



Full wwPDB X-ray Structure Validation Report

Dec 2, 2024 – 12:12 PM EST

PDB ID : 2JAH
Title : Biochemical and structural analysis of the Clavulanic acid dehydrogenase (CAD) from *Streptomyces clavuligerus*
Authors : MacKenzie, A.K.; Kershaw, N.J.; Hernandez, H.; Robinson, C.V.; Schofield, C.J.; Andersson, I.
Deposited on : 2006-11-28
Resolution : 1.80 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

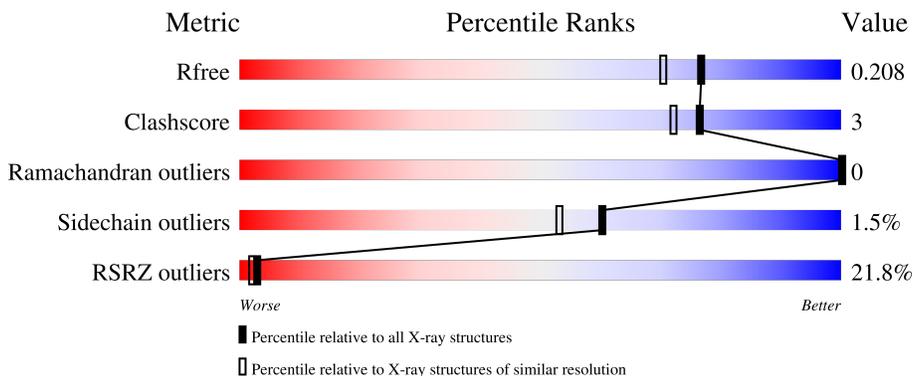
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	164625	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	247	
1	B	247	
1	C	247	
1	D	247	

2 Entry composition [i](#)

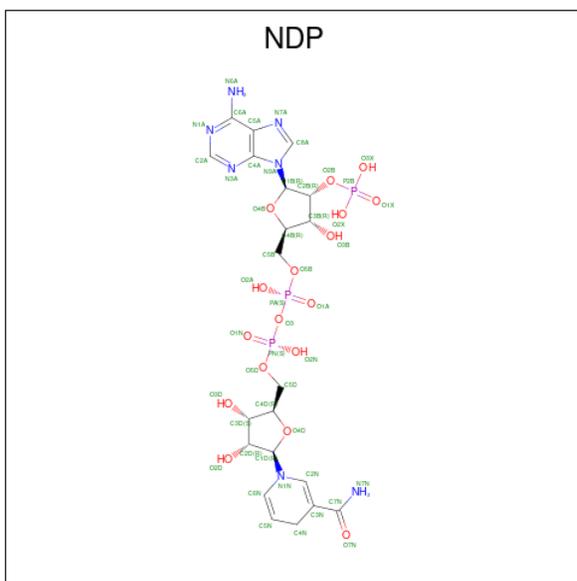
There are 3 unique types of molecules in this entry. The entry contains 8056 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CLAVULANIC ACID DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	245	Total 1840	C 1141	N 338	O 354	Se 7	0	1	0
1	B	245	Total 1840	C 1141	N 338	O 354	Se 7	0	1	0
1	C	246	Total 1858	C 1152	N 343	O 356	Se 7	0	2	0
1	D	245	Total 1832	C 1136	N 337	O 353	Se 6	0	0	0

- 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	
			Total	C	N	O			P
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

Continued on next page...

Continued from previous page...

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

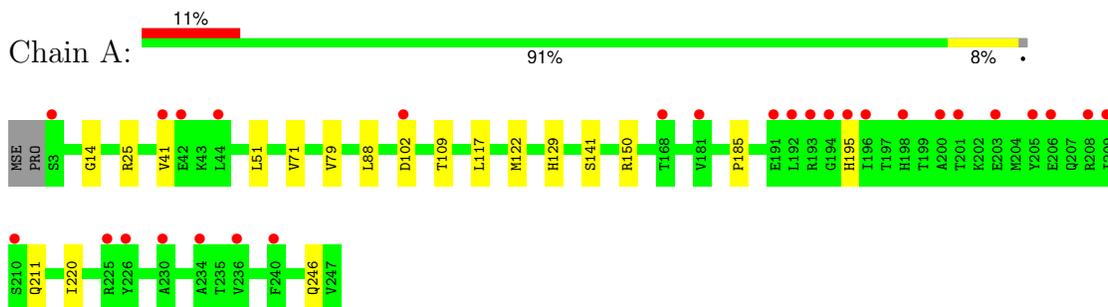
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	105	Total	O	0	0
			105	105		
3	C	131	Total	O	0	0
			131	131		
3	D	117	Total	O	0	0
			117	117		

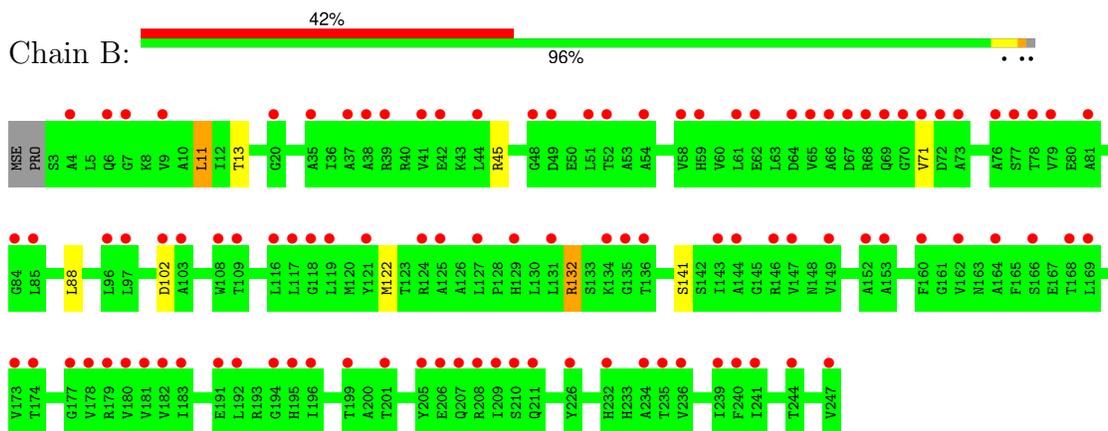
3 Residue-property plots

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. 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. 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.

