



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:52 PM UTC

PDB ID : 2JAP / pdb_00002jap
Title : Clavulanic Acid Dehydrogenase: Structural and Biochemical Analysis of the Final Step in the Biosynthesis of the beta-Lactamase Inhibitor Clavulanic acid
Authors : MacKenzie, A.K.; Kershaw, N.J.; Hernandez, H.; Robinson, C.V.; Schofield, C.J.; Andersson, I.
Deposited on : 2006-11-29
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

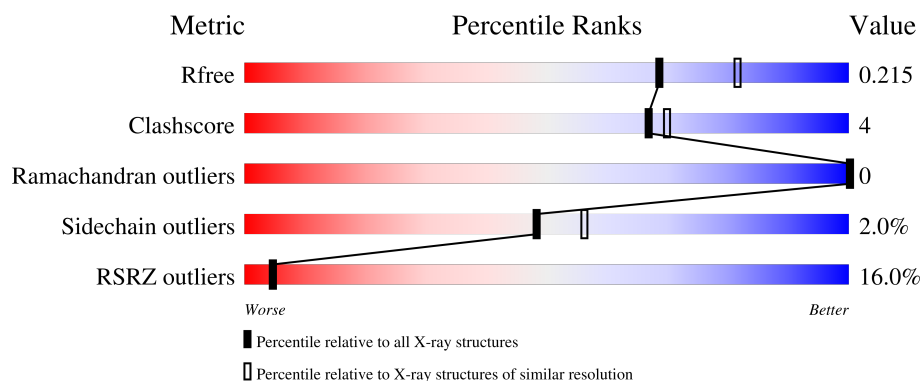
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

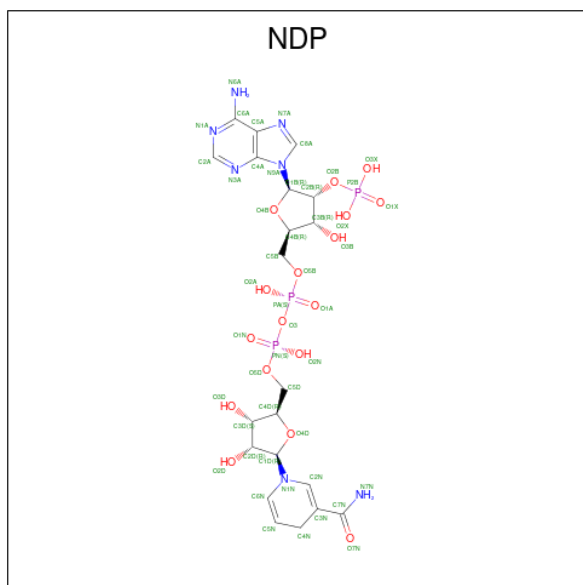
Mol	Chain	Length	Quality of chain
1	A	247	12% 93% 6% .
1	B	247	29% 89% 10% ..
1	C	247	8% 90% 10%
1	D	247	15% 93% 5% ..

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 CLAVALDEHYDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total 1832	C 1136	N 337	O 353	S 6	0	0	0
1	B	245	Total 1832	C 1136	N 337	O 353	S 6	0	0	0
1	C	246	Total 1850	C 1147	N 342	O 355	S 6	0	1	0
1	D	245	Total 1832	C 1136	N 337	O 353	S 6	0	0	0

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



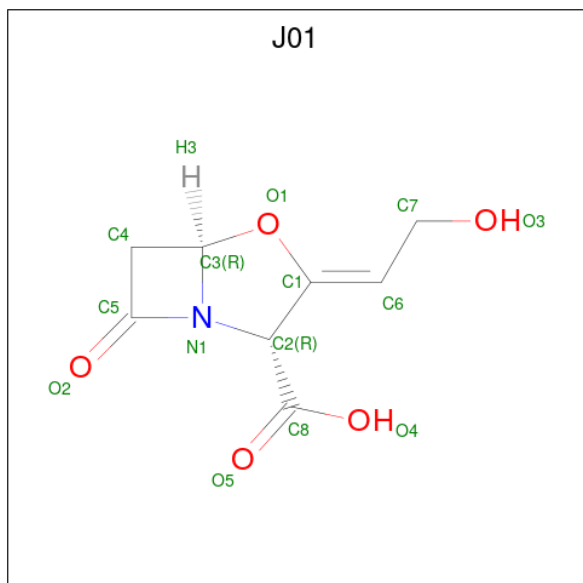
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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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 (2R,3Z,5R)-3-(2-HYDROXYETHYLIDENE)-7-OXO-4-OXA-1-AZABICYCLO[3.2.0]HEPTANE-2-CARBOXYLIC ACID (CCD ID: J01) (formula: C₈H₉NO₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			14	8	1	5			
3	B	1	Total	C	N	O		0	0
			14	8	1	5			
3	C	1	Total	C	N	O		0	0
			14	8	1	5			
3	D	1	Total	C	N	O		0	0
			14	8	1	5			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		
4	B	56	Total	O	0	0
			56	56		
4	C	73	Total	O	0	0
			73	73		

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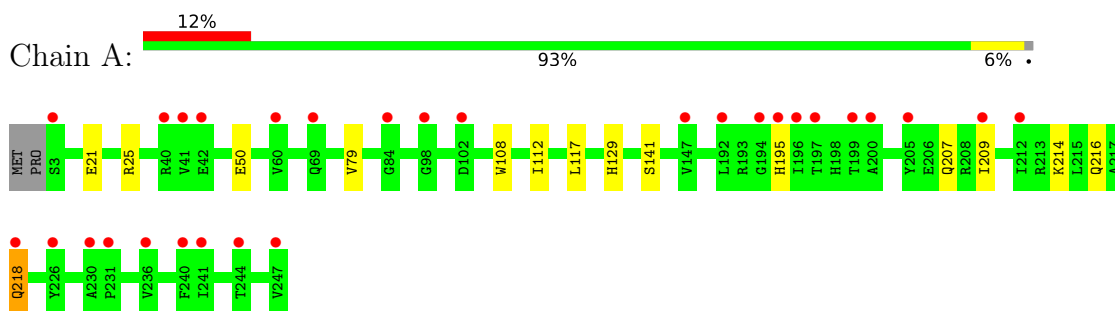
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	56	Total	O	0	0
			56	56		

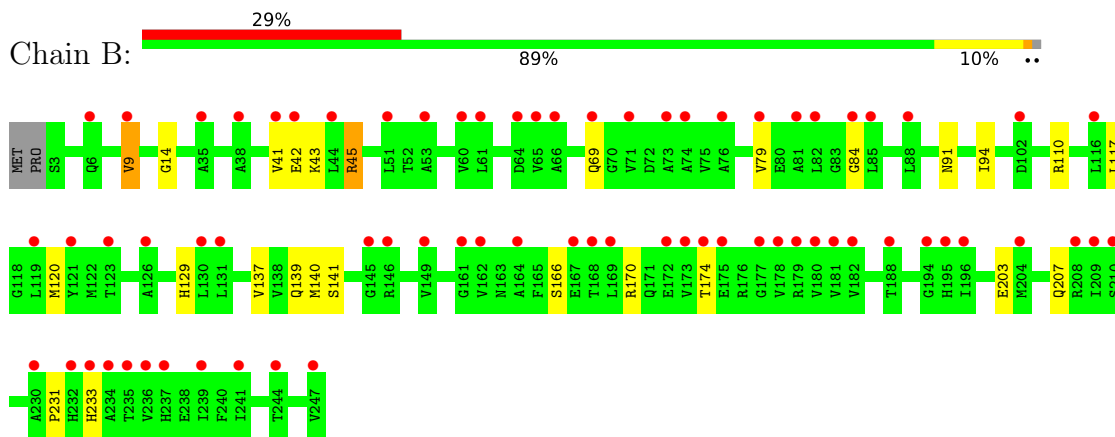
3 Residue-property plots [i](#)

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.

