



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:29 pm BST

PDB ID : 5C37
Title : Structure of the beta-ketoacyl reductase domain of human fatty acid synthase bound to a spiro-imidazolone inhibitor
Authors : Schubert, C.; Milligan, C.M.; Vo, K.; Grasberger, B.
Deposited on : 2015-06-17
Resolution : 2.30 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 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 : 2.11
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) : 2.11

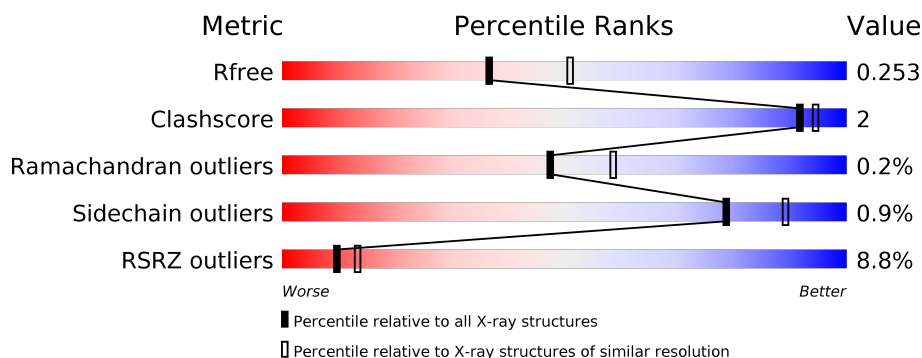
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	664	<div> <div>8%</div> <div>91%</div> <div>5%</div> </div>
1	C	664	<div> <div>9%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 19001 atoms, of which 9299 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.

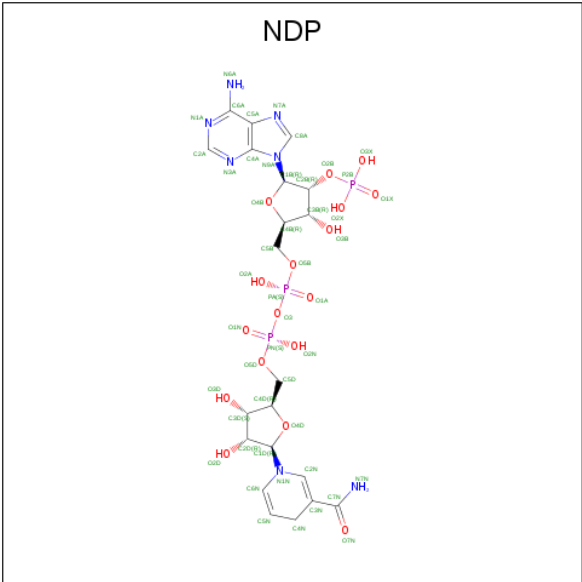
- Molecule 1 is a protein called Fatty acid synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	632	9294	2959	4617	822	872	24	0	0	0
1	C	624	9179	2922	4564	813	856	24	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

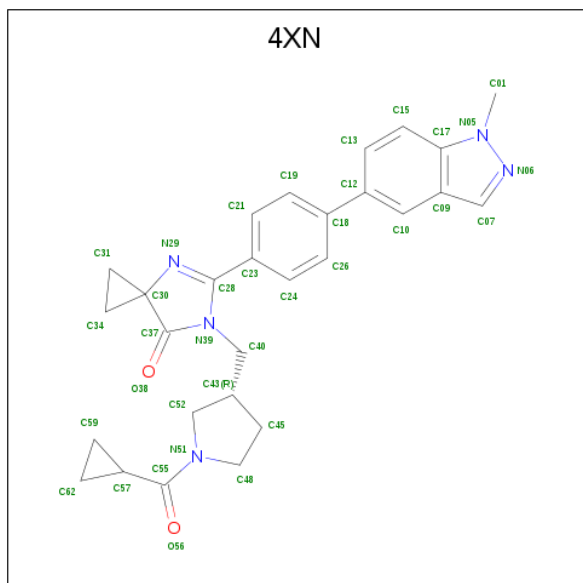
Chain	Residue	Modelled	Actual	Comment	Reference
A	1875	GLY	-	linker	UNP P49327
A	1876	GLY	-	linker	UNP P49327
A	1880	GLY	PHE	engineered mutation	UNP P49327
C	1875	GLY	-	linker	UNP P49327
C	1876	GLY	-	linker	UNP P49327
C	1880	GLY	PHE	engineered mutation	UNP P49327

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			74	21	26	7	17		
2	C	1	Total	C	H	N	O	0	0
			74	21	26	7	17		

- Molecule 3 is 6-{[(3R)-1-(cyclopropylcarbonyl)pyrrolidin-3-yl]methyl}-5-[4-(1-methyl-1H-indazol-5-yl)phenyl]-4,6-diazaspiro[2.4]hept-4-en-7-one (three-letter code: 4XN) (formula: C₂₈H₂₉N₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			64	28	29	5	2		
3	C	1	Total	C	H	N	O	0	0
			64	28	29	5	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl	0	0
			1 1		
4	C	2	Total Cl	0	0
			2 2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			14	3	8	3		

