.35	0.47
1:D:185:HIS:HD2	3:D:462:HOH:O	1.97	0.47
1:C:168:HIS:HE1	3:C:522:HOH:O	1.98	0.47
1:E:117:GLY:HA2	1:E:134:LEU:O	2.15	0.47
1:E:22:PHE:CE2	1:E:64:ILE:HD12	2.49	0.46
1:G:24:ARG:NE	3:G:408:HOH:O	2.48	0.46
1:C:185:HIS:HD2	3:C:477:HOH:O	1.99	0.46
1:A:117:GLY:HA2	1:A:134:LEU:O	2.16	0.46
1:F:117:GLY:HA2	1:F:134:LEU:O	2.15	0.46
1:B:25:LYS:HG3	1:B:151:VAL:HG22	1.98	0.46
1:H:67:GLN:O	2:H:301:NDP:H52N	2.15	0.46
1:E:67:GLN:O	2:E:301:NDP:H52N	2.16	0.45
1:H:242:ALA:HB3	1:H:243:PRO:HD3	1.98	0.45
1:C:117:GLY:HA2	1:C:134:LEU:O	2.16	0.45
1:I:117:GLY:HA2	1:I:134:LEU:O	2.16	0.44
1:H:75:GLN:NE2	2:H:301:NDP:H62A	2.15	0.44
1:B:218:LEU:HD13	3:B:415:HOH:O	2.18	0.44
1:C:242:ALA:HB3	1:C:243:PRO:HD3	2.00	0.44
1:E:11:LEU:HD11	1:E:31:VAL:HB	1.99	0.44
1:F:148:THR:O	1:F:151:VAL:HG12	2.17	0.44
1:B:117:GLY:HA2	1:B:134:LEU:O	2.18	0.44
1:E:27:HIS:HE1	3:E:559:HOH:O	1.99	0.44
1:G:117:GLY:HA2	1:G:134:LEU:O	2.16	0.43
1:G:242:ALA:HB3	1:G:243:PRO:HD3	1.99	0.43
1:D:78[B]:GLN:NE2	3:D:405:HOH:O	2.44	0.43
1:H:62:LEU:HD23	1:H:63:LEU:N	2.34	0.43
1:H:134:LEU:HD12	1:H:156:THR:HB	2.01	0.43
1:F:242:ALA:HB3	1:F:243:PRO:HD3	1.99	0.43
1:E:242:ALA:HB3	1:E:243:PRO:HD3	2.01	0.43
1:F:287:MET:O	1:F:288:LYS:CB	2.67	0.43
1:D:78[B]:GLN:HG3	3:D:522:HOH:O	2.18	0.43
1:G:272:GLU:HG2	3:G:579:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:HIS:HE1	3:F:435:HOH:O	2.01	0.42
1:H:11:LEU:HD11	1:H:31:VAL:HB	2.02	0.42
1:D:54:ASP:CG	3:D:613:HOH:O	2.62	0.42
1:H:121:ALA:O	2:H:301:NDP:H42N	2.20	0.42
1:B:242:ALA:HB3	1:B:243:PRO:HD3	2.02	0.42
1:D:42:LEU:HD22	1:D:42:LEU:N	2.35	0.42
1:F:247:GLU:CG	3:F:527:HOH:O	2.68	0.41
1:C:-3:GLN:NE2	3:C:405:HOH:O	2.42	0.41
1:C:125[B]:MET:SD	1:C:128:GLN:OE1	2.79	0.41
1:C:125[B]:MET:HE1	1:C:128:GLN:OE1	2.20	0.41
1:F:25:LYS:CG	1:F:151:VAL:HG21	2.43	0.41
1:G:168:HIS:HE1	3:G:429:HOH:O	2.03	0.41
1:D:75:GLN:O	1:D:79:GLN:HG3	2.21	0.41
1:G:247:GLU:CG	3:H:550:HOH:O	2.68	0.40
1:B:11:LEU:HD11	1:B:31:VAL:HB	2.04	0.40
1:E:42:LEU:HD22	1:E:42:LEU:N	2.37	0.40
1:A:261:PRO:HG2	1:B:261:PRO:HG2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:587:HOH:O	3:G:554:HOH:O[3_445]	2.06	0.14

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	286/294 (97%)	282 (99%)	4 (1%)	0	100	100
1	B	286/294 (97%)	282 (99%)	4 (1%)	0	100	100
1	C	292/294 (99%)	287 (98%)	5 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	288/294 (98%)	284 (99%)	4 (1%)	0	100	100
1	E	292/294 (99%)	288 (99%)	4 (1%)	0	100	100
1	F	287/294 (98%)	281 (98%)	6 (2%)	0	100	100
1	G	292/294 (99%)	285 (98%)	7 (2%)	0	100	100
1	H	279/294 (95%)	275 (99%)	4 (1%)	0	100	100
1	I	286/294 (97%)	282 (99%)	4 (1%)	0	100	100
All	All	2588/2646 (98%)	2546 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	210/221 (95%)	207 (99%)	3 (1%)	59	41
1	B	206/221 (93%)	201 (98%)	5 (2%)	43	19
1	C	215/221 (97%)	211 (98%)	4 (2%)	50	28
1	D	209/221 (95%)	205 (98%)	4 (2%)	50	28
1	E	213/221 (96%)	210 (99%)	3 (1%)	59	41
1	F	212/221 (96%)	209 (99%)	3 (1%)	59	41
1	G	215/221 (97%)	213 (99%)	2 (1%)	70	59
1	H	208/221 (94%)	202 (97%)	6 (3%)	37	14
1	I	212/221 (96%)	211 (100%)	1 (0%)	81	75
All	All	1900/1989 (96%)	1869 (98%)	31 (2%)	55	35

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	ARG
1	A	282	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	288	LYS
1	B	128	GLN
1	B	151	VAL
1	B	218	LEU
1	B	260	GLN
1	B	282	LEU
1	C	-3	GLN
1	C	78	GLN
1	C	108	LEU
1	C	282	LEU
1	D	78[A]	GLN
1	D	78[B]	GLN
1	D	108	LEU
1	D	194	ASN
1	E	151	VAL
1	E	260	GLN
1	E	282	LEU
1	F	250	GLN
1	F	260	GLN
1	F	282	LEU
1	G	250	GLN
1	G	282	LEU
1	H	62	LEU
1	H	92	LEU
1	H	134	LEU
1	H	151	VAL
1	H	235	LEU
1	H	238	GLN
1	I	265	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	27	HIS
1	A	40	GLN
1	A	116	HIS
1	A	128	GLN
1	A	168	HIS
1	A	204	GLN
1	B	3	ASN
1	B	27	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	116	HIS
1	B	168	HIS
1	B	185	HIS
1	B	204	GLN
1	B	214	GLN
1	C	3	ASN
1	C	27	HIS
1	C	67	GLN
1	C	116	HIS
1	C	168	HIS
1	C	185	HIS
1	C	204	GLN
1	C	244	ASN
1	D	27	HIS
1	D	67	GLN
1	D	110	HIS
1	D	116	HIS
1	D	128	GLN
1	D	168	HIS
1	D	185	HIS
1	D	204	GLN
1	D	217	ASN
1	E	27	HIS
1	E	116	HIS
1	E	168	HIS
1	E	185	HIS
1	E	204	GLN
1	E	214	GLN
1	E	217	ASN
1	F	116	HIS
1	F	128	GLN
1	F	168	HIS
1	F	204	GLN
1	F	244	ASN
1	F	250	GLN
1	G	3	ASN
1	G	21	GLN
1	G	27	HIS
1	G	67	GLN
1	G	116	HIS
1	G	168	HIS
1	G	185	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	204	GLN
1	G	244	ASN
1	H	33	ASN
1	H	75	GLN
1	H	116	HIS
1	H	168	HIS
1	H	185	HIS
1	H	204	GLN
1	I	21	GLN
1	I	116	HIS
1	I	168	HIS
1	I	204	GLN
1	I	222	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
2	NDP	H	301	-	51,52,52	0.74	1 (1%)	71,80,80	0.89	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	D	301	-	51,52,52	0.63	1 (1%)	71,80,80	0.88	3 (4%)
2	NDP	E	301	-	51,52,52	0.75	1 (1%)	71,80,80	0.82	1 (1%)
2	NDP	A	301	-	51,52,52	0.80	3 (5%)	71,80,80	0.84	3 (4%)
2	NDP	I	301	-	51,52,52	0.69	0	71,80,80	0.88	3 (4%)
2	NDP	C	301	-	51,52,52	0.92	2 (3%)	71,80,80	0.77	1 (1%)
2	NDP	B	301	-	51,52,52	0.67	1 (1%)	71,80,80	0.97	6 (8%)
2	NDP	G	301	-	51,52,52	0.78	2 (3%)	71,80,80	0.86	2 (2%)
2	NDP	F	301	-	51,52,52	0.90	3 (5%)	71,80,80	0.93	5 (7%)

