Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 03:35 PM EDT

PDB ID	:	6NNA
Title	:	Human Fatty Acid Synthase Psi/KR Tri-Domain with NADPH and Compound 22
Authors	:	Toms, A.V.; Martin, M.W.
Deposited on	:	2019-01-14
Resolution	:	2.26 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:

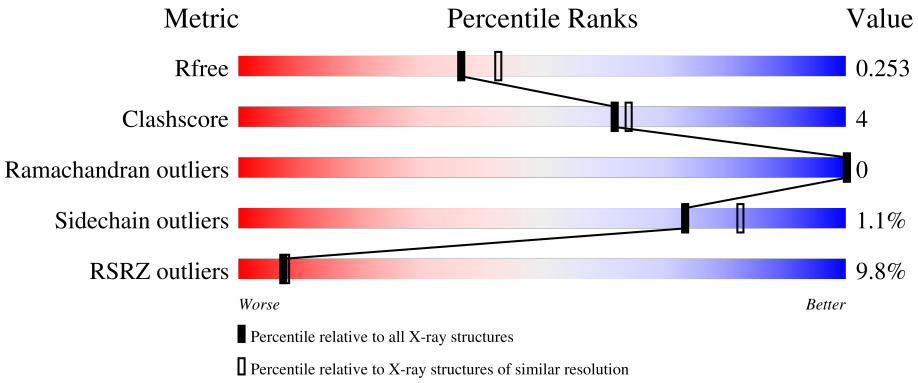
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 <=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	660	9% 83% 9% 8%
1	B	660	9% 82% 10% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10100 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.

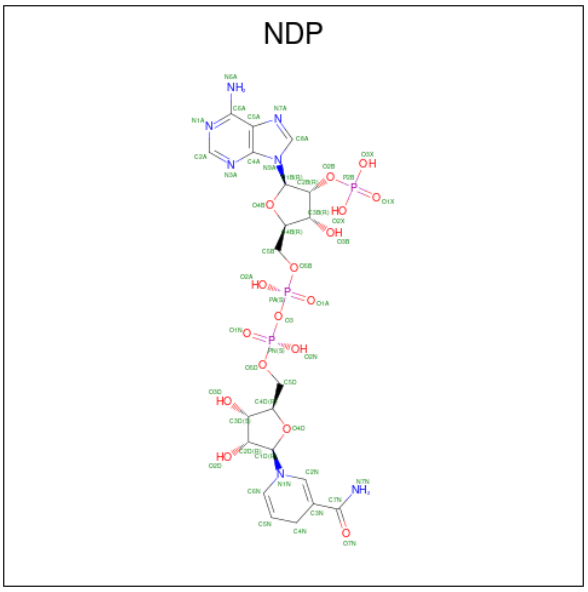
- Molecule 1 is a protein called Fatty acid synthase,Fatty acid synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	608	Total	As	C	N	O	S	0	2	0
			4653	1	2937	825	866	24			
1	B	608	Total	As	C	N	O	S	0	1	0
			4647	1	2933	823	866	24			

There are 16 discrepancies between the modelled and reference sequences:

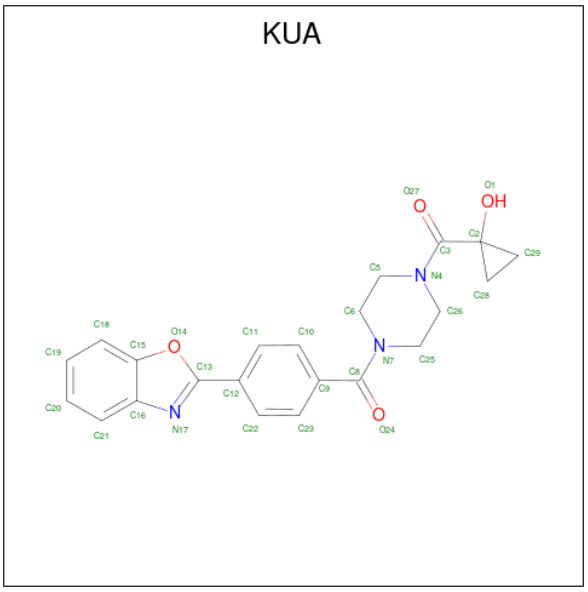
Chain	Residue	Modelled	Actual	Comment	Reference
A	1438	ALA	SER	engineered mutation	UNP P49327
A	1876	GLY	PRO	engineered mutation	UNP P49327
A	2115	HIS	-	expression tag	UNP P49327
A	2116	HIS	-	expression tag	UNP P49327
A	2117	HIS	-	expression tag	UNP P49327
A	2118	HIS	-	expression tag	UNP P49327
A	2119	HIS	-	expression tag	UNP P49327
A	2120	HIS	-	expression tag	UNP P49327
B	1438	ALA	SER	engineered mutation	UNP P49327
B	1876	GLY	PRO	engineered mutation	UNP P49327
B	2115	HIS	-	expression tag	UNP P49327
B	2116	HIS	-	expression tag	UNP P49327
B	2117	HIS	-	expression tag	UNP P49327
B	2118	HIS	-	expression tag	UNP P49327
B	2119	HIS	-	expression tag	UNP P49327
B	2120	HIS	-	expression tag	UNP P49327

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 3 is {4-[4-(1,3-benzoxazol-2-yl)benzene-1-carbonyl]piperazin-1-yl}(1-hydroxycyclopropyl)methanone (three-letter code: KUA) (formula: $C_{22}H_{21}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	22	3	4		

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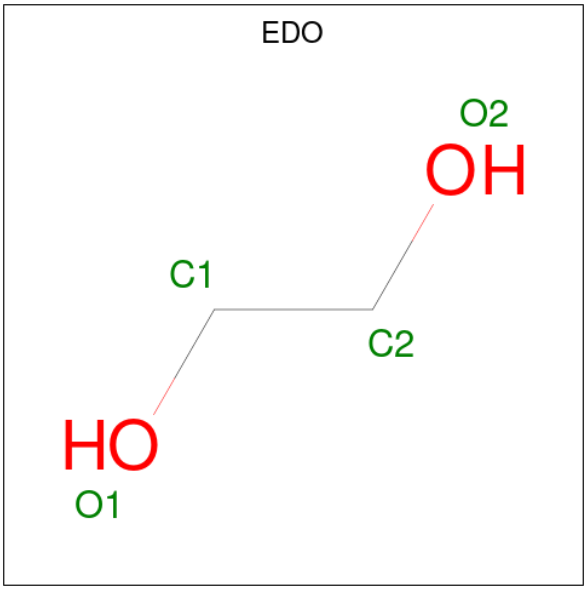
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 29 22 3 4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