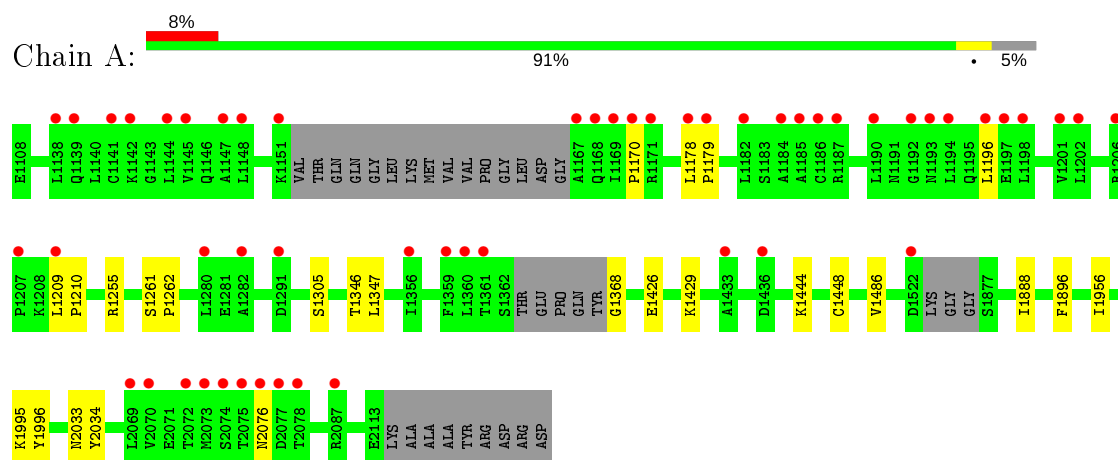
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	107	Total	O	0	0
			107	107		
6	C	128	Total	O	0	0
			128	128		

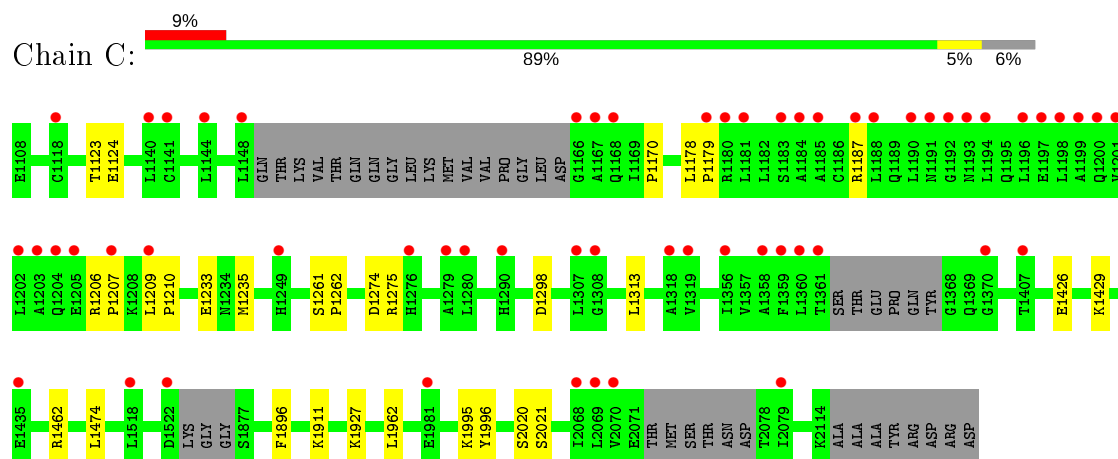
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Fatty acid synthase



• Molecule 1: Fatty acid synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.08 Å 80.52 Å 96.53 Å 90.00° 116.90° 90.00°	Depositor
Resolution (Å)	47.00 – 2.30 47.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.00-2.30) 92.9 (47.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.29 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.251 0.213 , 0.253	Depositor DCC
R_{free} test set	2032 reflections (3.57%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19001	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6230e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4XN, GOL, NDP, CL

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	0.22	0/4765	0.40	0/6484
1	C	0.22	0/4703	0.39	0/6397
All	All	0.22	0/9468	0.39	0/12881

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4677	4617	4616	12	0
1	C	4615	4564	4558	16	0
2	A	48	26	26	0	0
2	C	48	26	26	0	0
3	A	35	29	0	0	0
3	C	35	29	0	0	0
4	A	1	0	0	0	0
4	C	2	0	0	1	0
5	C	6	8	8	1	0
6	A	107	0	0	4	0
6	C	128	0	0	8	0
All	All	9702	9299	9234	29	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 2.

