



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:07 AM UTC

PDB ID : 4BB5 / pdb_00004bb5
Title : Free-Wilson and Structural Approaches to Co-optimising Human and Rodent Isoform Potency for 11b-Hydroxysteroid Dehydrogenase Type 1 11b-HSD1 Inhibitors
Authors : Goldberg, F.W.; Leach, A.G.; Scott, J.S.; Snelson, W.L.; Groombridge, S.D.; Donald, C.S.; Bennett, S.N.L.; Bodin, C.; Morentin Gutierrez, P.; Gyte, A.C.
Deposited on : 2012-09-20
Resolution : 2.20 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](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

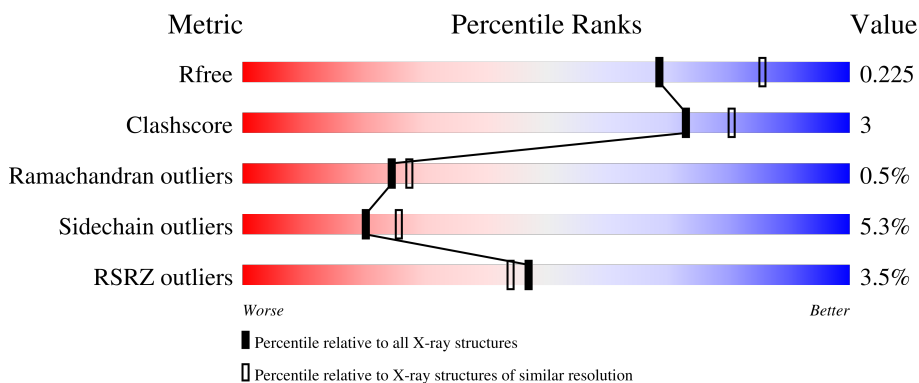
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	292	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 80% 9% • 10%</p>
1	B	292	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 81% 8% • 10%</p>
1	C	292	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 77% 9% • 13%</p>
1	D	292	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">4% 80% 8% • 10%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8641 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 CORTICOSTEROID 11-BETA-DEHYDROGENASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2023	1288	346	374	15	0	0	0
1	B	264	2032	1293	347	377	15	0	0	0
1	C	254	1943	1237	333	359	14	0	0	0
1	D	262	2015	1282	343	375	15	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	LEU	MET	conflict	UNP P28845
A	262	ARG	LEU	conflict	UNP P28845
A	272	SER	CYS	conflict	UNP P28845
A	278	GLU	PHE	conflict	UNP P28845
B	179	LEU	MET	conflict	UNP P28845
B	262	ARG	LEU	conflict	UNP P28845
B	272	SER	CYS	conflict	UNP P28845
B	278	GLU	PHE	conflict	UNP P28845
C	179	LEU	MET	conflict	UNP P28845
C	262	ARG	LEU	conflict	UNP P28845
C	272	SER	CYS	conflict	UNP P28845
C	278	GLU	PHE	conflict	UNP P28845
D	179	LEU	MET	conflict	UNP P28845
D	262	ARG	LEU	conflict	UNP P28845
D	272	SER	CYS	conflict	UNP P28845
D	278	GLU	PHE	conflict	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	24	4	3		
3	B	1	Total	C	N	O	0	0
			31	24	4	3		
3	C	1	Total	C	N	O	0	0
			31	24	4	3		
3	D	1	Total	C	N	O	0	0
			31	24	4	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	89	Total	O	0	0
			89	89		
4	C	90	Total	O	0	0
			90	90		
4	D	35	Total	O	0	0
			35	35		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.78Å 132.48Å 154.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.20 35.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.00-2.20) 99.6 (35.00-2.20)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.20Å)	Xtrriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.182 , 0.220 0.184 , 0.225	Depositor DCC
R_{free} test set	2607 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtrriage
Anisotropy	0.367	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8641	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, HD2

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	0.82	0/2057	1.27	3/2776 (0.1%)
1	B	0.83	0/2066	1.28	3/2788 (0.1%)
1	C	0.83	0/1974	1.25	3/2664 (0.1%)
1	D	0.79	0/2047	1.25	3/2760 (0.1%)
All	All	0.82	0/8144	1.26	12/10988 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ASN	CA-CB-CG	7.47	120.07	112.60
1	A	264	THR	N-CA-C	-6.77	103.97	111.82
1	C	94	GLU	N-CA-C	-5.50	106.07	112.89
1	B	94	GLU	N-CA-C	-5.49	106.08	112.89
1	D	285	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	94	GLU	N-CA-C	-5.29	106.32	112.89
1	A	62	VAL	N-CA-CB	5.26	118.84	112.10
1	D	95	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	268	ILE	N-CA-C	5.15	117.48	111.05
1	C	72	GLN	CA-C-N	5.07	127.48	120.29
1	C	72	GLN	C-N-CA	5.07	127.48	120.29
1	D	268	ILE	N-CA-C	5.04	117.35	111.05

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	2023	0	2070	20	0
1	B	2032	0	2076	17	0
1	C	1943	0	2000	20	0
1	D	2015	0	2059	17	0
2	A	48	0	25	2	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
3	A	31	0	34	2	0
3	B	31	0	34	1	0
3	C	31	0	34	1	0
3	D	31	0	34	2	0
4	A	98	0	0	1	0
4	B	89	0	0	1	0
4	C	90	0	0	1	0
4	D	35	0	0	1	0
All	All	8641	0	8441	54	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 3.

All (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HE2	1:B:140:MET:HE2	1.72	0.70
1:A:87:HIS:HD2	4:A:2007:HOH:O	1.79	0.66
1:C:129:PHE:HB3	1:D:197:ILE:HD11	1.79	0.64
1:D:216:GLY:HA3	1:D:259:ASP:OD1	1.97	0.64
1:C:197:ILE:HD11	1:D:129:PHE:HB3	1.79	0.63
1:A:197:ILE:HD11	1:B:129:PHE:HB3	1.81	0.61
1:A:129:PHE:HB3	1:B:197:ILE:HD11	1.85	0.58
1:C:140:MET:HE2	1:D:140:MET:HE2	1.88	0.56
3:A:1291:HD2:N4	3:A:1291:HD2:H281	2.22	0.54
1:C:129:PHE:HB3	1:D:197:ILE:CD1	2.37	0.54
1:C:197:ILE:CD1	1:D:129:PHE:HB3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:TYR:HB2	1:B:286:MET:HE2	1.90	0.54
1:D:87:HIS:HD2	4:D:2004:HOH:O	1.90	0.54
1:B:87:HIS:HD2	4:B:2014:HOH:O	1.90	0.53
3:D:1292:HD2:N4	3:D:1292:HD2:H281	2.25	0.51
1:C:216:GLY:HA3	1:C:259:ASP:OD1	2.12	0.50
1:A:273:ARG:HG3	1:B:175:VAL:HG22	1.94	0.50
1:C:171:LEU:HD22	1:C:216:GLY:HA2	1.94	0.49
1:A:72:GLN:HG3	1:A:88:TYR:CE2	2.47	0.49
1:B:101:GLN:HG3	1:C:123:ASN:OD1	2.13	0.49
1:A:129:PHE:HB3	1:B:197:ILE:CD1	2.43	0.48
1:A:223:ALA:O	1:A:227:VAL:HB	2.14	0.48
1:A:263:TRP:HE1	1:B:279:LEU:CD2	2.26	0.48
3:A:1291:HD2:H291	1:B:284:TYR:CE1	2.49	0.47
1:C:223:ALA:O	1:C:227:VAL:HB	2.14	0.47
1:D:217:LEU:HD21	1:D:227:VAL:HG11	1.96	0.47
1:A:197:ILE:CD1	1:B:129:PHE:HB3	2.45	0.47
1:C:197:ILE:HD11	1:D:129:PHE:CB	2.45	0.46
1:A:263:TRP:CD1	1:A:263:TRP:C	2.93	0.46
1:A:264:THR:HB	1:B:276:LEU:HD11	1.98	0.46
1:A:261:SER:HB3	1:A:264:THR:HG23	1.98	0.46
1:D:46:ILE:HG22	1:D:50:MET:HE2	1.98	0.45
3:B:1291:HD2:H281	3:B:1291:HD2:N4	2.32	0.45
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.98	0.45
1:B:223:ALA:O	1:B:227:VAL:HB	2.17	0.45
1:C:169:SER:O	2:C:1280:NAP:H6N	2.17	0.45
1:C:175:VAL:HG22	1:D:273:ARG:HG3	1.99	0.44
1:C:273:ARG:HG3	1:D:175:VAL:HG22	2.00	0.44
1:C:129:PHE:CB	1:D:197:ILE:HD11	2.46	0.44
1:A:248:GLY:HA3	1:A:256:VAL:CG2	2.46	0.44
1:C:279:LEU:HD21	1:D:263:TRP:HE3	1.83	0.43
1:D:180:VAL:HG21	3:D:1292:HD2:H122	2.00	0.43
1:A:263:TRP:HE1	1:B:279:LEU:HD21	1.83	0.43
1:C:248:GLY:HA3	1:C:256:VAL:HG21	2.02	0.42
1:A:169:SER:O	2:A:1290:NAP:H6N	2.20	0.42
1:A:185:ALA:HB2	1:B:193:PHE:HB2	2.02	0.42
1:C:87:HIS:HD2	4:C:2018:HOH:O	2.03	0.42
1:C:248:GLY:HA3	1:C:256:VAL:CG2	2.49	0.42
3:C:1281:HD2:H291	1:D:284:TYR:CE1	2.54	0.42
1:C:276:LEU:HD23	1:D:175:VAL:HG21	2.01	0.41
1:A:41:GLY:HA2	2:A:1290:NAP:H1B	2.01	0.41
1:A:133:ILE:HD11	1:B:152:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:PHE:CD2	1:C:247:LYS:HG2	2.56	0.41
1:B:232:HIS:CD2	1:B:232:HIS:N	2.89	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	261/292 (89%)	250 (96%)	11 (4%)	0	100	100
1	B	262/292 (90%)	251 (96%)	8 (3%)	3 (1%)	11	10
1	C	252/292 (86%)	243 (96%)	8 (3%)	1 (0%)	30	34
1	D	258/292 (88%)	247 (96%)	10 (4%)	1 (0%)	30	34
All	All	1033/1168 (88%)	991 (96%)	37 (4%)	5 (0%)	24	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	233	MET
1	D	283	SER
1	B	219	ASP
1	B	283	SER
1	C	219	ASP

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	220/245 (90%)	207 (94%)	13 (6%)	18	22
1	B	221/245 (90%)	210 (95%)	11 (5%)	22	28
1	C	211/245 (86%)	200 (95%)	11 (5%)	21	26
1	D	219/245 (89%)	208 (95%)	11 (5%)	22	28
All	All	871/980 (89%)	825 (95%)	46 (5%)	20	26