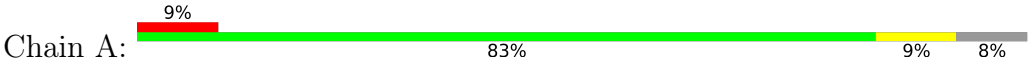
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	303	Total O 303 303	0	0
5	B	291	Total O 291 291	0	0

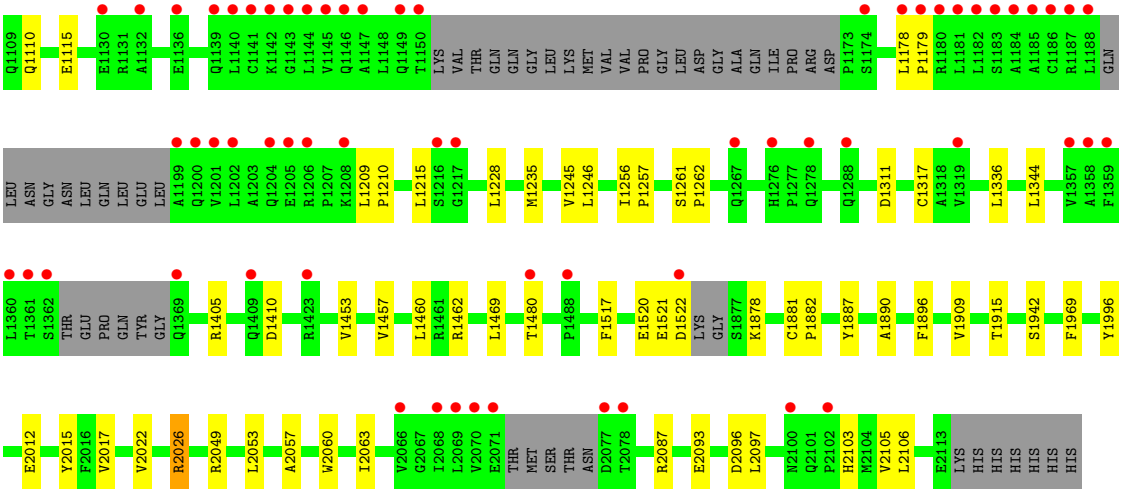
3 Residue-property plots (i)

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: Fatty acid synthase,Fatty acid synthase

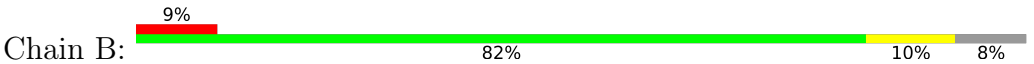
Chain A:

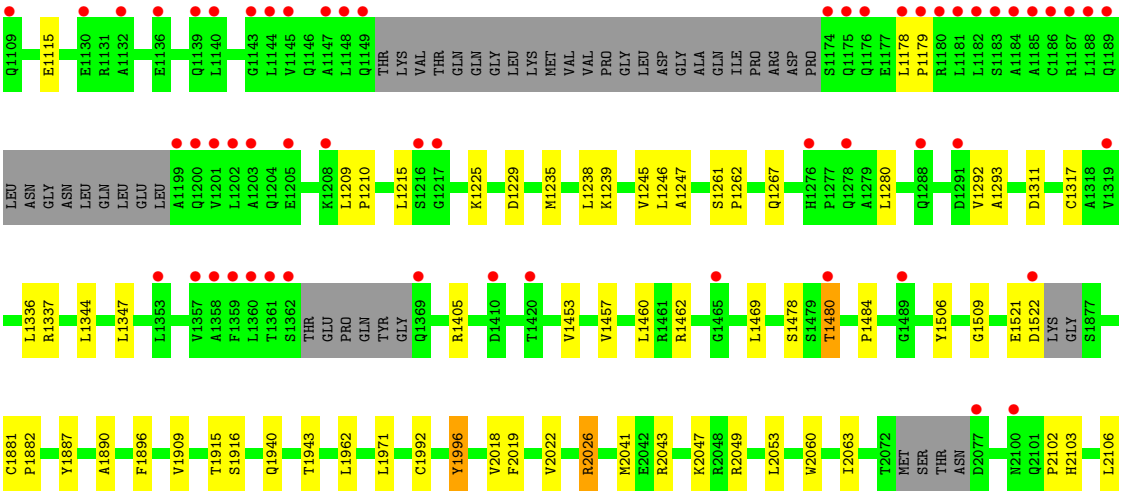




• Molecule 1: Fatty acid synthase,Fatty acid synthase

Chain B:






E213
LYS
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.11Å 85.74Å 86.47Å 65.57° 90.00° 87.00°	Depositor
Resolution (Å)	48.08 – 2.26 48.03 – 2.26	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.08-2.26) 97.3 (48.03-2.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.201 , 0.251 0.206 , 0.253	Depositor DCC
R_{free} test set	2646 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, NDP, CAF, KUA

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	0.65	0/4735	0.74	0/6419
1	B	0.66	0/4725	0.74	0/6405
All	All	0.65	0/9460	0.74	0/12824

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	4653	0	4679	39	0
1	B	4647	0	4671	44	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
4	A	28	0	42	4	0
4	B	24	0	36	6	0
5	A	303	0	0	4	0
5	B	291	0	0	0	0
All	All	10100	0	9480	83	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 4.