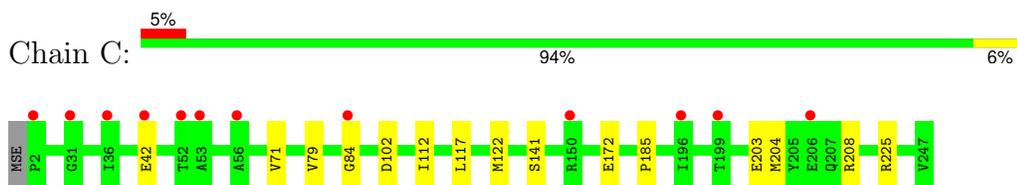
- Molecule 1: CLAVULANIC ACID DEHYDROGENASE



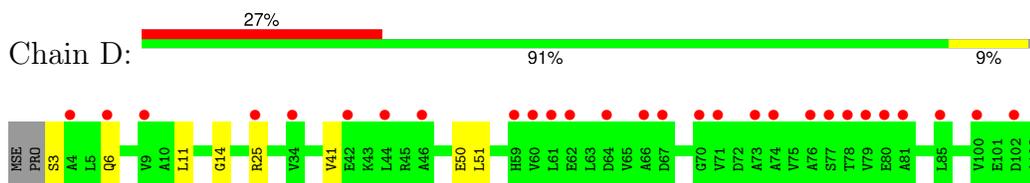
- Molecule 1: CLAVULANIC ACID DEHYDROGENASE

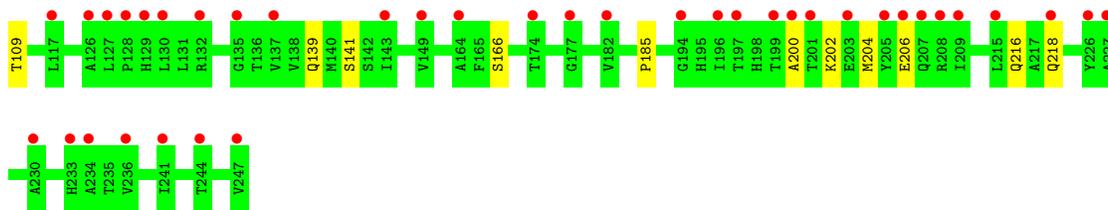


- Molecule 1: CLAVULANIC ACID DEHYDROGENASE



- Molecule 1: CLAVULANIC ACID DEHYDROGENASE





4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.75Å 122.63Å 126.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 1.80 29.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.92-1.80) 95.8 (29.92-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.182 , 0.209 0.182 , 0.208	Depositor DCC
R_{free} test set	4118 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtrriage
Anisotropy	0.086	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8056	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.93 % 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 2.9481e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/1854	0.60	0/2505
1	B	0.70	2/1854 (0.1%)	0.78	3/2505 (0.1%)
1	C	0.45	0/1873	0.61	0/2530
1	D	0.48	0/1846	0.60	0/2495
All	All	0.54	2/7427 (0.0%)	0.65	3/10035 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	ARG	CZ-NH1	19.21	1.58	1.33
1	B	45	ARG	NE-CZ	10.27	1.46	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	ARG	NE-CZ-NH1	17.71	129.16	120.30
1	B	45	ARG	NE-CZ-NH2	-17.03	111.78	120.30
1	B	11	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1840	0	1879	14	0
1	B	1840	0	1879	5	0
1	C	1858	0	1899	9	0
1	D	1832	0	1871	17	0
2	A	48	0	26	3	0
2	B	48	0	26	1	0
2	C	48	0	26	3	0
2	D	48	0	26	3	0
3	A	141	0	0	3	0
3	B	105	0	0	1	0
3	C	131	0	0	2	0
3	D	117	0	0	1	0
All	All	8056	0	7632	43	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 (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:GLN:HB3	1:D:218:GLN:OE1	1.72	0.89
1:D:218:GLN:H	1:D:218:GLN:CD	1.93	0.72
1:D:3:SER:HB2	1:D:6:GLN:CG	2.22	0.70
1:B:132:ARG:HG3	3:B:2042:HOH:O	1.92	0.69
1:D:3:SER:HB2	1:D:6:GLN:HG3	1.79	0.64
1:C:208:ARG:NH2	3:C:2104:HOH:O	2.31	0.62
1:D:3:SER:HB2	1:D:6:GLN:HG2	1.84	0.57
1:A:195:HIS:HE1	3:A:2141:HOH:O	1.89	0.56
1:C:71:VAL:HG13	1:C:122[B]:MSE:SE	2.56	0.55
1:B:71:VAL:HG13	1:B:122[B]:MSE:SE	2.57	0.54
1:D:202:LYS:O	1:D:206:GLU:HG3	2.07	0.54
1:A:109:THR:HG22	1:C:117:LEU:HD21	1.90	0.54
1:C:185:PRO:O	2:C:1248:NDP:H5N	2.09	0.52
1:A:141:SER:O	2:A:1248:NDP:H6N	2.09	0.52
1:D:25:ARG:NH1	1:D:50:GLU:OE1	2.43	0.51
1:C:204:MSE:HE2	3:C:2078:HOH:O	2.10	0.50
1:A:246:GLN:OE1	3:A:2135:HOH:O	2.19	0.49
1:D:185:PRO:O	2:D:1248:NDP:H5N	2.12	0.49
1:A:185:PRO:O	2:A:1248:NDP:H5N	2.12	0.49
1:A:71:VAL:HG13	1:A:122[B]:MSE:SE	2.63	0.48
1:D:218:GLN:CD	1:D:218:GLN:N	2.65	0.47
1:D:141:SER:O	2:D:1248:NDP:H6N	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:ALA:O	1:D:204:MSE:HG3	2.15	0.46
1:A:14:GLY:HA2	2:A:1248:NDP:H1B	1.98	0.46
1:D:14:GLY:HA2	2:D:1248:NDP:H1B	1.97	0.45
1:B:141:SER:O	2:B:1248:NDP:H6N	2.16	0.45
1:C:79:VAL:HG13	1:C:84:GLY:HA2	1.98	0.45
1:A:185:PRO:HB3	1:A:220:ILE:HD12	1.98	0.45
1:A:117:LEU:HD13	1:C:112:ILE:HD12	1.99	0.45
1:A:150:ARG:HD3	1:C:172:GLU:HA	1.99	0.44
1:A:88:LEU:HD21	1:A:122[A]:MSE:HG3	2.00	0.44
1:B:13:THR:CG2	1:B:122[B]:MSE:HE2	2.47	0.44
1:D:25:ARG:HD3	1:D:50:GLU:OE2	2.18	0.44
1:D:25:ARG:HG2	1:D:51:LEU:HD21	2.00	0.43
1:A:79:VAL:HG21	1:A:129:HIS:CE1	2.54	0.43
1:C:141:SER:O	2:C:1248:NDP:H6N	2.19	0.43
1:D:104:ASP:O	1:D:107:ASP:HB2	2.18	0.43
1:A:211:GLN:NE2	3:A:2115:HOH:O	2.53	0.42
1:B:88:LEU:HD21	1:B:122[A]:MSE:HG3	2.02	0.42
2:C:1248:NDP:O1N	2:C:1248:NDP:H2N	2.19	0.42
1:D:139:GLN:HG3	1:D:166:SER:OG	2.21	0.41
1:A:25:ARG:HG2	1:A:51:LEU:HD21	2.01	0.41
1:D:109:THR:HA	3:D:2045:HOH:O	2.21	0.41

