



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:20 AM EDT

PDB ID : 1QZR / pdb_00001qzr
Title : CRYSTAL STRUCTURE OF THE ATPASE REGION OF SACCHAROMYCES CEREVISIAE TOPOISOMERASE II BOUND TO ICRF-187 (DEXRAZOXANE)
Authors : Classen, S.; Olland, S.; Berger, J.M.
Deposited on : 2003-09-17
Resolution : 1.90 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

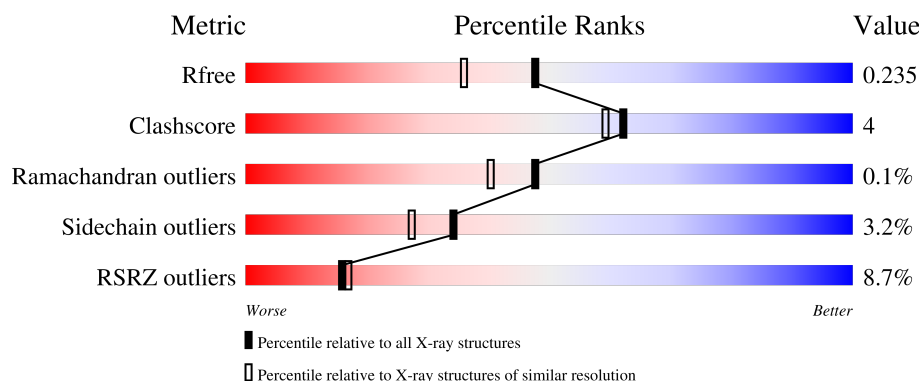
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	418	
1	B	418	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CDX	B	901[A]	X	-	-	-
4	CDX	B	901[B]	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6978 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 DNA topoisomerase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			3069	1954	520	580	15			
1	B	378	Total	C	N	O	S	0	0	0
			3041	1940	513	573	15			

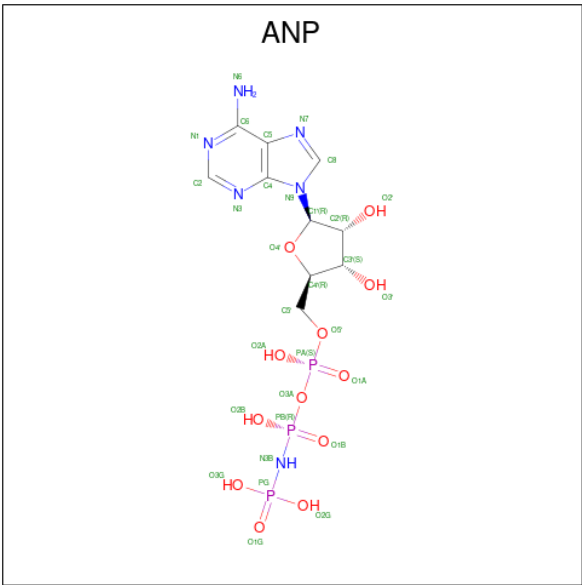
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	cloning artifact	UNP P06786
A	-3	HIS	-	cloning artifact	UNP P06786
A	-2	MET	-	cloning artifact	UNP P06786
A	-1	VAL	-	cloning artifact	UNP P06786
A	0	THR	-	cloning artifact	UNP P06786
B	-4	GLY	-	cloning artifact	UNP P06786
B	-3	HIS	-	cloning artifact	UNP P06786
B	-2	MET	-	cloning artifact	UNP P06786
B	-1	VAL	-	cloning artifact	UNP P06786
B	0	THR	-	cloning artifact	UNP P06786

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

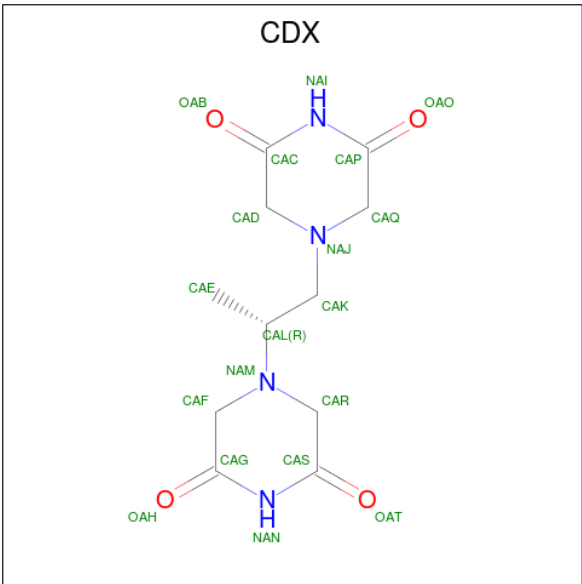
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is (S)-4,4'-(1-METHYL-1,2-ETHANEDIYL)BIS-2,6-PIPERAZINEDIONE (CCD ID: CDX) (formula: C₁₁H₁₆N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	1
			38	22	8	8		

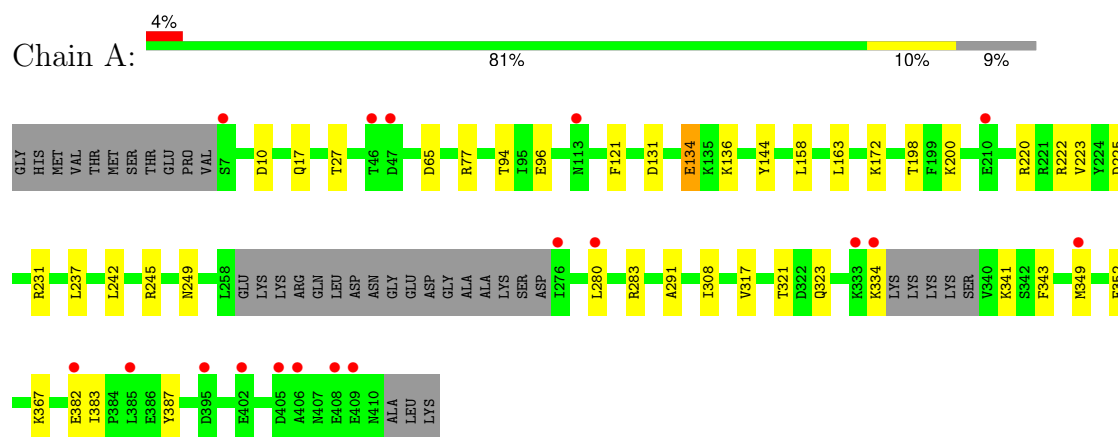
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	419	Total 419	O 419	0	0
5	B	347	Total 347	O 347	0	0

