



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:01 AM UTC

PDB ID : 3IRO / pdb_00003iro
Title : Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase complexed with NADPH and Q-8 antifolate
Authors : Chitnumsub, P.; Yuvaniyama, J.; Yuthavong, Y.
Deposited on : 2009-08-24
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

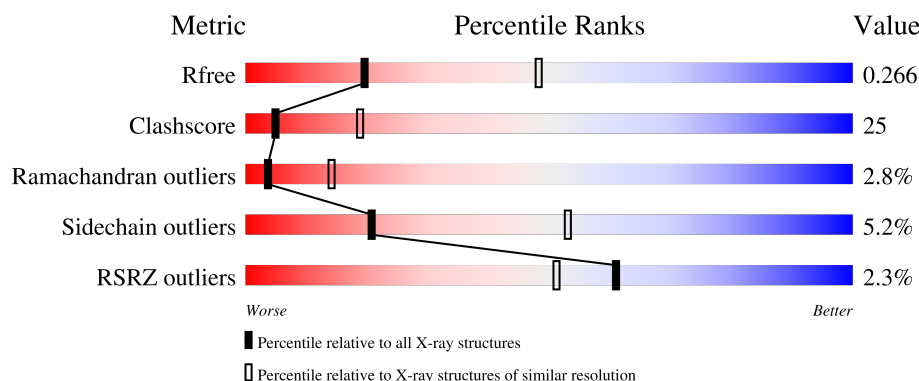
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	521	2% 52% 42% 5%
1	B	521	3% 49% 43% 7%
1	C	521	% 52% 40% 6%
1	D	521	2% 53% 40% 5%

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
5	ACT	A	809	-	-	X	-

2 Entry composition [i](#)

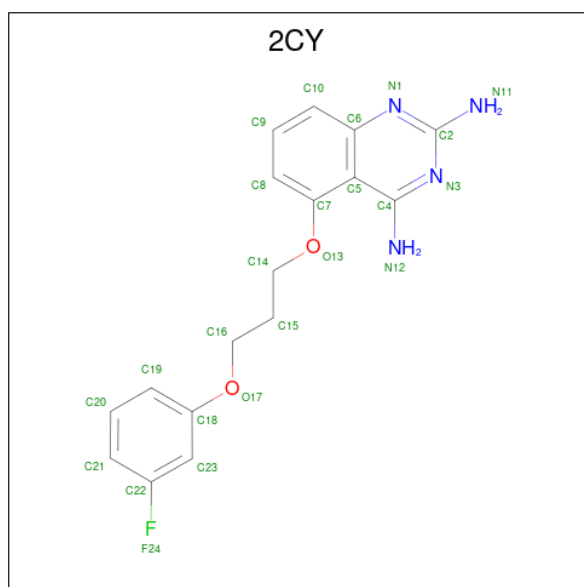
There are 7 unique types of molecules in this entry. The entry contains 16862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	0	0	0
			4124	2616	729	759	20			
1	B	515	Total	C	N	O	S	0	0	0
			4101	2602	725	755	19			
1	C	516	Total	C	N	O	S	0	0	0
			4107	2605	726	757	19			
1	D	513	Total	C	N	O	S	0	0	0
			4087	2594	723	752	18			

- Molecule 2 is 5-[3-(3-fluorophenoxy)propoxy]quinazoline-2,4-diamine (CCD ID: 2CY) (formula: C₁₇H₁₇FN₄O₂).



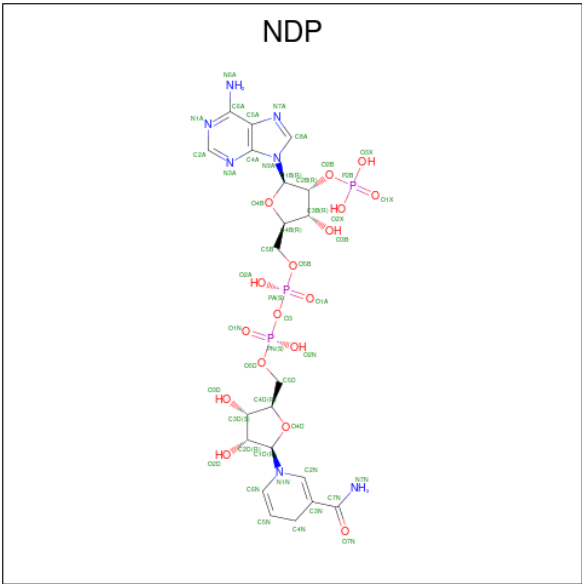
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	17	1	4	2		
2	B	1	Total	C	F	N	O	0	0
			24	17	1	4	2		