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	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
1	B	244/247 (99%)	241 (99%)	3 (1%)	0	100	100
1	C	246/247 (100%)	243 (99%)	3 (1%)	0	100	100
1	D	243/247 (98%)	239 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	977/988 (99%)	962 (98%)	15 (2%)	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	189/183 (103%)	187 (99%)	2 (1%)	70	65
1	B	189/183 (103%)	186 (98%)	3 (2%)	58	50
1	C	191/183 (104%)	187 (98%)	4 (2%)	48	38
1	D	188/183 (103%)	186 (99%)	2 (1%)	70	65
All	All	757/732 (103%)	746 (98%)	11 (2%)	60	53

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

Mol	Chain	Res	Type
1	A	41	VAL
1	A	102	ASP
1	B	11	LEU
1	B	102	ASP
1	B	132	ARG
1	C	42	GLU
1	C	102	ASP
1	C	203	GLU
1	C	225	ARG
1	D	11	LEU
1	D	41	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	195	HIS
1	A	211	GLN
1	A	246	GLN
1	B	91	ASN
1	B	195	HIS
1	B	207	GLN
1	B	211	GLN
1	C	91	ASN
1	C	195	HIS
1	D	91	ASN
1	D	151	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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	B	1248	-	47,52,52	1.61	5 (10%)	61,80,80	1.31	4 (6%)
2	NDP	C	1248	-	47,52,52	1.54	5 (10%)	61,80,80	1.39	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	A	1248	-	47,52,52	1.58	5 (10%)	61,80,80	1.27	4 (6%)
2	NDP	D	1248	-	47,52,52	1.59	6 (12%)	61,80,80	1.24	4 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	B	1248	-	-	5/30/77/77	0/5/5/5
2	NDP	C	1248	-	-	6/30/77/77	0/5/5/5
2	NDP	A	1248	-	-	4/30/77/77	0/5/5/5
2	NDP	D	1248	-	-	6/30/77/77	0/5/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1248	NDP	O7N-C7N	7.42	1.41	1.24
2	D	1248	NDP	O7N-C7N	7.28	1.41	1.24
2	A	1248	NDP	O7N-C7N	7.03	1.40	1.24
2	C	1248	NDP	O7N-C7N	6.95	1.40	1.24
2	D	1248	NDP	C2A-N3A	4.46	1.39	1.32
2	A	1248	NDP	C2A-N3A	4.43	1.39	1.32
2	B	1248	NDP	C2A-N3A	4.38	1.38	1.32
2	C	1248	NDP	C2A-N3A	4.14	1.38	1.32
2	B	1248	NDP	C2A-N1A	2.94	1.39	1.33
2	A	1248	NDP	C2A-N1A	2.79	1.38	1.33
2	D	1248	NDP	C2A-N1A	2.76	1.38	1.33
2	C	1248	NDP	C2A-N1A	2.52	1.38	1.33
2	D	1248	NDP	PN-O3	2.41	1.62	1.59
2	C	1248	NDP	PN-O3	2.40	1.62	1.59
2	A	1248	NDP	PN-O3	2.33	1.62	1.59
2	B	1248	NDP	PN-O3	2.30	1.62	1.59
2	B	1248	NDP	C6N-C5N	2.11	1.39	1.33
2	A	1248	NDP	C6N-C5N	2.04	1.39	1.33
2	C	1248	NDP	C6N-C5N	2.03	1.39	1.33
2	D	1248	NDP	C6N-C5N	2.02	1.39	1.33
2	D	1248	NDP	C2N-C3N	2.00	1.40	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1248	NDP	N3A-C2A-N1A	-6.69	119.59	128.67
2	B	1248	NDP	N3A-C2A-N1A	-6.57	119.75	128.67
2	D	1248	NDP	N3A-C2A-N1A	-5.99	120.54	128.67
2	A	1248	NDP	N3A-C2A-N1A	-5.79	120.82	128.67
2	C	1248	NDP	C6N-N1N-C2N	3.42	122.97	119.32
2	B	1248	NDP	C1D-N1N-C6N	-2.47	115.54	120.77
2	D	1248	NDP	O3-PN-O1N	-2.35	103.64	110.70
2	C	1248	NDP	C1D-N1N-C6N	-2.32	115.88	120.77
2	A	1248	NDP	C3N-C7N-N7N	2.30	121.76	117.67
2	A	1248	NDP	C6N-N1N-C2N	2.29	121.77	119.32
2	B	1248	NDP	C1B-N9A-C4A	-2.25	122.68	126.64
2	B	1248	NDP	C6N-N1N-C2N	2.25	121.73	119.32
2	D	1248	NDP	O4B-C1B-N9A	2.24	111.71	108.75
2	A	1248	NDP	C1D-N1N-C6N	-2.11	116.31	120.77
2	C	1248	NDP	C1B-N9A-C4A	-2.06	123.02	126.64
2	D	1248	NDP	O2N-PN-O3	2.04	112.79	107.27

There are no chirality outliers.

All (21) torsion outliers are listed below:

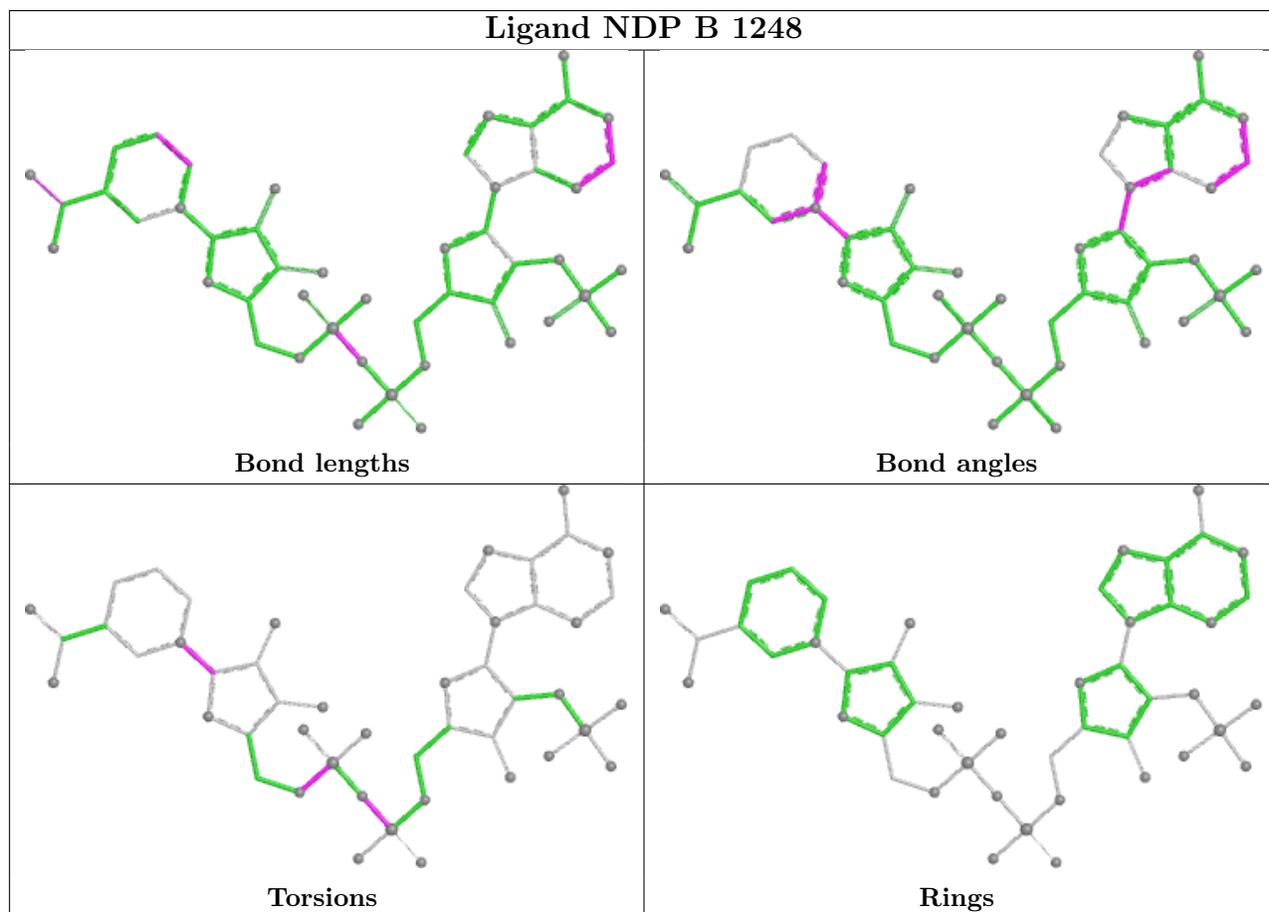
Mol	Chain	Res	Type	Atoms
2	A	1248	NDP	C5D-O5D-PN-O3
2	A	1248	NDP	C5D-O5D-PN-O1N
2	B	1248	NDP	C5D-O5D-PN-O3
2	B	1248	NDP	C5D-O5D-PN-O1N
2	B	1248	NDP	C5D-O5D-PN-O2N
2	C	1248	NDP	C5D-O5D-PN-O3
2	D	1248	NDP	C5D-O5D-PN-O3
2	D	1248	NDP	C5D-O5D-PN-O1N
2	D	1248	NDP	C5D-O5D-PN-O2N
2	A	1248	NDP	PN-O3-PA-O5B
2	B	1248	NDP	PN-O3-PA-O5B
2	C	1248	NDP	PN-O3-PA-O5B
2	D	1248	NDP	PN-O3-PA-O5B
2	A	1248	NDP	O4D-C1D-N1N-C6N
2	C	1248	NDP	O4D-C1D-N1N-C6N
2	B	1248	NDP	O4D-C1D-N1N-C6N
2	D	1248	NDP	O4D-C1D-N1N-C6N
2	C	1248	NDP	C5D-O5D-PN-O1N
2	D	1248	NDP	C2B-O2B-P2B-O2X
2	C	1248	NDP	C3B-C2B-O2B-P2B
2	C	1248	NDP	O4B-C4B-C5B-O5B

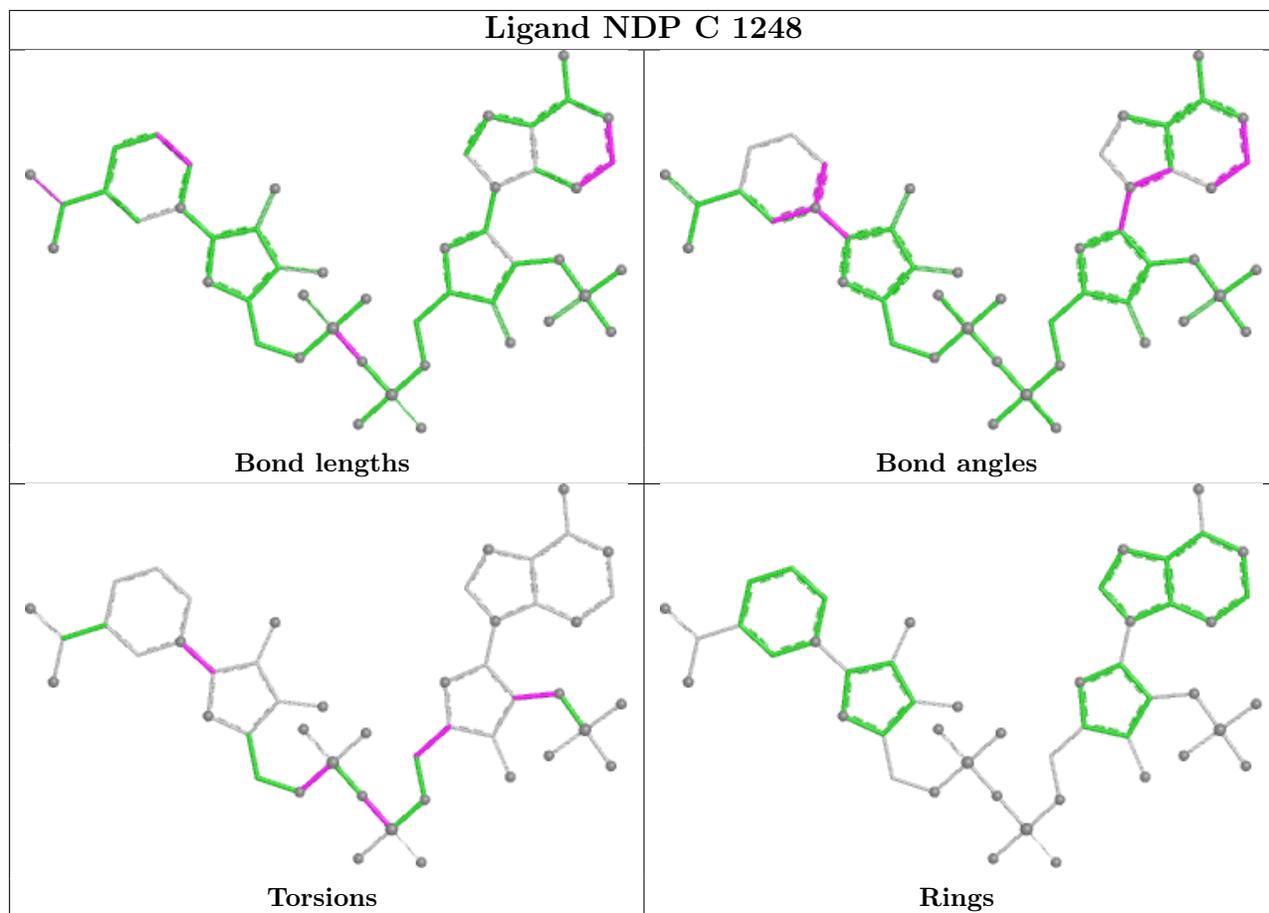
There are no ring outliers.