All (29) 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:C:1233:GLU:OE2	6:C:2301:HOH:O	2.03	0.76
1:C:1298:ASP:OD1	6:C:2302:HOH:O	2.05	0.73
1:A:1444:LYS:NZ	1:A:1486:VAL:O	2.22	0.73
4:C:2205:CL:CL	6:C:2424:HOH:O	2.43	0.73
1:A:1255:ARG:NH1	6:A:2301:HOH:O	2.22	0.70
1:C:1235:MET:O	6:C:2303:HOH:O	2.14	0.66
1:C:1123:THR:OG1	6:C:2304:HOH:O	2.14	0.65
1:C:1911:LYS:NZ	1:C:1962:LEU:O	2.29	0.65
1:A:1448:CYS:SG	6:A:2389:HOH:O	2.55	0.64
1:A:1426:GLU:OE1	1:A:1429:LYS:NZ	2.34	0.60
1:C:1124:GLU:OE2	5:C:2202:GOL:O1	2.20	0.59
1:C:1474:LEU:O	6:C:2305:HOH:O	2.18	0.55
1:C:1274:ASP:OD1	1:C:1275:ARG:N	2.42	0.52
1:C:1462:ARG:NH2	6:C:2303:HOH:O	2.46	0.49
1:A:1368:GLY:N	6:A:2308:HOH:O	2.47	0.47
1:A:1261:SER:N	1:A:1262:PRO:CD	2.78	0.47
1:A:1346:THR:OG1	1:A:1347:LEU:N	2.49	0.46
1:C:1178:LEU:HB3	1:C:1179:PRO:HD3	1.98	0.46
1:C:1209:LEU:N	1:C:1210:PRO:CD	2.79	0.46
1:C:1261:SER:N	1:C:1262:PRO:CD	2.79	0.46
1:A:2033:ASN:OD1	1:A:2034:TYR:N	2.49	0.46
1:A:1209:LEU:N	1:A:1210:PRO:CD	2.80	0.44
1:C:2020:SER:OG	1:C:2021:SER:N	2.51	0.42
1:A:1178:LEU:HB3	1:A:1179:PRO:HD3	2.02	0.42
1:A:1888:ILE:CD1	1:A:1956:ILE:HD13	2.51	0.41
1:C:1187:ARG:NE	6:C:2314:HOH:O	2.53	0.41
1:C:1206:ARG:N	1:C:1207:PRO:HD2	2.36	0.41
1:C:1426:GLU:OE1	1:C:1429:LYS:NZ	2.46	0.41
1:A:1305:SER:N	6:A:2305:HOH:O	2.53	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	624/664 (94%)	589 (94%)	33 (5%)	2 (0%)	41	50
1	C	614/664 (92%)	584 (95%)	29 (5%)	1 (0%)	47	58
All	All	1238/1328 (93%)	1173 (95%)	62 (5%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2076	ASN
1	C	1170	PRO
1	A	1170	PRO

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	488/548 (89%)	484 (99%)	4 (1%)	81	91
1	C	481/548 (88%)	476 (99%)	5 (1%)	76	87
All	All	969/1096 (88%)	960 (99%)	9 (1%)	78	89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1196	LEU
1	A	1896	PHE
1	A	1995	LYS

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Mol	Chain	Res	Type
1	A	1996	TYR
1	C	1313	LEU
1	C	1896	PHE
1	C	1927	LYS
1	C	1995	LYS
1	C	1996	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1204	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	4XN	C	2203	-	36,41,41	1.03	2 (5%)	49,63,63	1.63	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	C	2201	-	45,52,52	1.04	3 (6%)	53,80,80	0.96	2 (3%)
2	NDP	A	2201	-	45,52,52	1.03	3 (6%)	53,80,80	0.94	4 (7%)
3	4XN	A	2202	-	36,41,41	1.03	2 (5%)	49,63,63	1.63	8 (16%)
5	GOL	C	2202	-	5,5,5	0.32	0	5,5,5	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	4XN	C	2203	-	-	4/20/54/54	0/7/7/7
2	NDP	C	2201	-	-	10/30/77/77	0/5/5/5
2	NDP	A	2201	-	-	7/30/77/77	0/5/5/5
3	4XN	A	2202	-	-	4/20/54/54	0/7/7/7
5	GOL	C	2202	-	-	2/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2202	4XN	C37-N39	-2.41	1.34	1.38
3	C	2203	4XN	C37-N39	-2.33	1.34	1.38
2	C	2201	NDP	PN-O5D	2.32	1.68	1.59
2	A	2201	NDP	PA-O5B	2.30	1.68	1.59
2	C	2201	NDP	PA-O5B	2.28	1.68	1.59
2	A	2201	NDP	C8A-N7A	-2.27	1.30	1.34
2	A	2201	NDP	PN-O5D	2.25	1.68	1.59
3	C	2203	4XN	C15-C13	2.21	1.41	1.36
3	A	2202	4XN	C15-C13	2.07	1.41	1.36
2	C	2201	NDP	C8A-N7A	-2.06	1.31	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2203	4XN	N39-C28-N29	-6.07	111.15	116.09
3	A	2202	4XN	N39-C28-N29	-6.03	111.19	116.09
3	C	2203	4XN	C34-C30-C37	5.17	126.07	118.37
3	A	2202	4XN	C34-C30-C37	5.15	126.04	118.37
3	A	2202	4XN	C31-C30-C37	4.48	125.03	118.37
3	C	2203	4XN	C31-C30-C37	4.36	124.86	118.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2201	NDP	O4B-C1B-C2B	-2.97	101.44	106.59
3	C	2203	4XN	C40-N39-C37	2.68	126.01	123.53
3	C	2203	4XN	C45-C48-N51	2.57	106.31	103.28
3	C	2203	4XN	C40-N39-C28	-2.49	124.00	127.29
2	A	2201	NDP	O4B-C1B-C2B	-2.49	102.27	106.59
2	A	2201	NDP	O4B-C4B-C5B	2.42	117.33	109.37
3	A	2202	4XN	C40-N39-C37	2.39	125.74	123.53
3	A	2202	4XN	C45-C48-N51	2.31	106.01	103.28
3	C	2203	4XN	C09-C17-N05	-2.25	104.17	107.69
3	A	2202	4XN	C23-C28-N39	2.20	128.91	125.52
2	C	2201	NDP	C5A-C6A-N6A	2.18	123.67	120.35
3	A	2202	4XN	C40-N39-C28	-2.16	124.43	127.29
2	A	2201	NDP	O2B-C2B-C3B	-2.11	104.05	111.68
3	A	2202	4XN	C09-C17-N05	-2.10	104.41	107.69
2	A	2201	NDP	C5A-C6A-N6A	2.01	123.41	120.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2201	NDP	C5B-O5B-PA-O1A
5	C	2202	GOL	O1-C1-C2-C3
2	C	2201	NDP	C3D-C4D-C5D-O5D
5	C	2202	GOL	O1-C1-C2-O2
2	C	2201	NDP	O4D-C4D-C5D-O5D
2	A	2201	NDP	C1B-C2B-O2B-P2B
2	A	2201	NDP	C3B-C2B-O2B-P2B
2	C	2201	NDP	O4D-C1D-N1N-C6N
3	A	2202	4XN	C24-C23-C28-N29
2	C	2201	NDP	O4B-C4B-C5B-O5B
3	A	2202	4XN	C21-C23-C28-N29
3	C	2203	4XN	C24-C23-C28-N29
3	A	2202	4XN	C24-C23-C28-N39
3	A	2202	4XN	C21-C23-C28-N39
3	C	2203	4XN	C21-C23-C28-N39
3	C	2203	4XN	C24-C23-C28-N39
2	A	2201	NDP	O4D-C1D-N1N-C6N
3	C	2203	4XN	C21-C23-C28-N29
2	C	2201	NDP	C5B-O5B-PA-O3
2	C	2201	NDP	C2B-O2B-P2B-O2X
2	C	2201	NDP	C5B-O5B-PA-O2A
2	C	2201	NDP	C1B-C2B-O2B-P2B