All (83) 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:1110:GLN:HE22	1:A:2087:ARG:H	1.13	0.96
1:B:2103:HIS:ND1	4:B:2208:EDO:H22	1.94	0.83
1:A:1110:GLN:NE2	1:A:2087:ARG:H	1.78	0.81
1:B:1971:LEU:HD22	1:B:2019:PHE:CD2	2.34	0.61
1:A:2026:ARG:NH1	4:A:2207:EDO:O1	2.35	0.59
1:B:1971:LEU:HD22	1:B:2019:PHE:CG	2.38	0.58
1:B:1235:MET:SD	1:B:1311:ASP:HB3	2.44	0.58
1:B:2103:HIS:HB2	1:B:2106:LEU:HD21	1.85	0.58
1:A:1261:SER:OG	1:A:1262:PRO:HD3	2.04	0.57
1:B:1996:TYR:HB3	4:B:2205:EDO:H21	1.87	0.57
1:B:1317:CYS:SG	1:B:1344:LEU:HD11	2.45	0.56
1:B:1245:VAL:HG12	1:B:1246:LEU:HG	1.88	0.56
1:B:1992:CYS:HB3	4:B:2205:EDO:H21	1.87	0.55
1:A:2103:HIS:HB2	1:A:2106:LEU:HD21	1.88	0.54
1:B:2049:ARG:NH2	1:B:2102:PRO:O	2.40	0.54
1:A:1890:ALA:HA	1:A:1915:THR:OG1	2.08	0.54
1:B:1916:SER:O	1:B:1943:THR:HA	2.07	0.54
1:B:2026:ARG:NH1	4:B:2207:EDO:O2	2.42	0.53
1:B:1336:LEU:O	1:B:1405:ARG:NH1	2.42	0.53
1:A:2060:TRP:HB3	1:A:2063:ILE:HD11	1.90	0.52
1:B:1881:CAF:CE1	1:B:1882:PRO:HD2	2.39	0.52
1:B:1261:SER:OG	1:B:1262:PRO:HD3	2.10	0.52
1:B:1453:VAL:O	1:B:1457:VAL:HG23	2.10	0.52
1:A:1462[A]:ARG:NE	1:A:1462[A]:ARG:HA	2.26	0.51
1:B:1209:LEU:HG	1:B:1215:LEU:CD1	2.41	0.51
1:B:1209:LEU:O	1:B:1215:LEU:HD12	2.10	0.51
1:A:1245:VAL:HG12	1:A:1246:LEU:HG	1.93	0.50
1:B:1239:LYS:HD3	1:B:1267:GLN:HB2	1.93	0.50
1:B:2043:ARG:O	1:B:2047[A]:LYS:HG2	2.12	0.49
1:B:1215:LEU:CD2	1:B:1347:LEU:HD11	2.43	0.49
1:A:2012:GLU:OE2	5:A:2301:HOH:O	2.19	0.49
1:B:1460:LEU:HB3	1:B:1469:LEU:CD1	2.43	0.48
1:B:1225:LYS:NZ	1:B:1229:ASP:OD2	2.47	0.48
1:A:1915:THR:HA	1:A:1942:SER:O	2.14	0.48
1:B:1238:LEU:HD21	1:B:1462:ARG:NH1	2.29	0.47
1:A:1317:CYS:SG	1:A:1344:LEU:HD11	2.54	0.47
1:B:1178:LEU:HB3	1:B:1179:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1235:MET:SD	1:A:1311:ASP:HB3	2.55	0.47
1:B:1940:GLN:HG3	1:B:1962:LEU:HD11	1.97	0.46
1:A:1178:LEU:HB3	1:A:1179:PRO:HD3	1.97	0.46
1:A:1878:LYS:HE3	5:A:2416:HOH:O	2.16	0.46
1:A:1881:CAF:CE1	1:A:1882:PRO:HD2	2.45	0.46
1:B:1484:PRO:HD3	1:B:1506:TYR:CE2	2.51	0.46
1:A:1517:PHE:CZ	4:A:2204:EDO:H11	2.51	0.45
1:B:1521:GLU:O	1:B:1522:ASP:C	2.54	0.45
1:A:1969:PHE:HA	1:A:2017:VAL:O	2.17	0.45
1:B:1238:LEU:HD21	1:B:1462:ARG:HH12	1.82	0.44
1:A:1453:VAL:O	1:A:1457:VAL:HG23	2.16	0.44
1:A:1887:TYR:CE2	1:A:1909:VAL:HG22	2.52	0.44
1:B:1209:LEU:N	1:B:1210:PRO:CD	2.81	0.44
1:A:1460:LEU:HB3	1:A:1469:LEU:CD1	2.48	0.44
1:A:2093:GLU:HA	5:A:2416:HOH:O	2.17	0.44
1:B:1292:VAL:HG12	1:B:1293:ALA:O	2.18	0.43
1:B:1506:TYR:OH	1:B:1509:GLY:HA2	2.18	0.43
1:B:2022:VAL:HG23	1:B:2026:ARG:HG2	1.99	0.43
1:B:2060:TRP:HB3	1:B:2063:ILE:HD11	2.01	0.43
1:A:1209:LEU:N	1:A:1210:PRO:CD	2.82	0.42
1:A:1520:GLU:HG2	1:A:1521:GLU:H	1.83	0.42
1:A:1115:GLU:OE2	4:A:2207:EDO:C1	2.68	0.42
1:A:1228:LEU:HD11	1:A:1256:ILE:HG12	2.01	0.42
1:A:1336:LEU:O	1:A:1405:ARG:NH2	2.51	0.42
1:A:1881:CAF:CE1	1:A:2015:TYR:CE2	3.02	0.42
1:B:1115:GLU:OE2	4:B:2207:EDO:O2	2.27	0.42
1:A:1115:GLU:OE2	4:A:2207:EDO:H11	2.20	0.42
1:A:2022:VAL:HG23	1:A:2026:ARG:HG2	2.00	0.42
1:B:1890:ALA:HA	1:B:1915:THR:OG1	2.20	0.42
1:A:2022:VAL:CG2	1:A:2026:ARG:HG2	2.49	0.42
1:A:1522:ASP:HA	1:A:2097:LEU:HD21	2.02	0.41
1:B:1992:CYS:HB3	4:B:2205:EDO:C2	2.49	0.41
1:A:1878:LYS:CE	5:A:2416:HOH:O	2.67	0.41
1:B:1887:TYR:CE2	1:B:1909:VAL:HG22	2.56	0.41
1:B:2049:ARG:HD2	1:B:2053:LEU:O	2.21	0.41
1:A:2049:ARG:HD2	1:A:2053:LEU:O	2.21	0.41
1:A:2057:ALA:O	1:A:2105:VAL:HA	2.21	0.41
1:B:1311:ASP:OD1	1:B:1337:ARG:NE	2.47	0.41
1:A:1520:GLU:HG2	1:A:1521:GLU:N	2.36	0.41
1:A:1256:ILE:HB	1:A:1257:PRO:HD3	2.04	0.40
1:A:1261:SER:N	1:A:1262:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1522:ASP:HA	1:A:2097:LEU:CD2	2.52	0.40
1:B:1247:ALA:HB3	1:B:1280:LEU:HD21	2.02	0.40
1:B:1261:SER:N	1:B:1262:PRO:CD	2.85	0.40
1:B:2018:VAL:HG21	1:B:2041:MET:HB3	2.04	0.40
1:B:1478:SER:OG	1:B:1480:THR:HG22	2.22	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	597/660 (90%)	579 (97%)	18 (3%)	0	100	100
1	B	596/660 (90%)	579 (97%)	17 (3%)	0	100	100
All	All	1193/1320 (90%)	1158 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	504/547 (92%)	497 (99%)	7 (1%)	67	76
1	B	503/547 (92%)	499 (99%)	4 (1%)	81	88
All	All	1007/1094 (92%)	996 (99%)	11 (1%)	73	82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1215	LEU
1	A	1410	ASP
1	A	1480	THR
1	A	1896	PHE
1	A	1996	TYR
1	A	2026	ARG
1	A	2096	ASP
1	B	1480	THR
1	B	1896	PHE
1	B	1996	TYR
1	B	2026	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1110	GLN
1	A	1176	GLN
1	A	1482	HIS
1	B	1176	GLN
1	B	1906	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CAF	A	1881	1	3,9,10	0.67	0	1,12,14	0.26	0
1	CAF	B	1881	1	3,9,10	0.72	0	1,12,14	0.75	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
1	CAF	A	1881	1	-	0/0/8/10	-
1	CAF	B	1881	1	-	0/0/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1881	CAF	2	0
1	B	1881	CAF	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	$\#\|Z\| > 2$
4	EDO	B	2206	-	3,3,3	0.04	0	2,2,2	0.19	0
4	EDO	A	2209	-	3,3,3	0.08	0	2,2,2	0.19	0
2	NDP	A	2201	-	45,52,52	0.98	2 (4%)	53,80,80	1.24	6 (11%)
4	EDO	B	2203	-	3,3,3	0.11	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	A	2208	-	3,3,3	0.13	0	2,2,2	0.27	0
3	KUA	B	2202	-	28,33,33	1.05	2 (7%)	35,49,49	1.08	2 (5%)
4	EDO	B	2207	-	3,3,3	0.11	0	2,2,2	0.21	0
4	EDO	B	2208	-	3,3,3	0.05	0	2,2,2	0.30	0
4	EDO	A	2204	-	3,3,3	0.07	0	2,2,2	0.39	0
4	EDO	A	2205	-	3,3,3	0.14	0	2,2,2	0.31	0
4	EDO	B	2204	-	3,3,3	0.16	0	2,2,2	0.21	0
3	KUA	A	2202	-	28,33,33	1.06	2 (7%)	35,49,49	1.20	4 (11%)
4	EDO	B	2205	-	3,3,3	0.09	0	2,2,2	0.23	0
4	EDO	A	2206	-	3,3,3	0.14	0	2,2,2	0.09	0
4	EDO	A	2207	-	3,3,3	0.05	0	2,2,2	0.26	0
4	EDO	A	2203	-	3,3,3	0.06	0	2,2,2	0.28	0
2	NDP	B	2201	-	45,52,52	0.94	2 (4%)	53,80,80	1.25	8 (15%)