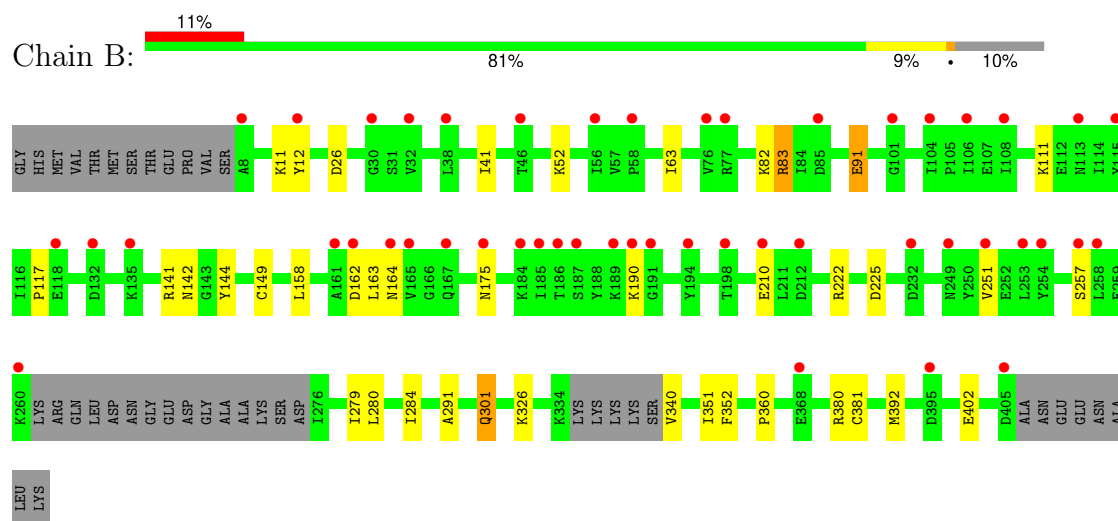
3 Residue-property plots [i](#)

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: DNA topoisomerase II



• Molecule 1: DNA topoisomerase II



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.55Å 71.44Å 215.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.18 – 1.90 45.18 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.8 (45.18-1.90) 90.8 (45.18-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.196 , 0.237 0.195 , 0.235	Depositor DCC
R_{free} test set	5512 reflections (8.41%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6978	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, CDX

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	0.62	0/3124	0.75	0/4216
1	B	0.58	0/3096	0.77	3/4179 (0.1%)
All	All	0.60	0/6220	0.76	3/8395 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ASN	N-CA-C	5.93	121.43	113.72
1	B	26	ASP	N-CA-C	5.45	116.90	111.07
1	B	83	ARG	N-CA-C	5.08	117.44	108.75

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	3069	0	3059	23	0
1	B	3041	0	3035	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	13	0	0
3	B	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	38	0	32	8	0
5	A	419	0	0	0	0
5	B	347	0	0	5	0
All	All	6978	0	6152	51	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 (51) 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:B:149:CYS:SG	5:B:1226:HOH:O	2.28	0.91
1:B:392:MET:HE2	1:B:392:MET:HA	1.56	0.85
1:A:245:ARG:H	1:A:249:ASN:HD22	1.30	0.79
1:B:91:GLU:H	1:B:91:GLU:CD	1.94	0.73
1:A:134:GLU:HG3	1:A:136:LYS:HE2	1.83	0.59
1:A:17:GLN:NE2	1:A:144:TYR:OH	2.38	0.56
4:B:901[B]:CDX:HAQ2	4:B:901[B]:CDX:HAE2	1.88	0.55
1:A:131:ASP:O	1:A:134:GLU:HG3	2.06	0.55
1:A:94:THR:HG22	1:A:200:LYS:HE2	1.89	0.54
1:A:121:PHE:CD2	1:A:158:LEU:HD22	2.43	0.53
1:B:251:VAL:CG1	1:B:279:ILE:HG21	2.39	0.52
4:B:901[B]:CDX:HAE2	4:B:901[B]:CDX:CAQ	2.39	0.52
1:A:323:GLN:HE22	1:A:383:ILE:H	1.58	0.51
1:B:11:LYS:HE3	1:B:12:TYR:CE2	2.46	0.50
1:B:222:ARG:O	1:B:225:ASP:HB2	2.11	0.49
1:B:63:ILE:O	5:B:1226:HOH:O	2.20	0.49
1:A:223:VAL:HG12	1:A:242:LEU:HD11	1.94	0.48
1:B:210:GLU:HG3	5:B:1162:HOH:O	2.14	0.48
1:B:91:GLU:CD	1:B:91:GLU:N	2.70	0.47
1:A:220:ARG:HG2	1:A:237:LEU:HD21	1.95	0.47
1:B:291:ALA:HB3	1:B:352:PHE:HB2	1.97	0.46
1:B:284:ILE:HG13	1:B:381:CYS:SG	2.55	0.46
1:B:392:MET:HA	1:B:392:MET:CE	2.38	0.46
1:A:280:LEU:HG	1:A:387:TYR:CE1	2.51	0.46
1:A:96:GLU:HG2	1:A:198:THR:HG23	1.98	0.45
1:A:323:GLN:NE2	1:A:383:ILE:H	2.13	0.45
1:A:323:GLN:HE22	1:A:382:GLU:HA	1.81	0.45
1:B:301:GLN:HE21	1:B:301:GLN:HB2	1.61	0.45
1:A:291:ALA:HB3	1:A:352:PHE:HB2	1.98	0.45
4:B:901[B]:CDX:HAF1	4:B:901[B]:CDX:HAK1	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ILE:C	5:B:1226:HOH:O	2.59	0.45
1:A:341:LYS:HD2	1:A:343:PHE:CE2	2.52	0.44
4:B:901[B]:CDX:HAK2	5:B:1252:HOH:O	2.17	0.44
1:A:317:VAL:O	1:A:321:THR:HG23	2.18	0.43
4:B:901[A]:CDX:HAF1	4:B:901[A]:CDX:HAK1	1.69	0.43
1:A:343:PHE:CD1	1:A:343:PHE:C	2.97	0.43
1:B:251:VAL:HG12	1:B:279:ILE:HG21	2.00	0.42
1:A:94:THR:CG2	1:A:200:LYS:HE2	2.49	0.42
1:A:231:ARG:HD3	1:A:283:ARG:NH2	2.35	0.42
1:B:144:TYR:CZ	4:B:901[A]:CDX:HAQ1	2.55	0.41
1:A:308:ILE:HD13	1:A:367:LYS:HD3	2.01	0.41
1:B:251:VAL:HG11	1:B:279:ILE:HG21	2.02	0.41
1:A:222:ARG:O	1:A:225:ASP:HB2	2.21	0.41
1:A:65:ASP:OD1	1:A:222:ARG:NE	2.49	0.41
1:B:117:PRO:HB3	1:B:158:LEU:CD2	2.50	0.40
1:A:27:THR:OG1	4:B:901[B]:CDX:HAE1	2.22	0.40
1:B:141:ARG:HD3	1:B:360:PRO:HD2	2.03	0.40
1:B:175:ASN:N	1:B:175:ASN:HD22	2.20	0.40
1:B:280:LEU:O	1:B:291:ALA:HA	2.21	0.40
1:B:82:LYS:HD2	1:B:82:LYS:HA	1.97	0.40
4:B:901[A]:CDX:CAQ	4:B:901[A]:CDX:HAE2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/418 (90%)	368 (98%)	8 (2%)	0	100	100
1	B	372/418 (89%)	362 (97%)	9 (2%)	1 (0%)	36	29
All	All	748/836 (90%)	730 (98%)	17 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	190	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	342/381 (90%)	335 (98%)	7 (2%)	48	46
1	B	339/381 (89%)	324 (96%)	15 (4%)	25	17
All	All	681/762 (89%)	659 (97%)	22 (3%)	34	27