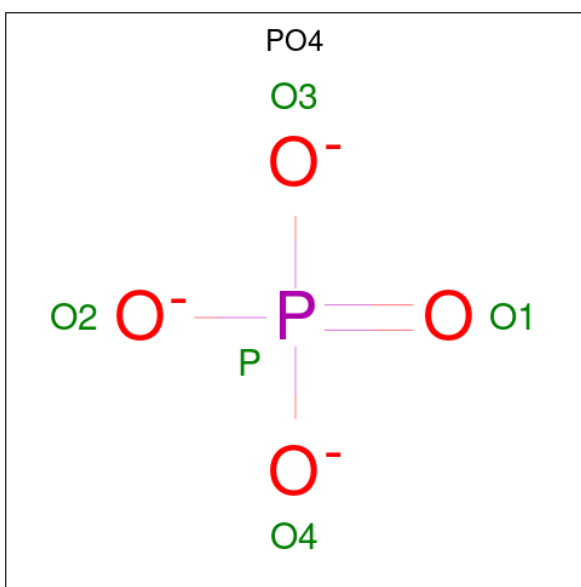
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	0	0
			24	17	1	4	2		
2	D	1	Total	C	F	N	O	0	0
			24	17	1	4	2		

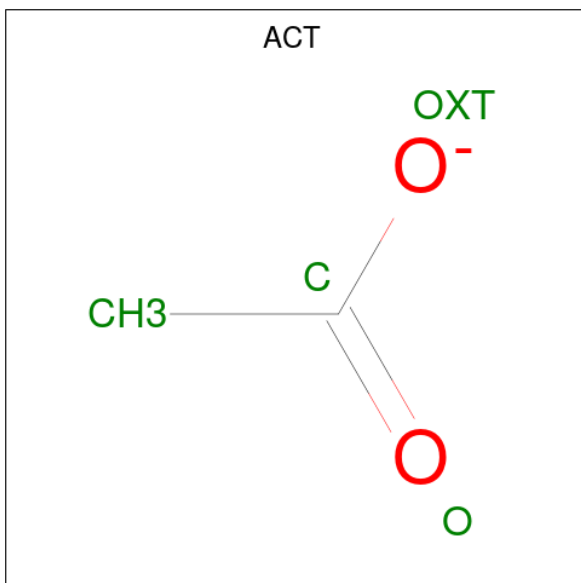
- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).





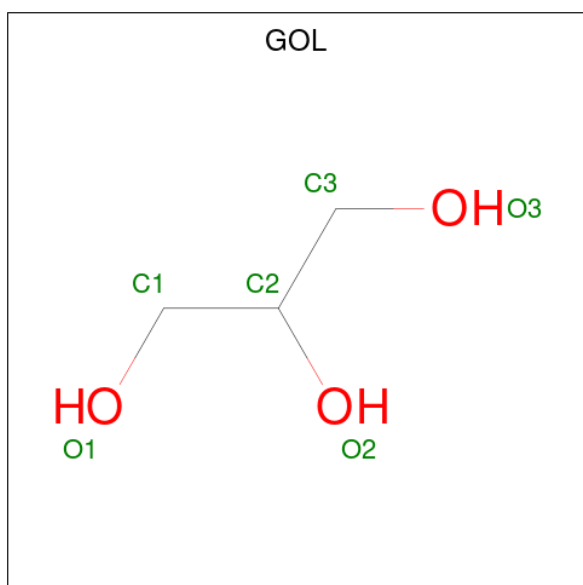
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