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
4	EDO	B	2206	-	-	1/1/1/1	-
4	EDO	A	2209	-	-	1/1/1/1	-
2	NDP	A	2201	-	-	5/30/77/77	0/5/5/5
4	EDO	B	2203	-	-	1/1/1/1	-
4	EDO	A	2208	-	-	1/1/1/1	-
3	KUA	B	2202	-	-	0/18/36/36	0/5/5/5
4	EDO	B	2207	-	-	0/1/1/1	-
4	EDO	B	2208	-	-	0/1/1/1	-
4	EDO	A	2204	-	-	0/1/1/1	-
4	EDO	A	2205	-	-	1/1/1/1	-
4	EDO	B	2204	-	-	1/1/1/1	-
3	KUA	A	2202	-	-	0/18/36/36	0/5/5/5
4	EDO	B	2205	-	-	0/1/1/1	-
4	EDO	A	2206	-	-	0/1/1/1	-
4	EDO	A	2207	-	-	1/1/1/1	-
4	EDO	A	2203	-	-	1/1/1/1	-
2	NDP	B	2201	-	-	6/30/77/77	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2201	NDP	C6N-C5N	3.33	1.39	1.33
2	A	2201	NDP	C5A-C4A	3.00	1.48	1.40
2	B	2201	NDP	C5A-C4A	2.91	1.48	1.40
3	B	2202	KUA	C29-C2	2.83	1.54	1.50
3	B	2202	KUA	C28-C2	2.59	1.53	1.50
3	A	2202	KUA	C28-C2	2.52	1.53	1.50
2	B	2201	NDP	C6N-C5N	2.36	1.37	1.33
3	A	2202	KUA	C29-C2	2.22	1.53	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2201	NDP	N3A-C2A-N1A	-3.97	122.48	128.68
2	A	2201	NDP	N3A-C2A-N1A	-3.77	122.78	128.68
3	A	2202	KUA	C26-N4-C5	3.70	119.75	112.62
3	B	2202	KUA	C26-N4-C5	3.35	119.07	112.62
3	A	2202	KUA	C13-N17-C16	2.61	108.95	103.78
2	A	2201	NDP	C3N-C7N-N7N	2.58	122.25	117.67
3	A	2202	KUA	C10-C11-C12	-2.41	117.66	121.13
2	A	2201	NDP	O2A-PA-O1A	2.39	124.06	112.24
3	A	2202	KUA	C12-C13-N17	2.37	126.74	123.56
2	B	2201	NDP	C2A-N1A-C6A	2.29	122.66	118.75
2	B	2201	NDP	O2B-P2B-O1X	-2.27	100.65	109.39
2	A	2201	NDP	C2A-N1A-C6A	2.24	122.59	118.75
2	B	2201	NDP	O2X-P2B-O1X	2.18	119.22	110.68
3	B	2202	KUA	C10-C11-C12	-2.16	118.02	121.13
2	B	2201	NDP	O2A-PA-O1A	2.16	122.91	112.24
2	A	2201	NDP	O7N-C7N-C3N	-2.15	116.85	120.90
2	B	2201	NDP	O7N-C7N-C3N	-2.14	116.88	120.90
2	A	2201	NDP	O2B-P2B-O1X	-2.12	101.22	109.39
2	B	2201	NDP	O3X-P2B-O2X	2.08	115.59	107.64
2	B	2201	NDP	O2N-PN-O1N	2.01	122.16	112.24

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2201	NDP	C5D-O5D-PN-O1N
2	B	2201	NDP	C5D-O5D-PN-O1N
4	B	2204	EDO	O1-C1-C2-O2
4	A	2207	EDO	O1-C1-C2-O2
4	B	2206	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	2205	EDO	O1-C1-C2-O2
4	A	2208	EDO	O1-C1-C2-O2
4	B	2203	EDO	O1-C1-C2-O2
2	B	2201	NDP	O4D-C1D-N1N-C6N
4	A	2203	EDO	O1-C1-C2-O2
2	B	2201	NDP	C5D-O5D-PN-O3
2	A	2201	NDP	O4D-C1D-N1N-C6N
2	A	2201	NDP	C5D-O5D-PN-O2N
2	B	2201	NDP	C5D-O5D-PN-O2N
4	A	2209	EDO	O1-C1-C2-O2
2	A	2201	NDP	O4B-C4B-C5B-O5B
2	A	2201	NDP	C5D-O5D-PN-O3
2	B	2201	NDP	O4B-C4B-C5B-O5B
2	B	2201	NDP	C2N-C3N-C7N-N7N

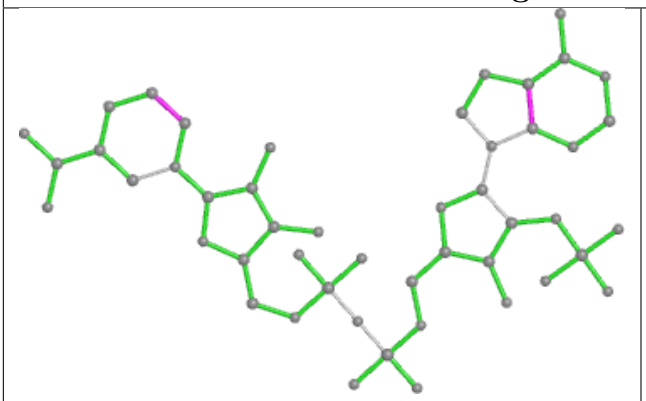
There are no ring outliers.