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
2	NDP	H	301	-	-	4/34/77/77	0/5/5/5
2	NDP	D	301	-	-	2/34/77/77	0/5/5/5
2	NDP	E	301	-	-	4/34/77/77	0/5/5/5
2	NDP	A	301	-	-	4/34/77/77	0/5/5/5
2	NDP	I	301	-	-	3/34/77/77	0/5/5/5
2	NDP	C	301	-	-	5/34/77/77	0/5/5/5
2	NDP	B	301	-	-	4/34/77/77	0/5/5/5
2	NDP	G	301	-	-	4/34/77/77	0/5/5/5
2	NDP	F	301	-	-	1/34/77/77	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NDP	P2B-O2B	4.23	1.66	1.59
2	C	301	NDP	P2B-O2B	3.71	1.66	1.59
2	C	301	NDP	PN-O3	3.34	1.63	1.59
2	E	301	NDP	P2B-O2B	3.11	1.65	1.59
2	H	301	NDP	P2B-O2B	2.68	1.64	1.59
2	A	301	NDP	P2B-O2B	2.63	1.64	1.59
2	A	301	NDP	PA-O3	2.60	1.62	1.59
2	G	301	NDP	P2B-O2B	2.57	1.64	1.59
2	A	301	NDP	PN-O3	2.51	1.62	1.59
2	G	301	NDP	PN-O3	2.45	1.62	1.59
2	B	301	NDP	PN-O3	2.41	1.62	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	NDP	P2B-O2B	2.35	1.63	1.59
2	F	301	NDP	PN-O3	2.23	1.61	1.59
2	F	301	NDP	PA-O3	2.10	1.61	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	NDP	P2B-O2B-C2B	-3.27	114.71	123.43
2	C	301	NDP	C3B-C2B-C1B	-2.84	97.37	102.81
2	A	301	NDP	O2A-PA-O1A	2.68	124.93	112.44
2	A	301	NDP	C3B-C2B-C1B	-2.66	97.72	102.81
2	H	301	NDP	C3B-C2B-C1B	-2.64	97.75	102.81
2	B	301	NDP	P2B-O2B-C2B	-2.62	116.42	123.43
2	D	301	NDP	C3N-C7N-N7N	2.60	122.29	117.67
2	G	301	NDP	P2B-O2B-C2B	-2.60	116.49	123.43
2	D	301	NDP	C3B-C2B-C1B	-2.60	97.83	102.81
2	B	301	NDP	C3N-C7N-N7N	2.51	122.12	117.67
2	G	301	NDP	C3B-C2B-C1B	-2.47	98.08	102.81
2	D	301	NDP	P2B-O2B-C2B	-2.31	117.25	123.43
2	E	301	NDP	C3B-C2B-C1B	-2.28	98.44	102.81
2	H	301	NDP	O7N-C7N-C3N	-2.27	116.62	120.90
2	H	301	NDP	P2B-O2B-C2B	-2.25	117.43	123.43
2	I	301	NDP	O2A-PA-O1A	2.23	122.81	112.44
2	B	301	NDP	C3B-C2B-C1B	-2.21	98.58	102.81
2	A	301	NDP	P2B-O2B-C2B	-2.19	117.58	123.43
2	B	301	NDP	O2B-P2B-O1X	-2.18	101.56	109.33
2	F	301	NDP	O2X-P2B-O2B	-2.15	97.47	105.85
2	B	301	NDP	O2A-PA-O1A	2.13	122.38	112.44
2	B	301	NDP	O7N-C7N-C3N	-2.13	116.89	120.90
2	I	301	NDP	C3B-C2B-C1B	-2.06	98.86	102.81
2	F	301	NDP	C3N-C7N-N7N	2.05	121.30	117.67
2	F	301	NDP	O2A-PA-O1A	2.04	121.95	112.44
2	H	301	NDP	C3N-C7N-N7N	2.03	121.28	117.67
2	F	301	NDP	C3B-C2B-C1B	-2.03	98.93	102.81
2	I	301	NDP	C3N-C7N-N7N	2.01	121.24	117.67

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NDP	C5D-O5D-PN-O1N
2	B	301	NDP	C5D-O5D-PN-O1N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	301	NDP	C5D-O5D-PN-O1N
2	G	301	NDP	C5D-O5D-PN-O1N
2	C	301	NDP	C5D-O5D-PN-O3
2	F	301	NDP	O4D-C1D-N1N-C6N
2	B	301	NDP	C2B-O2B-P2B-O2X
2	C	301	NDP	C2B-O2B-P2B-O3X
2	D	301	NDP	O4D-C1D-N1N-C6N
2	E	301	NDP	O4D-C1D-N1N-C6N
2	C	301	NDP	O4D-C1D-N1N-C6N
2	G	301	NDP	O4D-C1D-N1N-C6N
2	A	301	NDP	O4D-C1D-N1N-C6N
2	B	301	NDP	O4D-C1D-N1N-C6N
2	H	301	NDP	O4D-C1D-N1N-C6N
2	I	301	NDP	O4D-C1D-N1N-C6N
2	A	301	NDP	C2B-O2B-P2B-O1X
2	E	301	NDP	PN-O3-PA-O1A
2	E	301	NDP	PN-O3-PA-O2A
2	H	301	NDP	C2D-C1D-N1N-C6N
2	B	301	NDP	C2D-C1D-N1N-C6N
2	C	301	NDP	C2D-C1D-N1N-C6N
2	A	301	NDP	C2D-C1D-N1N-C6N
2	E	301	NDP	C2D-C1D-N1N-C6N
2	G	301	NDP	C2D-C1D-N1N-C6N
2	I	301	NDP	C2D-C1D-N1N-C6N
2	G	301	NDP	C2B-O2B-P2B-O2X
2	I	301	NDP	C1B-C2B-O2B-P2B
2	H	301	NDP	PN-O3-PA-O2A
2	D	301	NDP	O4B-C4B-C5B-O5B
2	H	301	NDP	O4B-C4B-C5B-O5B

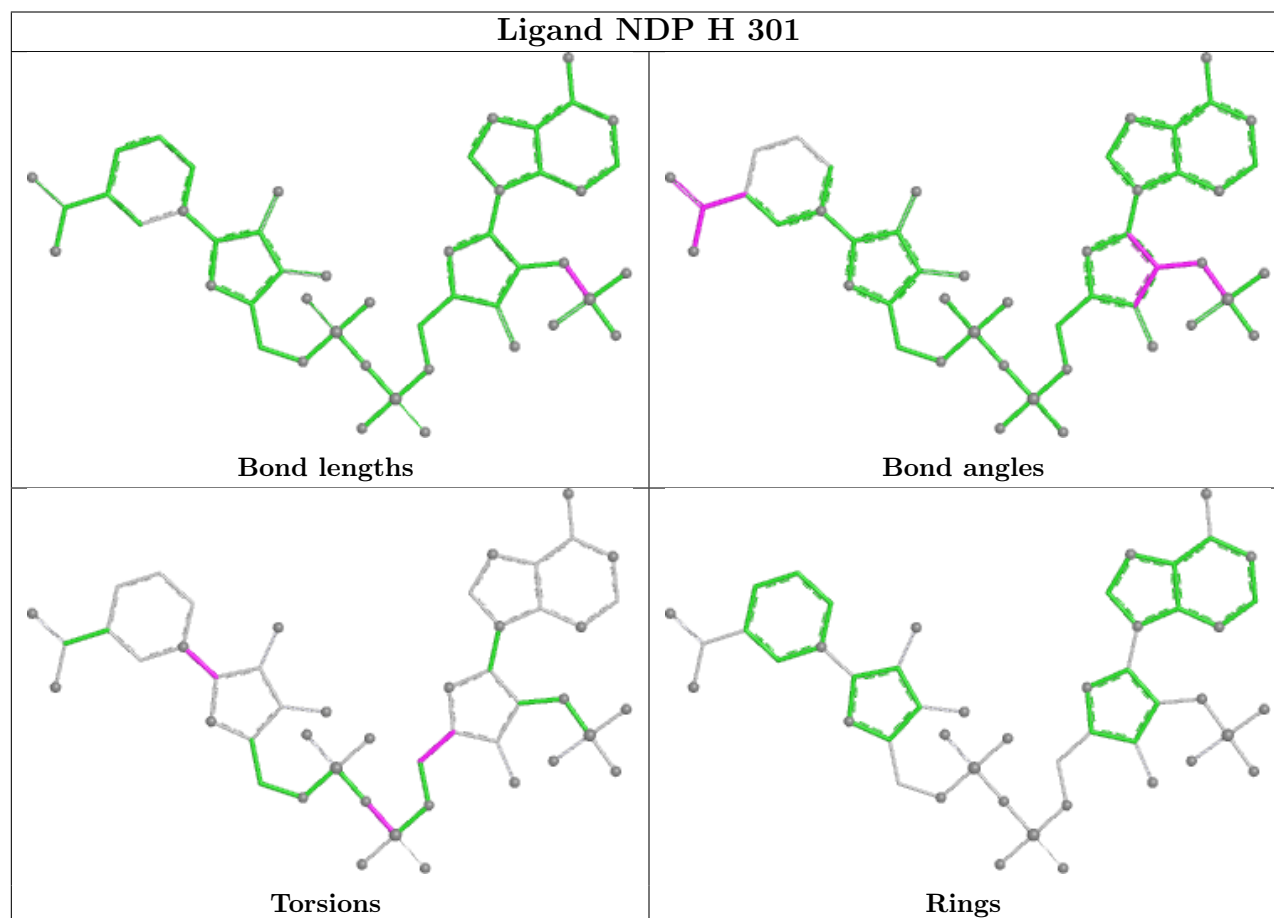
There are no ring outliers.