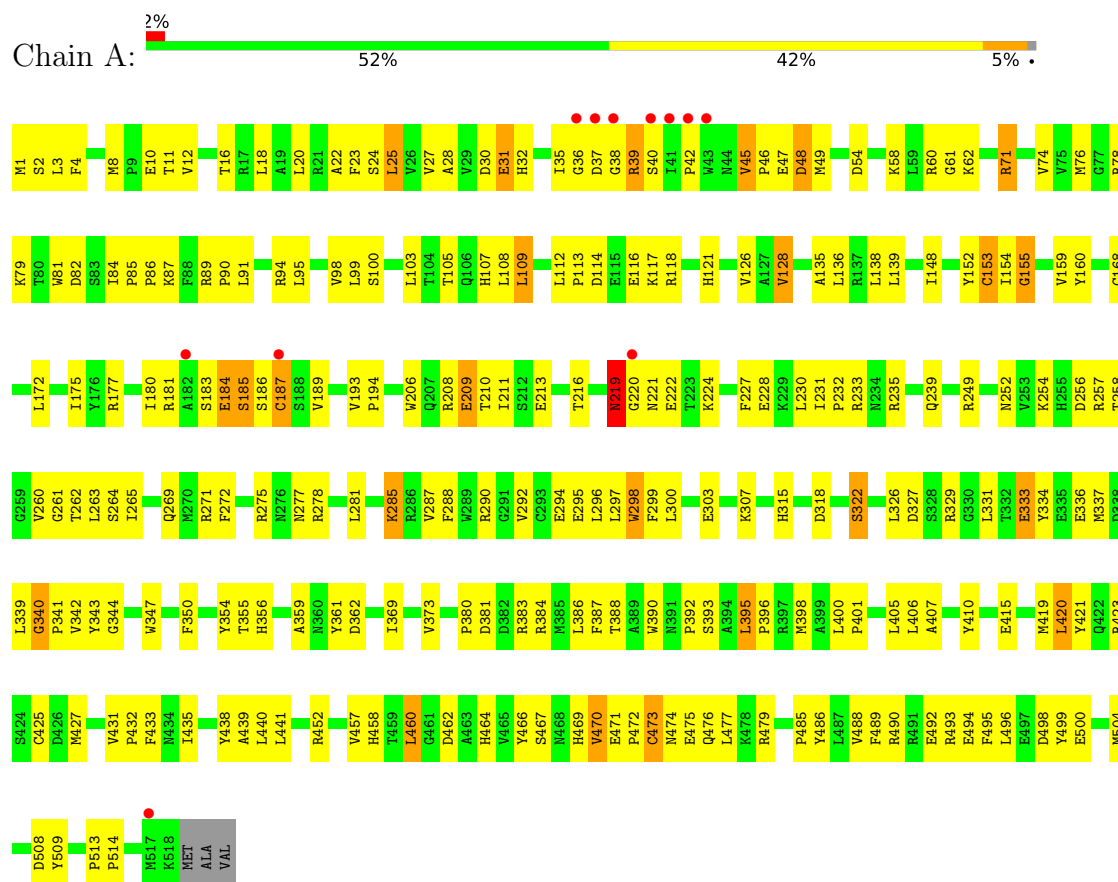
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	23	Total 23	O 23	0	0
7	B	12	Total 12	O 12	0	0
7	C	23	Total 23	O 23	0	0
7	D	25	Total 25	O 25	0	0

3 Residue-property plots

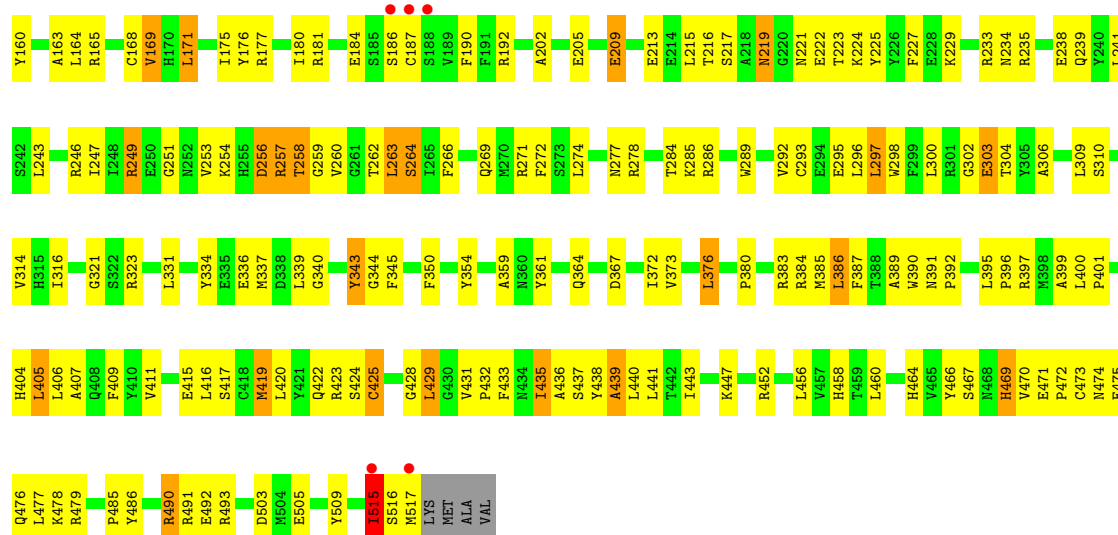
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bifunctional dihydrofolate reductase-thymidylate synthase