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASP
1	A	77	ARG
1	A	134	GLU
1	A	163	LEU
1	A	172	LYS
1	A	334	LYS
1	A	349	MET
1	B	41	ILE
1	B	52	LYS
1	B	83	ARG
1	B	91	GLU
1	B	111	LYS
1	B	162	ASP
1	B	163	LEU
1	B	164	ASN
1	B	257	SER
1	B	301	GLN
1	B	326	LYS
1	B	340	VAL
1	B	351	ILE
1	B	380	ARG
1	B	402	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	17	GLN
1	A	35	GLN
1	A	89	HIS
1	A	93	HIS
1	A	167	GLN
1	A	249	ASN
1	A	300	GLN
1	A	323	GLN
1	A	389	ASN
1	A	410	ASN
1	B	89	HIS
1	B	142	ASN
1	B	167	GLN
1	B	175	ASN
1	B	234	ASN
1	B	249	ASN
1	B	300	GLN
1	B	301	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 ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	CDX	B	901[B]	-	19,20,20	0.90	0	25,28,28	1.97	7 (28%)
4	CDX	B	901[A]	-	19,20,20	0.94	0	25,28,28	2.01	7 (28%)
3	ANP	A	902	2	33,33,33	2.11	13 (39%)	45,52,52	1.76	8 (17%)
3	ANP	B	903	2	33,33,33	2.29	13 (39%)	45,52,52	1.77	9 (20%)

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	CDX	B	901[B]	-	1/1/7/9	3/8/32/32	0/2/2/2
3	ANP	B	903	2	-	4/18/38/38	0/3/3/3
3	ANP	A	902	2	-	4/18/38/38	0/3/3/3
4	CDX	B	901[A]	-	1/1/7/9	5/8/32/32	0/2/2/2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	ANP	PA-O3A	-6.62	1.52	1.59
3	A	902	ANP	PA-O3A	-5.99	1.53	1.59
3	B	903	ANP	PB-O3A	-5.66	1.52	1.59
3	B	903	ANP	C5-C4	4.40	1.46	1.39
3	A	902	ANP	PB-O3A	-4.25	1.53	1.59
3	A	902	ANP	C5-C4	4.10	1.46	1.39
3	B	903	ANP	PB-O1B	3.58	1.51	1.46
3	B	903	ANP	C5-N7	-2.76	1.34	1.39
3	A	902	ANP	PG-O1G	2.74	1.50	1.46
3	A	902	ANP	PG-O2G	-2.73	1.49	1.56
3	A	902	ANP	PB-O2B	-2.63	1.49	1.56
3	B	903	ANP	C5-C6	2.62	1.48	1.41
3	A	902	ANP	C5-C6	2.59	1.48	1.41
3	A	902	ANP	C5-N7	-2.58	1.34	1.39
3	A	902	ANP	PG-O3G	-2.40	1.50	1.56
3	B	903	ANP	PB-O2B	-2.39	1.50	1.56
3	B	903	ANP	C8-N7	2.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	ANP	PG-O2G	-2.33	1.50	1.56
3	A	902	ANP	C4-N9	-2.29	1.32	1.37
3	A	902	ANP	C6-N6	2.24	1.39	1.34
3	B	903	ANP	PG-O3G	-2.23	1.50	1.56
3	B	903	ANP	C4-N9	-2.18	1.33	1.37
3	B	903	ANP	C6-N6	2.18	1.39	1.34
3	A	902	ANP	C8-N7	2.14	1.35	1.31
3	A	902	ANP	PB-O1B	2.10	1.49	1.46
3	B	903	ANP	PG-O1G	2.09	1.49	1.46