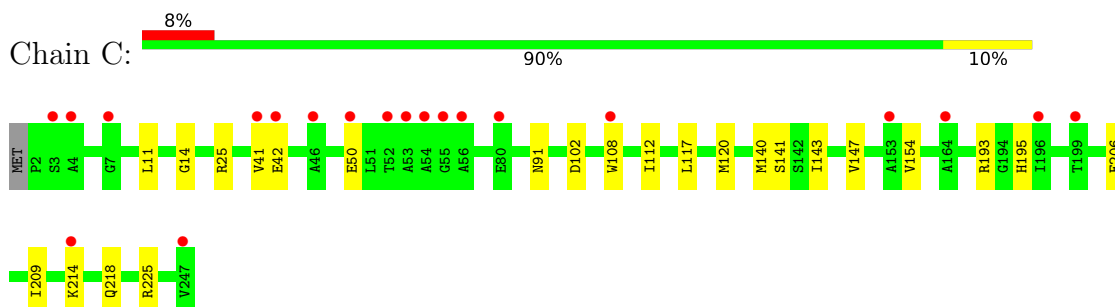
• Molecule 1: CLAVALDEHYDE DEHYDROGENASE



• Molecule 1: CLAVALDEHYDE DEHYDROGENASE

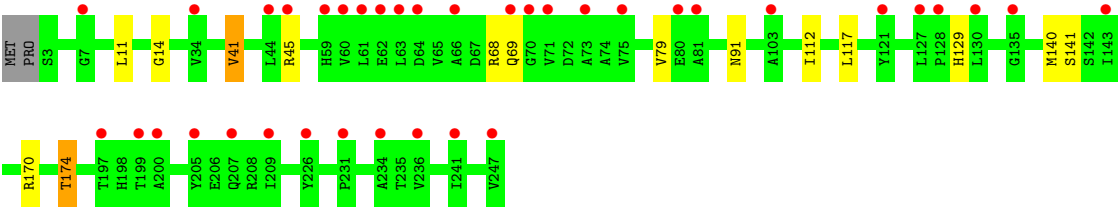


• Molecule 1: CLAVALDEHYDE DEHYDROGENASE



• Molecule 1: CLAVALDEHYDE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.08Å 123.42Å 126.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.86 – 2.10 34.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.86-2.10) 99.2 (34.86-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.216 0.184 , 0.215	Depositor DCC
R_{free} test set	2713 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7847	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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 44.18 % 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 1.5838e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: J01, 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	0.59	0/1852	0.84	0/2513
1	B	0.59	1/1852 (0.1%)	0.83	0/2513
1	C	0.58	0/1871	0.84	0/2538
1	D	0.57	0/1852	0.82	0/2513
All	All	0.58	1/7427 (0.0%)	0.83	0/10077

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	ARG	NE-CZ	7.70	1.41	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	45	ARG	Sidechain

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	1832	0	1871	14	0
1	B	1832	0	1871	13	0
1	C	1850	0	1891	12	0
1	D	1832	0	1871	8	0
2	A	48	0	26	5	0
2	B	48	0	26	5	0
2	C	48	0	26	5	0
2	D	48	0	26	5	0
3	A	14	0	8	4	0
3	B	14	0	8	3	0
3	C	14	0	8	3	0
3	D	14	0	8	3	0
4	A	68	0	0	2	0
4	B	56	0	0	0	0
4	C	73	0	0	1	0
4	D	56	0	0	0	0
All	All	7847	0	7640	56	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 (56) 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)
2:A:1248:NDP:H41N	3:A:1249:J01:H7C1	1.53	0.89
2:C:1248:NDP:H41N	3:C:1249:J01:H7C1	1.58	0.85
2:A:1248:NDP:C4N	3:A:1249:J01:H7C1	2.21	0.71
2:C:1248:NDP:C4N	3:C:1249:J01:H7C1	2.21	0.70
2:B:1248:NDP:H41N	3:B:1249:J01:H7C1	1.73	0.70
1:C:209:ILE:HD12	1:C:214:LYS:HE2	1.77	0.66
1:A:216:GLN:HB3	1:A:218:GLN:HE21	1.59	0.66
1:A:141:SER:O	2:A:1248:NDP:H6N	1.97	0.65
1:D:68:ARG:HH12	1:D:69:GLN:HE21	1.48	0.60
1:A:218:GLN:H	1:A:218:GLN:CD	2.11	0.59
2:B:1248:NDP:C4N	3:B:1249:J01:H7C1	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HD12	1:A:214:LYS:HE2	1.85	0.56
2:A:1248:NDP:C3N	3:A:1249:J01:H7C1	2.36	0.56
2:D:1248:NDP:H41N	3:D:1249:J01:H7C1	1.87	0.56
1:C:14:GLY:HA2	2:C:1248:NDP:H1B	1.87	0.55
2:C:1248:NDP:C3N	3:C:1249:J01:H7C1	2.36	0.55
2:D:1248:NDP:C3N	3:D:1249:J01:H7C1	2.37	0.55
1:B:120:MET:HE1	1:D:112:ILE:HD11	1.89	0.53
1:B:141:SER:O	2:B:1248:NDP:H6N	2.08	0.52
1:C:141:SER:O	2:C:1248:NDP:H6N	2.10	0.52
1:D:14:GLY:HA2	2:D:1248:NDP:H1B	1.92	0.51
1:D:141:SER:O	2:D:1248:NDP:H6N	2.11	0.51
1:C:195:HIS:HE1	4:C:2070:HOH:O	1.95	0.50
1:C:25:ARG:NH1	1:C:50:GLU:OE2	2.45	0.50
1:C:91:ASN:HD22	1:C:140:MET:HG2	1.78	0.49
2:D:1248:NDP:C4N	3:D:1249:J01:H7C1	2.43	0.49
1:B:9:VAL:HG11	1:B:84:GLY:O	2.13	0.48
2:B:1248:NDP:C3N	3:B:1249:J01:H7C1	2.43	0.48
1:B:231:PRO:HB2	1:B:233:HIS:CE1	2.48	0.48
2:A:1248:NDP:H41N	3:A:1249:J01:C7	2.35	0.48
1:C:143:ILE:HG12	1:C:147:VAL:CG2	2.44	0.48
1:C:193:ARG:NE	1:C:206:GLU:OE2	2.44	0.47
1:A:117:LEU:HD13	1:C:112:ILE:HD12	1.95	0.47
1:B:117:LEU:HA	1:B:120:MET:HE3	1.97	0.47
1:B:203:GLU:O	1:B:207:GLN:HG2	2.15	0.47
1:D:79:VAL:HG21	1:D:129:HIS:CE1	2.50	0.46
1:D:91:ASN:HD22	1:D:140:MET:HG2	1.82	0.45
1:B:79:VAL:HG21	1:B:129:HIS:CD2	2.51	0.45
1:D:170:ARG:O	1:D:174:THR:HB	2.17	0.45
1:A:25:ARG:HH12	1:A:50:GLU:CD	2.24	0.44
1:B:91:ASN:HD22	1:B:140:MET:HG2	1.83	0.43
1:A:79:VAL:HG21	1:A:129:HIS:CE1	2.53	0.43
1:D:41:VAL:O	1:D:45:ARG:HG3	2.19	0.43
1:A:214:LYS:HE3	4:A:2049:HOH:O	2.17	0.42
1:A:195:HIS:HE1	4:A:2062:HOH:O	2.02	0.42
1:B:139:GLN:HG3	1:B:166:SER:OG	2.20	0.42
1:A:207:GLN:HA	1:A:207:GLN:OE1	2.20	0.41
1:A:112:ILE:HD12	1:C:117:LEU:HD13	2.03	0.41
1:C:108:TRP:CD1	1:C:154:VAL:HG21	2.56	0.41
1:A:218:GLN:CD	1:A:218:GLN:N	2.77	0.41
1:A:108:TRP:CZ3	1:C:120:MET:HB3	2.56	0.41
1:B:94:ILE:HD11	1:B:110:ARG:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:GLU:OE2	1:A:25:ARG:NH2	2.52	0.40
1:B:42:GLU:HG2	1:B:43:LYS:N	2.36	0.40
1:B:170:ARG:O	1:B:174:THR:HB	2.21	0.40
1:B:14:GLY:HA2	2:B:1248:NDP:H1B	2.03	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	243/247 (98%)	238 (98%)	5 (2%)	0	100	100
1	B	243/247 (98%)	238 (98%)	5 (2%)	0	100	100
1	C	245/247 (99%)	239 (98%)	6 (2%)	0	100	100
1	D	243/247 (98%)	238 (98%)	5 (2%)	0	100	100
All	All	974/988 (99%)	953 (98%)	21 (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	188/190 (99%)	187 (100%)	1 (0%)	81	88
1	B	188/190 (99%)	184 (98%)	4 (2%)	47	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	190/190 (100%)	184 (97%)	6 (3%)	34	38
1	D	188/190 (99%)	184 (98%)	4 (2%)	47	54
All	All	754/760 (99%)	739 (98%)	15 (2%)	48	56