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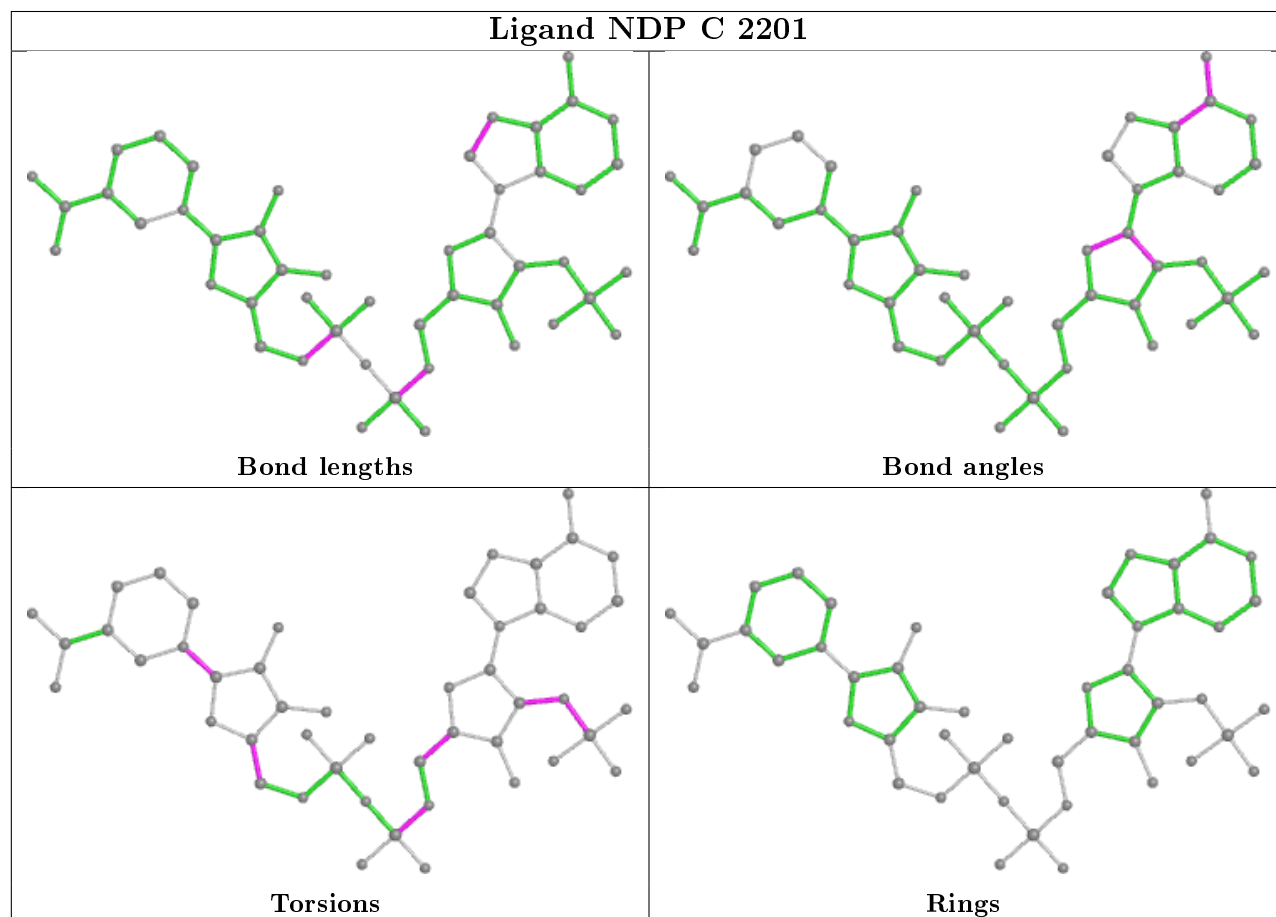
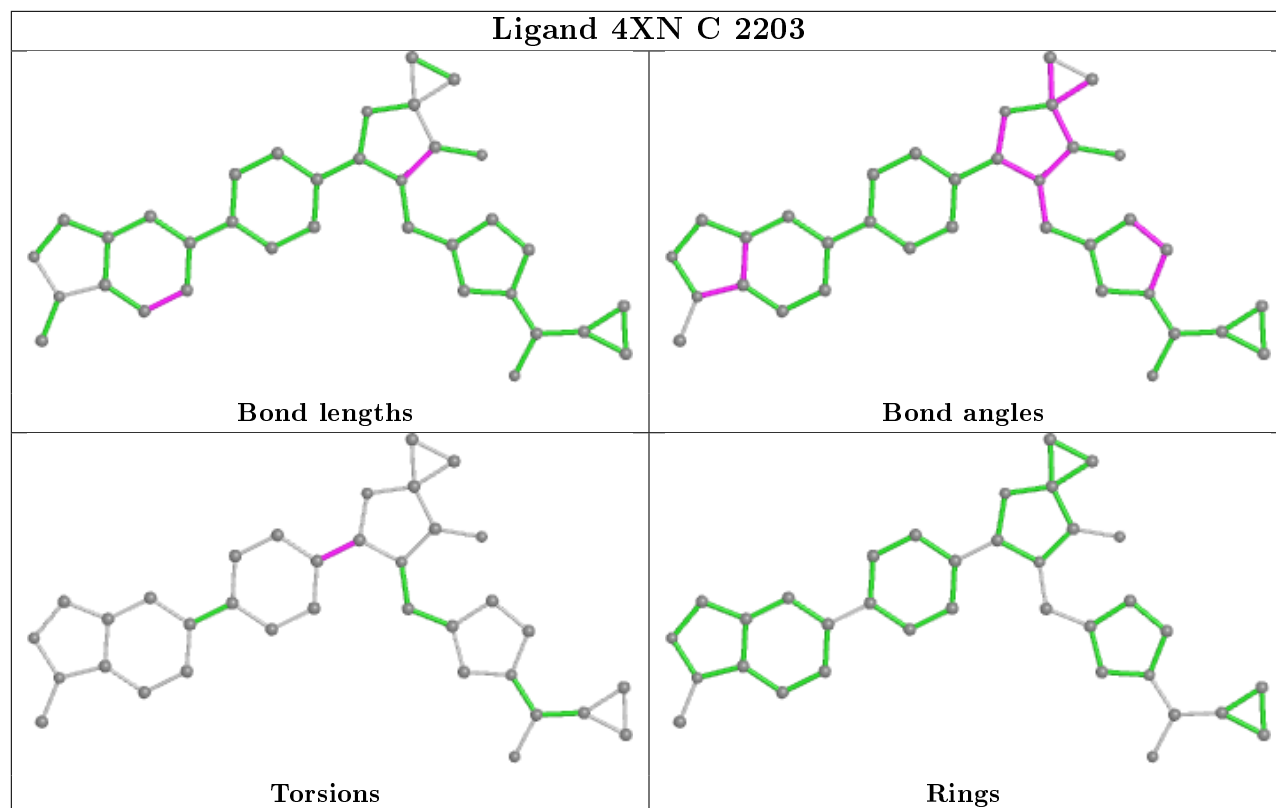
Mol	Chain	Res	Type	Atoms
2	C	2201	NDP	C3B-C2B-O2B-P2B
2	A	2201	NDP	C4B-C5B-O5B-PA
2	A	2201	NDP	O4D-C4D-C5D-O5D
2	A	2201	NDP	O4B-C4B-C5B-O5B
2	A	2201	NDP	C3D-C4D-C5D-O5D