5 monomers are involved in 10 short contacts:

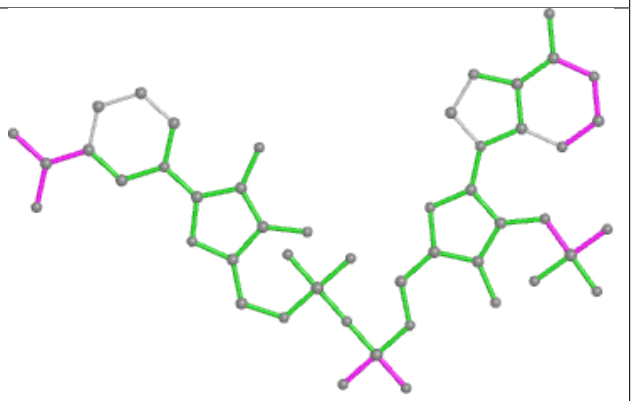
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2207	EDO	2	0
4	B	2208	EDO	1	0
4	A	2204	EDO	1	0
4	B	2205	EDO	3	0
4	A	2207	EDO	3	0

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 then 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.

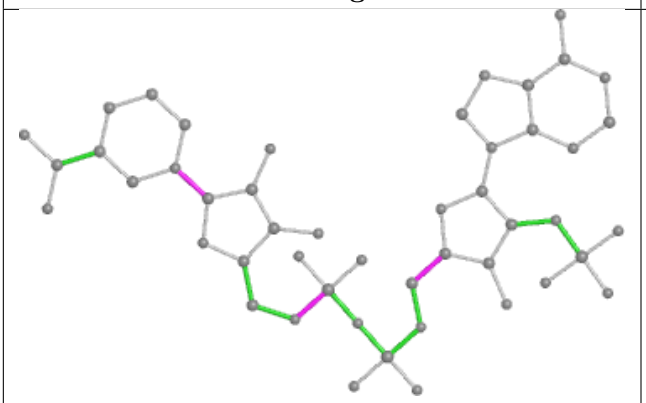
Ligand NDP A 2201



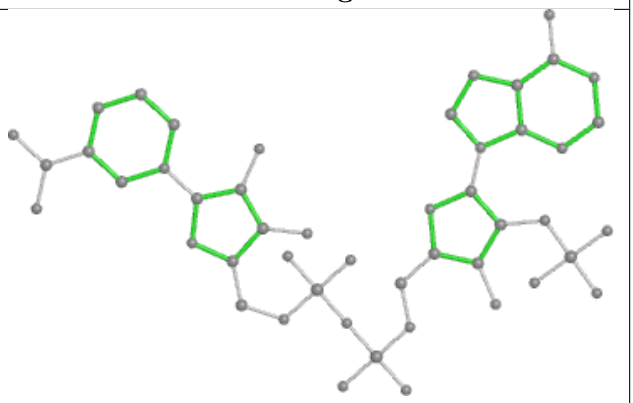
Bond lengths



Bond angles

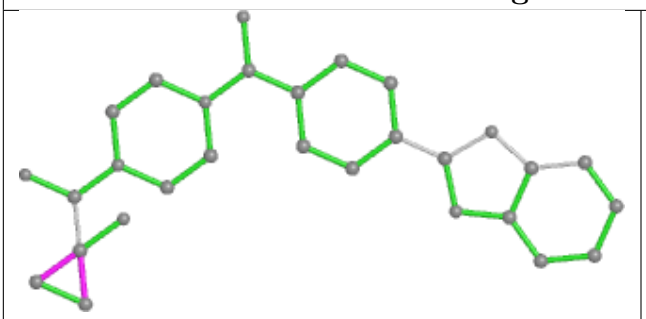


Torsions

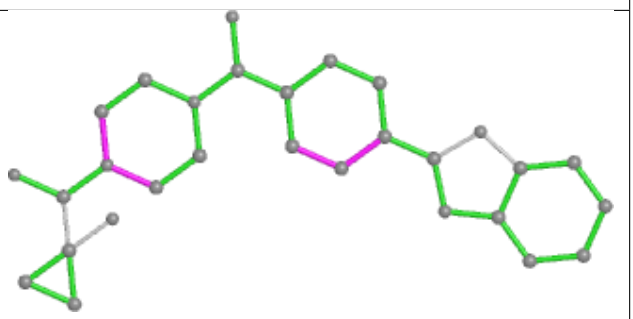


Rings

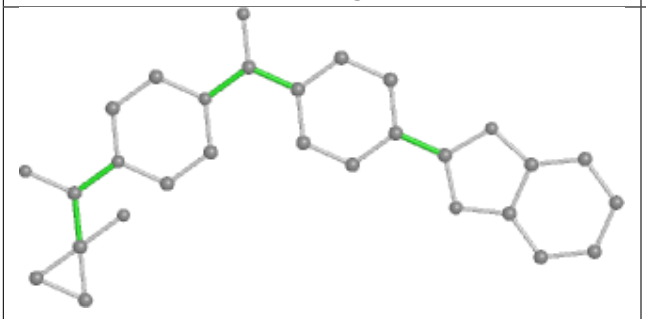
Ligand KUA B 2202



Bond lengths



Bond angles



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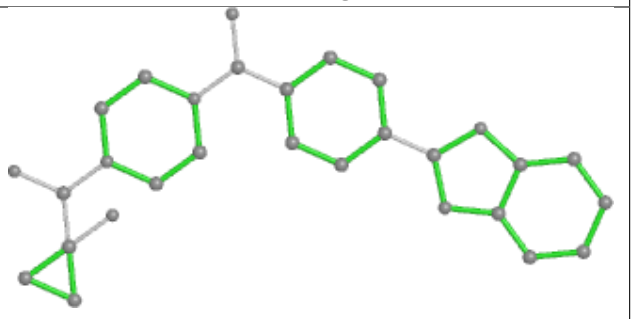
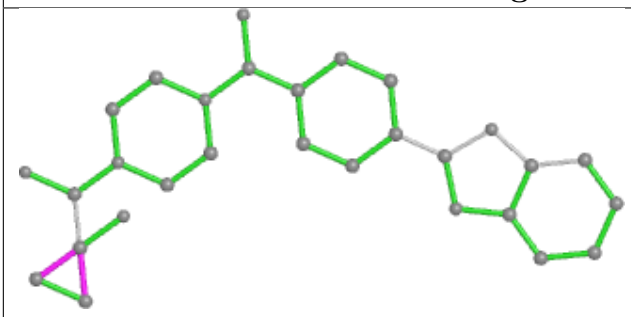
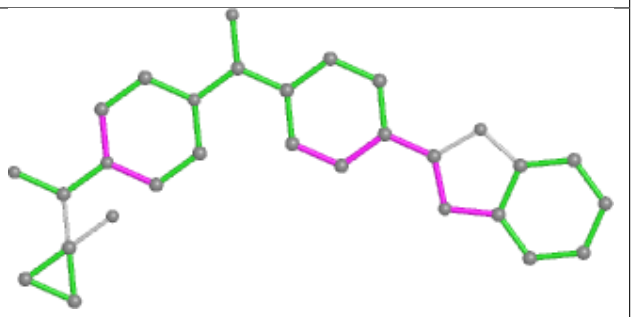