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
1	B	9	VAL
1	B	41	VAL
1	B	69	GLN
1	B	137	VAL
1	C	11	LEU
1	C	41	VAL
1	C	42	GLU
1	C	102	ASP
1	C	218	GLN
1	C	225	ARG
1	D	11	LEU
1	D	41	VAL
1	D	117	LEU
1	D	174	THR

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
1	A	151	ASN
1	A	218	GLN
1	B	69	GLN
1	B	91	ASN
1	B	129	HIS
1	B	218	GLN
1	C	91	ASN
1	C	195	HIS
1	D	69	GLN
1	D	91	ASN
1	D	218	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NDP	A	1248	-	51,52,52	1.50	5 (9%)	71,80,80	1.55	10 (14%)
3	J01	B	1249	-	11,15,15	1.74	3 (27%)	11,22,22	3.56	5 (45%)
3	J01	A	1249	-	11,15,15	1.74	3 (27%)	11,22,22	3.44	5 (45%)
2	NDP	D	1248	-	51,52,52	1.52	7 (13%)	71,80,80	1.50	10 (14%)
3	J01	D	1249	-	11,15,15	1.64	1 (9%)	11,22,22	3.19	5 (45%)
2	NDP	C	1248	-	51,52,52	1.49	6 (11%)	71,80,80	1.55	8 (11%)
3	J01	C	1249	-	11,15,15	1.66	3 (27%)	11,22,22	3.37	5 (45%)
2	NDP	B	1248	-	51,52,52	1.55	7 (13%)	71,80,80	1.55	9 (12%)

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	A	1248	-	-	5/34/77/77	0/5/5/5
3	J01	B	1249	-	-	1/7/31/31	0/2/2/2
3	J01	A	1249	-	-	1/7/31/31	0/2/2/2
2	NDP	D	1248	-	-	10/34/77/77	0/5/5/5
3	J01	D	1249	-	-	1/7/31/31	0/2/2/2
2	NDP	C	1248	-	-	8/34/77/77	0/5/5/5
3	J01	C	1249	-	-	1/7/31/31	0/2/2/2
2	NDP	B	1248	-	-	7/34/77/77	0/5/5/5

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1248	NDP	O7N-C7N	7.45	1.41	1.24
2	B	1248	NDP	O7N-C7N	7.35	1.41	1.24
2	D	1248	NDP	O7N-C7N	7.31	1.41	1.24
2	A	1248	NDP	O7N-C7N	7.19	1.41	1.24
3	B	1249	J01	O1-C1	4.25	1.45	1.38
3	D	1249	J01	O1-C1	4.23	1.45	1.38
3	A	1249	J01	O1-C1	3.98	1.45	1.38
3	C	1249	J01	O1-C1	3.74	1.44	1.38
2	B	1248	NDP	C2A-N1A	3.17	1.39	1.33
2	D	1248	NDP	C2A-N1A	2.91	1.39	1.33
2	C	1248	NDP	C2A-N1A	2.89	1.39	1.33
2	A	1248	NDP	C2A-N1A	2.89	1.39	1.33
2	D	1248	NDP	C2A-N3A	2.72	1.38	1.33
2	D	1248	NDP	PA-O3	2.71	1.62	1.59
2	A	1248	NDP	C2A-N3A	2.65	1.38	1.33
2	B	1248	NDP	C2A-N3A	2.64	1.38	1.33
2	A	1248	NDP	PN-O3	2.63	1.62	1.59
2	B	1248	NDP	PA-O3	2.52	1.62	1.59
3	A	1249	J01	C4-C5	-2.51	1.49	1.52
3	A	1249	J01	C2-C8	-2.48	1.50	1.53
2	C	1248	NDP	C2A-N3A	2.45	1.38	1.33
2	B	1248	NDP	PN-O3	2.40	1.62	1.59
3	C	1249	J01	C2-C8	-2.37	1.50	1.53
2	D	1248	NDP	PN-O3	2.36	1.62	1.59
2	A	1248	NDP	C8A-N7A	2.32	1.36	1.31
3	B	1249	J01	C4-C5	-2.31	1.49	1.52
3	C	1249	J01	C4-C5	-2.20	1.50	1.52
2	B	1248	NDP	C8A-N7A	2.18	1.35	1.31
2	C	1248	NDP	PN-O3	2.10	1.61	1.59
2	C	1248	NDP	PA-O3	2.09	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1248	NDP	C8A-N7A	2.07	1.35	1.31
2	D	1248	NDP	C8A-N7A	2.03	1.35	1.31
2	D	1248	NDP	C6N-C5N	2.03	1.39	1.33
3	B	1249	J01	C2-C8	-2.02	1.50	1.53
2	B	1248	NDP	C6N-C5N	2.01	1.39	1.33