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	145	LEU
1	A	160	GLN
1	A	175	VAL
1	A	227	VAL
1	A	233	MET
1	A	240	GLU
1	A	263	TRP
1	A	264	THR
1	A	266	LEU
1	A	276	LEU
1	A	278	GLU
1	A	279	LEU
1	B	97	THR
1	B	127	ASN
1	B	145	LEU
1	B	175	VAL
1	B	207	ASN
1	B	227	VAL
1	B	234	GLN
1	B	262	ARG
1	B	278	GLU
1	B	279	LEU
1	B	285	ASN
1	C	97	THR
1	C	145	LEU
1	C	171	LEU
1	C	175	VAL
1	C	205	ARG
1	C	207	ASN
1	C	227	VAL

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Mol	Chain	Res	Type
1	C	234	GLN
1	C	266	LEU
1	C	278	GLU
1	C	279	LEU
1	D	145	LEU
1	D	160	GLN
1	D	175	VAL
1	D	180	VAL
1	D	205	ARG
1	D	207	ASN
1	D	227	VAL
1	D	233	MET
1	D	266	LEU
1	D	278	GLU
1	D	279	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	87	HIS
1	A	123	ASN
1	A	127	ASN
1	A	207	ASN
1	A	253	GLN
1	A	270	ASN
1	B	72	GLN
1	B	87	HIS
1	B	123	ASN
1	B	127	ASN
1	B	130	HIS
1	B	135	HIS
1	B	207	ASN
1	B	253	GLN
1	B	270	ASN
1	C	87	HIS
1	C	101	GLN
1	C	127	ASN
1	C	130	HIS
1	C	135	HIS
1	C	207	ASN
1	C	270	ASN

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Mol	Chain	Res	Type
1	D	77	HIS
1	D	87	HIS
1	D	101	GLN
1	D	123	ASN
1	D	127	ASN
1	D	130	HIS
1	D	160	GLN
1	D	207	ASN
1	D	270	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	HD2	B	1291	-	36,36,36	1.24	2 (5%)	45,54,54	1.21	5 (11%)
3	HD2	A	1291	-	36,36,36	1.11	2 (5%)	45,54,54	1.65	7 (15%)
2	NAP	A	1290	-	50,52,52	3.49	23 (46%)	71,80,80	2.58	30 (42%)
3	HD2	D	1292	-	36,36,36	1.11	3 (8%)	45,54,54	1.53	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	B	1290	-	50,52,52	3.83	29 (58%)	71,80,80	2.90	33 (46%)
3	HD2	C	1281	-	36,36,36	1.17	2 (5%)	45,54,54	1.56	9 (20%)
2	NAP	D	1291	-	50,52,52	3.45	27 (54%)	71,80,80	2.94	36 (50%)
2	NAP	C	1280	-	50,52,52	3.40	25 (50%)	71,80,80	2.72	33 (46%)

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	HD2	B	1291	-	-	3/16/61/61	0/7/6/6
3	HD2	A	1291	-	-	4/16/61/61	0/7/6/6
2	NAP	A	1290	-	-	6/35/67/67	0/5/5/5
3	HD2	D	1292	-	-	3/16/61/61	0/7/6/6
2	NAP	B	1290	-	-	4/35/67/67	0/5/5/5
3	HD2	C	1281	-	-	3/16/61/61	0/7/6/6
2	NAP	D	1291	-	-	5/35/67/67	0/5/5/5
2	NAP	C	1280	-	-	6/35/67/67	0/5/5/5

All (113) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1290	NAP	C4N-C3N	9.96	1.54	1.39
2	C	1280	NAP	C4N-C3N	9.29	1.53	1.39
2	A	1290	NAP	C4N-C3N	9.09	1.53	1.39
2	A	1290	NAP	PA-O3	8.46	1.68	1.59
2	D	1291	NAP	C4N-C3N	8.28	1.52	1.39
2	B	1290	NAP	C3B-C4B	8.27	1.74	1.53
2	D	1291	NAP	O4B-C4B	7.96	1.62	1.45
2	B	1290	NAP	O4B-C4B	7.80	1.62	1.45
2	A	1290	NAP	C3B-C4B	7.32	1.71	1.53
2	A	1290	NAP	O4B-C4B	7.05	1.60	1.45
2	B	1290	NAP	C2N-N1N	7.04	1.42	1.35
2	C	1280	NAP	C2N-N1N	6.95	1.42	1.35
2	B	1290	NAP	C3D-C4D	6.86	1.70	1.53
2	D	1291	NAP	C3B-C4B	6.78	1.70	1.53
2	D	1291	NAP	C2N-N1N	6.73	1.42	1.35
2	B	1290	NAP	C5B-C4B	6.71	1.71	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1280	NAP	C3B-C4B	6.55	1.69	1.53
2	C	1280	NAP	O4B-C4B	6.49	1.59	1.45
2	B	1290	NAP	O3D-C3D	6.25	1.58	1.43
2	A	1290	NAP	C2N-N1N	6.15	1.41	1.35
2	C	1280	NAP	C3D-C4D	6.14	1.68	1.53
2	A	1290	NAP	C3D-C4D	6.07	1.68	1.53
2	B	1290	NAP	PA-O3	6.07	1.66	1.59
3	B	1291	HD2	C5-N7	5.86	1.41	1.34
2	D	1291	NAP	C3D-C4D	5.78	1.67	1.53
2	C	1280	NAP	C5B-C4B	5.76	1.68	1.51
2	D	1291	NAP	C8A-N9A	5.69	1.47	1.37
2	A	1290	NAP	O7N-C7N	-5.61	1.13	1.24
3	C	1281	HD2	C5-N7	5.42	1.41	1.34
2	A	1290	NAP	C5B-C4B	5.39	1.67	1.51
2	B	1290	NAP	C6A-N1A	5.37	1.50	1.35
2	C	1280	NAP	C7N-N7N	5.33	1.42	1.33
2	D	1291	NAP	C5B-C4B	5.25	1.67	1.51
2	D	1291	NAP	C6A-N1A	5.25	1.50	1.35
2	B	1290	NAP	O4B-C1B	-5.04	1.30	1.42
2	C	1280	NAP	C6A-N1A	5.02	1.49	1.35
2	B	1290	NAP	C2D-C3D	-5.01	1.39	1.53
2	D	1291	NAP	C2B-C1B	4.95	1.65	1.53
3	A	1291	HD2	C5-N7	4.91	1.40	1.34
2	B	1290	NAP	O7N-C7N	-4.84	1.15	1.24
2	A	1290	NAP	C6A-N1A	4.79	1.49	1.35
2	C	1280	NAP	C8A-N9A	4.77	1.45	1.37
2	A	1290	NAP	C2D-C3D	-4.71	1.40	1.53
2	B	1290	NAP	O4D-C1D	-4.63	1.34	1.40
2	D	1291	NAP	O3D-C3D	4.62	1.54	1.43
2	A	1290	NAP	C5A-N7A	-4.61	1.30	1.39
2	B	1290	NAP	C8A-N9A	4.59	1.45	1.37
2	A	1290	NAP	C2B-C1B	4.48	1.64	1.53
3	D	1292	HD2	C5-N7	4.46	1.39	1.34
2	D	1291	NAP	O4B-C1B	-4.40	1.31	1.42
2	D	1291	NAP	O7N-C7N	-4.40	1.15	1.24
2	C	1280	NAP	O3D-C3D	4.37	1.53	1.43
2	A	1290	NAP	O4B-C1B	-4.32	1.32	1.42
2	B	1290	NAP	C2B-C1B	4.25	1.63	1.53
2	C	1280	NAP	C2D-C3D	-4.10	1.42	1.53
2	C	1280	NAP	PA-O3	4.04	1.63	1.59
2	C	1280	NAP	C2B-C1B	3.96	1.62	1.53
2	D	1291	NAP	C2N-C3N	3.94	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1291	NAP	PA-O3	3.82	1.63	1.59
2	A	1290	NAP	O4D-C1D	-3.82	1.35	1.40
2	C	1280	NAP	C2N-C3N	3.79	1.45	1.39
2	C	1280	NAP	O4B-C1B	-3.77	1.33	1.42
2	D	1291	NAP	C2D-C3D	-3.71	1.43	1.53
2	A	1290	NAP	C2N-C3N	3.69	1.44	1.39
2	C	1280	NAP	C5A-C6A	3.68	1.51	1.41
2	B	1290	NAP	C2N-C3N	3.63	1.44	1.39
2	A	1290	NAP	C8A-N9A	3.57	1.43	1.37
2	B	1290	NAP	PN-O3	3.53	1.63	1.59
2	D	1291	NAP	C5A-C6A	3.44	1.50	1.41
2	C	1280	NAP	C6N-C5N	3.29	1.45	1.38
2	D	1291	NAP	O4D-C1D	-3.22	1.36	1.40
2	D	1291	NAP	C4A-N3A	3.05	1.40	1.34
2	C	1280	NAP	C5A-C4A	3.05	1.44	1.39
2	B	1290	NAP	O4D-C4D	2.92	1.51	1.45
2	A	1290	NAP	C4A-N9A	-2.91	1.31	1.37
2	D	1291	NAP	C7N-N7N	2.89	1.38	1.33
2	C	1280	NAP	C2A-N1A	2.86	1.39	1.33
2	D	1291	NAP	C6N-C5N	2.86	1.44	1.38
2	D	1291	NAP	O4D-C4D	2.83	1.51	1.45
2	B	1290	NAP	C7N-N7N	2.83	1.38	1.33
2	A	1290	NAP	O3D-C3D	2.83	1.50	1.43
2	B	1290	NAP	C5A-N7A	-2.77	1.34	1.39
2	B	1290	NAP	C4A-N9A	-2.70	1.32	1.37
2	C	1280	NAP	C5A-N7A	-2.61	1.34	1.39
3	D	1292	HD2	C2-C3	-2.60	1.38	1.41
3	C	1281	HD2	C2-C3	-2.56	1.38	1.41
2	D	1291	NAP	C1B-N9A	2.55	1.53	1.46
2	D	1291	NAP	C4A-N9A	-2.54	1.32	1.37
2	C	1280	NAP	C1B-N9A	2.51	1.53	1.46
2	B	1290	NAP	C5D-C4D	-2.51	1.44	1.51
2	C	1280	NAP	P2B-O2B	2.50	1.63	1.59
2	D	1291	NAP	P2B-O1X	2.49	1.58	1.50
2	C	1280	NAP	O4D-C4D	2.49	1.50	1.45
2	B	1290	NAP	O2D-C2D	2.48	1.49	1.43
2	C	1280	NAP	C4A-N9A	-2.48	1.32	1.37
3	A	1291	HD2	C2-C3	-2.46	1.38	1.41
2	B	1290	NAP	C3N-C7N	-2.45	1.46	1.50
2	D	1291	NAP	PN-O3	-2.42	1.56	1.59
2	A	1290	NAP	O4D-C4D	2.39	1.50	1.45
2	A	1290	NAP	O2D-C2D	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1280	NAP	PA-O2A	-2.33	1.44	1.55
2	B	1290	NAP	O3B-C3B	-2.28	1.37	1.43
2	B	1290	NAP	P2B-O1X	2.20	1.57	1.50
2	B	1290	NAP	PA-O5B	-2.18	1.50	1.59
3	B	1291	HD2	C2-C3	-2.15	1.39	1.41
2	D	1291	NAP	O3B-C3B	-2.11	1.37	1.43
2	B	1290	NAP	C5A-C6A	2.11	1.46	1.41
2	A	1290	NAP	C5A-C6A	2.11	1.46	1.41
2	A	1290	NAP	C6N-C5N	2.06	1.42	1.38
2	A	1290	NAP	PA-O5B	-2.04	1.51	1.59
2	B	1290	NAP	PN-O1N	-2.03	1.43	1.50
2	D	1291	NAP	PA-O5B	-2.02	1.51	1.59
3	D	1292	HD2	C31-C27	-2.01	1.49	1.52