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	ANP	C5-C4-N3	-5.34	119.36	126.72
3	A	902	ANP	C5-C4-N3	-5.10	119.70	126.72
4	B	901[A]	CDX	CAC-CAD-NAJ	-4.56	106.13	112.58
4	B	901[B]	CDX	CAC-CAD-NAJ	-4.50	106.21	112.58
4	B	901[A]	CDX	CAE-CAL-NAM	-4.38	107.05	114.45
3	B	903	ANP	N3-C4-N9	4.32	134.52	127.17
3	A	902	ANP	N3-C4-N9	4.31	134.50	127.17
4	B	901[B]	CDX	CAE-CAL-NAM	-4.28	107.21	114.45
4	B	901[B]	CDX	CAP-CAQ-NAJ	-4.14	106.73	112.58
4	B	901[A]	CDX	CAP-CAQ-NAJ	-3.95	107.00	112.58
3	B	903	ANP	C2-N3-C4	3.77	121.04	111.83
3	B	903	ANP	N3-C2-N1	-3.77	122.88	128.58
3	A	902	ANP	N3-C2-N1	-3.67	123.03	128.58
3	A	902	ANP	C2-N3-C4	3.59	120.60	111.83
4	B	901[A]	CDX	CAL-CAK-NAJ	-3.45	108.37	113.70
3	A	902	ANP	C4-N9-C8	3.24	109.14	105.74
3	B	903	ANP	C4-C5-N7	-2.93	107.23	110.58
4	B	901[B]	CDX	CAQ-NAJ-CAD	-2.83	106.87	109.88
3	A	902	ANP	C4-C5-N7	-2.76	107.42	110.58
3	B	903	ANP	C4-N9-C8	2.75	108.62	105.74
3	A	902	ANP	N9-C8-N7	-2.58	110.28	113.94
3	A	902	ANP	C5-N7-C8	2.48	107.36	103.45
3	B	903	ANP	C5-N7-C8	2.41	107.24	103.45
4	B	901[B]	CDX	CAF-NAM-CAR	-2.35	107.24	109.99
4	B	901[B]	CDX	CAL-CAK-NAJ	-2.33	110.10	113.70
4	B	901[A]	CDX	CAF-NAM-CAR	-2.26	107.35	109.99
4	B	901[A]	CDX	CAQ-NAJ-CAD	-2.23	107.51	109.88
3	B	903	ANP	N9-C8-N7	-2.23	110.77	113.94
4	B	901[A]	CDX	OAO-CAP-NAI	2.09	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	903	ANP	O2B-PB-O3A	2.06	111.52	104.64
4	B	901[B]	CDX	OAO-CAP-NAI	2.03	123.42	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	901[A]	CDX	CAL
4	B	901[B]	CDX	CAL

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	ANP	PB-N3B-PG-O1G
3	A	902	ANP	PG-N3B-PB-O1B
3	A	902	ANP	PA-O3A-PB-O2B
3	B	903	ANP	PB-N3B-PG-O1G
3	B	903	ANP	PG-N3B-PB-O1B
3	B	903	ANP	PA-O3A-PB-O2B
4	B	901[A]	CDX	NAJ-CAK-CAL-CAE
4	B	901[A]	CDX	CAK-CAL-NAM-CAR
4	B	901[A]	CDX	CAK-CAL-NAM-CAF
4	B	901[A]	CDX	CAE-CAL-NAM-CAR
4	B	901[A]	CDX	CAE-CAL-NAM-CAF
4	B	901[B]	CDX	NAJ-CAK-CAL-CAE
4	B	901[B]	CDX	CAK-CAL-NAM-CAF
4	B	901[B]	CDX	CAE-CAL-NAM-CAF
3	A	902	ANP	PA-O3A-PB-O1B
3	B	903	ANP	PA-O3A-PB-O1B

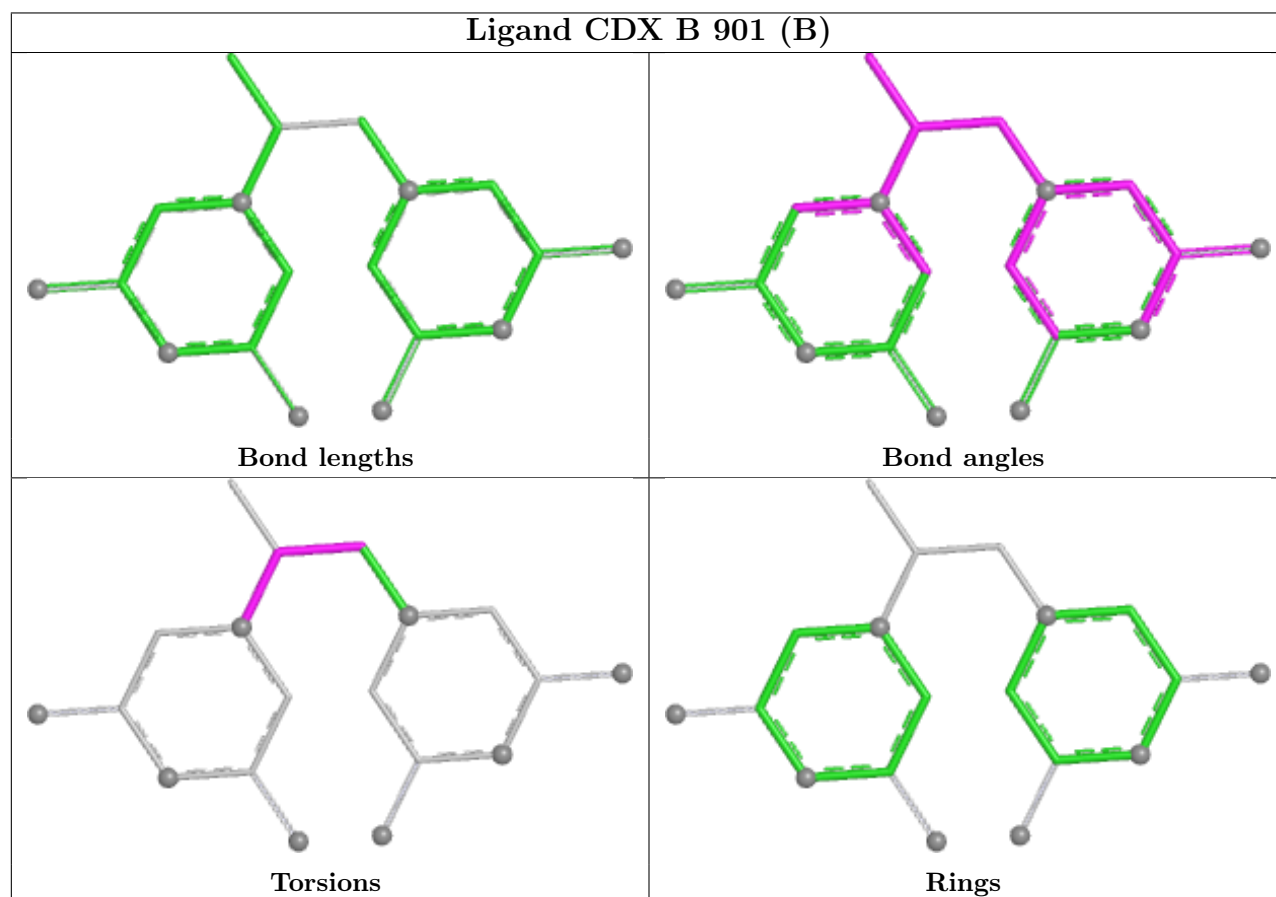
There are no ring outliers.