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1249	J01	C4-C5-N1	7.24	98.37	92.52
3	A	1249	J01	C4-C5-N1	6.73	97.96	92.52
3	C	1249	J01	C4-C5-N1	6.49	97.77	92.52
2	C	1248	NDP	N3A-C2A-N1A	-6.06	119.41	128.58
2	B	1248	NDP	N3A-C2A-N1A	-6.02	119.47	128.58
3	D	1249	J01	C4-C5-N1	6.01	97.38	92.52
2	A	1248	NDP	N3A-C2A-N1A	-5.78	119.83	128.58
2	D	1248	NDP	N3A-C2A-N1A	-5.51	120.24	128.58
3	A	1249	J01	O2-C5-C4	-5.50	131.13	136.78
3	B	1249	J01	O2-C5-C4	-5.42	131.22	136.78
3	D	1249	J01	O2-C5-C4	-5.23	131.41	136.78
3	C	1249	J01	O2-C5-C4	-5.08	131.56	136.78
3	B	1249	J01	C3-C4-C5	-4.74	81.70	85.20
3	C	1249	J01	C3-C4-C5	-4.41	81.93	85.20
3	A	1249	J01	C3-C4-C5	-4.41	81.94	85.20
2	D	1248	NDP	N9A-C8A-N7A	-4.30	107.83	113.94
2	C	1248	NDP	N9A-C8A-N7A	-4.30	107.83	113.94
2	B	1248	NDP	N9A-C8A-N7A	-4.18	108.00	113.94
3	B	1249	J01	C3-N1-C5	-4.16	86.35	93.30
3	D	1249	J01	C3-C4-C5	-4.04	82.21	85.20
3	A	1249	J01	C3-N1-C5	-3.93	86.75	93.30
3	C	1249	J01	C3-N1-C5	-3.92	86.75	93.30
2	A	1248	NDP	C5A-C4A-N3A	-3.92	121.32	126.72
2	C	1248	NDP	C5A-C4A-N3A	-3.89	121.36	126.72
3	D	1249	J01	C3-N1-C5	-3.87	86.84	93.30
3	C	1249	J01	C2-N1-C5	-3.86	113.36	125.00
2	A	1248	NDP	N9A-C8A-N7A	-3.81	108.53	113.94
2	D	1248	NDP	C5A-C4A-N3A	-3.80	121.48	126.72
3	B	1249	J01	C2-N1-C5	-3.70	113.85	125.00
2	B	1248	NDP	C5A-C4A-N3A	-3.68	121.65	126.72
2	D	1248	NDP	C5A-N7A-C8A	3.66	109.21	103.45
2	C	1248	NDP	C5A-N7A-C8A	3.59	109.09	103.45
3	A	1249	J01	C2-N1-C5	-3.57	114.24	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1248	NDP	C5A-N7A-C8A	3.42	108.82	103.45
3	D	1249	J01	C2-N1-C5	-3.35	114.89	125.00
2	C	1248	NDP	C2A-N3A-C4A	3.33	119.95	111.83
2	A	1248	NDP	C2A-N3A-C4A	3.31	119.91	111.83
2	B	1248	NDP	C2A-N3A-C4A	3.26	119.80	111.83
2	A	1248	NDP	C5A-N7A-C8A	3.24	108.54	103.45
2	D	1248	NDP	C2A-N3A-C4A	3.03	119.22	111.83
2	B	1248	NDP	C4A-N9A-C8A	2.76	108.64	105.74
2	A	1248	NDP	C6N-N1N-C2N	2.76	122.27	119.32
2	B	1248	NDP	N3A-C4A-N9A	2.73	131.81	127.17
2	D	1248	NDP	N3A-C4A-N9A	2.64	131.65	127.17
2	C	1248	NDP	N3A-C4A-N9A	2.62	131.62	127.17
2	C	1248	NDP	C4A-C5A-N7A	-2.59	107.62	110.58
2	C	1248	NDP	C4A-N9A-C8A	2.57	108.43	105.74
2	B	1248	NDP	O7N-C7N-C3N	-2.55	116.10	120.90
2	D	1248	NDP	C4A-N9A-C8A	2.54	108.40	105.74
2	D	1248	NDP	C4A-C5A-N7A	-2.53	107.69	110.58
2	A	1248	NDP	N3A-C4A-N9A	2.45	131.34	127.17
2	A	1248	NDP	C4A-C5A-N7A	-2.44	107.80	110.58
2	A	1248	NDP	C1D-N1N-C6N	-2.28	115.96	120.77
2	B	1248	NDP	C4A-C5A-N7A	-2.26	108.00	110.58
2	D	1248	NDP	O4D-C1D-N1N	2.12	112.14	108.08
2	A	1248	NDP	O2A-PA-O3	2.05	112.80	107.27
2	D	1248	NDP	C1D-N1N-C6N	-2.00	116.53	120.77

There are no chirality outliers.

All (34) 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	A	1248	NDP	C5D-O5D-PN-O2N
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	C5B-O5B-PA-O1A
2	C	1248	NDP	C5D-O5D-PN-O3
2	D	1248	NDP	C5D-O5D-PN-O3
3	A	1249	J01	C1-C6-C7-O3
3	B	1249	J01	C1-C6-C7-O3
3	C	1249	J01	C1-C6-C7-O3
3	D	1249	J01	C1-C6-C7-O3

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Mol	Chain	Res	Type	Atoms
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	B	1248	NDP	O4D-C1D-N1N-C6N
2	C	1248	NDP	O4D-C1D-N1N-C6N
2	C	1248	NDP	C5B-O5B-PA-O2A
2	C	1248	NDP	C5D-O5D-PN-O1N
2	D	1248	NDP	C5B-O5B-PA-O1A
2	D	1248	NDP	C5B-O5B-PA-O2A
2	D	1248	NDP	C5D-O5D-PN-O1N
2	D	1248	NDP	O4D-C1D-N1N-C6N
2	B	1248	NDP	C2B-O2B-P2B-O2X
2	C	1248	NDP	C2B-O2B-P2B-O2X
2	B	1248	NDP	C2B-O2B-P2B-O1X
2	D	1248	NDP	C2B-O2B-P2B-O1X
2	D	1248	NDP	O4B-C4B-C5B-O5B
2	D	1248	NDP	C2B-O2B-P2B-O2X
2	D	1248	NDP	C2B-O2B-P2B-O3X
2	C	1248	NDP	O4B-C4B-C5B-O5B