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1291	NAP	N3A-C2A-N1A	-7.58	117.11	128.58
2	B	1290	NAP	C2B-C1B-N9A	-7.28	101.77	113.75
2	A	1290	NAP	C2B-C1B-N9A	-7.17	101.95	113.75
2	C	1280	NAP	O3X-P2B-O2X	6.92	133.76	107.80
2	D	1291	NAP	C2B-C1B-N9A	-6.82	102.53	113.75
2	B	1290	NAP	C5N-C6N-N1N	6.80	129.65	120.38
2	D	1291	NAP	O3X-P2B-O2X	6.66	132.78	107.80
2	A	1290	NAP	O3X-P2B-O2X	6.29	131.38	107.80
2	B	1290	NAP	O3B-C3B-C4B	-6.17	93.35	111.08
2	C	1280	NAP	O3B-C3B-C4B	-6.10	93.56	111.08
2	B	1290	NAP	N3A-C2A-N1A	-6.08	119.38	128.58
2	B	1290	NAP	O3X-P2B-O2X	5.97	130.19	107.80
3	C	1281	HD2	C31-C27-N7	-5.69	105.23	112.03
2	A	1290	NAP	N3A-C2A-N1A	-5.67	120.00	128.58
2	A	1290	NAP	O4B-C1B-C2B	-5.67	96.82	106.59
3	A	1291	HD2	C5-N7-C27	-5.58	115.65	124.32
2	D	1291	NAP	O3B-C3B-C4B	-5.47	95.38	111.08
2	C	1280	NAP	C2B-C1B-N9A	-5.44	104.81	113.75
3	A	1291	HD2	C31-C27-N7	-5.29	105.70	112.03
2	D	1291	NAP	C5N-C6N-N1N	5.26	127.56	120.38
2	C	1280	NAP	O2B-P2B-O1X	-5.21	90.76	109.33
2	D	1291	NAP	O3D-C3D-C4D	-5.11	96.39	111.08
2	D	1291	NAP	O2X-P2B-O1X	-5.10	90.95	110.83
2	A	1290	NAP	O4B-C4B-C5B	-5.09	93.02	109.33
2	C	1280	NAP	N3A-C2A-N1A	-5.09	120.88	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1290	NAP	O3D-C3D-C4D	-5.04	96.60	111.08
2	B	1290	NAP	O2X-P2B-O1X	-5.00	91.34	110.83
2	C	1280	NAP	O5B-C5B-C4B	-4.95	92.15	108.99
2	D	1291	NAP	O4B-C1B-C2B	-4.90	98.15	106.59
2	C	1280	NAP	O2X-P2B-O1X	-4.88	91.82	110.83
2	D	1291	NAP	O3X-P2B-O1X	-4.88	91.82	110.83
2	C	1280	NAP	O3-PA-O1A	-4.81	96.22	110.70
2	B	1290	NAP	C6N-C5N-C4N	-4.76	112.59	119.45
2	C	1280	NAP	O3D-C3D-C4D	-4.58	97.94	111.08
2	D	1291	NAP	N9A-C8A-N7A	-4.57	107.46	113.94
2	A	1290	NAP	C5N-C6N-N1N	4.54	126.57	120.38
2	B	1290	NAP	O5B-C5B-C4B	-4.50	93.65	108.99
2	B	1290	NAP	C4D-O4D-C1D	-4.50	105.80	109.92
2	D	1291	NAP	O4B-C4B-C5B	-4.50	94.92	109.33
2	C	1280	NAP	O4B-C4B-C5B	-4.46	95.06	109.33
2	A	1290	NAP	O2X-P2B-O1X	-4.45	93.50	110.83
3	D	1292	HD2	C31-C27-N7	-4.45	106.72	112.03
2	A	1290	NAP	C2A-N1A-C6A	4.44	126.03	118.73
2	D	1291	NAP	O5B-C5B-C4B	-4.37	94.11	108.99
2	B	1290	NAP	O2B-P2B-O1X	-4.34	93.87	109.33
2	A	1290	NAP	O5B-C5B-C4B	-4.27	94.46	108.99
2	B	1290	NAP	O4B-C4B-C5B	-4.20	95.87	109.33
2	C	1280	NAP	O4B-C1B-C2B	-4.19	99.37	106.59
2	C	1280	NAP	O2N-PN-O1N	4.18	131.87	112.44
3	D	1292	HD2	C12-C8-C3	-4.03	108.58	114.39
2	D	1291	NAP	C2A-N3A-C4A	4.01	121.61	111.83
2	B	1290	NAP	N9A-C8A-N7A	-3.99	108.27	113.94
2	B	1290	NAP	O2B-C2B-C3B	-3.97	97.44	111.68
2	D	1291	NAP	O2B-P2B-O1X	-3.96	95.22	109.33
3	C	1281	HD2	C5-N7-C27	-3.96	118.17	124.32
2	A	1290	NAP	O3B-C3B-C4B	-3.94	99.77	111.08
2	D	1291	NAP	C2A-N1A-C6A	3.93	125.18	118.73
2	A	1290	NAP	O3-PA-O1A	-3.87	99.08	110.70
2	B	1290	NAP	O3X-P2B-O1X	-3.81	96.00	110.83
2	B	1290	NAP	C2A-N1A-C6A	3.71	124.82	118.73
2	D	1291	NAP	C6N-C5N-C4N	-3.69	114.13	119.45
2	C	1280	NAP	C2A-N1A-C6A	3.68	124.77	118.73
3	B	1291	HD2	C12-C8-C3	-3.65	109.12	114.39
2	C	1280	NAP	C3N-C7N-N7N	-3.60	113.30	117.74
3	D	1292	HD2	C5-N7-C27	-3.58	118.75	124.32
3	B	1291	HD2	C31-C27-N7	-3.58	107.76	112.03
2	C	1280	NAP	C5N-C6N-N1N	3.56	125.24	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1291	NAP	O3-PA-O1A	-3.55	100.02	110.70
2	D	1291	NAP	C6N-N1N-C2N	-3.53	118.87	121.88
2	B	1290	NAP	O4B-C4B-C3B	-3.53	98.15	105.15
3	C	1281	HD2	C12-C8-C9	3.52	108.90	102.87
2	C	1280	NAP	O2B-C2B-C3B	-3.51	99.09	111.68
2	B	1290	NAP	C2N-N1N-C1D	3.50	126.86	119.13
2	A	1290	NAP	O2B-P2B-O1X	-3.39	97.25	109.33
2	A	1290	NAP	O3D-C3D-C4D	-3.32	101.54	111.08
2	C	1280	NAP	O3X-P2B-O1X	-3.31	97.93	110.83
2	C	1280	NAP	C6N-N1N-C1D	-3.31	113.23	119.73
3	A	1291	HD2	C12-C8-C3	-3.29	109.65	114.39
2	D	1291	NAP	O2N-PN-O1N	3.23	127.48	112.44
2	B	1290	NAP	O4B-C1B-C2B	-3.21	101.07	106.59
3	D	1292	HD2	O14-C13-N15	3.20	128.55	122.47
2	C	1280	NAP	O2A-PA-O1A	3.20	127.33	112.44
2	C	1280	NAP	O7N-C7N-N7N	3.19	127.23	122.62
2	D	1291	NAP	C2N-N1N-C1D	3.11	126.00	119.13
2	B	1290	NAP	C2A-N3A-C4A	3.10	119.40	111.83
2	B	1290	NAP	C6N-N1N-C1D	-3.09	113.67	119.73
3	D	1292	HD2	C12-C8-C9	3.08	108.14	102.87
2	D	1291	NAP	O2X-P2B-O2B	3.07	117.81	105.85
2	A	1290	NAP	O2B-C2B-C3B	-3.07	100.67	111.68
2	D	1291	NAP	O7N-C7N-N7N	3.06	127.03	122.62
2	C	1280	NAP	C4D-O4D-C1D	-3.05	107.14	109.92
2	B	1290	NAP	O7N-C7N-N7N	3.04	127.01	122.62
2	D	1291	NAP	C4D-O4D-C1D	-3.02	107.16	109.92
2	A	1290	NAP	O3X-P2B-O1X	-3.02	99.09	110.83
2	C	1280	NAP	C2N-N1N-C1D	2.99	125.74	119.13
2	A	1290	NAP	C2A-N3A-C4A	2.90	118.92	111.83
2	A	1290	NAP	C4D-O4D-C1D	-2.90	107.27	109.92
2	A	1290	NAP	C5A-N7A-C8A	2.88	107.97	103.45
2	D	1291	NAP	C5B-C4B-C3B	-2.87	104.89	115.21
2	A	1290	NAP	O7N-C7N-C3N	-2.85	116.12	119.60
2	B	1290	NAP	C5B-C4B-C3B	-2.84	105.00	115.21
3	D	1292	HD2	C9-C8-C3	-2.84	110.30	114.39
2	A	1290	NAP	N9A-C8A-N7A	-2.83	109.91	113.94
2	B	1290	NAP	C6N-N1N-C2N	-2.83	119.47	121.88
2	D	1291	NAP	O2B-C2B-C3B	-2.83	101.52	111.68
2	B	1290	NAP	C2D-C3D-C4D	-2.82	97.16	102.61
2	C	1280	NAP	N9A-C8A-N7A	-2.80	109.96	113.94
2	A	1290	NAP	C6N-C5N-C4N	-2.79	115.42	119.45
2	C	1280	NAP	C2A-N3A-C4A	2.79	118.64	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1291	NAP	O2N-PN-O3	-2.73	99.90	107.27
2	B	1290	NAP	C5N-C4N-C3N	2.71	123.03	120.36
2	C	1280	NAP	O2X-P2B-O2B	2.70	116.36	105.85
2	B	1290	NAP	O2X-P2B-O2B	2.70	116.35	105.85
3	C	1281	HD2	C12-C8-C3	-2.68	110.52	114.39
3	C	1281	HD2	O14-C13-N15	2.64	127.49	122.47
2	B	1290	NAP	C4A-N9A-C1B	-2.63	120.48	126.63
2	D	1291	NAP	O4B-C4B-C3B	-2.62	99.96	105.15
2	C	1280	NAP	C6N-C5N-C4N	-2.61	115.69	119.45
2	B	1290	NAP	O5D-PN-O1N	2.58	119.16	108.94
2	D	1291	NAP	C5N-C4N-C3N	2.58	122.90	120.36
2	A	1290	NAP	O2N-PN-O1N	2.56	124.37	112.44
3	A	1291	HD2	C12-C8-C9	2.56	107.26	102.87
2	D	1291	NAP	C4A-N9A-C1B	-2.54	120.69	126.63
2	B	1290	NAP	C1B-N9A-C8A	2.53	132.70	127.09
2	D	1291	NAP	C5A-N7A-C8A	2.52	107.41	103.45
2	A	1290	NAP	C2N-N1N-C1D	2.52	124.69	119.13
2	A	1290	NAP	C6N-N1N-C2N	-2.48	119.76	121.88
2	A	1290	NAP	O4B-C4B-C3B	-2.48	100.24	105.15
3	C	1281	HD2	N6-C5-N4	-2.45	124.05	126.42
2	B	1290	NAP	O7N-C7N-C3N	-2.45	116.60	119.60
2	C	1280	NAP	C5A-N7A-C8A	2.39	107.20	103.45
3	C	1281	HD2	C21-C16-C17	2.37	112.14	108.79
2	C	1280	NAP	C4B-O4B-C1B	2.34	114.64	109.47
2	D	1291	NAP	C6N-N1N-C1D	-2.34	115.13	119.73
2	A	1290	NAP	C2B-C3B-C4B	-2.33	96.99	101.99
2	B	1290	NAP	O2N-PN-O1N	2.32	123.26	112.44
2	D	1291	NAP	C3N-C7N-N7N	-2.30	114.90	117.74
2	C	1280	NAP	C1B-N9A-C8A	2.28	132.16	127.09
2	C	1280	NAP	C2B-C3B-C4B	-2.23	97.20	101.99
2	A	1290	NAP	O7N-C7N-N7N	2.23	125.84	122.62
3	A	1291	HD2	C2-C13-N15	-2.21	111.87	116.67
2	B	1290	NAP	C5A-N7A-C8A	2.20	106.91	103.45
3	A	1291	HD2	C9-C8-C3	-2.19	111.23	114.39
2	C	1280	NAP	C4A-N9A-C1B	-2.17	121.55	126.63
2	A	1290	NAP	C6N-N1N-C1D	-2.13	115.55	119.73
2	D	1291	NAP	C6A-C5A-C4A	-2.13	114.27	117.18
3	C	1281	HD2	C9-C8-C3	-2.12	111.33	114.39
2	C	1280	NAP	O2N-PN-O3	-2.12	101.54	107.27
2	D	1291	NAP	O2D-C2D-C3D	-2.09	105.11	111.82
3	B	1291	HD2	C11-C12-C8	2.09	108.43	104.79
2	D	1291	NAP	O3-PN-O1N	-2.08	104.44	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1291	HD2	C10-C9-C8	2.08	108.41	104.79
2	D	1291	NAP	C4A-N9A-C8A	2.07	107.91	105.74
3	C	1281	HD2	C2-C13-N15	-2.06	112.20	116.67
3	B	1291	HD2	C12-C8-C9	2.06	106.40	102.87
3	B	1291	HD2	O14-C13-N15	2.05	126.37	122.47
2	A	1290	NAP	C1B-N9A-C8A	2.03	131.59	127.09
2	A	1290	NAP	P2B-O2B-C2B	2.02	128.84	123.43
2	C	1280	NAP	O4B-C1B-N9A	2.02	111.97	108.09
3	D	1292	HD2	C2-C13-N15	-2.01	112.30	116.67