There are no ring outliers.

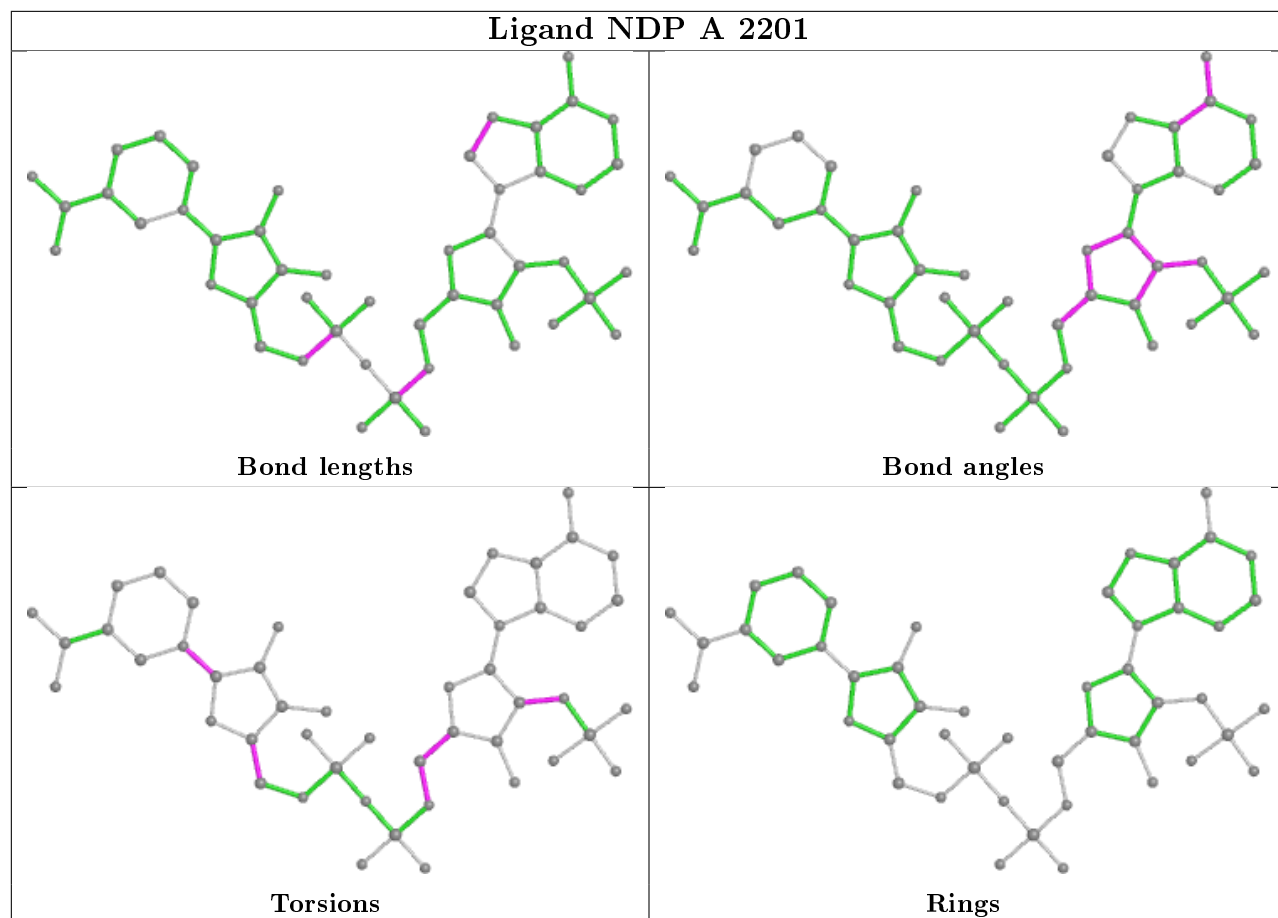
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2202	GOL	1	0