2 monomers are involved in 8 short contacts:

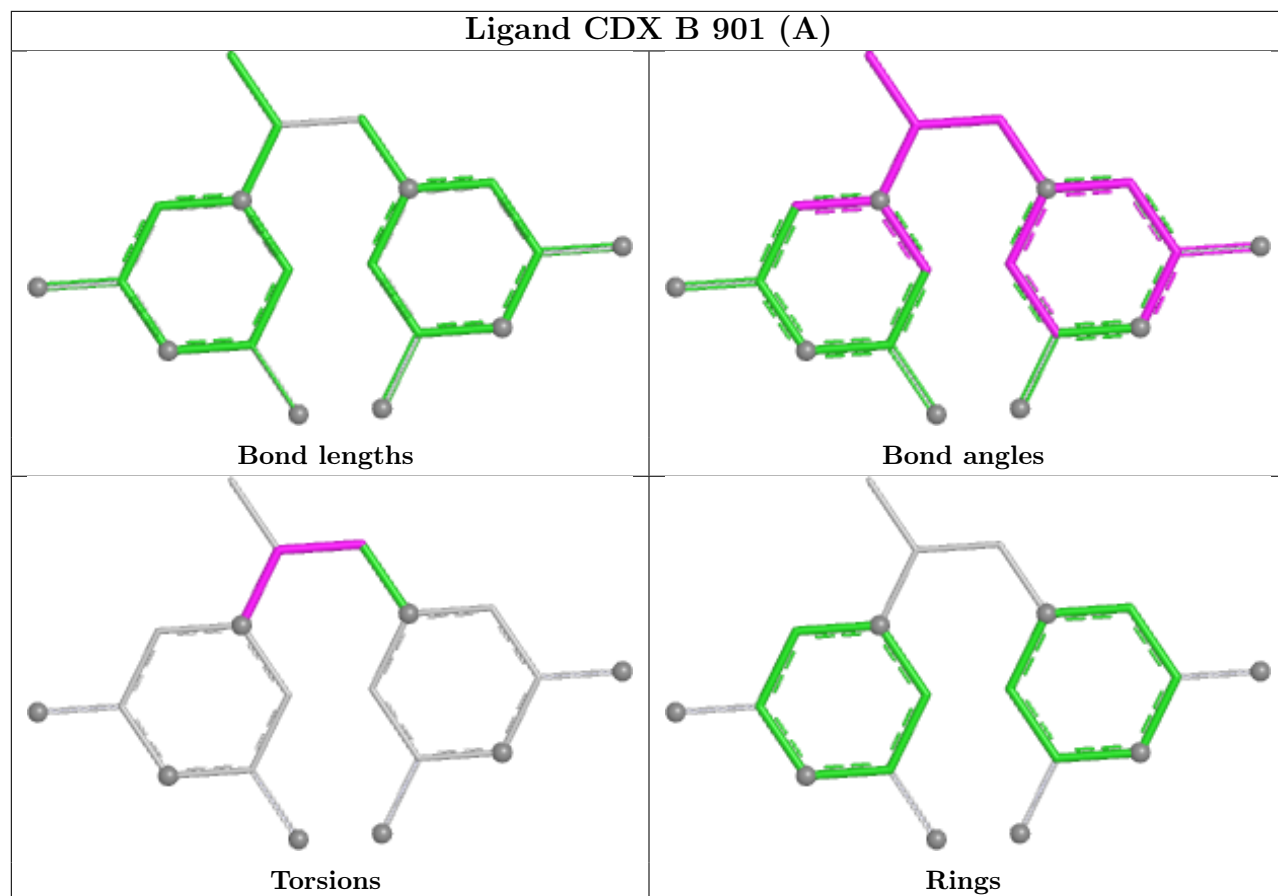
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	901[B]	CDX	5	0
4	B	901[A]	CDX	3	0