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1290	NAP	C5D-O5D-PN-O3
2	A	1290	NAP	C5D-O5D-PN-O1N
2	B	1290	NAP	C5D-O5D-PN-O3
2	B	1290	NAP	C5D-O5D-PN-O1N
2	C	1280	NAP	C5D-O5D-PN-O3
2	C	1280	NAP	C5D-O5D-PN-O1N
2	D	1291	NAP	C5D-O5D-PN-O3
2	D	1291	NAP	C5D-O5D-PN-O1N
3	A	1291	HD2	N4-C5-N7-C27
3	A	1291	HD2	N6-C5-N7-C27
3	A	1291	HD2	C28-C27-N7-C5
3	B	1291	HD2	N4-C5-N7-C27
3	B	1291	HD2	N6-C5-N7-C27
3	B	1291	HD2	C28-C27-N7-C5
3	C	1281	HD2	N4-C5-N7-C27
3	C	1281	HD2	N6-C5-N7-C27
3	C	1281	HD2	C28-C27-N7-C5
3	D	1292	HD2	N4-C5-N7-C27
3	D	1292	HD2	N6-C5-N7-C27
3	D	1292	HD2	C28-C27-N7-C5
2	C	1280	NAP	PN-O3-PA-O1A
2	A	1290	NAP	C5D-O5D-PN-O2N
2	C	1280	NAP	C5D-O5D-PN-O2N
2	A	1290	NAP	PN-O3-PA-O2A
2	B	1290	NAP	PN-O3-PA-O1A
2	B	1290	NAP	PN-O3-PA-O2A
2	C	1280	NAP	PN-O3-PA-O2A
2	D	1291	NAP	PN-O3-PA-O2A

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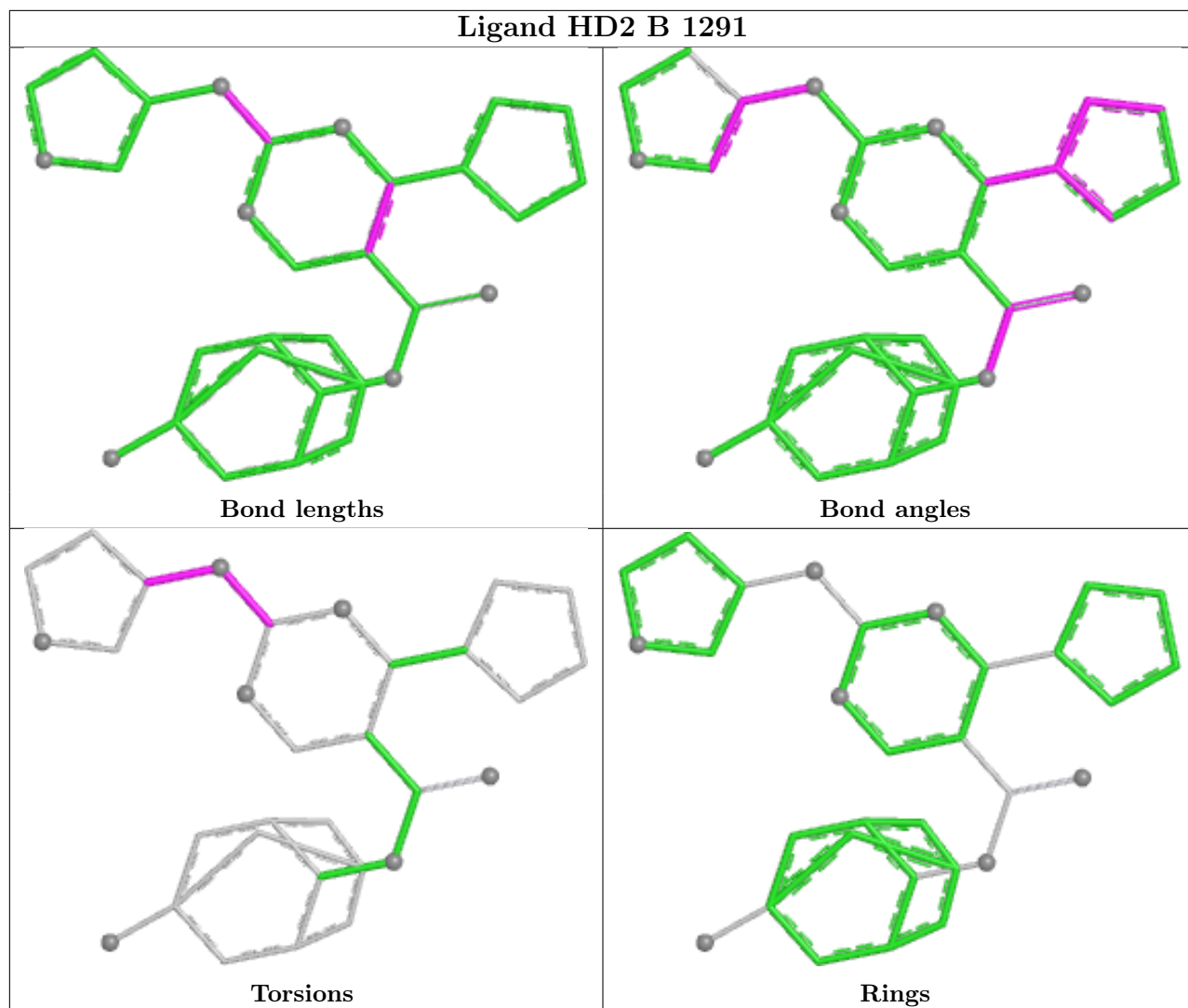
Mol	Chain	Res	Type	Atoms
2	A	1290	NAP	C2B-O2B-P2B-O1X
2	C	1280	NAP	C2B-O2B-P2B-O1X
2	A	1290	NAP	PN-O3-PA-O1A
3	A	1291	HD2	C21-C16-N15-C13
2	D	1291	NAP	O4B-C4B-C5B-O5B
2	D	1291	NAP	PN-O3-PA-O1A

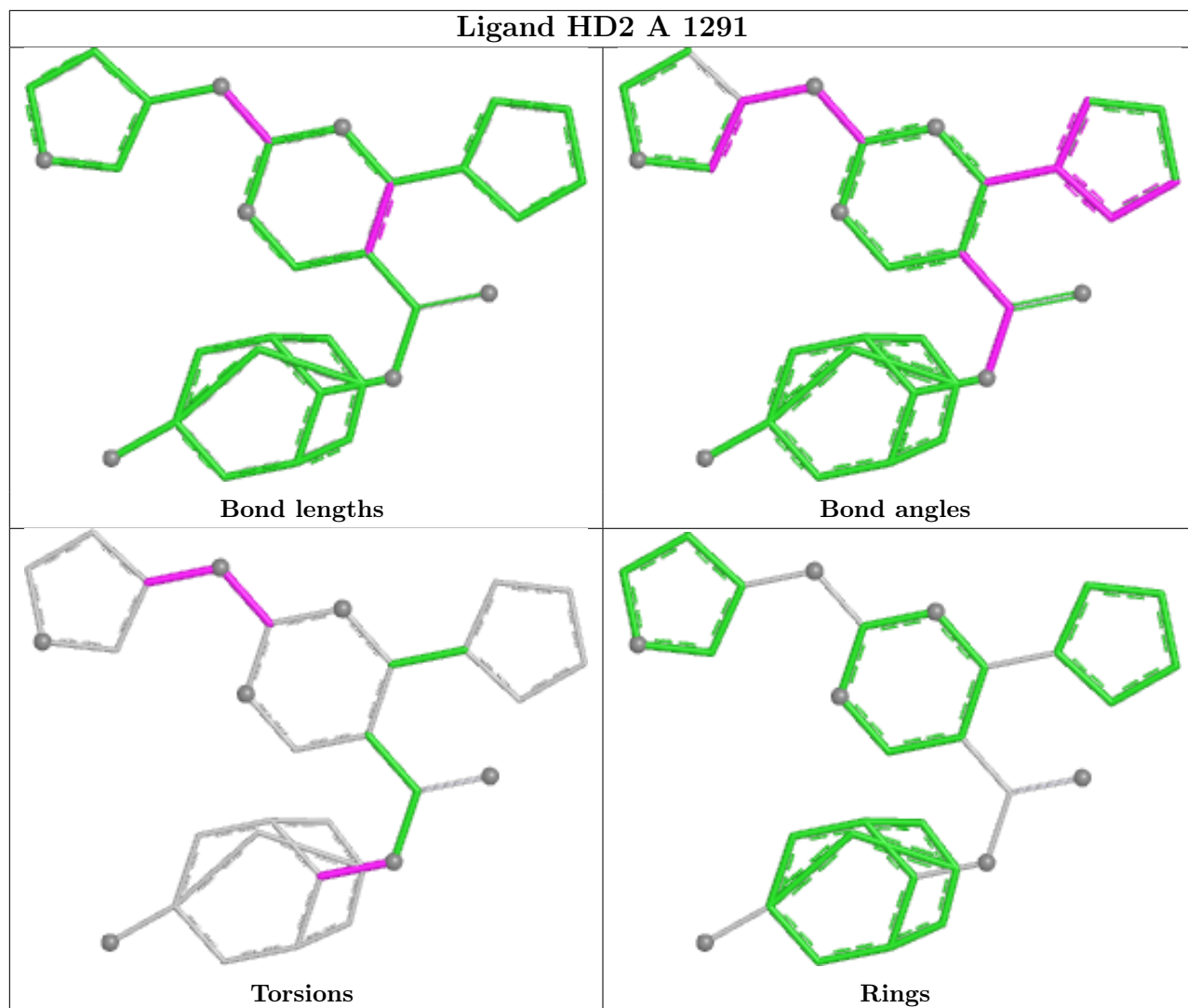
There are no ring outliers.