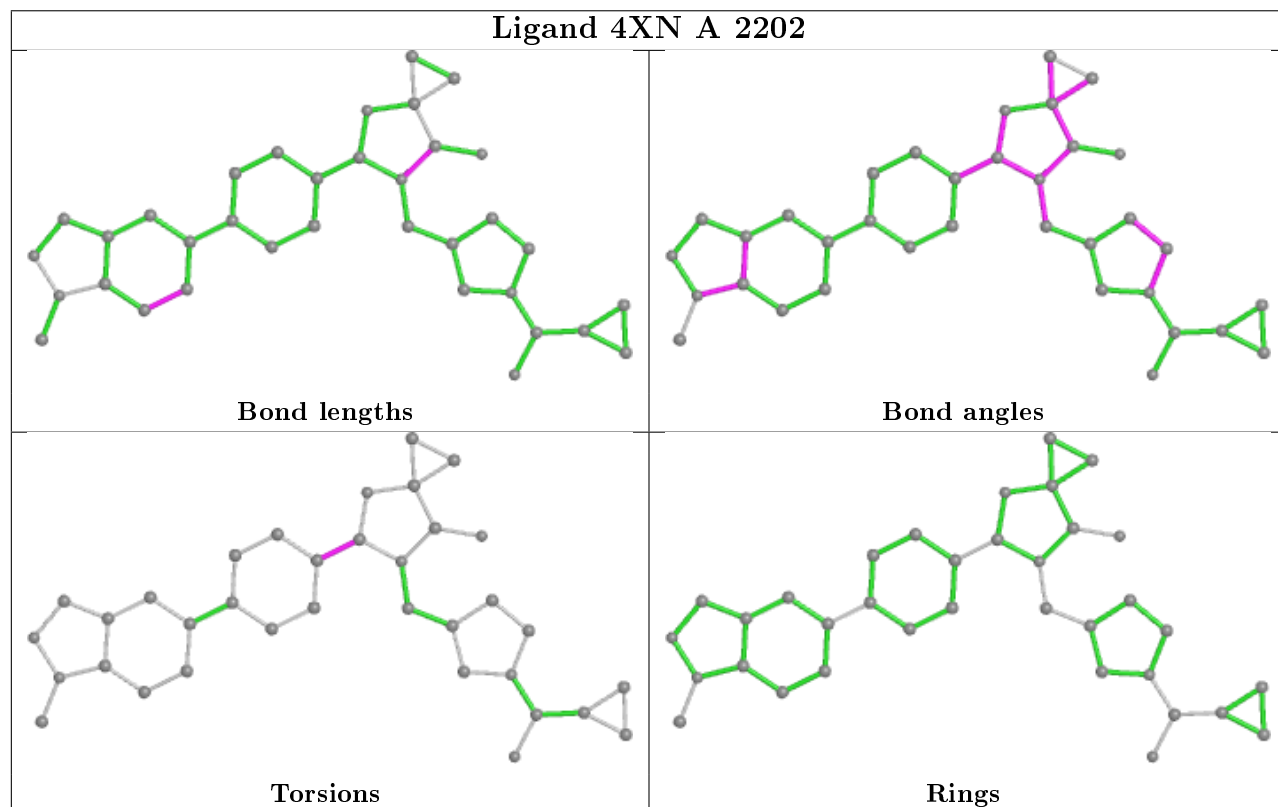
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand NDP A 2201