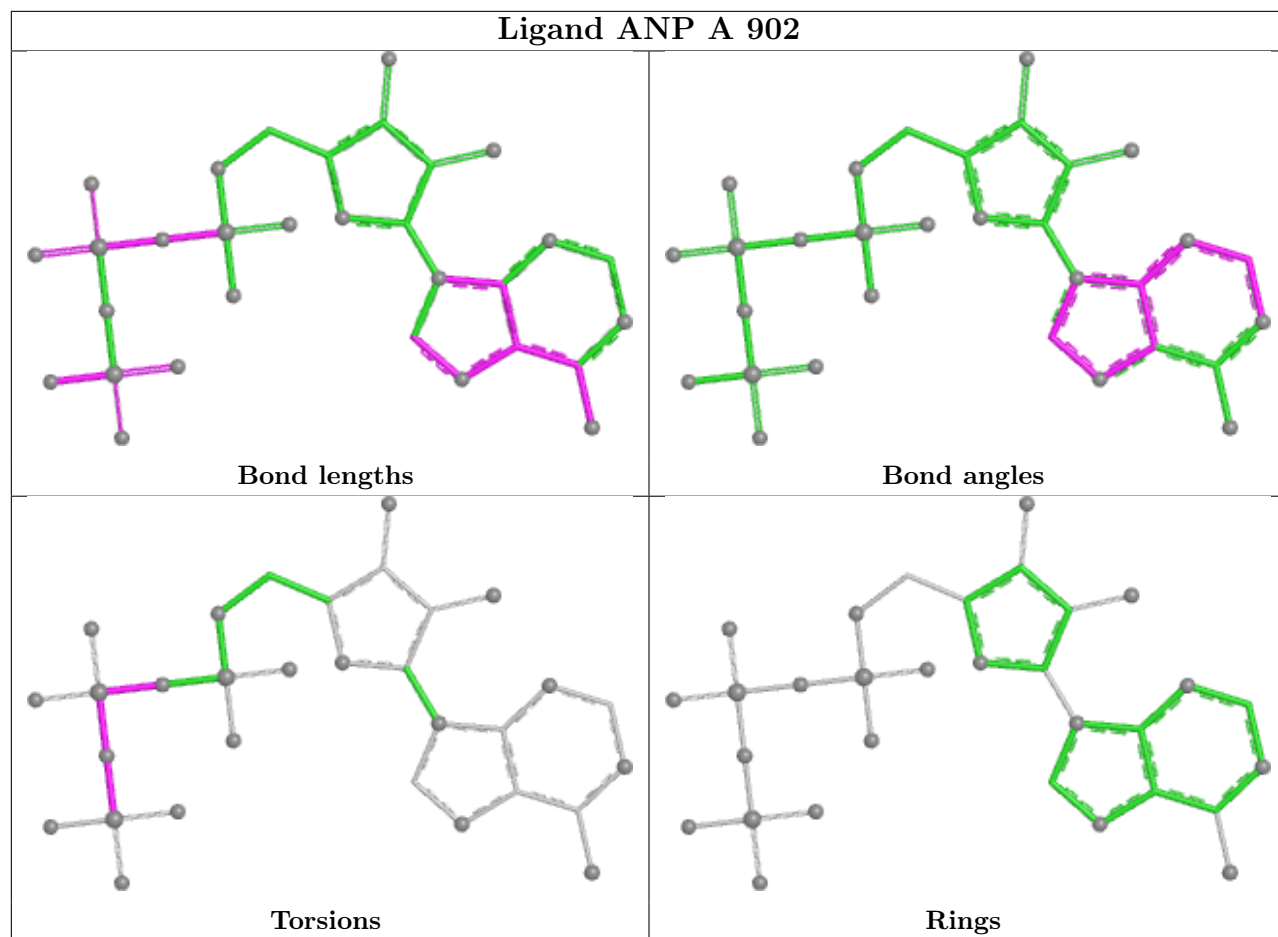
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

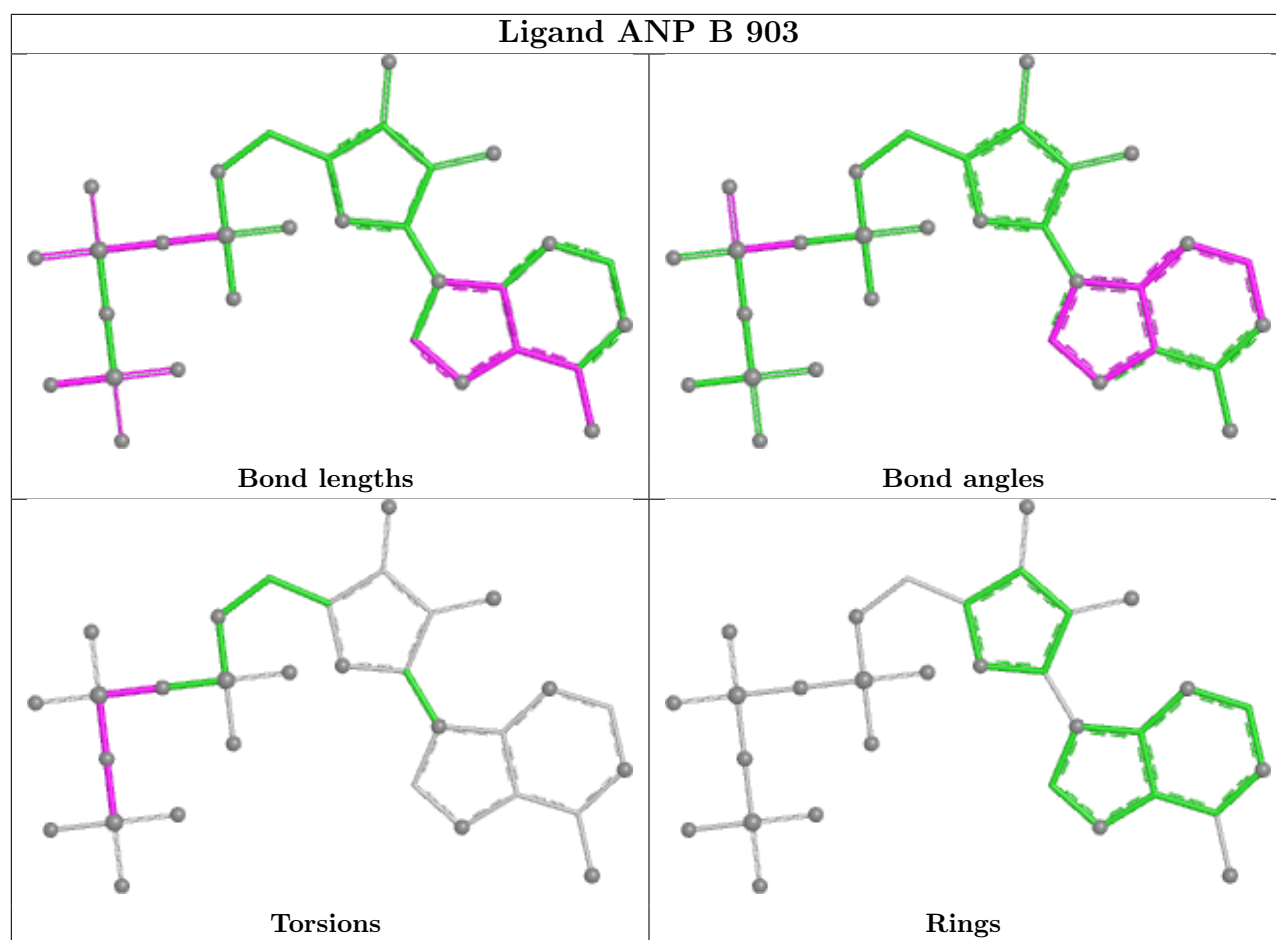
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