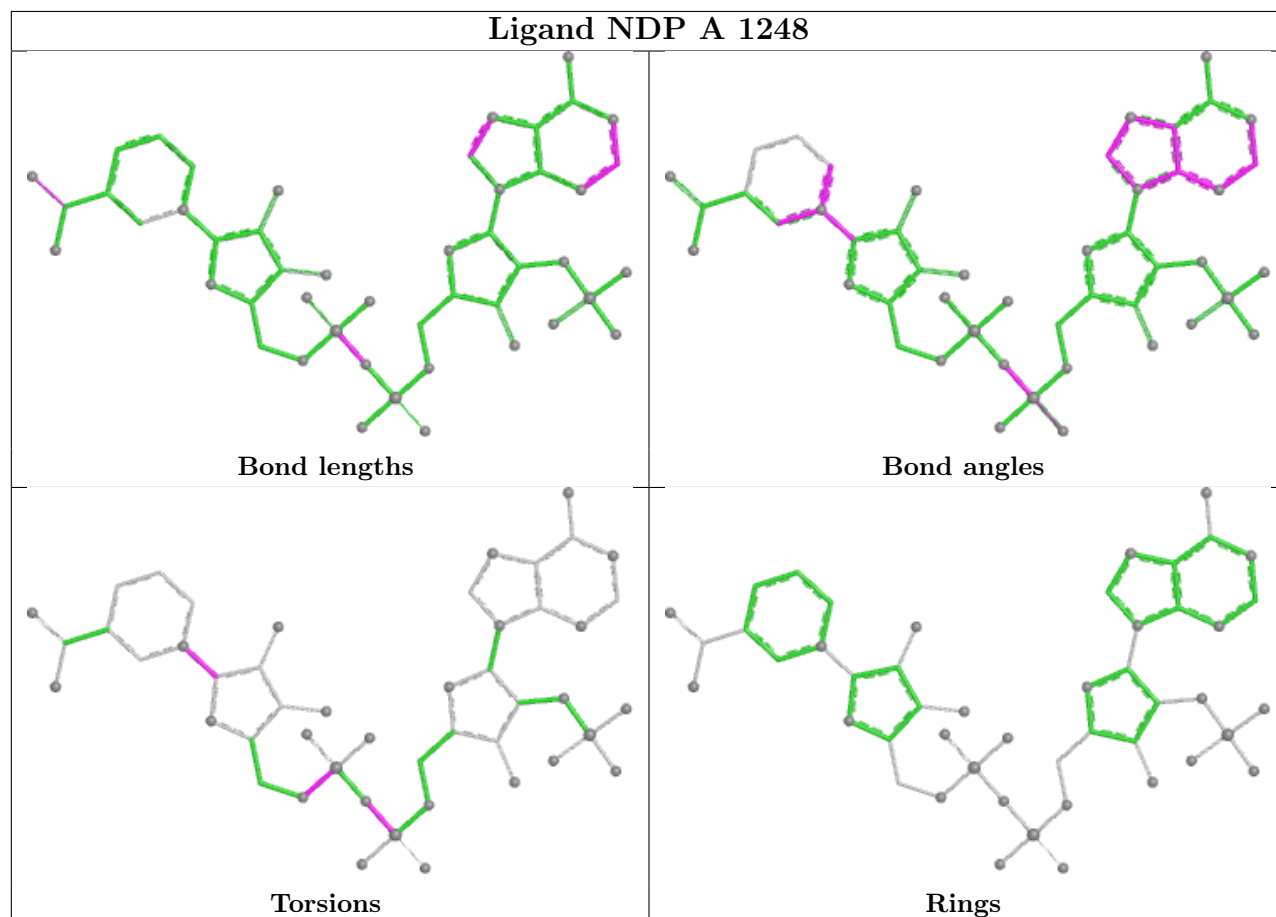
There are no ring outliers.

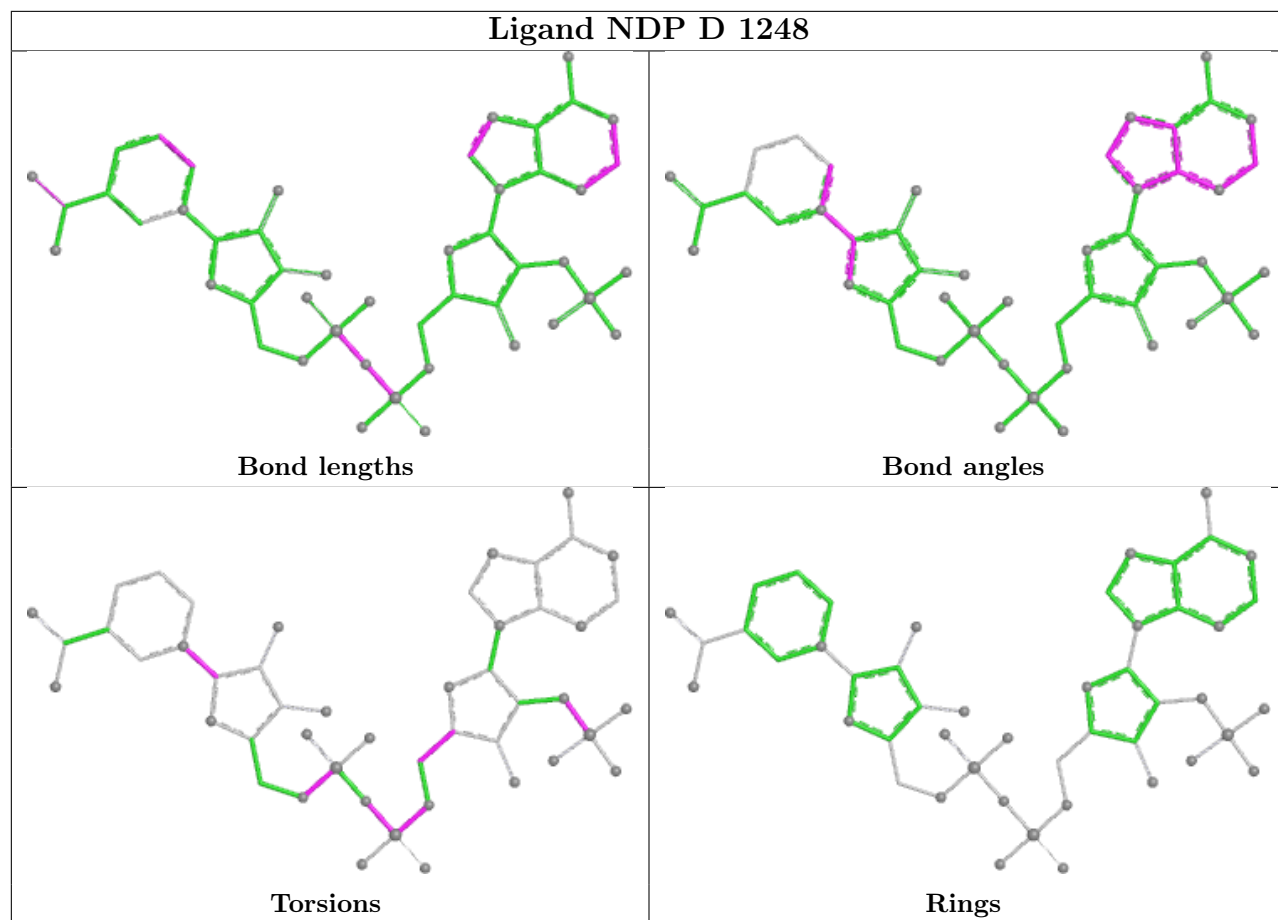
8 monomers are involved in 20 short contacts:

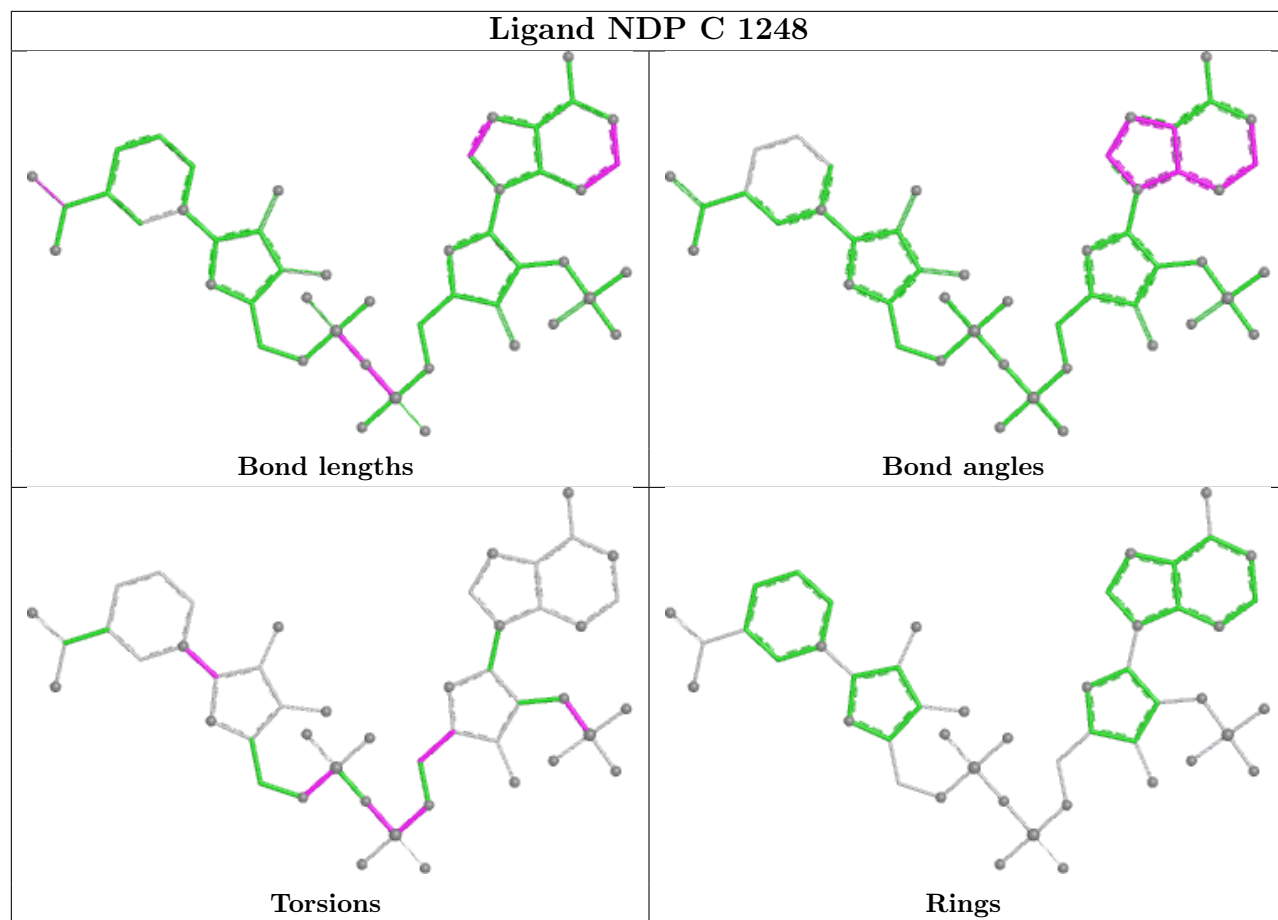
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1248	NDP	5	0
3	B	1249	J01	3	0
3	A	1249	J01	4	0
2	D	1248	NDP	5	0
3	D	1249	J01	3	0
2	C	1248	NDP	5	0
3	C	1249	J01	3	0
2	B	1248	NDP	5	0