Ligand 4XN A 2202



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	632/664 (95%)	0.58	53 (8%) 11 15	29, 60, 110, 157	0
1	C	624/664 (93%)	0.65	57 (9%) 9 12	30, 56, 109, 179	0
All	All	1256/1328 (94%)	0.61	110 (8%) 10 13	29, 58, 110, 179	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2070	VAL	14.4
1	C	1166	GLY	8.4
1	C	1196	LEU	8.3
1	A	1202	LEU	7.4
1	A	2075	THR	6.7
1	C	1360	LEU	6.1
1	C	1191	ASN	5.3
1	C	1167	ALA	5.2
1	A	1182	LEU	5.2
1	A	2074	SER	5.2
1	C	1197	GLU	4.9
1	A	1185	ALA	4.7
1	C	1144	LEU	4.7
1	C	1184	ALA	4.6
1	C	1198	LEU	4.5
1	A	2070	VAL	4.4
1	C	1192	GLY	4.3
1	C	1204	GLN	4.2
1	A	1179	PRO	4.1
1	A	1141	CYS	4.1
1	A	2076	ASN	4.1
1	C	1276	HIS	4.1
1	C	1203	ALA	4.0
1	C	1201	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1144	LEU	3.9
1	C	1370	GLY	3.8
1	C	1181	LEU	3.8
1	A	1145	VAL	3.8
1	C	1187	ARG	3.8
1	C	1200	GLN	3.7
1	A	1193	ASN	3.7
1	A	1184	ALA	3.7
1	A	1360	LEU	3.6
1	C	1202	LEU	3.6
1	A	1148	LEU	3.6
1	A	1169	ILE	3.5
1	C	1194	LEU	3.5
1	C	1359	PHE	3.4
1	A	1359	PHE	3.4
1	C	1308	GLY	3.4
1	C	2068	ILE	3.3
1	A	1186	CYS	3.2
1	A	1201	VAL	3.2
1	A	1139	GLN	3.2
1	C	1183	SER	3.2
1	A	1147	ALA	3.2
1	C	1407	THR	3.1
1	C	1193	ASN	3.1
1	C	1361	THR	3.1
1	C	1356	ILE	3.1
1	C	1205	GLU	3.1
1	A	2077	ASP	3.0
1	C	1168	GLN	3.0
1	C	1141	CYS	3.0
1	C	1522	ASP	3.0
1	C	1249	HIS	3.0
1	A	1171	ARG	2.9
1	C	1207	PRO	2.9
1	C	1319	VAL	2.8
1	A	1178	LEU	2.8
1	A	1138	LEU	2.8
1	C	1358	ALA	2.7
1	A	1194	LEU	2.7
1	C	2069	LEU	2.7
1	A	2078	THR	2.7
1	C	1435	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1199	ALA	2.7
1	C	1209	LEU	2.7
1	C	1188	LEU	2.7
1	A	1522	ASP	2.7
1	C	1140	LEU	2.6
1	A	1206	ARG	2.6
1	A	2087	ARG	2.6
1	A	1142	LYS	2.6
1	A	1151	LYS	2.6
1	A	2069	LEU	2.6
1	A	1207	PRO	2.5
1	C	1190	LEU	2.5
1	C	1180	ARG	2.5
1	A	1170	PRO	2.5
1	A	1356	ILE	2.4
1	C	1148	LEU	2.3
1	C	1280	LEU	2.3
1	A	1280	LEU	2.3
1	A	1192	GLY	2.3
1	A	1361	THR	2.3
1	A	1187	ARG	2.3
1	A	1190	LEU	2.3
1	A	1168	GLN	2.3
1	A	2072	THR	2.2
1	A	1282	ALA	2.2
1	C	1179	PRO	2.2
1	C	1279	ALA	2.2
1	C	1318	ALA	2.2
1	C	1290	HIS	2.2
1	A	2073	MET	2.2
1	A	1198	LEU	2.2
1	A	1197	GLU	2.1
1	C	1118	CYS	2.1
1	C	1185	ALA	2.1
1	A	1209	LEU	2.1
1	C	1307	LEU	2.1
1	A	1167	ALA	2.1
1	A	1433	ALA	2.1
1	A	1291	ASP	2.1
1	A	1436	ASP	2.0
1	A	1196	LEU	2.0
1	C	1518	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	2079	ILE	2.0
1	C	1981	GLU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

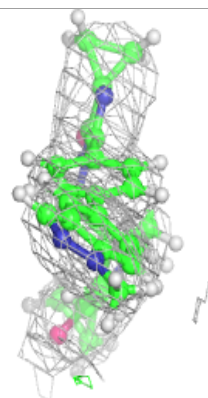
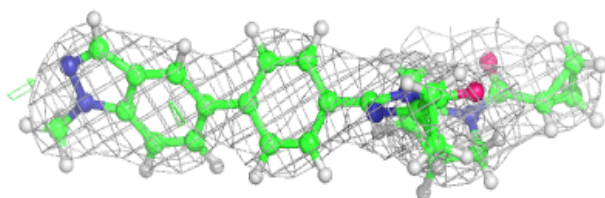
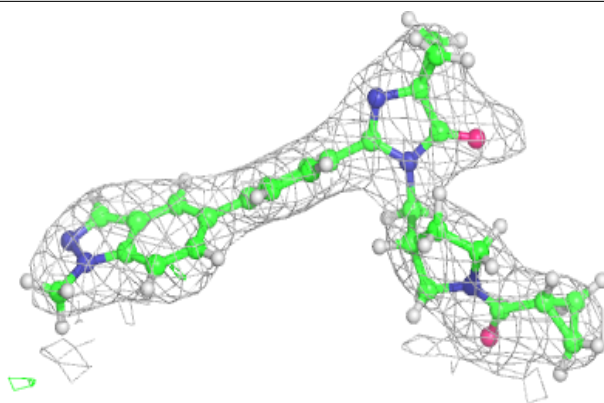
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	C	2204	1/1	0.66	0.14	69,69,69,69	0
5	GOL	C	2202	6/6	0.86	0.21	51,61,67,72	0
4	CL	A	2203	1/1	0.89	0.23	69,69,69,69	0
4	CL	C	2205	1/1	0.94	0.19	77,77,77,77	0
3	4XN	C	2203	35/35	0.95	0.14	40,50,60,61	0
3	4XN	A	2202	35/35	0.96	0.15	29,41,52,52	0
2	NDP	C	2201	48/48	0.96	0.14	36,47,61,61	0
2	NDP	A	2201	48/48	0.97	0.13	33,48,63,69	0