Rings

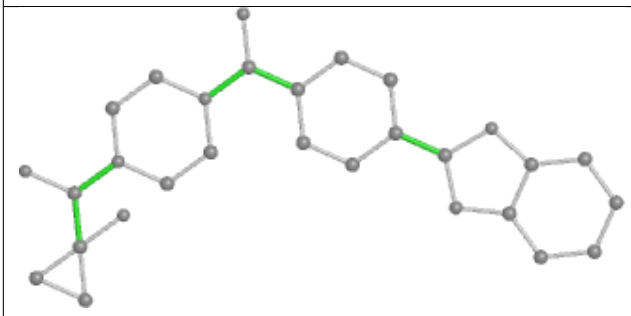
Ligand KUA A 2202



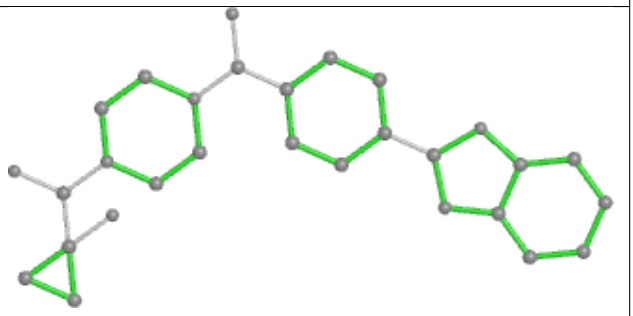
Bond lengths



Bond angles

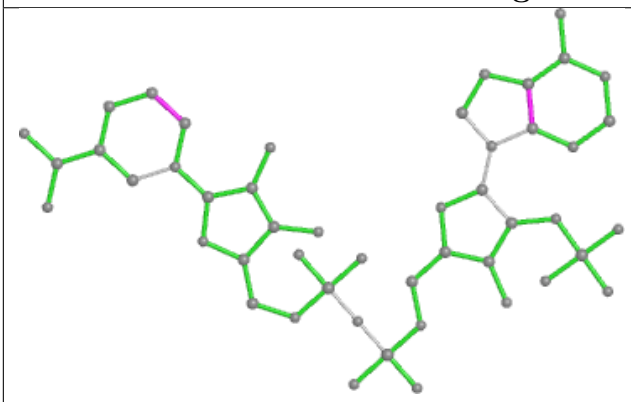


Torsions

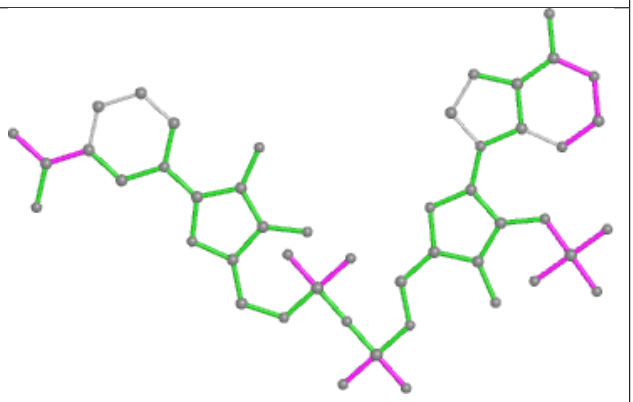


Rings

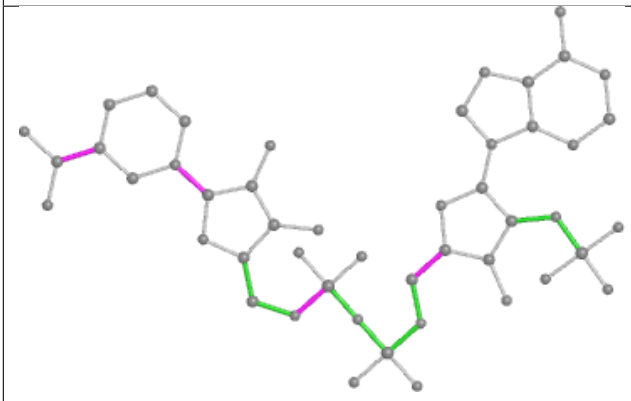
Ligand NDP B 2201



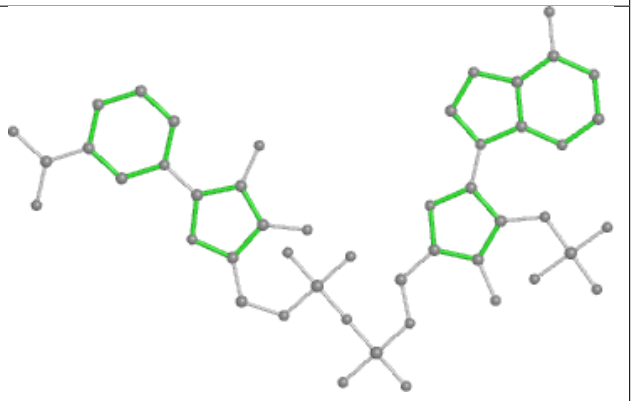
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	607/660 (91%)	0.59	62 (10%) 6 6	18, 33, 77, 104	0
1	B	607/660 (91%)	0.60	57 (9%) 8 9	17, 32, 74, 121	0
All	All	1214/1320 (91%)	0.60	119 (9%) 7 8	17, 33, 78, 121	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1187	ARG	8.9
1	B	1362	SER	8.2
1	B	1183	SER	8.2
1	B	1201	VAL	7.9
1	B	1202	LEU	7.8
1	A	1150	THR	7.7
1	A	2071	GLU	7.1
1	A	1187	ARG	6.6
1	A	2077	ASP	6.5
1	B	1188	LEU	6.2
1	A	1185	ALA	6.1
1	B	1185	ALA	6.0
1	B	1200	GLN	5.9
1	B	1360	LEU	5.7
1	B	1174	SER	5.6
1	B	1140	LEU	5.5
1	B	1184	ALA	5.4
1	A	1359	PHE	5.3
1	A	1360	LEU	5.2
1	B	1359	PHE	5.2
1	A	1369	GLN	5.2
1	B	1145	VAL	5.1
1	A	1183	SER	4.8
1	B	1182	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	1200	GLN	4.7
1	A	1358	ALA	4.6
1	B	1149	GLN	4.5
1	B	1175	GLN	4.4
1	A	1357	VAL	4.4
1	A	1149	GLN	4.4
1	A	1202	LEU	4.4
1	B	1276	HIS	4.3
1	A	1199	ALA	4.3
1	A	1143	GLY	4.3
1	A	1145	VAL	4.2
1	B	1369	GLN	4.2
1	A	1361	THR	4.2
1	A	1180	ARG	4.2
1	B	1357	VAL	4.2
1	B	1180	ARG	4.2
1	B	2100	ASN	4.2
1	A	1184	ALA	4.1
1	A	1206	ARG	4.0
1	A	1130	GLU	4.0
1	B	1186	CYS	4.0
1	B	1189	GLN	4.0
1	B	1147	ALA	3.9
1	A	1140	LEU	3.8
1	A	1174	SER	3.8
1	B	1361	THR	3.7
1	B	1148	LEU	3.7
1	A	1146	GLN	3.6
1	B	1205	GLU	3.6
1	A	1188	LEU	3.5
1	A	1205	GLU	3.5
1	B	1420	THR	3.4
1	A	1216	SER	3.4
1	A	1201	VAL	3.4
1	B	1288	GLN	3.4
1	A	2070	VAL	3.4
1	A	1488	PRO	3.4
1	A	2066	VAL	3.3
1	B	1278	GLN	3.3
1	A	2100	ASN	3.3
1	A	1288	GLN	3.3
1	A	1147	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1181	LEU	3.3
1	A	1319	VAL	3.2
1	B	1410	ASP	3.2
1	A	1132	ALA	3.2
1	B	1358	ALA	3.2
1	B	1179	PRO	3.2
1	A	1204	GLN	3.2
1	A	1362	SER	3.1
1	A	1141	CYS	3.1
1	A	1181	LEU	3.0