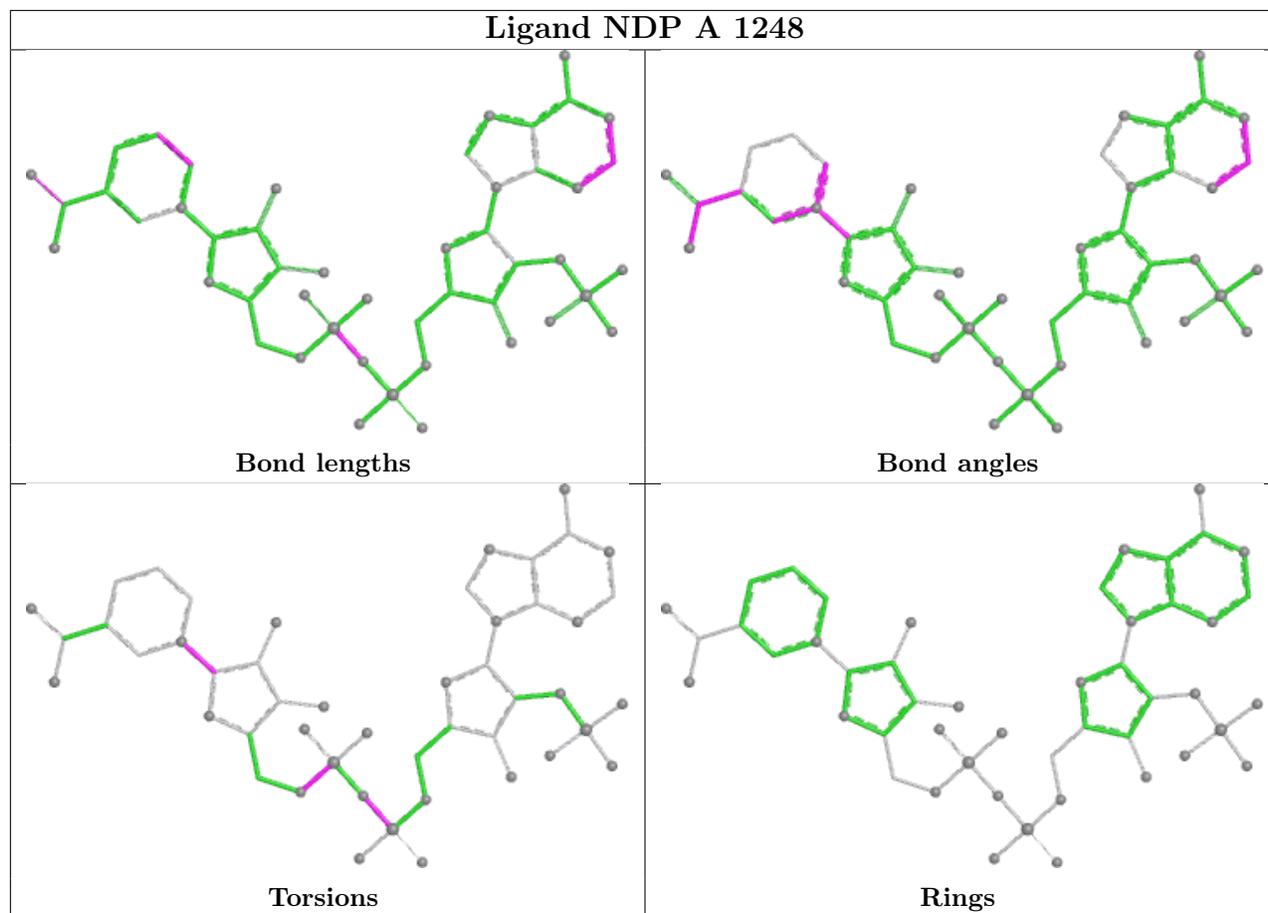
4 monomers are involved in 10 short contacts:

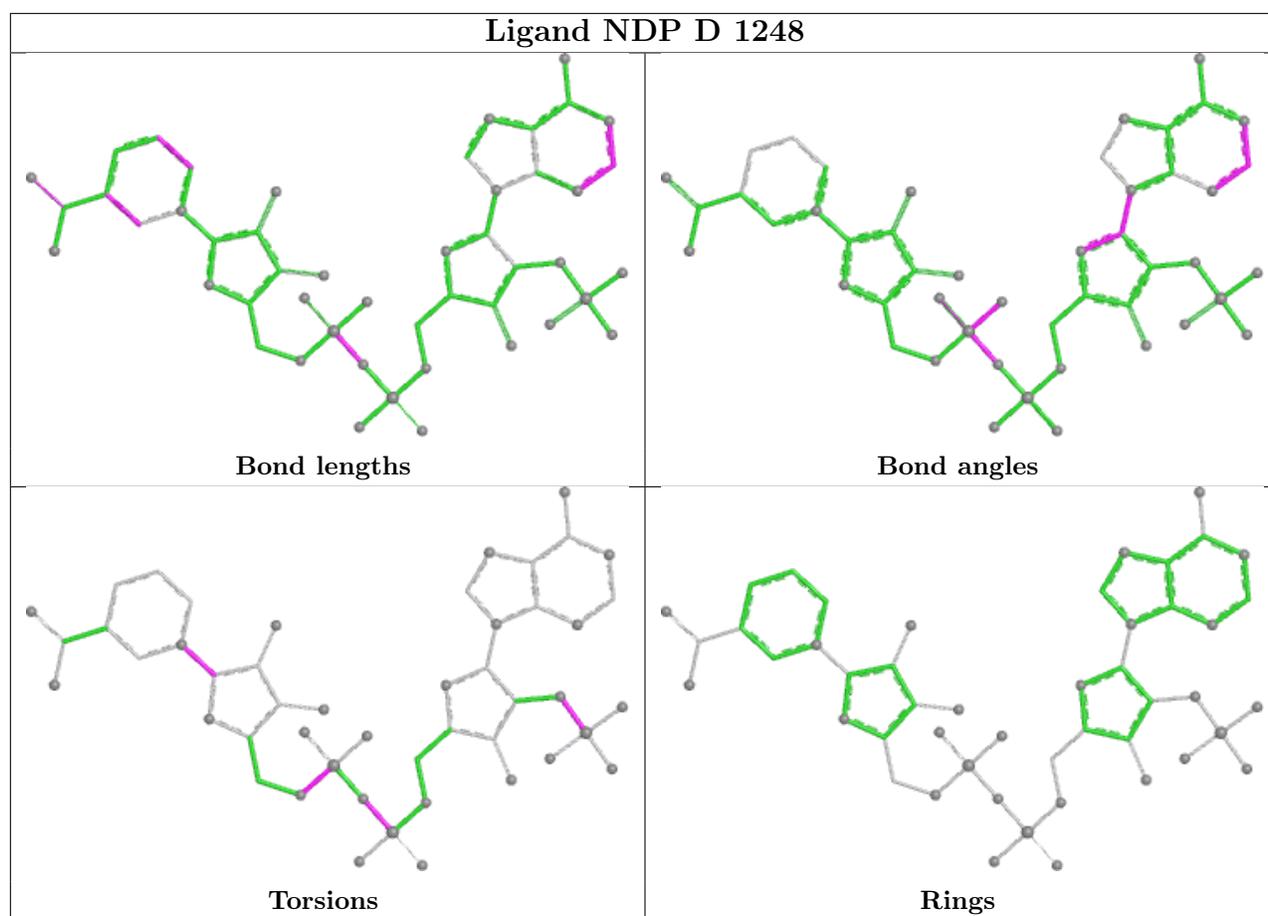
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1248	NDP	1	0
2	C	1248	NDP	3	0
2	A	1248	NDP	3	0
2	D	1248	NDP	3	0