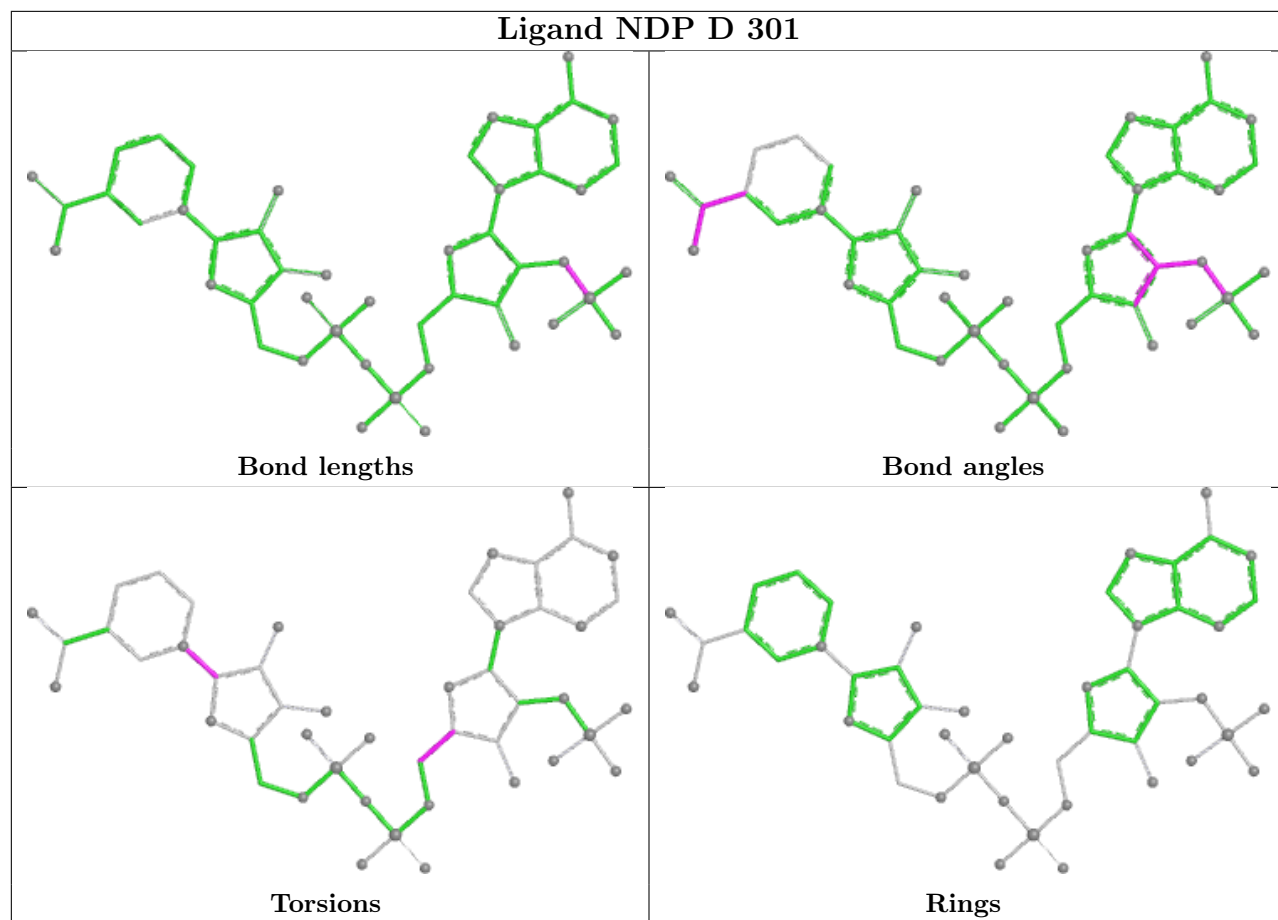
3 monomers are involved in 5 short contacts:

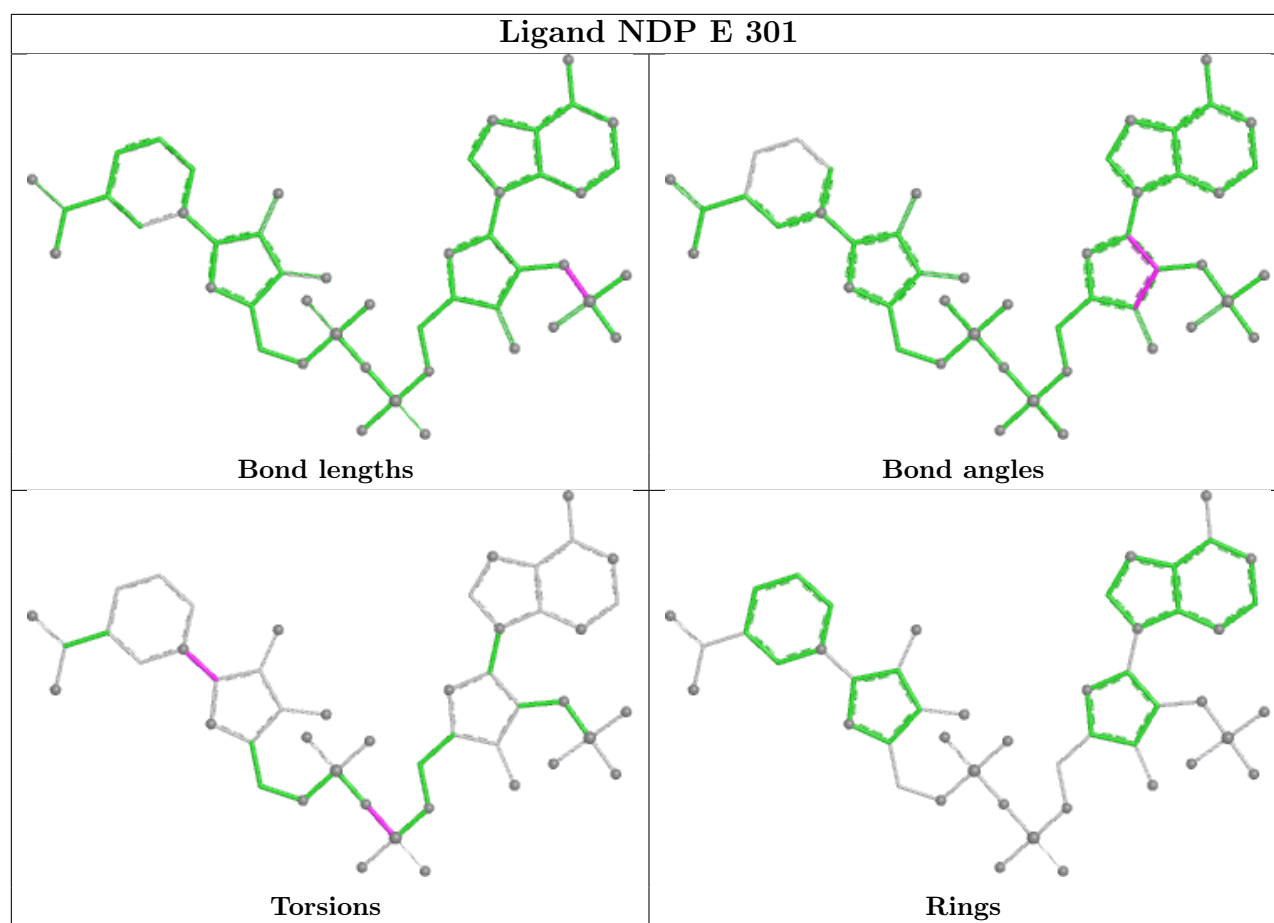
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	301	NDP	3	0
2	D	301	NDP	1	0
2	E	301	NDP	1	0