1	A	1276	HIS	3.0
1	B	1319	VAL	3.0
1	B	1143	GLY	3.0
1	A	1139	GLN	2.9
1	A	1186	CYS	2.9
1	A	1278	GLN	2.9
1	A	1182	LEU	2.9
1	B	1130	GLU	2.8
1	B	1139	GLN	2.8
1	A	1522	ASP	2.7
1	A	1179	PRO	2.7
1	B	1208	LYS	2.7
1	A	2069	LEU	2.6
1	A	1409	GLN	2.6
1	B	1144	LEU	2.6
1	B	1132	ALA	2.6
1	B	1176	GLN	2.5
1	B	1178	LEU	2.5
1	B	1522	ASP	2.5
1	B	1353	LEU	2.5
1	A	2068	ILE	2.3
1	A	2102	PRO	2.3
1	B	1480	THR	2.3
1	A	1144	LEU	2.3
1	B	1216	SER	2.3
1	A	1136	GLU	2.3
1	B	1203	ALA	2.3
1	B	1217	GLY	2.2
1	B	1109	GLN	2.2
1	B	1291	ASP	2.2
1	B	1489	GLY	2.2
1	A	1267	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1217	GLY	2.1
1	B	2077	ASP	2.1
1	A	1142	LYS	2.1
1	A	1423	ARG	2.1
1	A	1480	THR	2.1
1	A	2078	THR	2.0
1	B	1199	ALA	2.0
1	B	1136	GLU	2.0
1	A	1208	LYS	2.0
1	A	1178	LEU	2.0
1	B	1465	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CAF	B	1881	10/11	0.94	0.14	27,29,38,39	0
1	CAF	A	1881	10/11	0.97	0.12	28,30,35,37	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	2208	4/4	0.66	0.24	50,54,55,58	0
4	EDO	B	2207	4/4	0.75	0.25	46,50,51,56	0
4	EDO	A	2207	4/4	0.78	0.22	36,40,40,43	0
4	EDO	A	2203	4/4	0.82	0.18	53,54,54,55	0
4	EDO	A	2208	4/4	0.82	0.17	50,52,52,52	0

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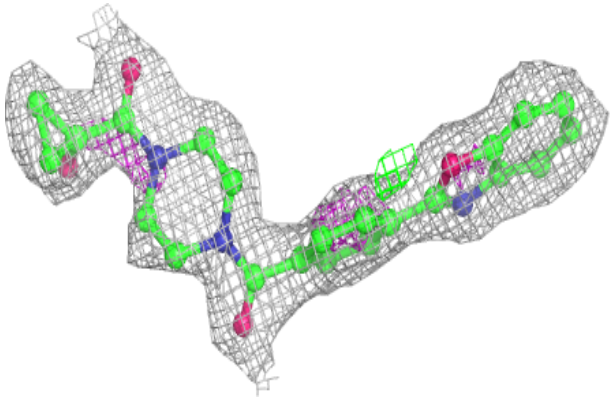
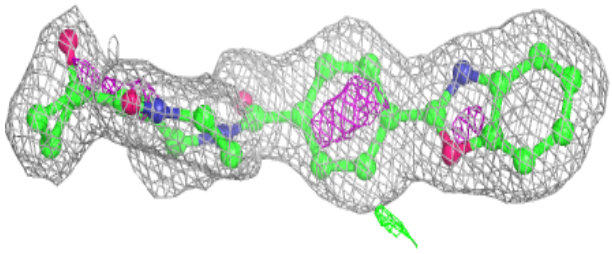
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	2205	4/4	0.84	0.20	54,57,57,57	0
4	EDO	B	2205	4/4	0.85	0.18	39,40,41,43	0
4	EDO	A	2209	4/4	0.86	0.24	38,39,40,41	0
4	EDO	B	2206	4/4	0.89	0.23	46,47,49,53	0
4	EDO	A	2206	4/4	0.90	0.17	46,46,47,49	0
3	KUA	A	2202	29/29	0.90	0.17	21,23,27,28	0
4	EDO	B	2203	4/4	0.90	0.21	36,37,38,40	0
4	EDO	B	2204	4/4	0.90	0.17	33,34,34,34	0
4	EDO	A	2204	4/4	0.91	0.19	39,40,40,41	0
3	KUA	B	2202	29/29	0.91	0.16	18,21,25,25	0
2	NDP	B	2201	48/48	0.95	0.12	16,21,28,31	0
2	NDP	A	2201	48/48	0.95	0.12	17,22,30,32	0

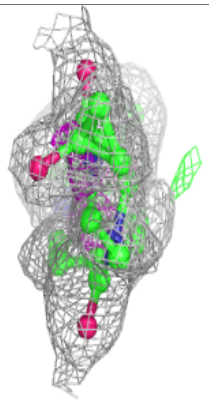
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KUA 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)