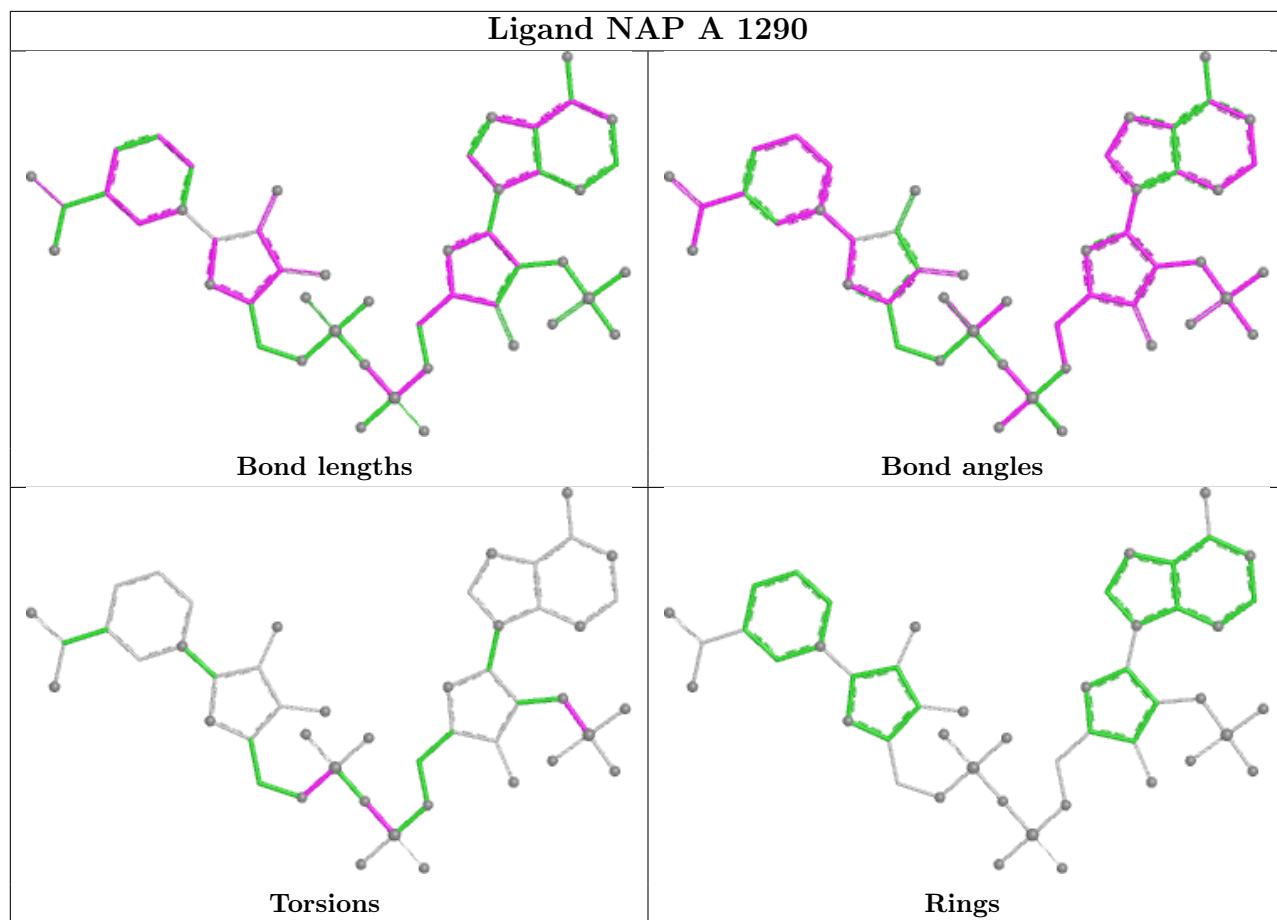
6 monomers are involved in 9 short contacts:

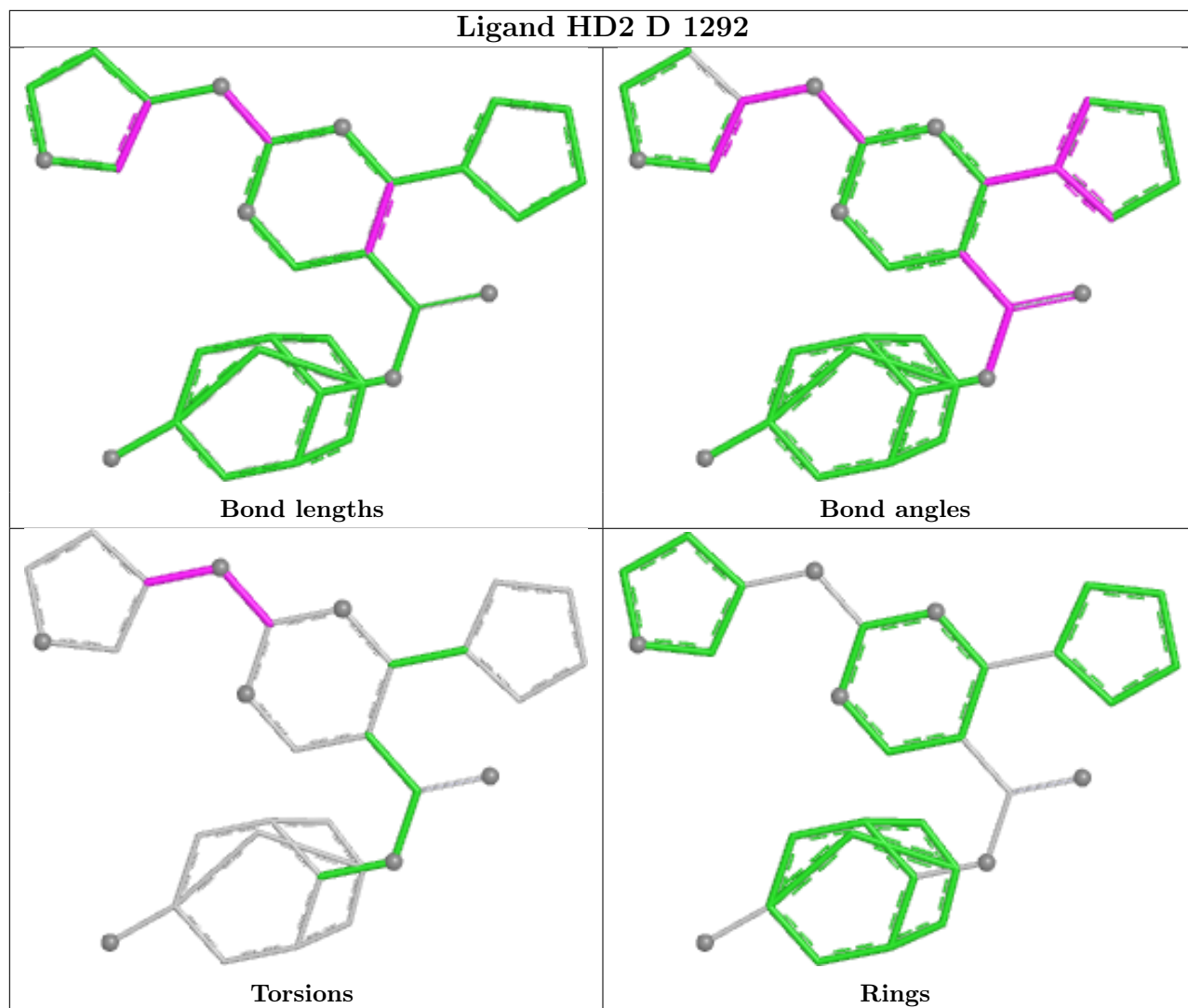
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1291	HD2	1	0
3	A	1291	HD2	2	0
2	A	1290	NAP	2	0
3	D	1292	HD2	2	0
3	C	1281	HD2	1	0
2	C	1280	NAP	1	0