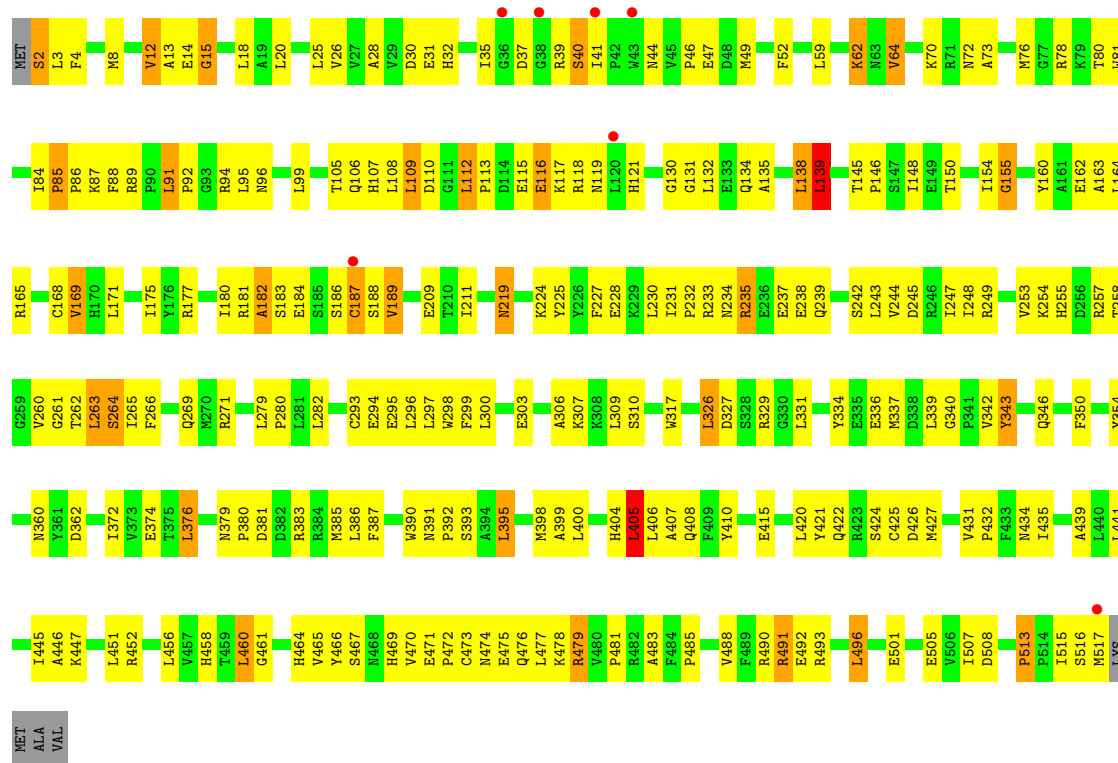


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



VAL	I435	A436	S437	Y438	A439	L440	L441	A448	R452	P453	G454	E455	L456	L460	A463	Y466	H469	E470	E471	P472	C473	E474	E475	K478	P485	Y486	F489	R490	E491	E492	R493	E494	F495	L496	E497	D498	M504	E505	Y509	Y512	P513	P514	I515	SER	MET	LYS	MET	ALA								
	D338	L339	G340	P341	Y342	Y343	Q346	W347	R348	H349	F350	Y354	T355	H356	N360	Y361	D362	D367	L376	N379	M385	L386	A389	W390	N391	P392	L395	P396	R397	M398	A399	H404	L405	L406	A407	Q408	F409	E415	L416	L420	C425	G430	V431	F432	F433	N434										
	H255	D256	R257	T258	G259	T262	L263	S264	F266	N270	R271	F272	S273	L274	R275	N276	R277	R278	T283	T284	F288	V292	L296	L297	W298	F299	L300	R301	G302	E303	K307	K308	L309	S310	D311	K312	H315	D318	S322	F325	L326	D327	S328	E333	E336	M337										
	A163	L164	R165	V169	L171	L172	L175	Y176	R177	T178	R181	E184	S185	C187	S188	V193	P194	E195	A201	Q207	R208	E209	H210	T210	A218	N219	G220	N221	Y225	L228	L229	L230	L232	R233	N234	R235	E236	E237	L241	S242	T246	R247	I248	R249	V253	K254										
	R89	P90	L91	L95	N96	V97	V98	L99	S100	S101	T102	L103	T104	T105	Q106	H107	L108	L109	D110	G111	L112	P113	D114	E115	E116	K117	R118	N119	L120	H121	A122	G131	L132	E133	Q134	A135	L136	R137	L138	L139	A140	S141	Y144	T145	P146	S147	I148	E149	T150	V151	Y152	G153	I154	G155	G156	E162

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.54Å 165.94Å 84.72Å 90.00° 113.41° 90.00°	Depositor
Resolution (Å)	45.07 – 2.80 45.07 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (45.07-2.80) 95.0 (45.07-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.206 , 0.277 0.198 , 0.266	Depositor DCC
R_{free} test set	2478 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16862	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: NDP, ACT, 2CY, PO4, GOL

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	0/4224	0.99	15/5729 (0.3%)
1	B	0.46	0/4201	1.02	19/5700 (0.3%)
1	C	0.46	0/4207	1.00	19/5708 (0.3%)