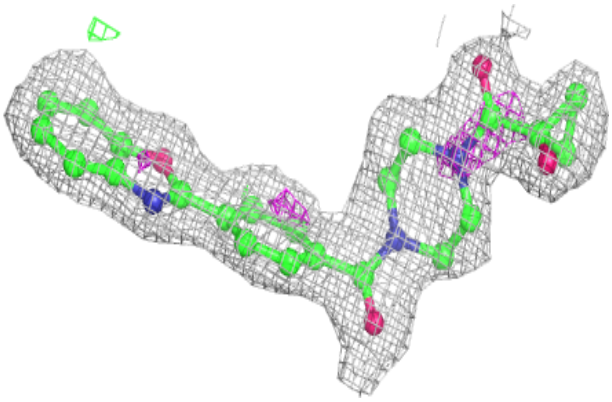


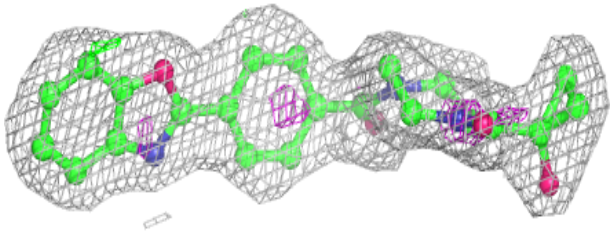


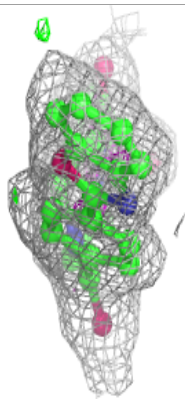


Electron density around KUA B 2202:

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

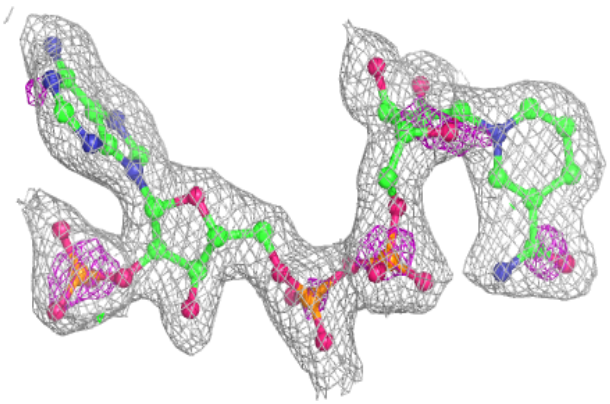


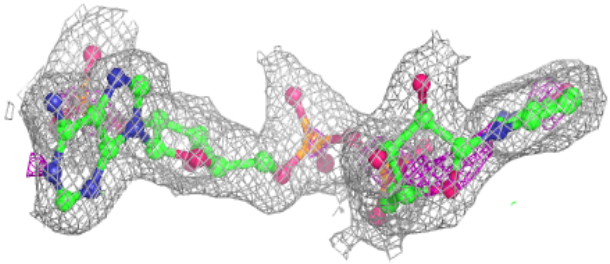


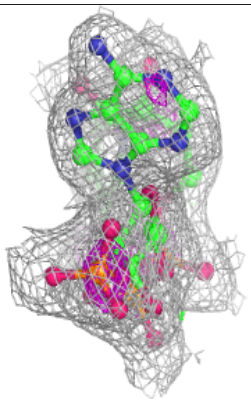


Electron density around NDP B 2201:

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

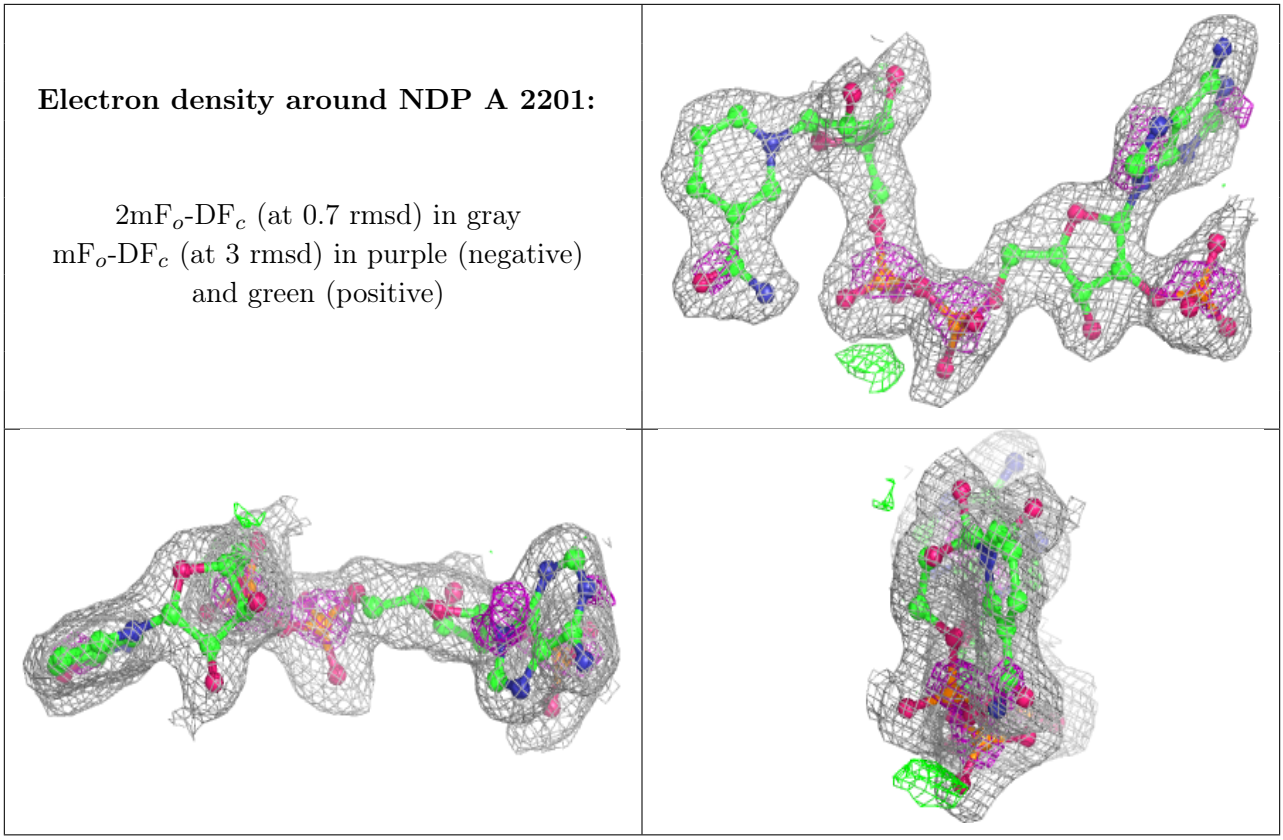






Electron density around NDP A 2201:

$2mF_o$-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.