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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Warning: The R factor obtained from EDS is 0.277, which does not match the depositor's R factor of 0.182. Please interpret the results in this section carefully.

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	239/247 (96%)	1.03	28 (11%) 10 9	19, 22, 30, 38	0
1	B	239/247 (96%)	1.91	103 (43%) 1 0	19, 23, 29, 35	0
1	C	240/247 (97%)	0.85	12 (5%) 35 32	13, 23, 29, 36	1 (0%)
1	D	239/247 (96%)	1.54	66 (27%) 2 1	18, 23, 30, 35	0
All	All	957/988 (96%)	1.33	209 (21%) 3 2	13, 23, 30, 38	1 (0%)

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	VAL	4.6
1	B	70	GLY	4.1
1	B	66	ALA	4.1
1	B	177	GLY	3.8
1	B	235	THR	3.8
1	B	6	GLN	3.8
1	B	38	ALA	3.7
1	B	35	ALA	3.7
1	B	44	LEU	3.6
1	B	71	VAL	3.6
1	B	79	VAL	3.5
1	B	81	ALA	3.5
1	C	53	ALA	3.5
1	A	194	GLY	3.5
1	D	71	VAL	3.4
1	B	61	LEU	3.4
1	B	59	HIS	3.4
1	B	9	VAL	3.4
1	D	247	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	70	GLY	3.3
1	D	64	ASP	3.3
1	A	196	ILE	3.3
1	B	69	GLN	3.3
1	D	218	GLN	3.3
1	B	164	ALA	3.2
1	D	79	VAL	3.2
1	D	76	ALA	3.2
1	D	81	ALA	3.2
1	A	236	VAL	3.1
1	B	210	SER	3.1
1	B	143	ILE	3.1
1	B	247	VAL	3.1
1	B	244	THR	3.1
1	D	42	GLU	3.0
1	A	205	TYR	3.0
1	B	226	TYR	3.0
1	B	234	ALA	3.0
1	B	207	GLN	3.0
1	B	76	ALA	3.0
1	D	126	ALA	3.0
1	C	42	GLU	3.0
1	B	52	THR	3.0
1	C	56	ALA	2.9
1	B	119	LEU	2.9
1	B	169	LEU	2.9
1	D	73	ALA	2.9
1	D	77	SER	2.9
1	B	209	ILE	2.9
1	A	42	GLU	2.9
1	B	208	ARG	2.9
1	A	192	LEU	2.8
1	B	37	ALA	2.8
1	B	103	ALA	2.8
1	B	102	ASP	2.8
1	D	85	LEU	2.8
1	D	149	VAL	2.8
1	B	67	ASP	2.8
1	B	241	ILE	2.8
1	B	147	VAL	2.7
1	B	73	ALA	2.7
1	D	199	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	51	LEU	2.7
1	B	41	VAL	2.7
1	B	78	THR	2.7
1	B	211	GLN	2.7
1	D	67	ASP	2.7
1	D	61	LEU	2.7
1	B	58	VAL	2.6
1	B	162	VAL	2.6
1	A	102	ASP	2.6
1	B	232	HIS	2.6
1	D	226	TYR	2.6
1	D	203	GLU	2.6
1	D	208	ARG	2.6
1	D	44	LEU	2.6
1	B	174	THR	2.6
1	B	182	VAL	2.6
1	D	80	GLU	2.6
1	D	205	TYR	2.6
1	A	208	ARG	2.6
1	D	128	PRO	2.6
1	B	239	ILE	2.6
1	D	143	ILE	2.6
1	D	137	VAL	2.5
1	A	209	ILE	2.5
1	A	201	THR	2.5
1	B	84	GLY	2.5
1	B	195	HIS	2.5
1	B	131	LEU	2.5
1	D	117	LEU	2.5
1	D	194	GLY	2.5
1	A	198	HIS	2.5
1	B	173	VAL	2.5
1	B	205	TYR	2.5
1	C	206	GLU	2.5
1	B	85	LEU	2.5
1	B	153	ALA	2.5
1	A	191	GLU	2.5
1	B	206	GLU	2.5
1	A	193	ARG	2.4
1	A	44	LEU	2.4
1	B	196	ILE	2.4
1	A	200	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	206	GLU	2.4
1	B	166	SER	2.4
1	B	236	VAL	2.4
1	B	240	PHE	2.4
1	A	226	TYR	2.4
1	A	168	THR	2.4
1	D	127	LEU	2.4
1	D	196	ILE	2.4
1	D	209	ILE	2.4
1	B	4	ALA	2.4
1	B	77	SER	2.4
1	B	129	HIS	2.4
1	B	149	VAL	2.4
1	B	192	LEU	2.4
1	B	183	ILE	2.4
1	B	168	THR	2.4
1	D	78	THR	2.4
1	B	116	LEU	2.3
1	B	117	LEU	2.3
1	A	234	ALA	2.3
1	B	49	ASP	2.3
1	A	203	GLU	2.3
1	D	206	GLU	2.3
1	B	68	ARG	2.3
1	C	52	THR	2.3
1	D	130	LEU	2.3
1	B	72	ASP	2.3
1	D	200	ALA	2.3
1	B	62	GLU	2.3
1	B	179	ARG	2.3
1	B	121	TYR	2.3
1	D	66	ALA	2.3
1	B	136	THR	2.3
1	D	174	THR	2.3
1	D	182	VAL	2.3
1	D	59	HIS	2.3
1	D	6	GLN	2.3
1	B	97	LEU	2.3
1	D	132	ARG	2.2
1	B	194	GLY	2.2
1	D	177	GLY	2.2
1	D	201	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	240	PHE	2.2
1	B	160	PHE	2.2
1	A	230	ALA	2.2
1	D	46	ALA	2.2
1	B	180	VAL	2.2
1	D	34	VAL	2.2
1	C	31	GLY	2.2
1	D	4	ALA	2.2
1	D	74	ALA	2.2
1	D	230	ALA	2.2
1	A	195	HIS	2.2
1	B	124	ARG	2.2
1	D	197	THR	2.2
1	D	244	THR	2.2
1	B	191	GLU	2.2
1	C	150[A]	ARG	2.2
1	D	102	ASP	2.1
1	A	3	SER	2.1
1	B	134	LYS	2.1
1	B	181	VAL	2.1
1	B	127	LEU	2.1
1	B	152	ALA	2.1
1	D	233	HIS	2.1
1	D	234	ALA	2.1
1	C	196	ILE	2.1
1	A	210	SER	2.1
1	B	7	GLY	2.1
1	C	84	GLY	2.1
1	B	65	VAL	2.1
1	D	60	VAL	2.1
1	D	100	VAL	2.1
1	B	146	ARG	2.1
1	B	54	ALA	2.1
1	B	96	LEU	2.1
1	C	2	PRO	2.1
1	C	36	ILE	2.1
1	B	199	THR	2.1
1	B	48	GLY	2.1
1	B	118	GLY	2.1
1	B	135	GLY	2.1
1	A	181	VAL	2.1
1	B	64	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	227	ALA	2.1
1	B	42	GLU	2.1
1	B	109	THR	2.1
1	B	201	THR	2.1
1	C	199	THR	2.1
1	D	62	GLU	2.1
1	A	225	ARG	2.1
1	B	39	ARG	2.1
1	D	9	VAL	2.0
1	B	144	ALA	2.0
1	D	164	ALA	2.0
1	D	207	GLN	2.0
1	D	241	ILE	2.0
1	D	25	ARG	2.0
1	B	108	TRP	2.0
1	D	129	HIS	2.0
1	B	20	GLY	2.0
1	D	135	GLY	2.0
1	A	41	VAL	2.0
1	B	125	ALA	2.0
1	D	236	VAL	2.0
1	D	215	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