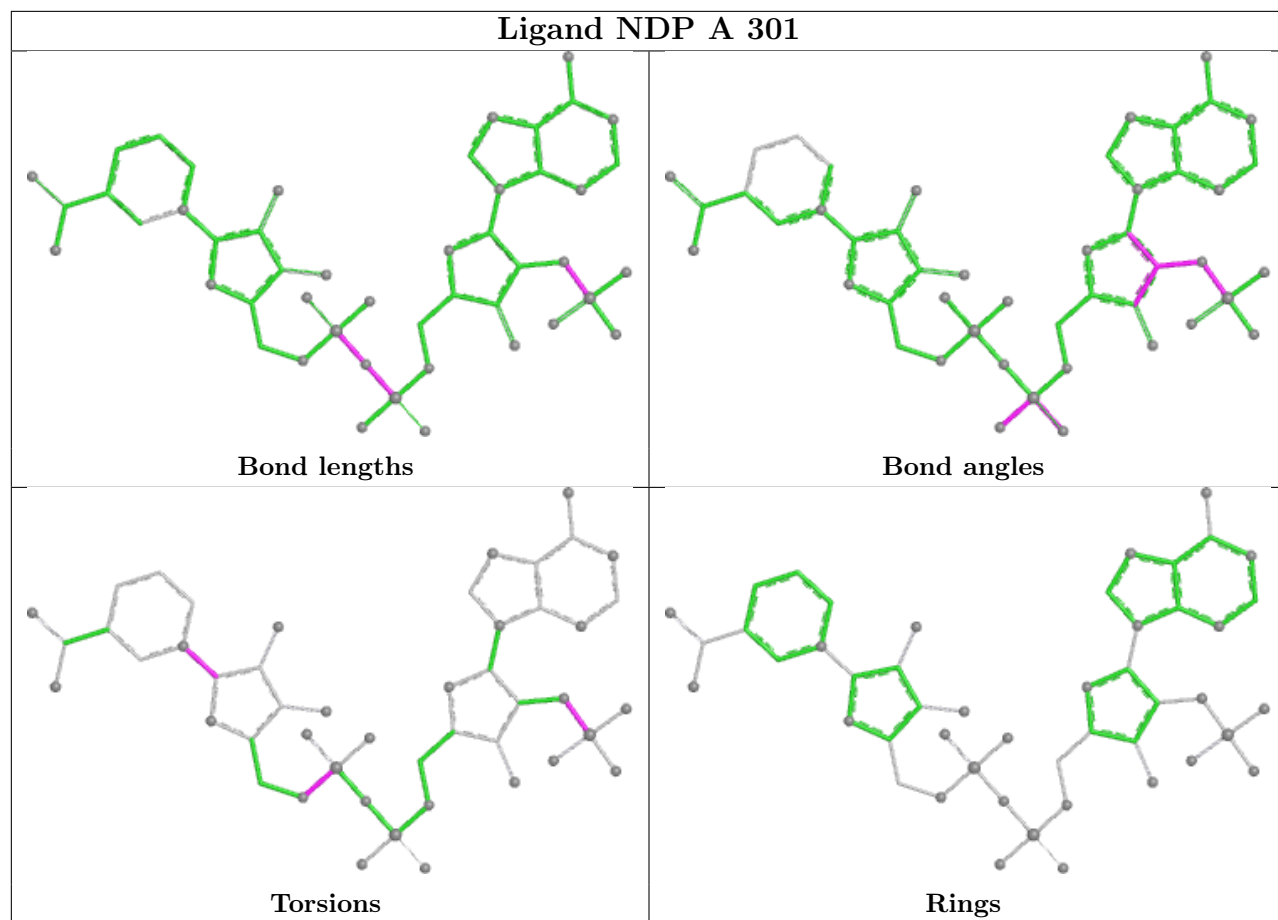
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

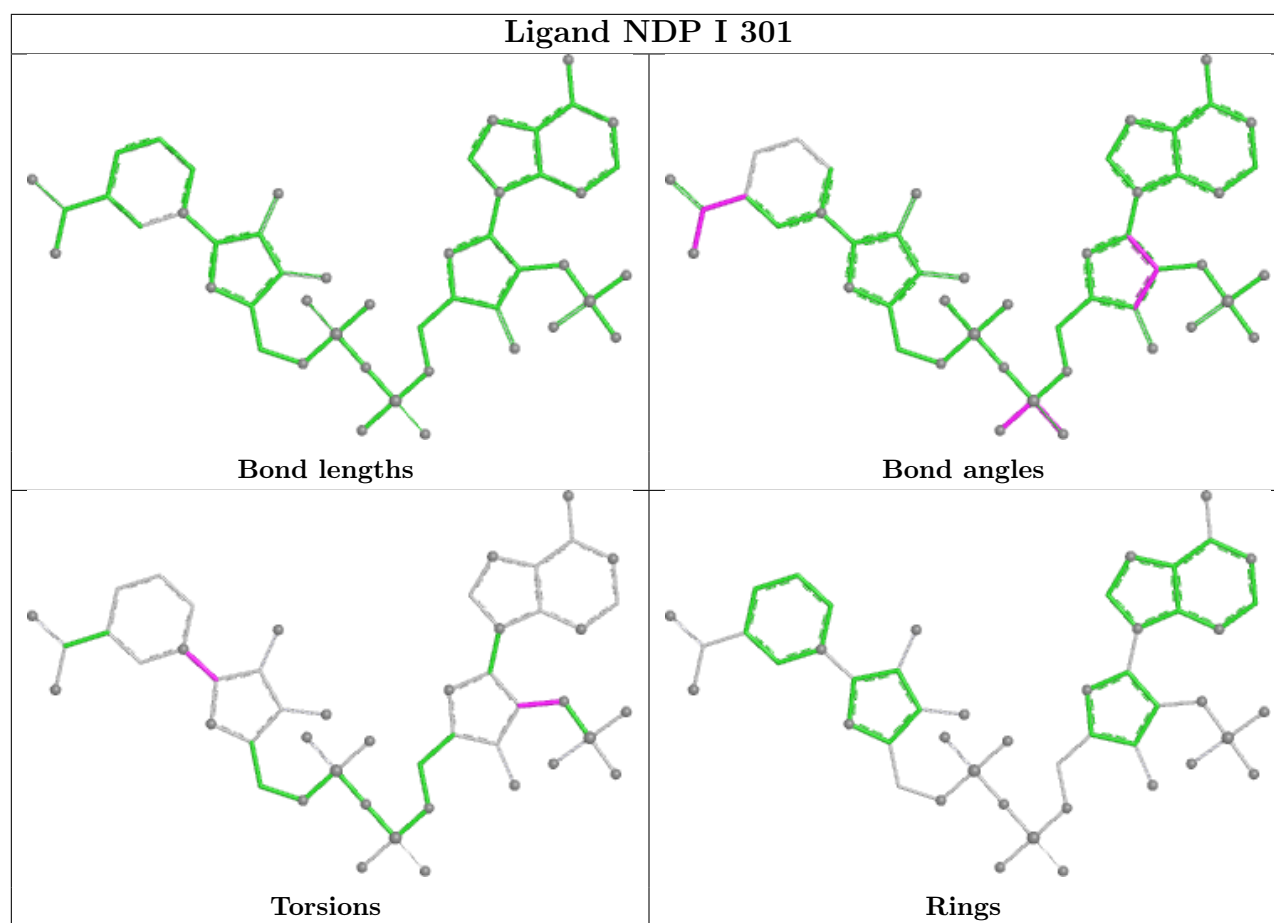
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