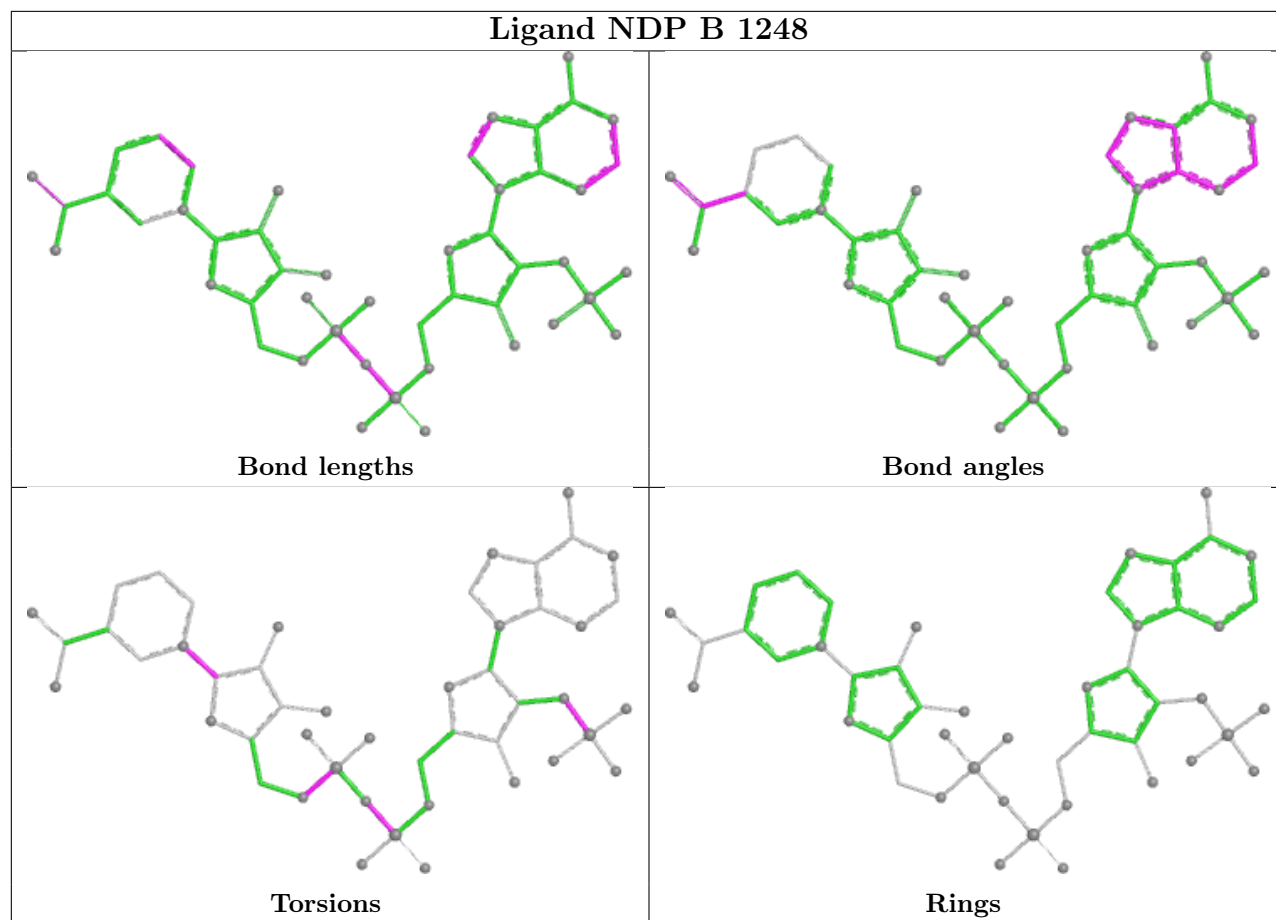
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	245/247 (99%)	1.07	29 (11%) 9 9	30, 32, 36, 40	0
1	B	245/247 (99%)	1.64	71 (28%) 1 1	30, 32, 35, 41	0
1	C	246/247 (99%)	1.02	20 (8%) 18 19	16, 32, 36, 42	1 (0%)
1	D	245/247 (99%)	1.29	37 (15%) 5 5	29, 32, 36, 39	0
All	All	981/988 (99%)	1.26	157 (16%) 5 5	16, 32, 36, 42	1 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	SER	4.1
1	B	81	ALA	3.7
1	D	73	ALA	3.7
1	B	41	VAL	3.6
1	B	168	THR	3.6
1	B	169	LEU	3.5
1	B	164	ALA	3.5
1	A	192	LEU	3.5
1	B	35	ALA	3.5
1	C	199	THR	3.2
1	B	196	ILE	3.2
1	B	235	THR	3.2
1	B	76	ALA	3.1
1	C	53	ALA	3.1
1	C	56	ALA	3.1
1	A	42	GLU	3.1
1	B	244	THR	3.0
1	B	234	ALA	3.0
1	A	195	HIS	3.0
1	A	199	THR	3.0
1	D	199	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	66	ALA	3.0
1	C	42	GLU	3.0
1	C	80	GLU	3.0
1	A	196	ILE	3.0
1	A	3	SER	2.9
1	D	247	VAL	2.9
1	D	62	GLU	2.9
1	B	195	HIS	2.8
1	A	194	GLY	2.8
1	B	51	LEU	2.8
1	B	71	VAL	2.8
1	B	162	VAL	2.8
1	D	209	ILE	2.8
1	D	70	GLY	2.8
1	B	42	GLU	2.8
1	B	194	GLY	2.8
1	D	61	LEU	2.8
1	C	196	ILE	2.8
1	D	241	ILE	2.8
1	B	61	LEU	2.7
1	B	116	LEU	2.7
1	B	69	GLN	2.7
1	B	180	VAL	2.7
1	B	178	VAL	2.7
1	B	64	ASP	2.7
1	D	103	ALA	2.7
1	D	234	ALA	2.7
1	B	204	MET	2.7
1	B	173	VAL	2.7
1	D	80	GLU	2.6
1	D	44	LEU	2.6
1	A	247	VAL	2.6
1	A	84	GLY	2.6
1	B	84	GLY	2.6
1	C	4	ALA	2.6
1	C	54	ALA	2.6
1	A	244	THR	2.6
1	D	207	GLN	2.6
1	B	131	LEU	2.6
1	D	130	LEU	2.6
1	A	40	ARG	2.5
1	A	197	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	9	VAL	2.5
1	B	236	VAL	2.5
1	A	230	ALA	2.5
1	B	6	GLN	2.5
1	B	126	ALA	2.5
1	C	108	TRP	2.5
1	B	177	GLY	2.5
1	B	241	ILE	2.5
1	C	41	VAL	2.5
1	D	45	ARG	2.5
1	B	181	VAL	2.4
1	D	121	TYR	2.4
1	D	69	GLN	2.4
1	B	102	ASP	2.4
1	D	205	TYR	2.4
1	B	53	ALA	2.4
1	D	81	ALA	2.4
1	C	55	GLY	2.4
1	D	200	ALA	2.4
1	B	85	LEU	2.4
1	D	75	VAL	2.4
1	D	143	ILE	2.4
1	D	236	VAL	2.4
1	C	164	ALA	2.3
1	B	44	LEU	2.3
1	B	88	LEU	2.3
1	B	209	ILE	2.3
1	B	230	ALA	2.3
1	C	46	ALA	2.3
1	C	153	ALA	2.3
1	C	3	SER	2.3
1	B	65	VAL	2.3
1	B	38	ALA	2.3
1	D	135	GLY	2.3
1	B	119	LEU	2.3
1	A	218	GLN	2.2
1	A	240	PHE	2.2
1	B	239	ILE	2.2
1	A	236	VAL	2.2
1	B	79	VAL	2.2
1	D	34	VAL	2.2
1	D	64	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	73	ALA	2.2
1	D	63	LEU	2.2
1	B	121	TYR	2.2
1	D	226	TYR	2.2
1	D	59	HIS	2.2
1	C	52	THR	2.2
1	A	60	VAL	2.2
1	A	147	VAL	2.2
1	B	130	LEU	2.2
1	B	233	HIS	2.2
1	B	146	ARG	2.2
1	D	128	PRO	2.2
1	A	41	VAL	2.2
1	C	7	GLY	2.2
1	A	200	ALA	2.2
1	B	74	ALA	2.2
1	B	237	HIS	2.2
1	B	172	GLU	2.1
1	C	50	GLU	2.1
1	C	247	VAL	2.1
1	D	71	VAL	2.1
1	B	232	HIS	2.1
1	D	66	ALA	2.1
1	A	209	ILE	2.1
1	A	98	GLY	2.1
1	B	60	VAL	2.1
1	B	145	GLY	2.1
1	D	7	GLY	2.1
1	D	127	LEU	2.1
1	A	226	TYR	2.1
1	D	197	THR	2.1
1	C	214	LYS	2.1
1	A	231	PRO	2.1
1	B	182	VAL	2.1
1	B	247	VAL	2.1
1	D	60	VAL	2.1
1	B	167	GLU	2.0
1	A	212	ILE	2.0
1	A	241	ILE	2.0
1	B	149	VAL	2.0
1	B	175	GLU	2.0
1	A	69	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	2.0
1	A	102	ASP	2.0
1	B	179	ARG	2.0
1	B	208	ARG	2.0
1	B	123	THR	2.0
1	B	174	THR	2.0
1	B	188	THR	2.0
1	D	231	PRO	2.0
1	B	161	GLY	2.0
1	A	205	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