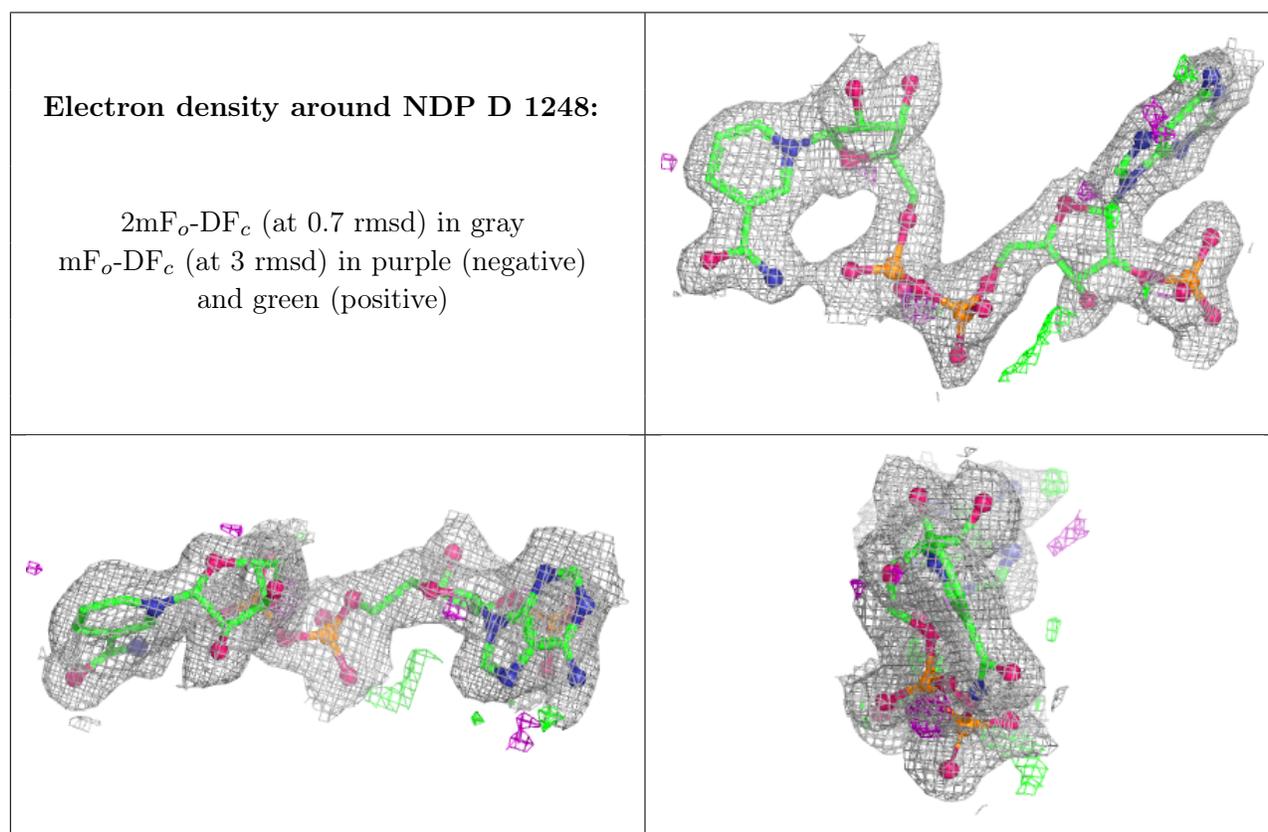
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NDP	D	1248	48/48	0.89	0.10	20,23,25,25	0

Continued on next page...

Continued from previous page...