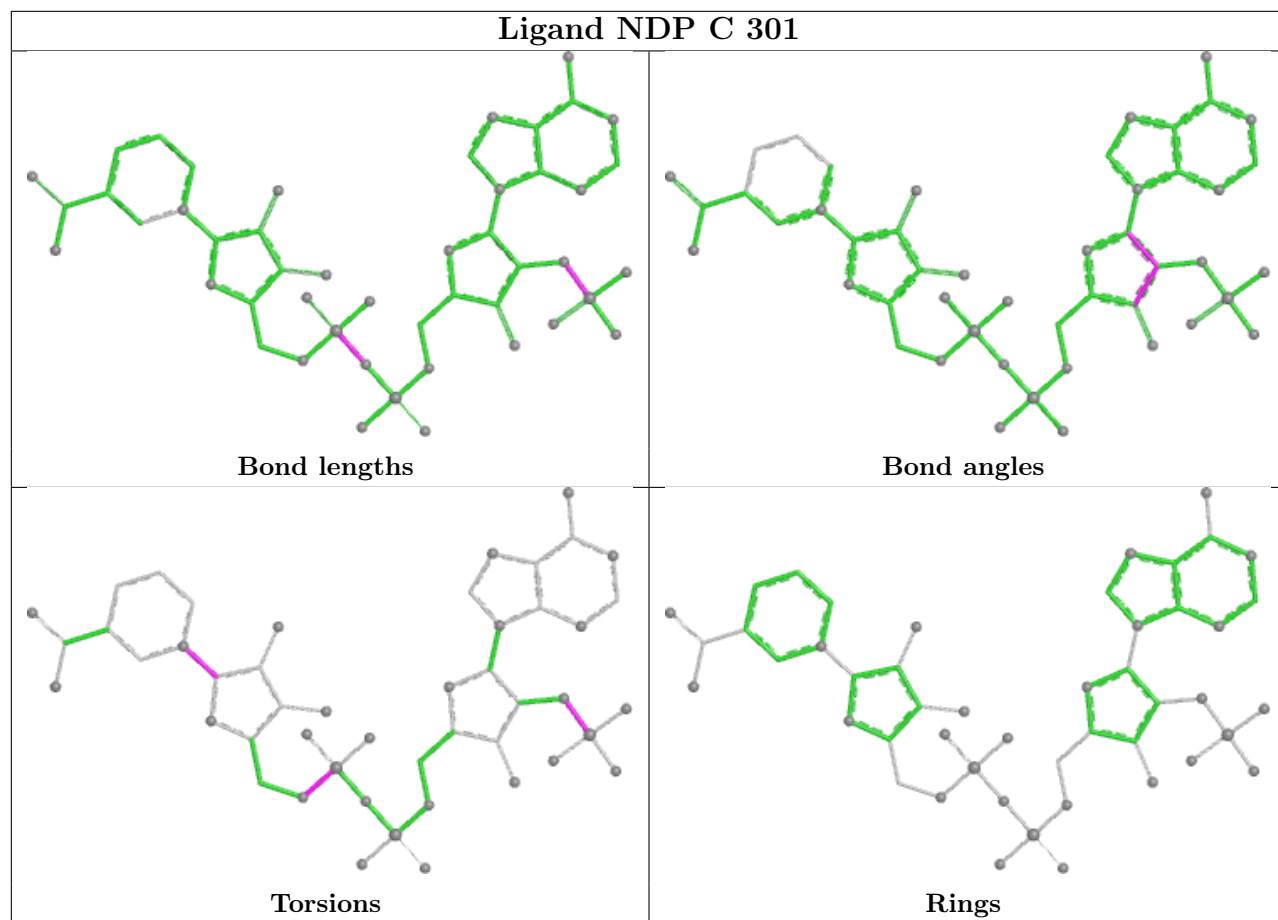


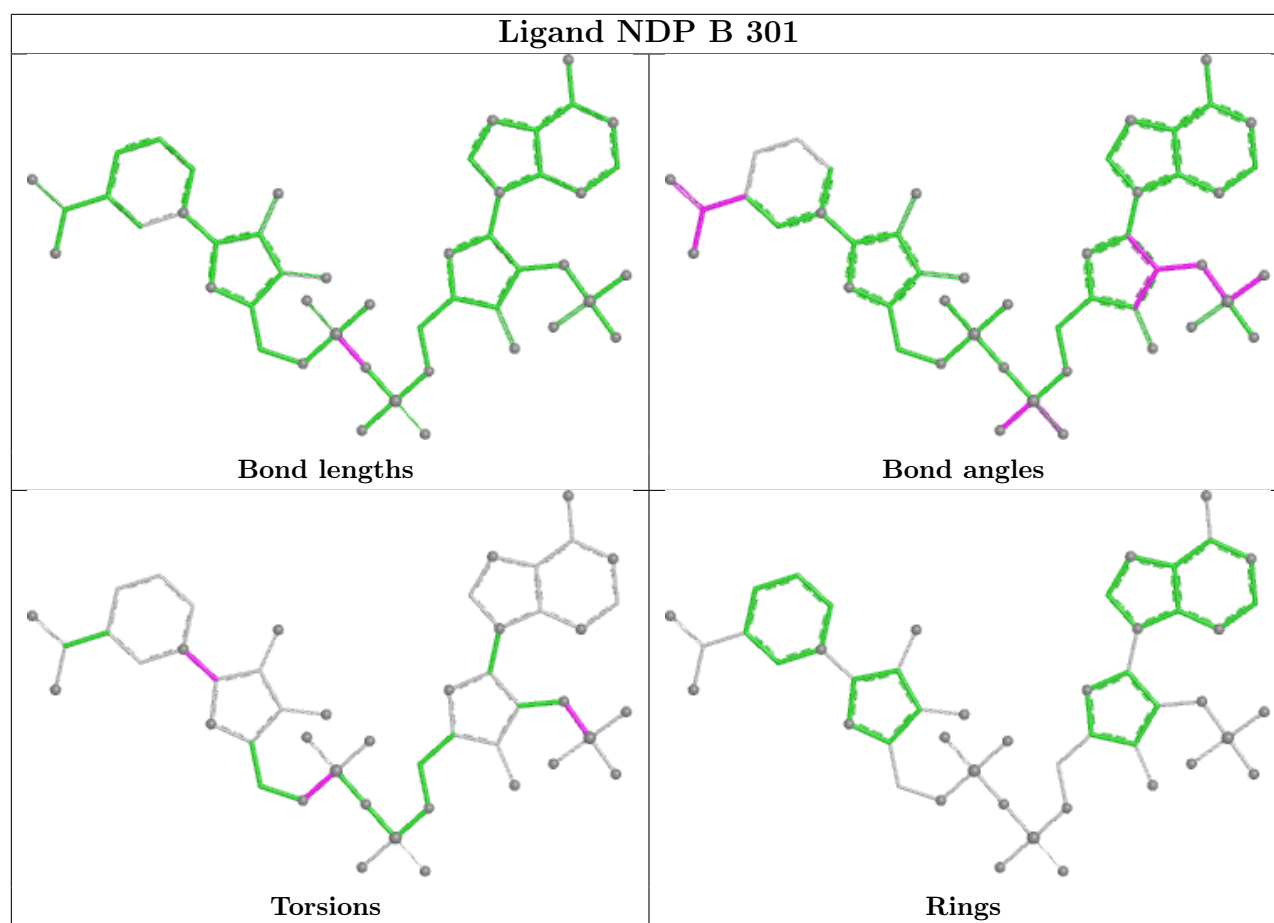


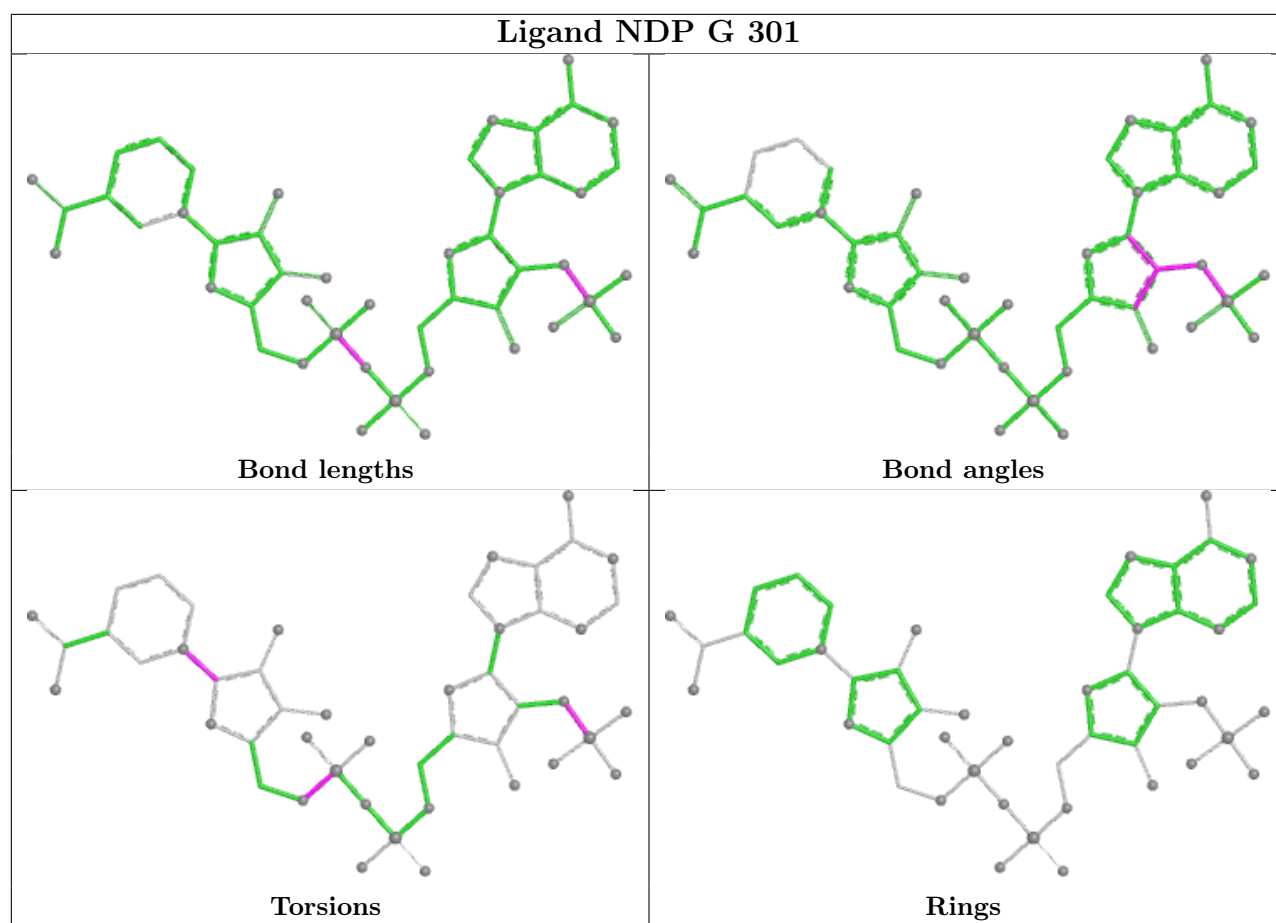


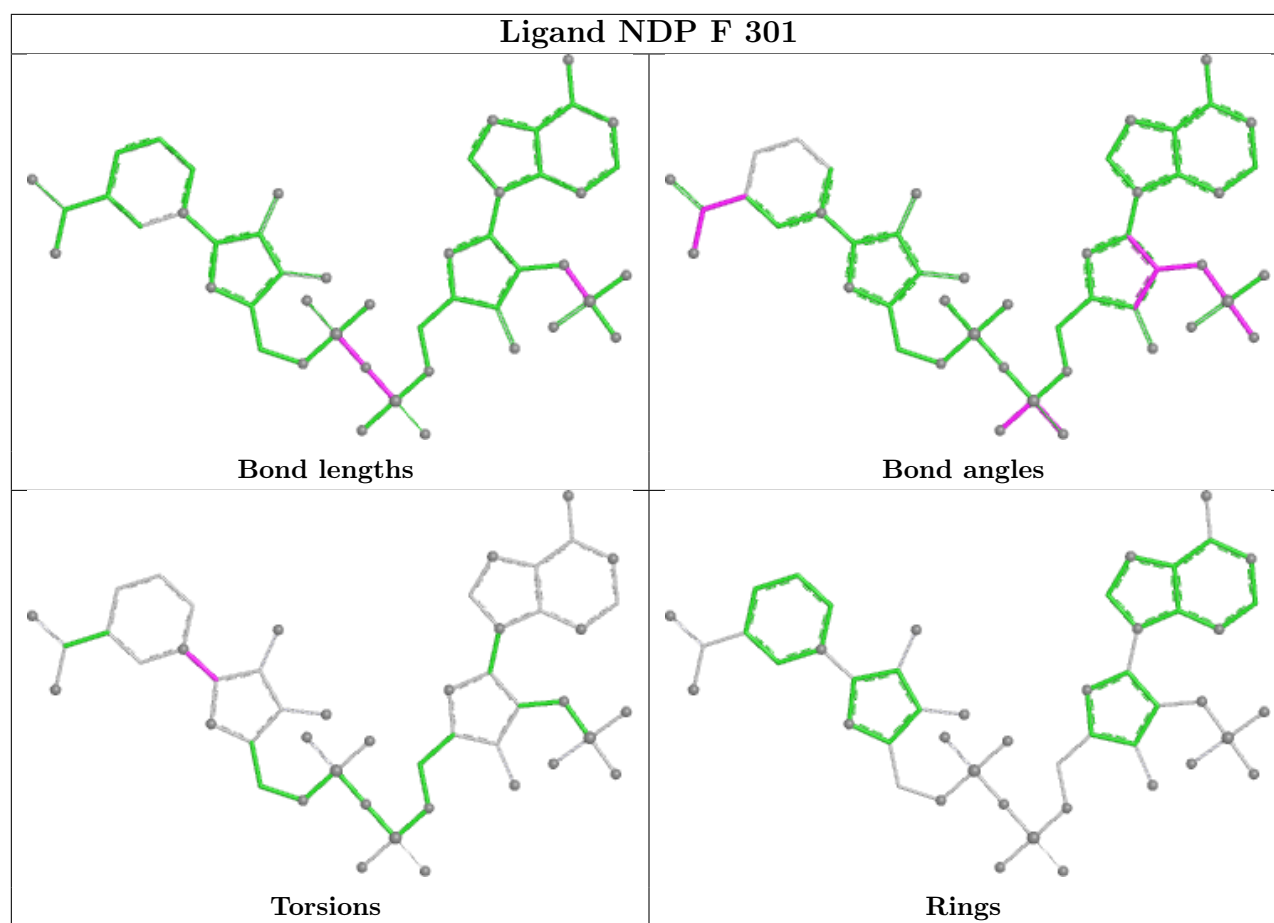












5.7 Other polymers [i](#)

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	287/294 (97%)	0.01	6 (2%) 63 70	13, 26, 44, 67	1 (0%)
1	B	288/294 (97%)	0.15	12 (4%) 40 49	18, 26, 48, 82	0
1	C	293/294 (99%)	-0.08	6 (2%) 65 72	18, 24, 41, 69	1 (0%)
1	D	288/294 (97%)	-0.04	7 (2%) 59 68	13, 24, 43, 65	2 (0%)
1	E	293/294 (99%)	0.19	10 (3%) 48 56	15, 27, 53, 77	1 (0%)
1	F	288/294 (97%)	0.26	7 (2%) 59 68	15, 30, 48, 69	1 (0%)
1	G	293/294 (99%)	0.22	11 (3%) 44 53	16, 28, 46, 76	1 (0%)
1	H	281/294 (95%)	0.19	11 (3%) 43 52	17, 28, 47, 77	2 (0%)
1	I	288/294 (97%)	0.03	6 (2%) 63 70	18, 26, 45, 69	0
All	All	2599/2646 (98%)	0.10	76 (2%) 53 62	13, 27, 47, 82	9 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	-1	PRO	5.3
1	G	0	ALA	4.9
1	E	-1	PRO	4.8
1	C	-5	LEU	4.7
1	G	-4	PHE	4.3
1	E	-4	PHE	4.1
1	H	233	SER	3.9
1	H	238	GLN	3.9
1	E	0	ALA	3.9
1	E	-3	GLN	3.9
1	A	233	SER	3.8
1	E	-2	GLY	3.8
1	A	2	ALA	3.6
1	H	239	ALA	3.5