Ligand CDX B 901 (A)







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	382/418 (91%)	0.28	18 (4%) 36 39	13, 20, 32, 79	0
1	B	378/418 (90%)	0.88	48 (12%) 8 8	14, 22, 31, 52	0
All	All	760/836 (90%)	0.58	66 (8%) 16 17	13, 21, 31, 79	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	VAL	5.4
1	B	186	THR	4.5
1	B	162	ASP	4.3
1	B	104	ILE	4.2
1	B	12	TYR	3.8
1	B	191	GLY	3.8
1	B	164	ASN	3.7
1	B	405	ASP	3.5
1	A	334	LYS	3.4
1	B	258	LEU	3.3
1	A	402	GLU	3.1
1	B	118	GLU	3.1
1	A	46	THR	3.1
1	B	113	ASN	3.1
1	A	113	ASN	3.0
1	B	232	ASP	3.0
1	A	276	ILE	3.0
1	A	280	LEU	2.9
1	A	47	ASP	2.9
1	A	349	MET	2.9
1	B	161	ALA	2.8
1	B	187	SER	2.8
1	A	385	LEU	2.8
1	A	210	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	38	LEU	2.7
1	B	185	ILE	2.7
1	A	409	GLU	2.6
1	B	132	ASP	2.6
1	A	406	ALA	2.6
1	B	8	ALA	2.6
1	B	190	LYS	2.6
1	A	382	GLU	2.5
1	B	198	THR	2.5
1	B	46	THR	2.5
1	B	249	ASN	2.4
1	B	257	SER	2.4
1	B	101	GLY	2.4
1	A	405	ASP	2.3
1	A	333	LYS	2.3
1	B	167	GLN	2.3
1	B	30	GLY	2.3
1	B	189	LYS	2.3
1	B	58	PRO	2.2
1	B	56	ILE	2.2
1	B	108	ILE	2.2
1	B	253	LEU	2.2
1	B	210	GLU	2.2
1	B	85	ASP	2.2
1	B	395	ASP	2.2
1	A	408	GLU	2.2
1	B	368	GLU	2.2
1	B	184	LYS	2.2
1	B	260	LYS	2.2
1	B	106	ILE	2.1
1	B	212	ASP	2.1
1	B	135	LYS	2.1
1	B	115	TYR	2.1
1	A	395	ASP	2.1
1	B	32	VAL	2.1
1	B	76	VAL	2.1
1	B	194	TYR	2.1
1	B	77	ARG	2.1
1	B	251	VAL	2.1
1	A	7	SER	2.0
1	B	175	ASN	2.0
1	B	254	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](#)

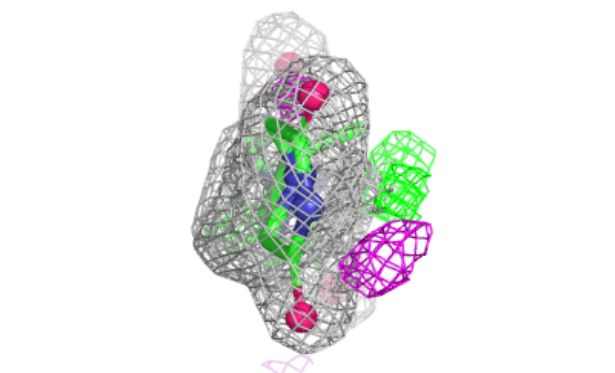
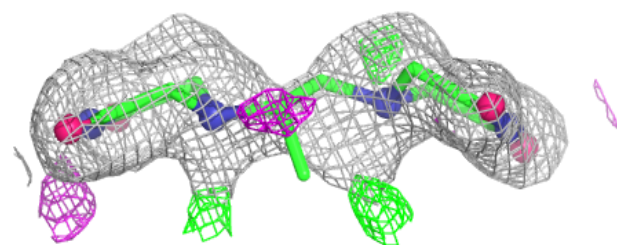
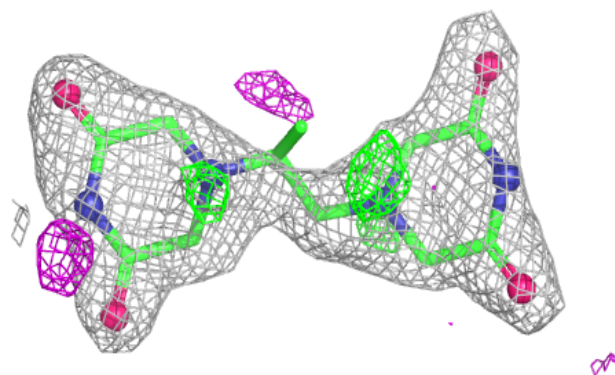
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	CDX	B	901[A]	19/19	0.85	0.21	54,55,57,58	19
4	CDX	B	901[B]	19/19	0.85	0.21	54,56,57,58	19
3	ANP	B	903	31/31	0.96	0.08	24,30,38,39	0
2	MG	B	905	1/1	0.97	0.05	25,25,25,25	0
3	ANP	A	902	31/31	0.98	0.06	20,23,26,29	0
2	MG	A	904	1/1	0.98	0.03	23,23,23,23	0