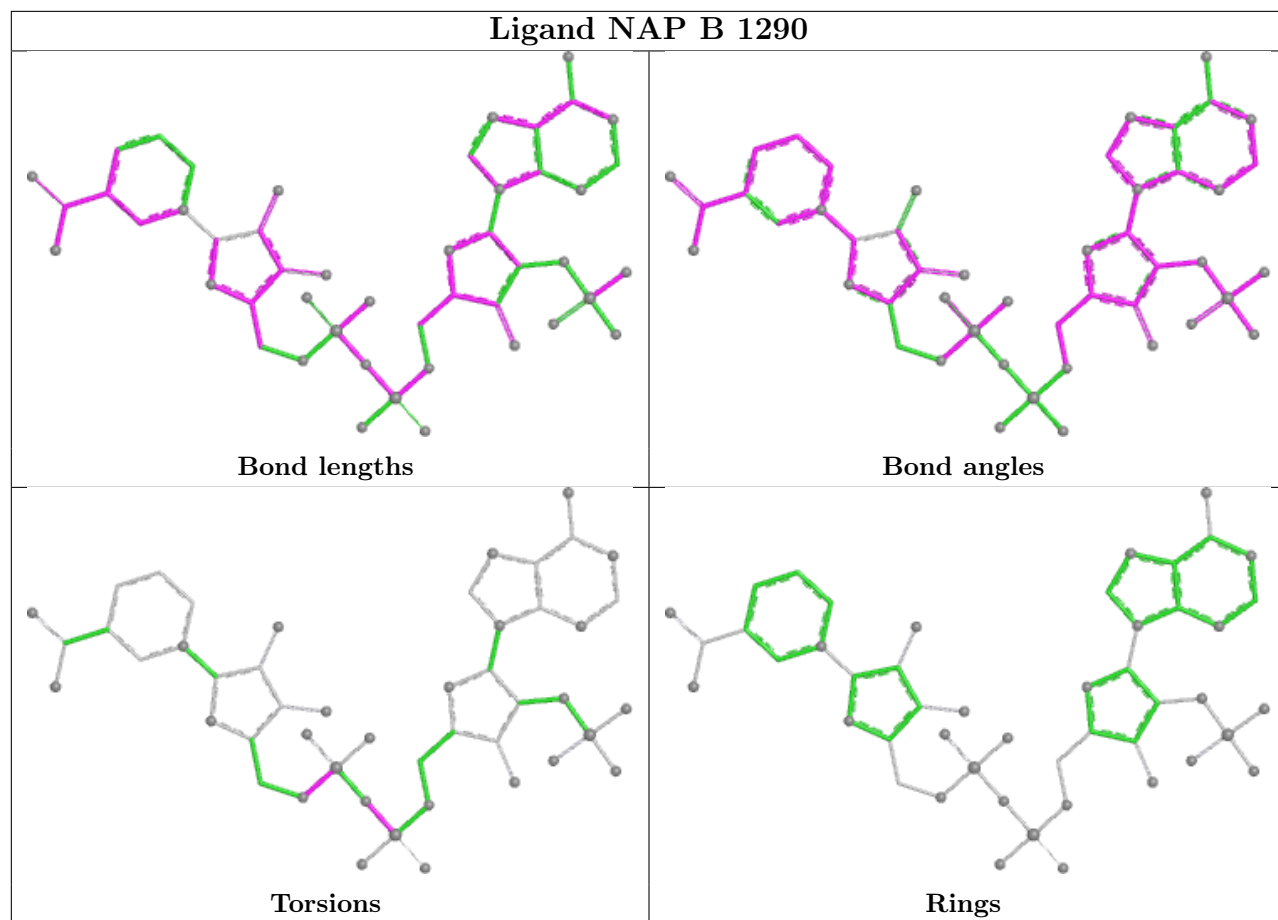
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