1	C	-1	PRO	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	241	ALA	3.5
1	B	239	ALA	3.4
1	H	129	PRO	3.3
1	B	230	ASP	3.3
1	B	237	MET	3.2
1	D	230	ASP	3.2
1	G	2	ALA	3.2
1	G	-3	GLN	3.1
1	H	237	MET	3.1
1	F	288	LYS	3.0
1	D	231	GLY	3.0
1	A	230	ASP	2.9
1	H	4	SER	2.8
1	F	1	MET	2.8
1	B	233	SER	2.7
1	G	-2	GLY	2.7
1	G	288	LYS	2.7
1	F	124	PHE	2.7
1	C	0	ALA	2.7
1	G	124	PHE	2.6
1	E	231	GLY	2.6
1	A	232	GLY	2.6
1	D	237	MET	2.6
1	I	237	MET	2.6
1	E	86	ALA	2.6
1	H	124	PHE	2.5
1	B	130	ASP	2.5
1	D	2	ALA	2.5
1	A	231	GLY	2.5
1	E	129	PRO	2.5
1	B	229	GLY	2.5
1	C	130	ASP	2.4
1	E	232	GLY	2.4
1	G	86	ALA	2.4
1	B	238	GLN	2.4
1	B	241	ALA	2.4
1	D	288	LYS	2.4
1	I	288	LYS	2.3
1	I	230	ASP	2.3
1	A	288	LYS	2.3
1	B	231	GLY	2.3
1	I	231	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	218	LEU	2.2
1	D	233	SER	2.2
1	G	1	MET	2.2
1	I	1	MET	2.2
1	F	129	PRO	2.2
1	C	128	GLN	2.2
1	B	288	LYS	2.2
1	H	240	LYS	2.2
1	I	236	ASP	2.1
1	H	215	HIS	2.1
1	H	218	LEU	2.1
1	F	45	ILE	2.1
1	B	232	GLY	2.1
1	F	2	ALA	2.1
1	F	44	ALA	2.1
1	B	1	MET	2.1
1	G	51	PRO	2.1
1	C	-4	PHE	2.1
1	D	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