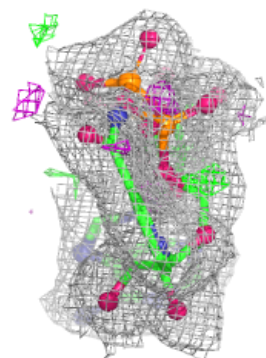
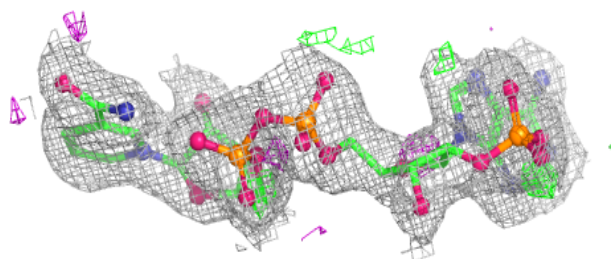
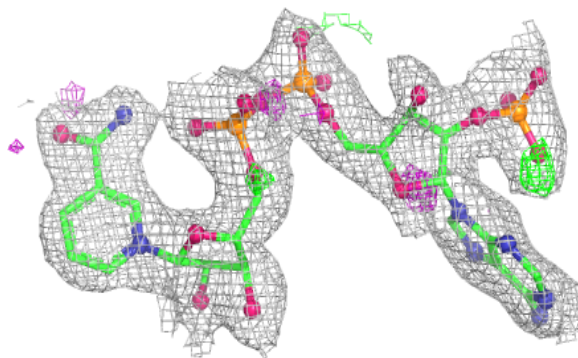
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	J01	B	1249	14/14	0.80	0.14	37,41,42,42	0
3	J01	D	1249	14/14	0.85	0.12	37,41,42,42	0
3	J01	C	1249	14/14	0.86	0.12	42,45,46,46	0
3	J01	A	1249	14/14	0.86	0.11	36,41,41,42	0
2	NDP	D	1248	48/48	0.88	0.10	32,34,35,35	0
2	NDP	B	1248	48/48	0.89	0.09	28,31,34,35	0
2	NDP	C	1248	48/48	0.91	0.09	29,32,34,35	0
2	NDP	A	1248	48/48	0.91	0.10	29,33,35,35	0

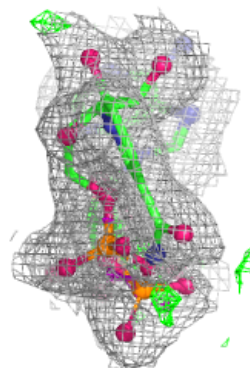
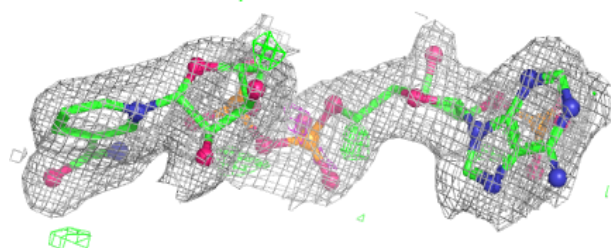
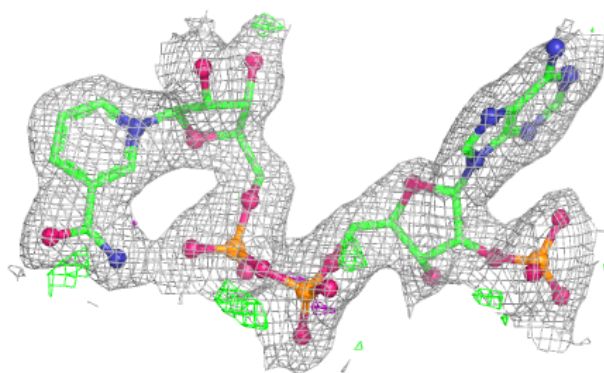
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP D 1248:

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

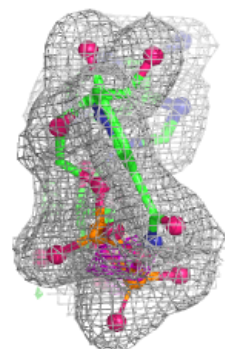
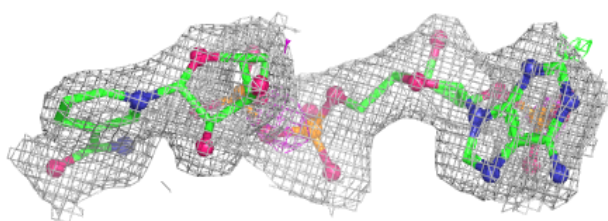
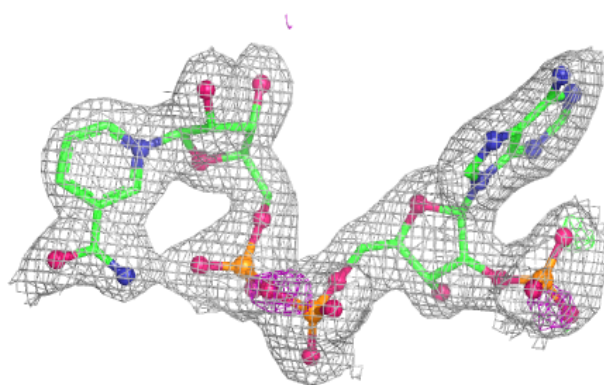
**Electron density around NDP B 1248:**

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

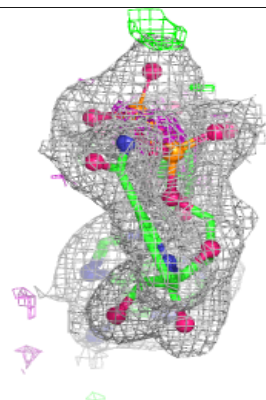
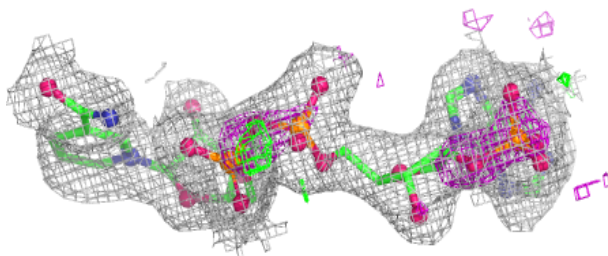
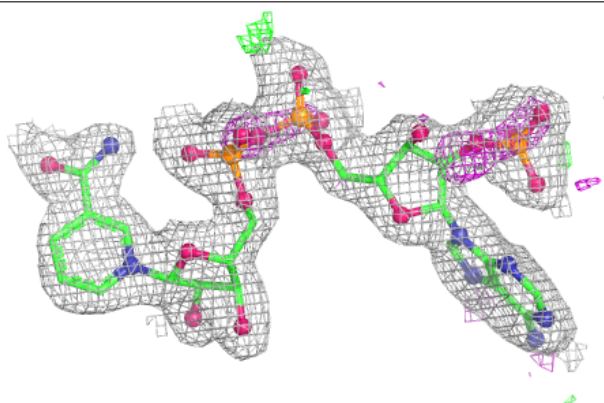


Electron density around NDP C 1248:

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

**Electron density around NDP A 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.