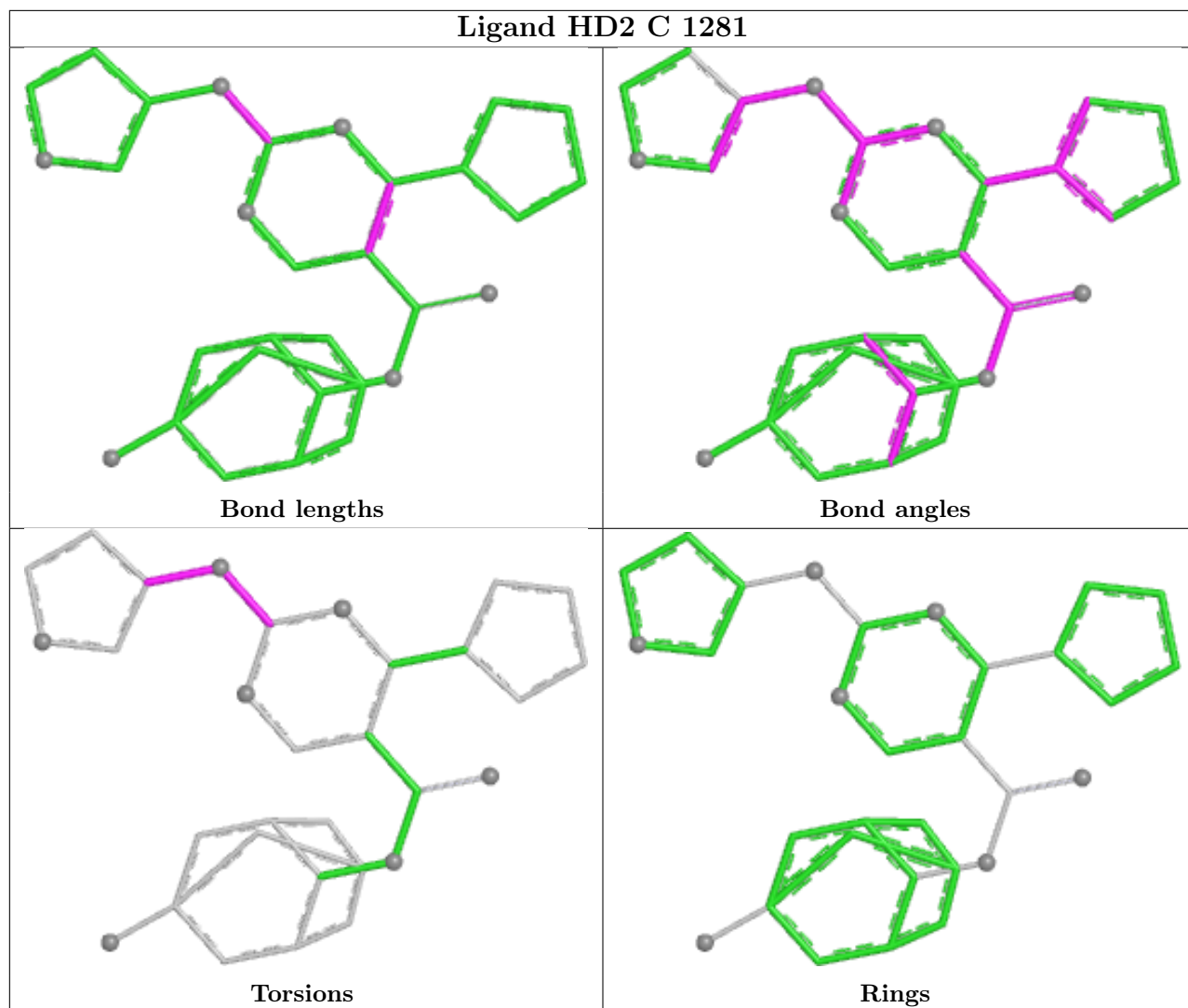


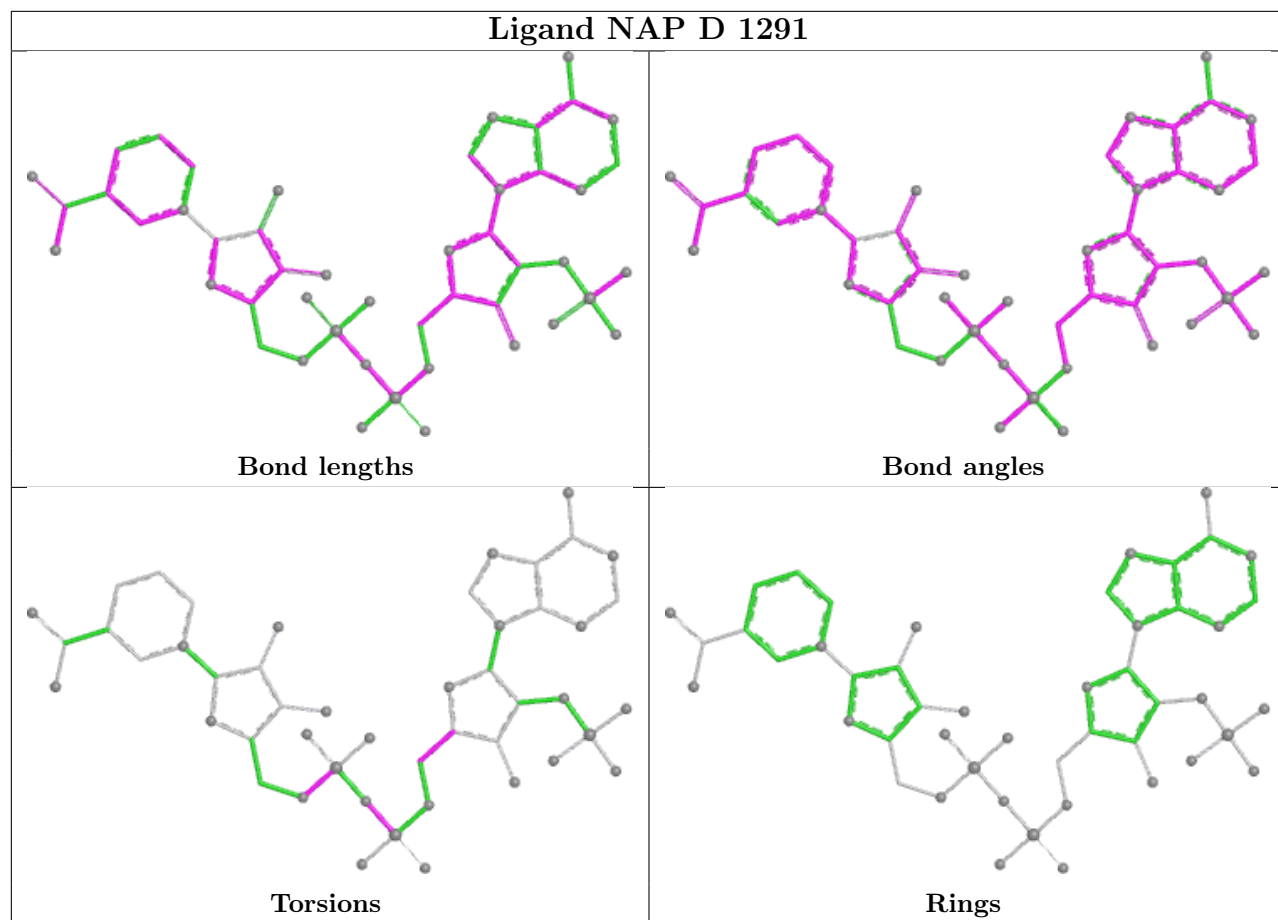


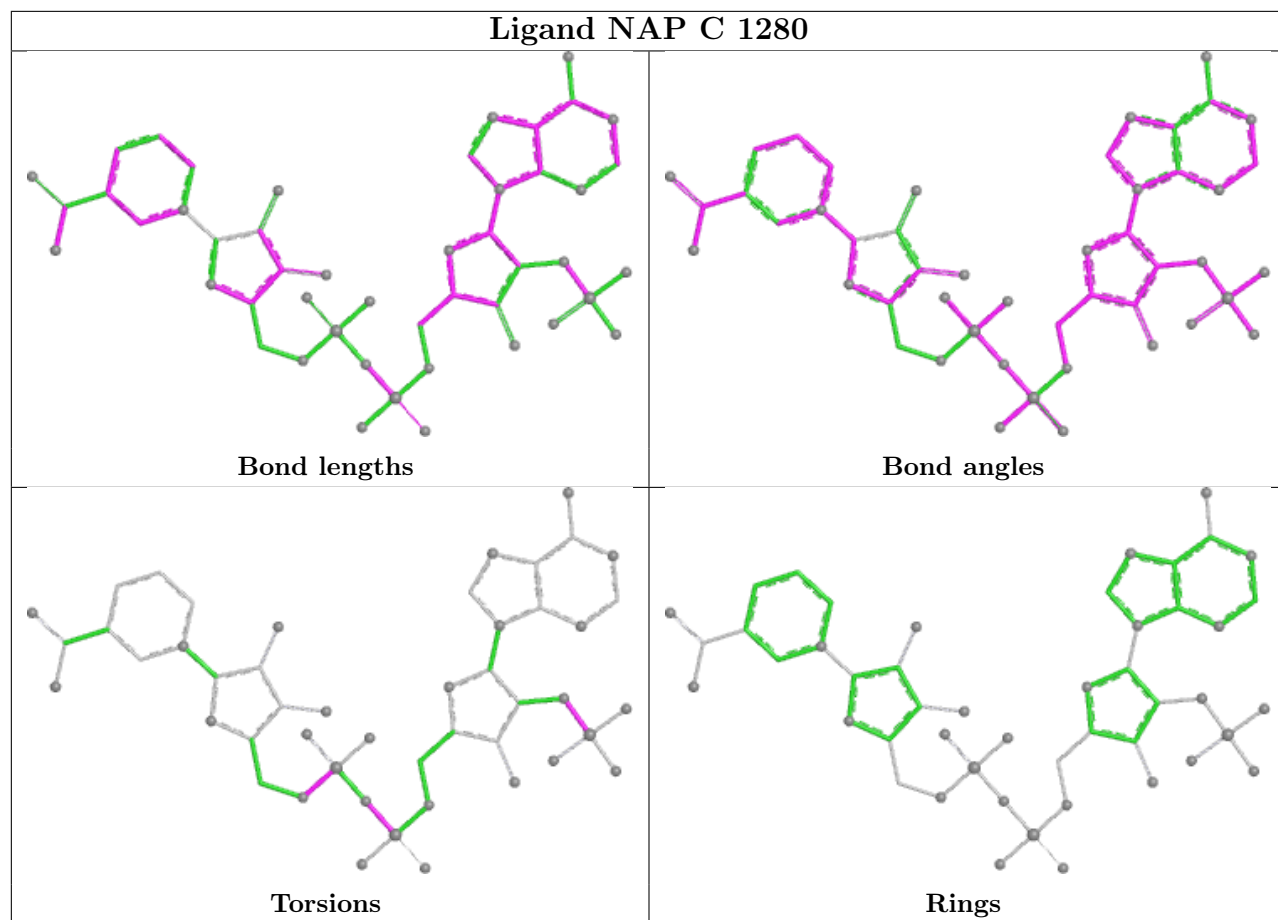












5.7 Other polymers [\(i\)](#)

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	263/292 (90%)	0.04	14 (5%) 32 29	5, 21, 49, 69	0
1	B	264/292 (90%)	-0.18	9 (3%) 48 45	6, 18, 52, 68	0
1	C	254/292 (86%)	-0.27	3 (1%) 76 74	9, 17, 42, 74	0
1	D	262/292 (89%)	0.34	11 (4%) 40 37	10, 30, 58, 71	0
All	All	1043/1168 (89%)	-0.02	37 (3%) 47 44	5, 22, 52, 74	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	279	LEU	5.9
1	A	263	TRP	5.4
1	D	233	MET	4.9
1	D	229	GLY	4.2
1	A	280	TYR	3.9
1	D	290	ILE	3.7
1	D	284	TYR	3.3
1	A	232	HIS	3.2
1	A	283	SER	3.2
1	A	284	TYR	3.0
1	A	282	THR	3.0
1	D	283	SER	3.0
1	B	283	SER	2.9
1	A	259	ASP	2.9
1	B	280	TYR	2.8
1	A	260	SER	2.7
1	A	261	SER	2.7
1	B	279	LEU	2.7
1	D	280	TYR	2.7
1	A	287	ASP	2.7
1	D	282	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	69	GLU	2.6
1	B	205	ARG	2.5
1	A	233	MET	2.5
1	D	227	VAL	2.4
1	B	285	ASN	2.4
1	B	286	MET	2.4
1	B	284	TYR	2.3
1	D	287	ASP	2.2
1	C	259	ASP	2.2
1	C	266	LEU	2.2
1	D	279	LEU	2.1
1	B	232	HIS	2.1
1	A	27	PHE	2.1
1	A	262	ARG	2.1
1	B	281	SER	2.1
1	D	108	LYS	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.

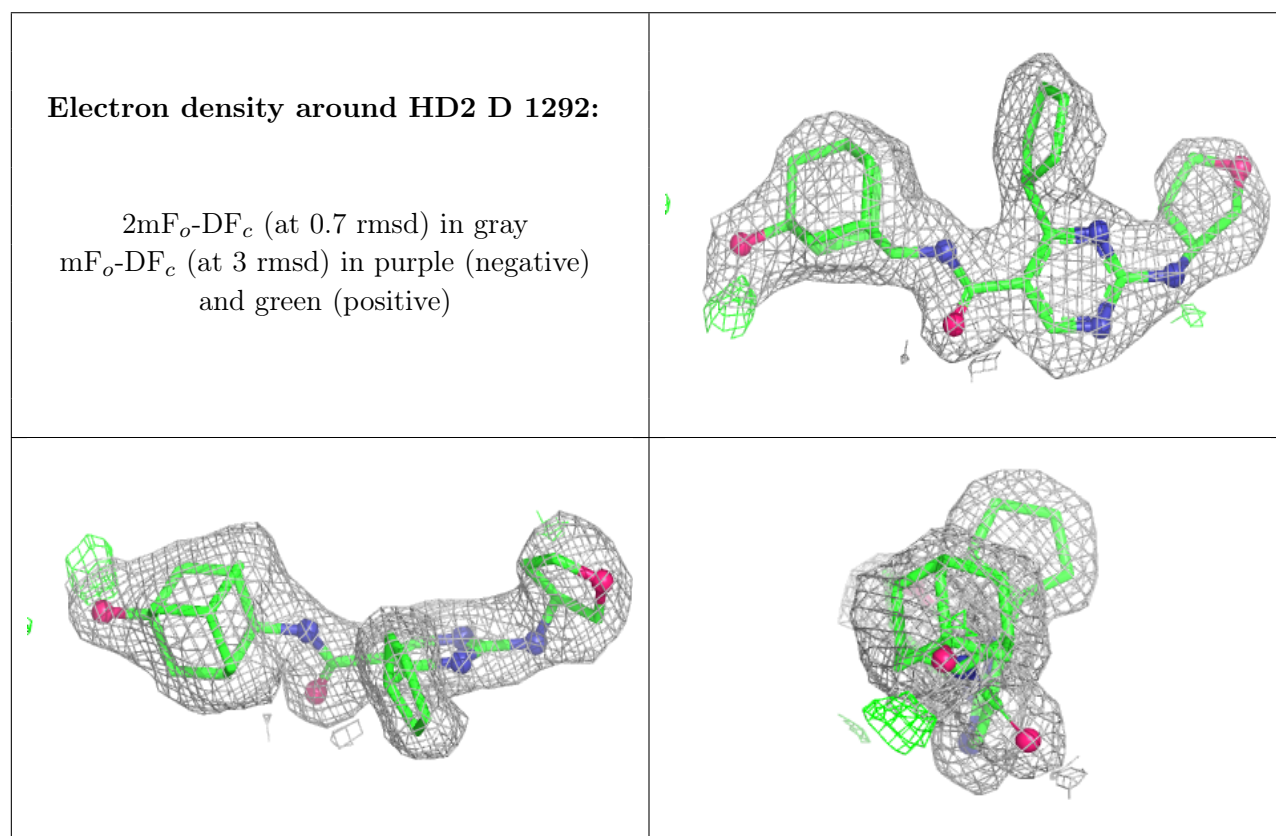
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HD2	D	1292	31/31	0.91	0.09	21,28,41,45	0
3	HD2	C	1281	31/31	0.93	0.08	10,16,36,40	0
3	HD2	A	1291	31/31	0.93	0.08	15,21,42,44	0
3	HD2	B	1291	31/31	0.94	0.07	12,15,39,43	0
2	NAP	D	1291	48/48	0.96	0.06	15,21,31,33	0
2	NAP	C	1280	48/48	0.98	0.05	7,12,16,21	0
2	NAP	A	1290	48/48	0.98	0.04	5,14,19,22	0

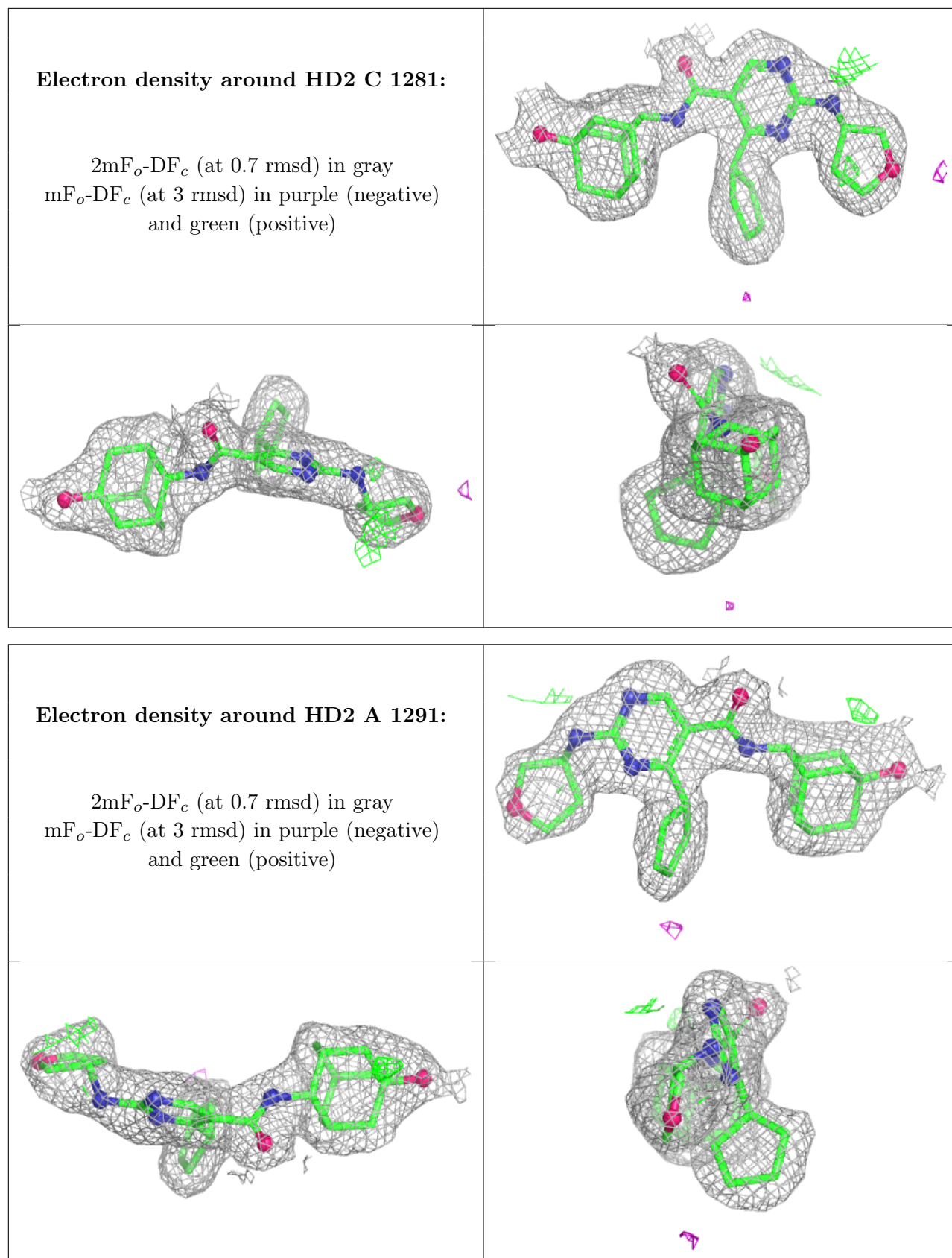
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAP	B	1290	48/48	0.99	0.04	5,10,14,22	0