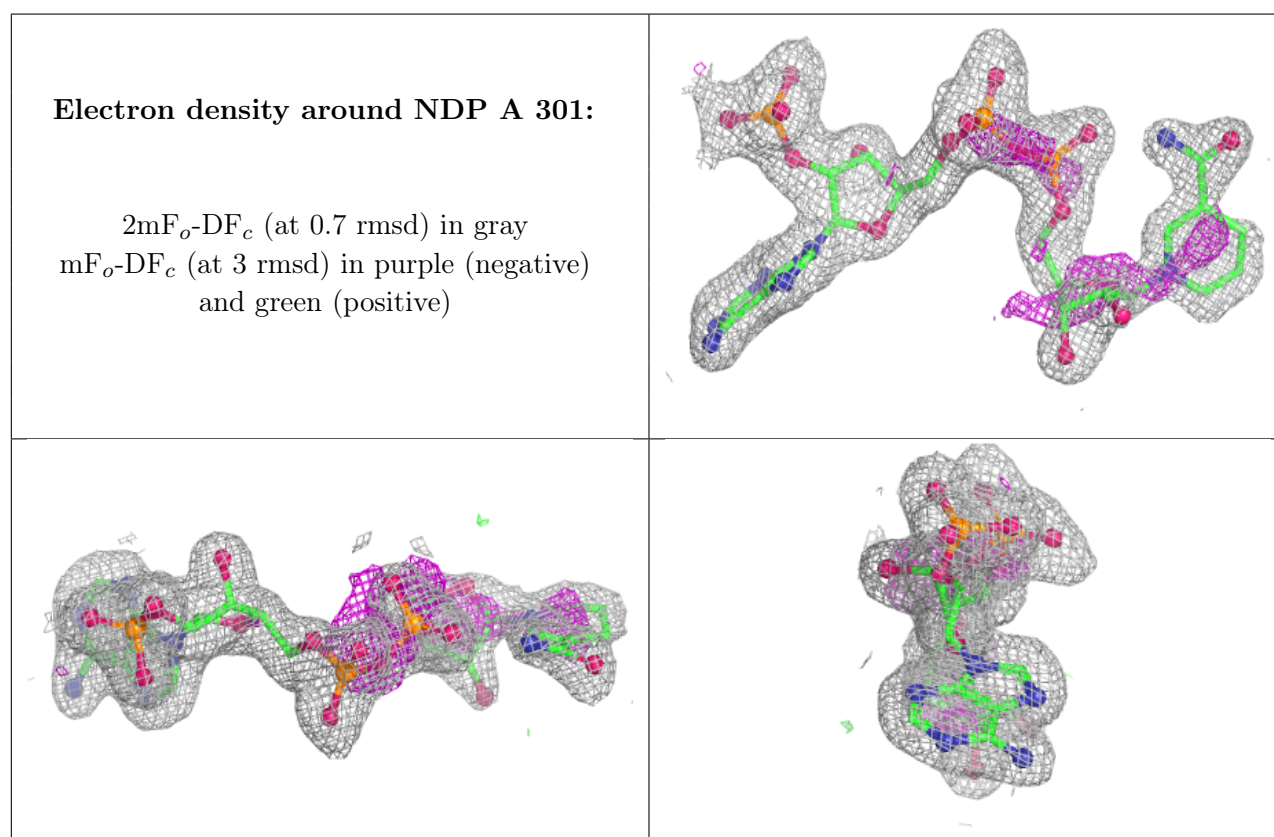
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	A	301	48/48	0.94	0.09	27,36,54,54	0
2	NDP	G	301	48/48	0.94	0.08	30,36,46,50	0
2	NDP	F	301	48/48	0.95	0.08	32,37,46,49	0
2	NDP	I	301	48/48	0.95	0.08	25,32,46,50	0

Continued on next page...

Continued from previous page...

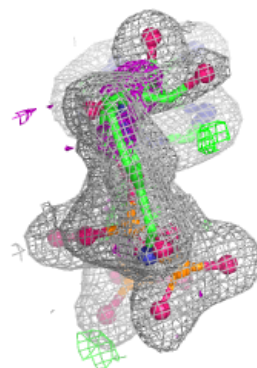
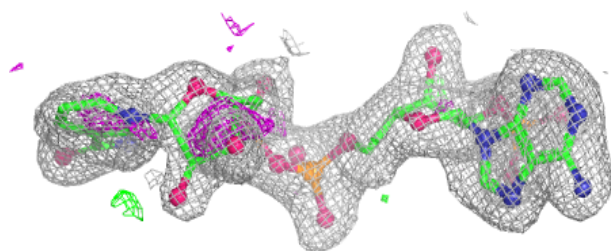
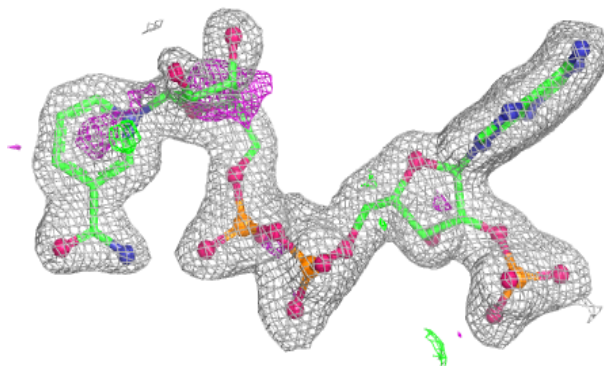
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDP	C	301	48/48	0.96	0.07	23,30,37,38	0
2	NDP	B	301	48/48	0.96	0.07	24,31,38,39	0
2	NDP	H	301	48/48	0.98	0.04	19,23,25,26	0
2	NDP	D	301	48/48	0.99	0.04	16,19,21,23	0
2	NDP	E	301	48/48	0.99	0.04	20,23,27,28	0

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.

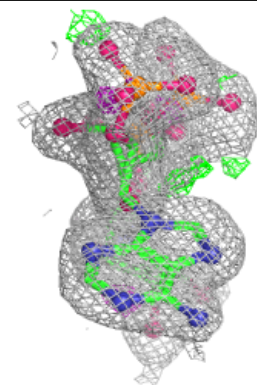
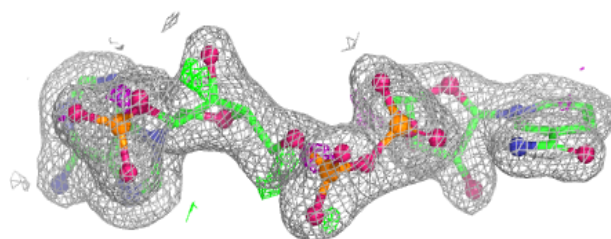
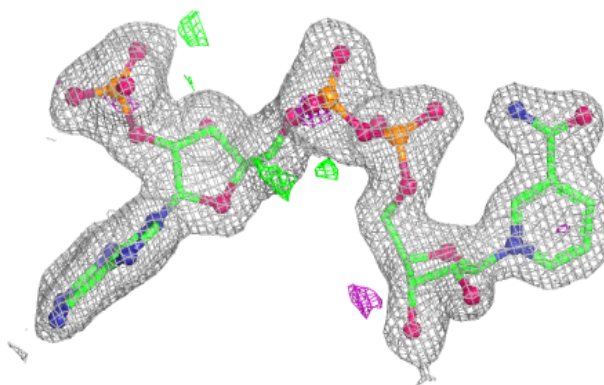


Electron density around NDP G 301:

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

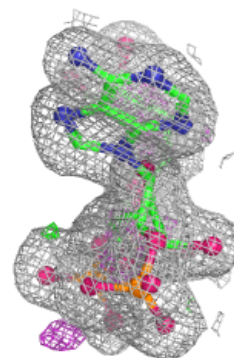
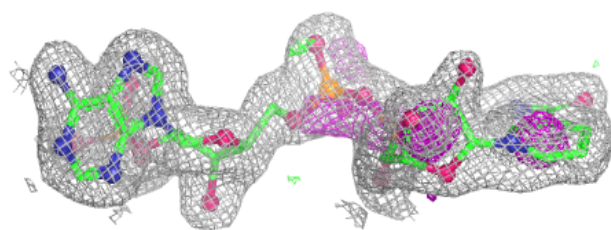
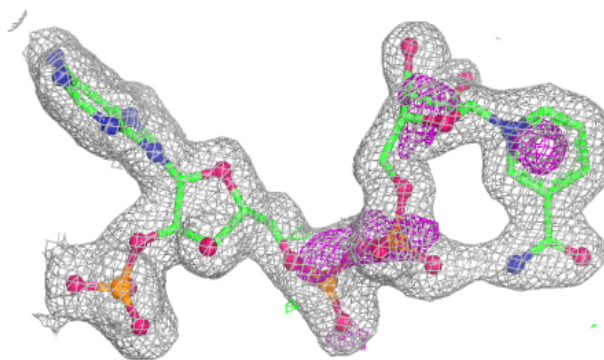
**Electron density around NDP F 301:**