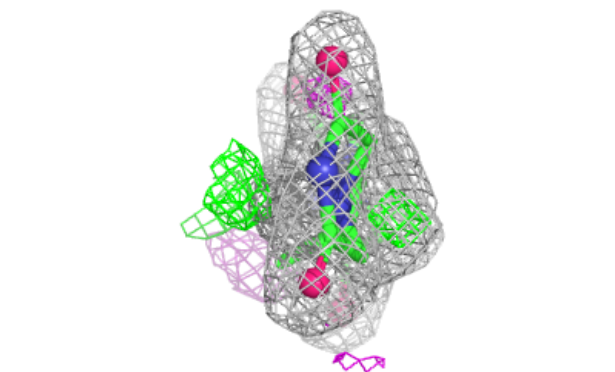
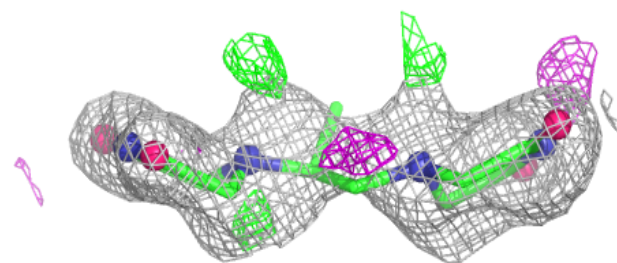
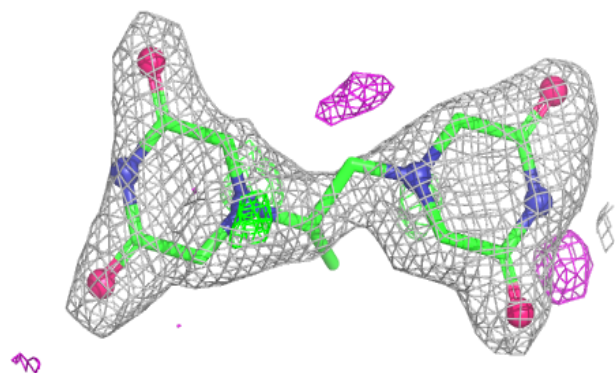
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CDX B 901 (A):

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

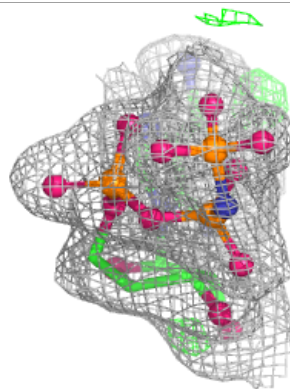
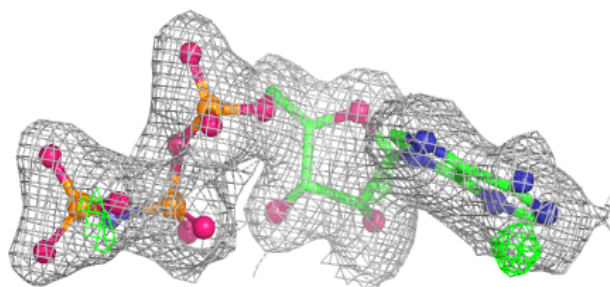
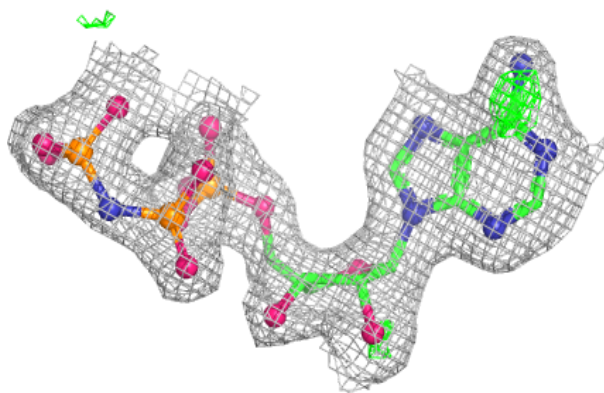
**Electron density around CDX B 901 (B):**

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

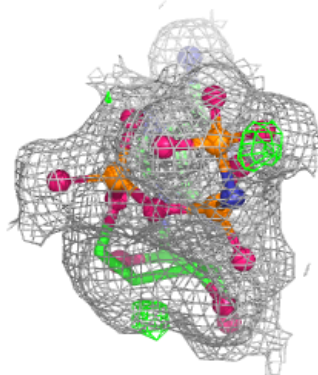
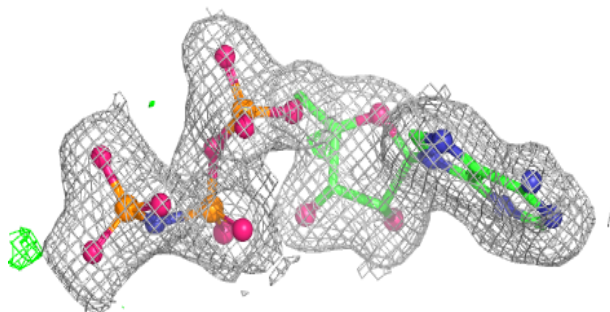
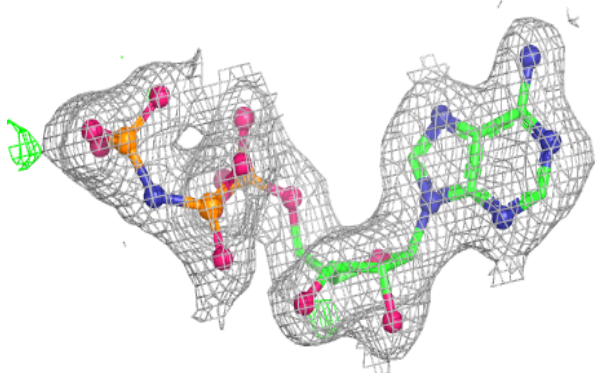


Electron density around ANP B 903:

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

**Electron density around ANP A 902:**

$2mF_o-DF_c$ (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.