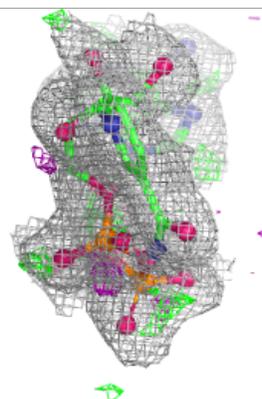
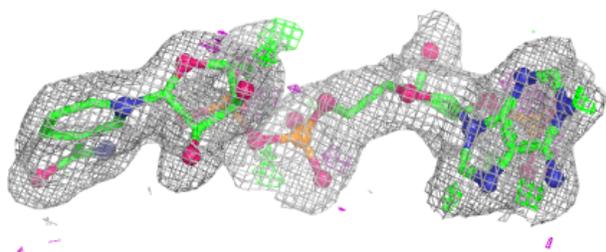
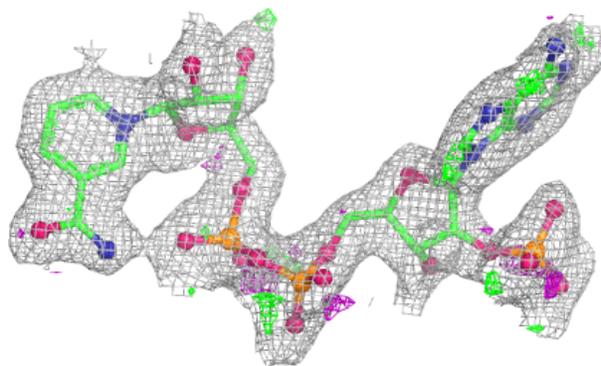
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NDP	B	1248	48/48	0.90	0.11	19,22,23,24	0
2	NDP	C	1248	48/48	0.93	0.09	19,22,24,25	0
2	NDP	A	1248	48/48	0.93	0.10	21,24,25,27	0

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

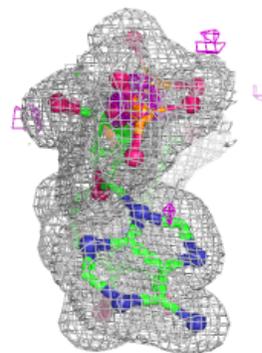
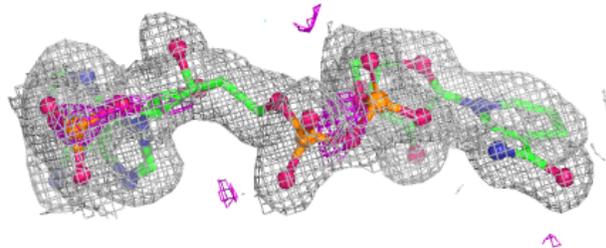
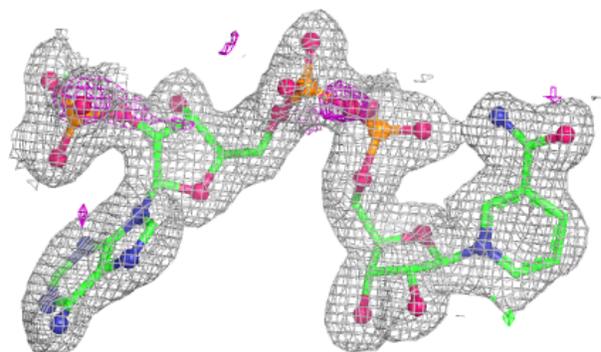


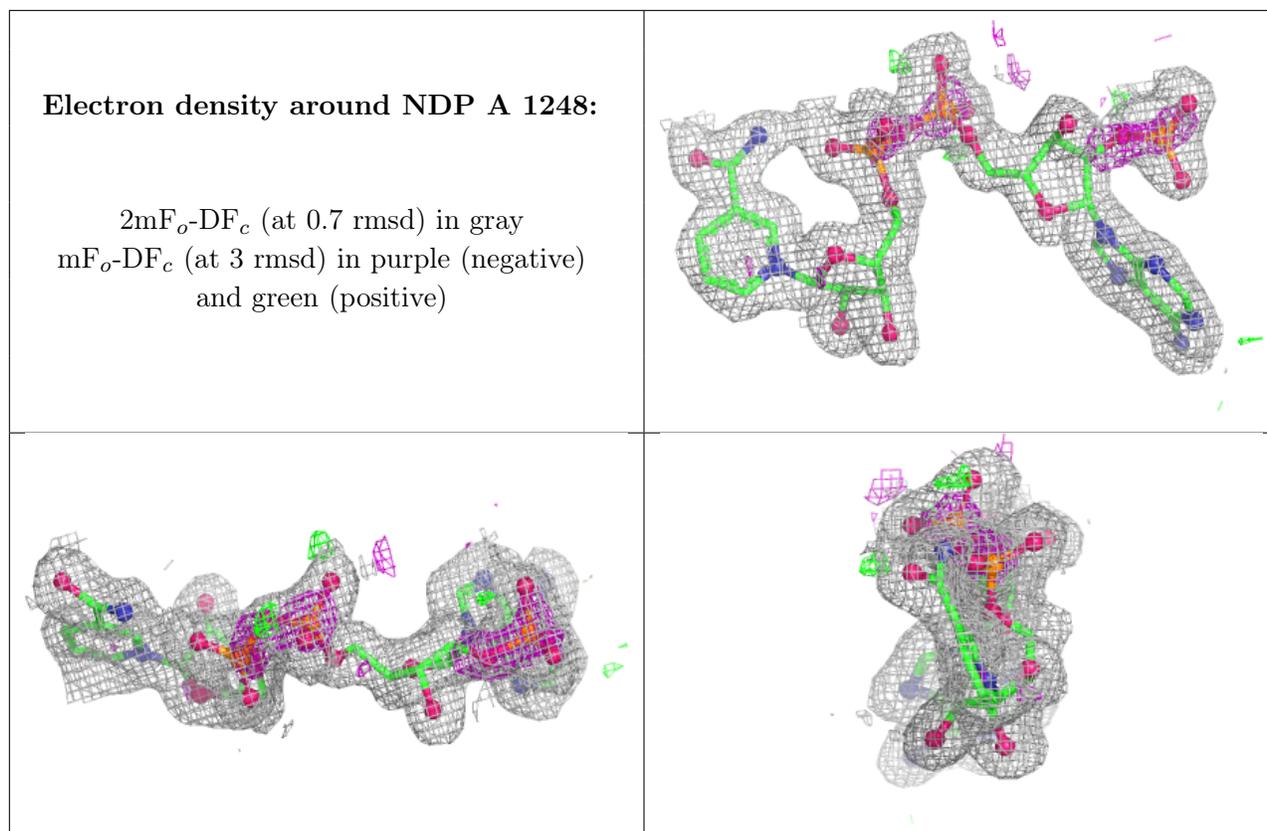
Electron density around NDP B 1248:

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

**Electron density around NDP C 1248:**

$2mF_o-DF_c$ (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.