1	D	0.47	0/4187	1.01	17/5682 (0.3%)
All	All	0.46	0/16819	1.00	70/22819 (0.3%)

There are no bond length outliers.

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	GLY	N-CA-C	9.92	125.01	110.63
1	D	209	GLU	N-CA-C	-9.24	100.32	111.69
1	D	154	ILE	N-CA-C	8.88	120.60	112.17
1	C	138	LEU	N-CA-C	-8.71	101.47	110.97
1	A	209	GLU	N-CA-C	-8.08	101.54	111.40

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	4124	0	4085	191	0
1	B	4101	0	4055	252	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4107	0	4060	216	0
1	D	4087	0	4041	203	0
2	A	24	0	17	1	0
2	B	24	0	17	2	0
2	C	24	0	17	1	0
2	D	24	0	17	3	0
3	A	48	0	26	1	0
3	B	48	0	26	5	0
3	C	48	0	26	4	0
3	D	48	0	26	5	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
4	C	10	0	0	1	0
5	A	12	0	9	2	0
5	B	4	0	3	0	0
5	C	8	0	6	0	0
5	D	16	0	12	1	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
7	A	23	0	0	1	0
7	B	12	0	0	0	0
7	C	23	0	0	1	0
7	D	25	0	0	0	0
All	All	16862	0	16459	836	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 25.

The worst 5 of 836 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ASP:HB3	1:C:40:SER:HB3	1.40	1.02
1:C:62:LYS:HE2	1:C:64:VAL:HB	1.41	1.00
1:A:329:ARG:HH12	1:A:400:LEU:HA	1.35	0.90
1:C:116:GLU:HA	1:C:119:ASN:ND2	1.87	0.90
1:C:233:ARG:NH1	1:C:235:ARG:HH12	1.70	0.89

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	516/521 (99%)	463 (90%)	39 (8%)	14 (3%)	4	15
1	B	513/521 (98%)	466 (91%)	33 (6%)	14 (3%)	4	15
1	C	514/521 (99%)	453 (88%)	46 (9%)	15 (3%)	3	13
1	D	511/521 (98%)	448 (88%)	49 (10%)	14 (3%)	4	15
All	All	2054/2084 (99%)	1830 (89%)	167 (8%)	57 (3%)	4	14

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLY
1	B	12	VAL
1	B	113	PRO
1	B	516	SER
1	C	182	ALA

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	444/446 (100%)	426 (96%)	18 (4%)	27	62
1	B	441/446 (99%)	416 (94%)	25 (6%)	18	49
1	C	442/446 (99%)	419 (95%)	23 (5%)	21	53
1	D	439/446 (98%)	413 (94%)	26 (6%)	18	48
All	All	1766/1784 (99%)	1674 (95%)	92 (5%)	21	53