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

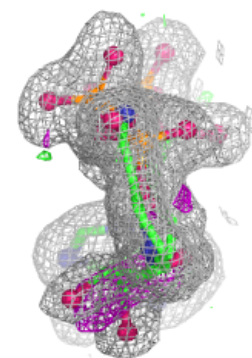
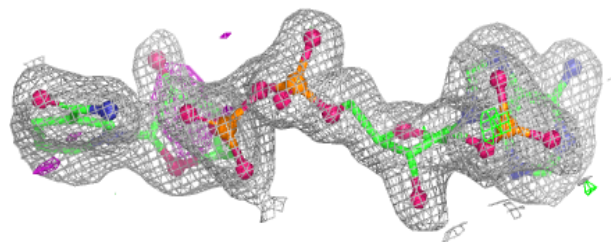
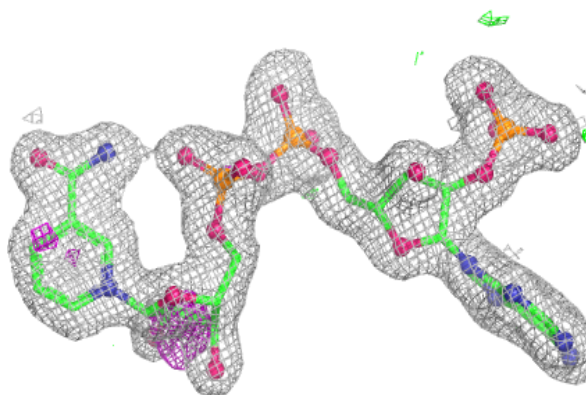


Electron density around NDP I 301:

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

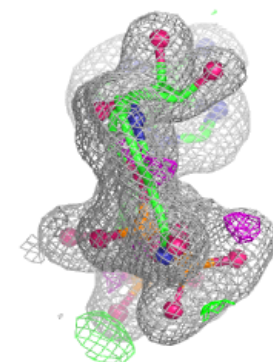
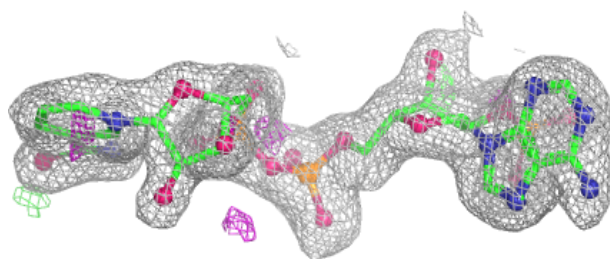
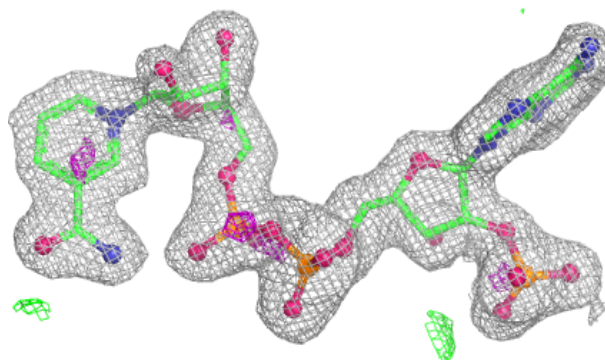
**Electron density around NDP C 301:**

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

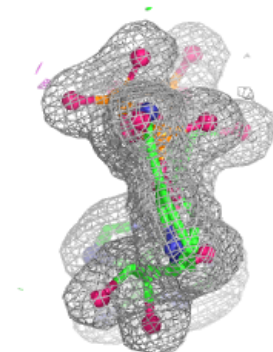
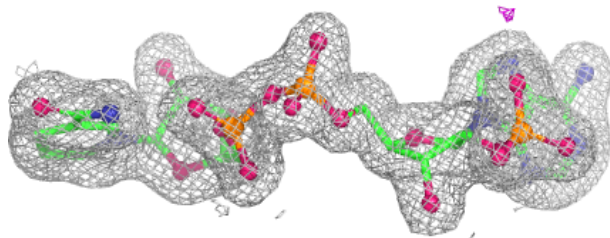
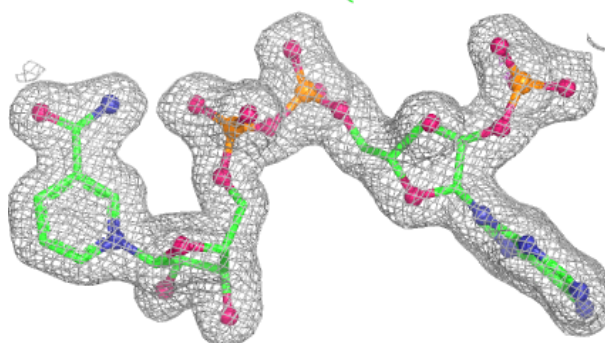


Electron density around NDP B 301:

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

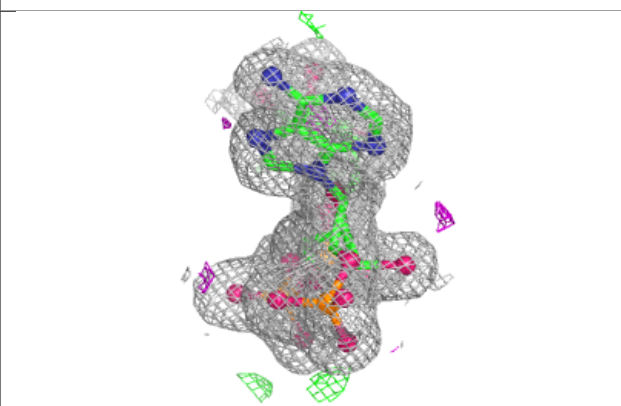
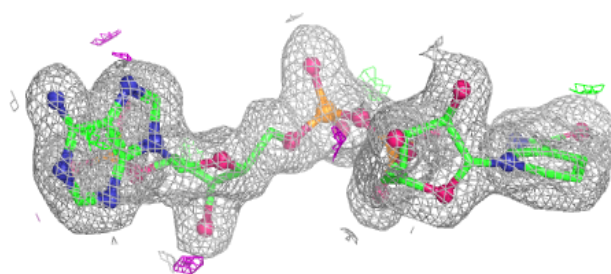
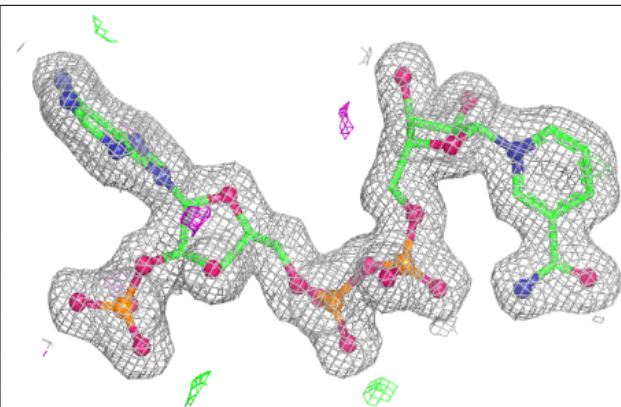
**Electron density around NDP H 301:**

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

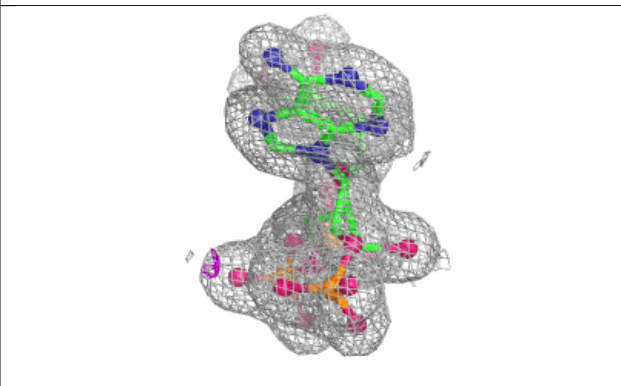
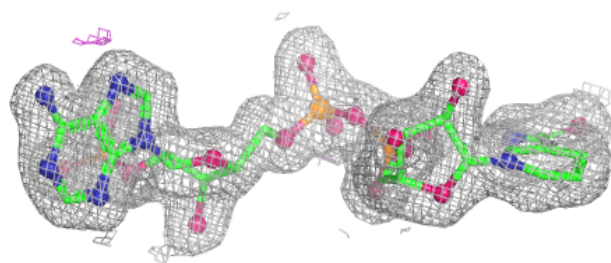
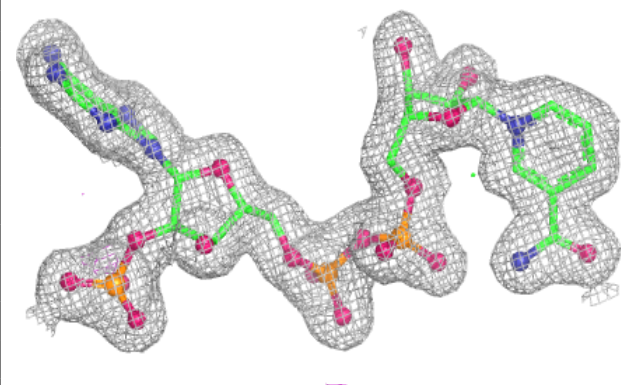


Electron density around NDP D 301:

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

**Electron density around NDP E 301:**

$2mF_o-DF_c$ (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.