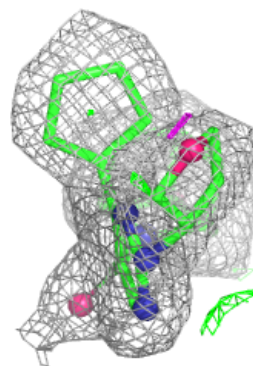
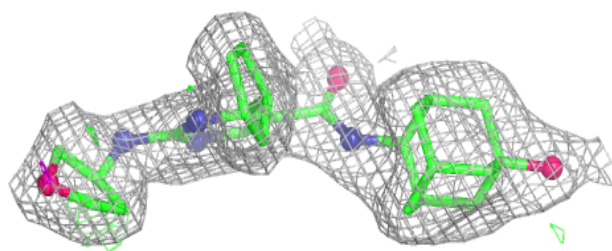
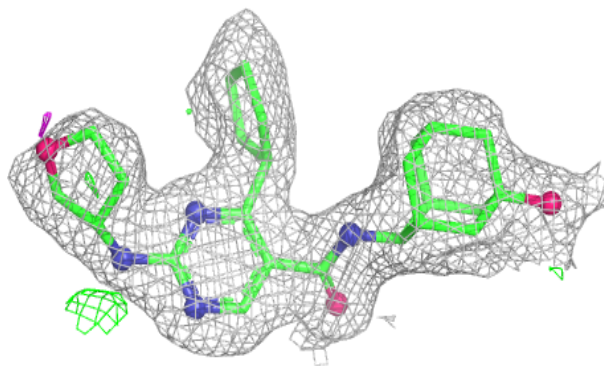
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



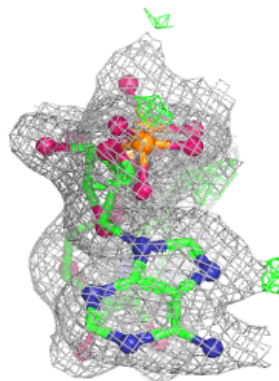
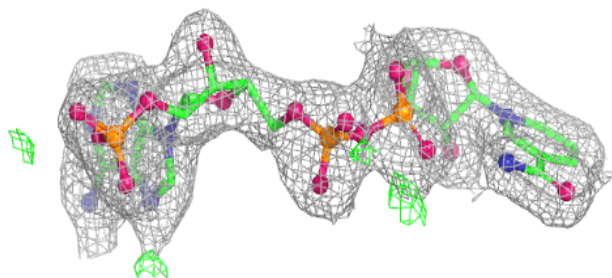
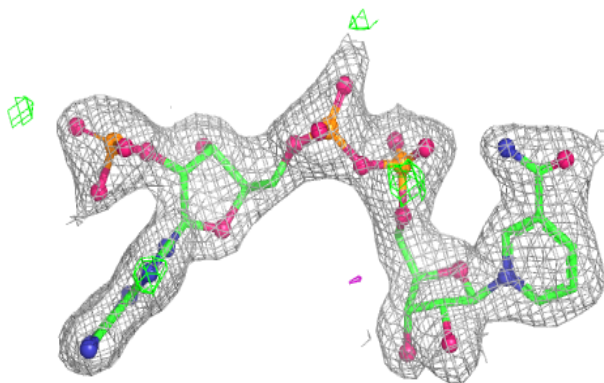


Electron density around HD2 B 1291:

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

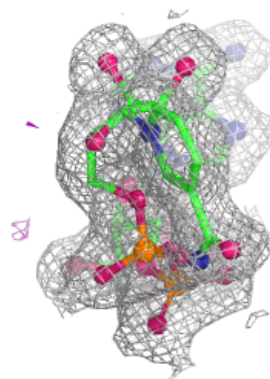
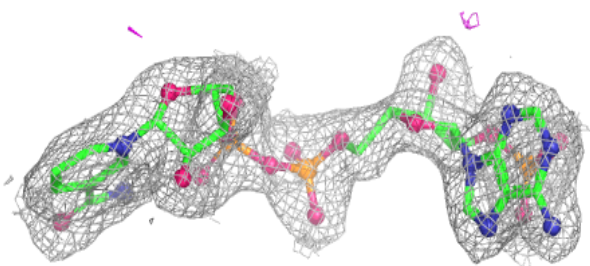
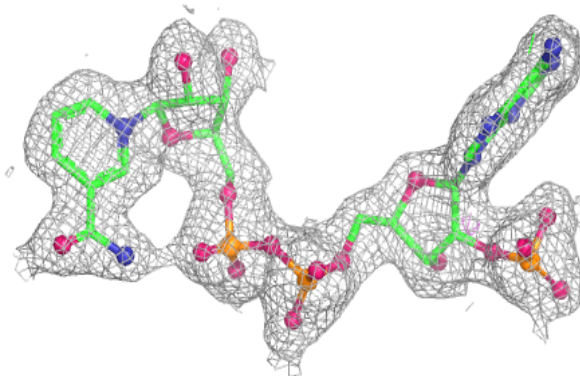
**Electron density around NAP D 1291:**

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

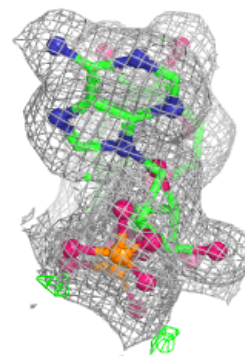
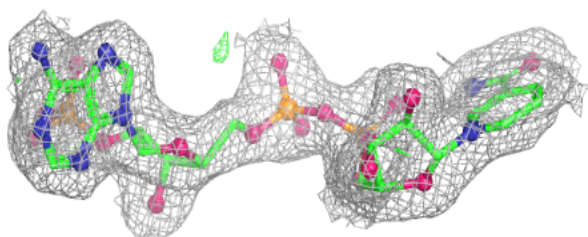
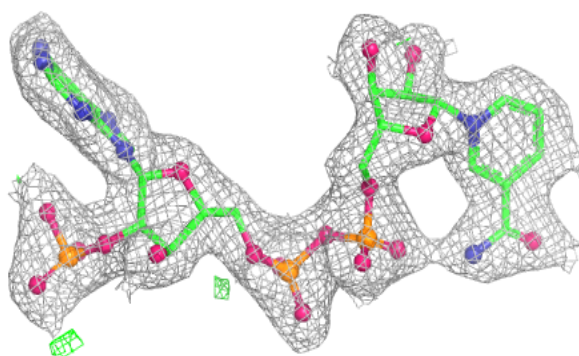


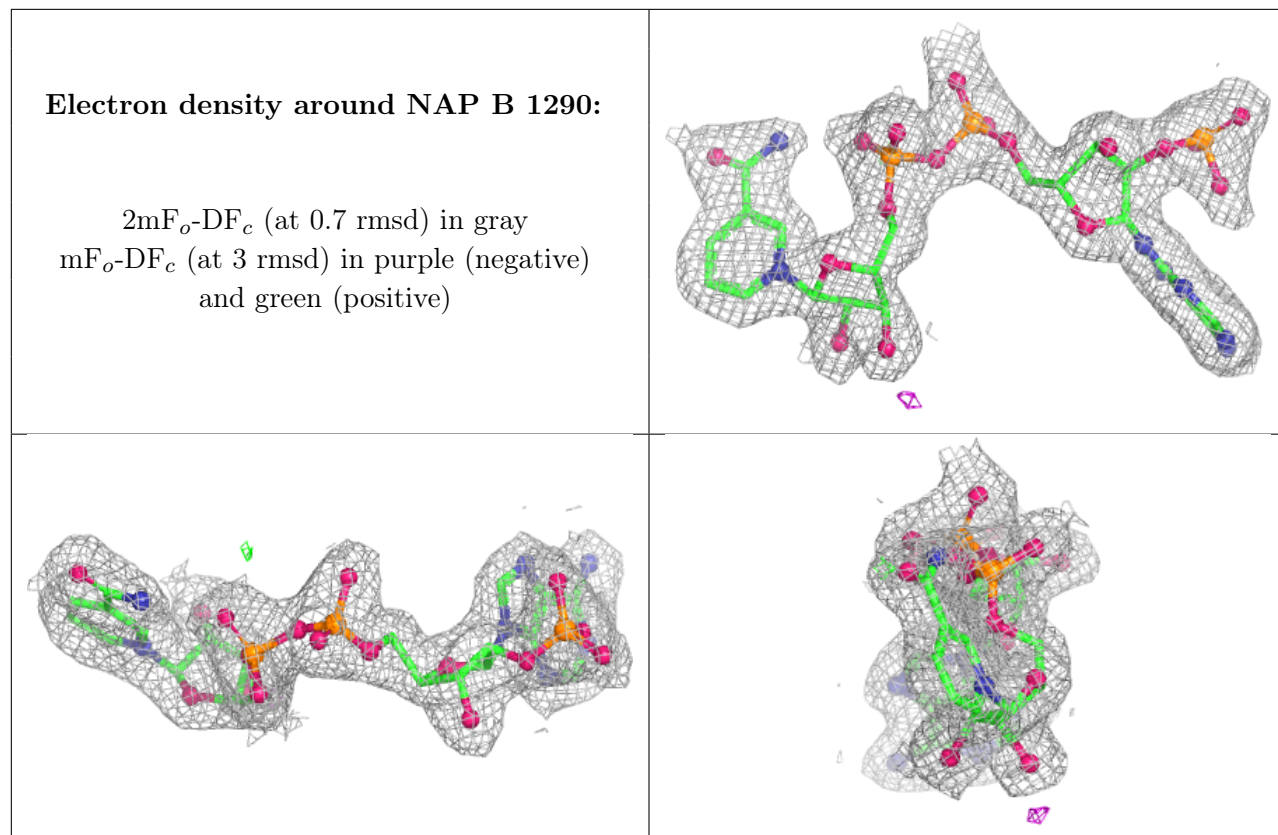
Electron density around NAP C 1280:

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

**Electron density around NAP A 1290:**

$2mF_o-DF_c$ (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.