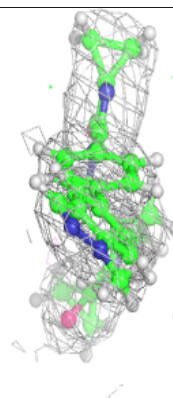
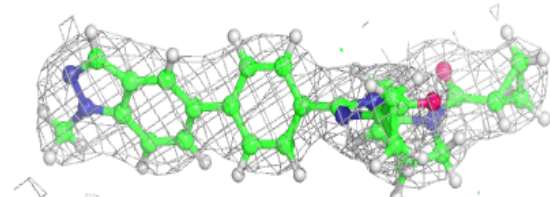
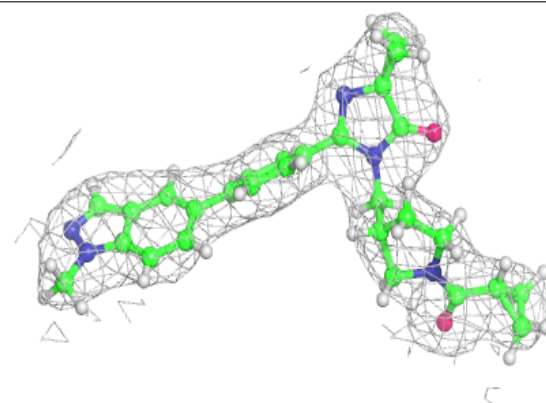
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4XN C 2203:

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

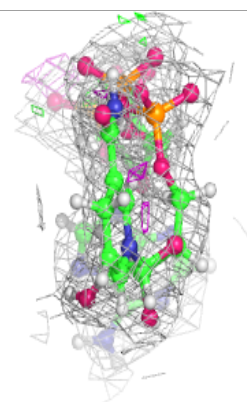
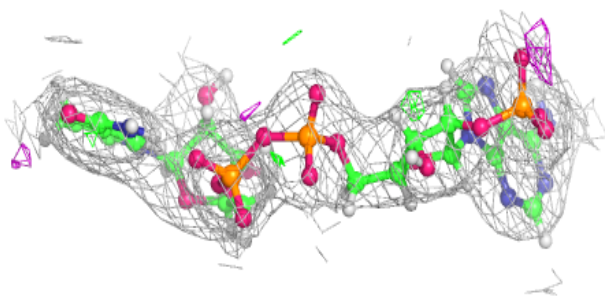
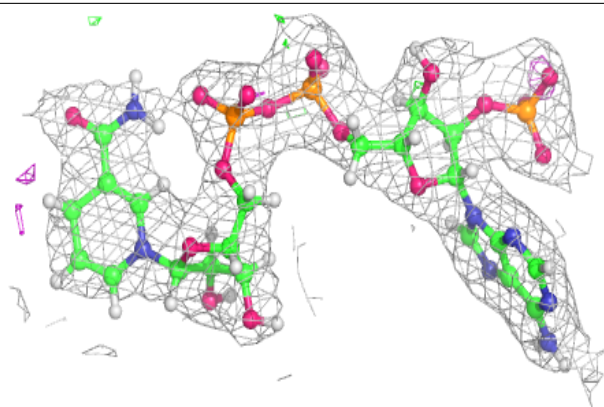
**Electron density around 4XN A 2202:**

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

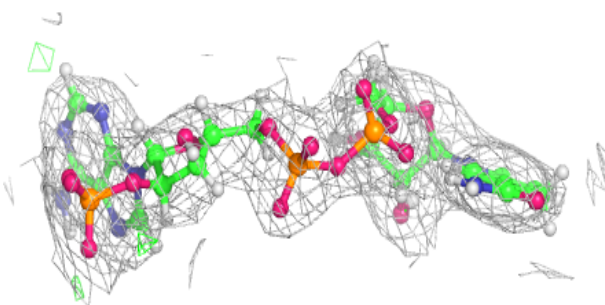
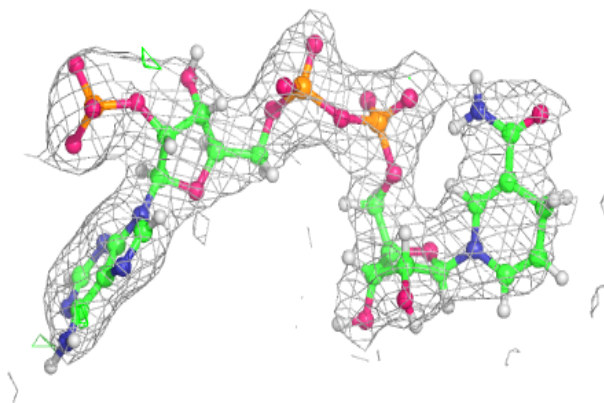


Electron density around NDP C 2201:

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

**Electron density around NDP A 2201:**

$2mF_o-DF_c$ (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.