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	374	GLU
1	D	106	GLN
1	C	395	LEU
1	C	496	LEU
1	D	146	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	422	GLN
1	D	129	ASN
1	C	464	HIS
1	C	476	GLN
1	D	207	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	PO4	B	801	-	4,4,4	2.38	1 (25%)	6,6,6	0.95	0
6	GOL	B	806	-	5,5,5	0.52	0	5,5,5	0.22	0
3	NDP	C	703	-	51,52,52	1.71	12 (23%)	71,80,80	1.60	14 (19%)
2	2CY	A	601	-	26,26,26	2.19	10 (38%)	35,35,35	1.79	7 (20%)
6	GOL	C	805	-	5,5,5	0.46	0	5,5,5	0.31	0
5	ACT	D	815	-	3,3,3	0.62	0	3,3,3	1.36	0
3	NDP	A	701	-	51,52,52	1.77	11 (21%)	71,80,80	1.50	13 (18%)
4	PO4	C	804	-	4,4,4	2.68	1 (25%)	6,6,6	0.88	0
2	2CY	C	603	-	26,26,26	2.16	11 (42%)	35,35,35	1.80	8 (22%)
3	NDP	D	704	-	51,52,52	1.75	11 (21%)	71,80,80	1.56	13 (18%)
5	ACT	A	809	-	3,3,3	0.64	0	3,3,3	1.36	0
5	ACT	D	810	-	3,3,3	0.38	0	3,3,3	1.46	0
5	ACT	D	816	-	3,3,3	0.50	0	3,3,3	1.44	0
2	2CY	B	602	-	26,26,26	2.21	11 (42%)	35,35,35	1.76	7 (20%)
5	ACT	A	807	-	3,3,3	0.58	0	3,3,3	1.40	0
5	ACT	B	811	-	3,3,3	0.80	0	3,3,3	1.45	0
5	ACT	C	812	-	3,3,3	0.53	0	3,3,3	1.30	0
5	ACT	D	814	-	3,3,3	0.69	0	3,3,3	1.33	0
4	PO4	A	802	-	4,4,4	2.58	1 (25%)	6,6,6	0.91	0
5	ACT	C	813	-	3,3,3	0.69	0	3,3,3	1.39	0
4	PO4	C	803	-	4,4,4	2.64	1 (25%)	6,6,6	0.90	0
2	2CY	D	604	-	26,26,26	2.20	11 (42%)	35,35,35	1.78	8 (22%)
3	NDP	B	702	-	51,52,52	1.67	11 (21%)	71,80,80	1.60	13 (18%)
5	ACT	A	808	-	3,3,3	0.60	0	3,3,3	1.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	806	-	-	0/4/4/4	-
2	2CY	C	603	-	-	3/8/8/8	0/3/3/3
3	NDP	C	703	-	-	2/34/77/77	0/5/5/5
2	2CY	B	602	-	-	3/8/8/8	0/3/3/3
3	NDP	D	704	-	-	10/34/77/77	0/5/5/5
3	NDP	B	702	-	-	2/34/77/77	0/5/5/5
2	2CY	A	601	-	-	5/8/8/8	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	805	-	-	0/4/4/4	-
2	2CY	D	604	-	-	2/8/8/8	0/3/3/3
3	NDP	A	701	-	-	5/34/77/77	0/5/5/5

The worst 5 of 92 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	2CY	O17-C18	-5.11	1.26	1.37
4	C	804	PO4	P-O1	5.09	1.62	1.50
2	D	604	2CY	O17-C18	-5.08	1.26	1.37
4	C	803	PO4	P-O1	5.01	1.62	1.50
3	A	701	NDP	C4N-C3N	-4.92	1.40	1.50

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	2CY	N1-C2-N3	-5.58	120.12	127.21
2	D	604	2CY	N1-C2-N3	-5.48	120.24	127.21
2	A	601	2CY	N1-C2-N3	-5.41	120.33	127.21
2	B	602	2CY	N1-C2-N3	-5.38	120.36	127.21
3	B	702	NDP	C1D-N1N-C2N	-4.76	113.31	121.14

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	704	NDP	C5D-O5D-PN-O1N
2	C	603	2CY	O13-C14-C15-C16
2	D	604	2CY	O13-C14-C15-C16
2	B	602	2CY	O13-C14-C15-C16
2	A	601	2CY	C15-C14-O13-C7

There are no ring outliers.

12 monomers are involved in 27 short contacts:

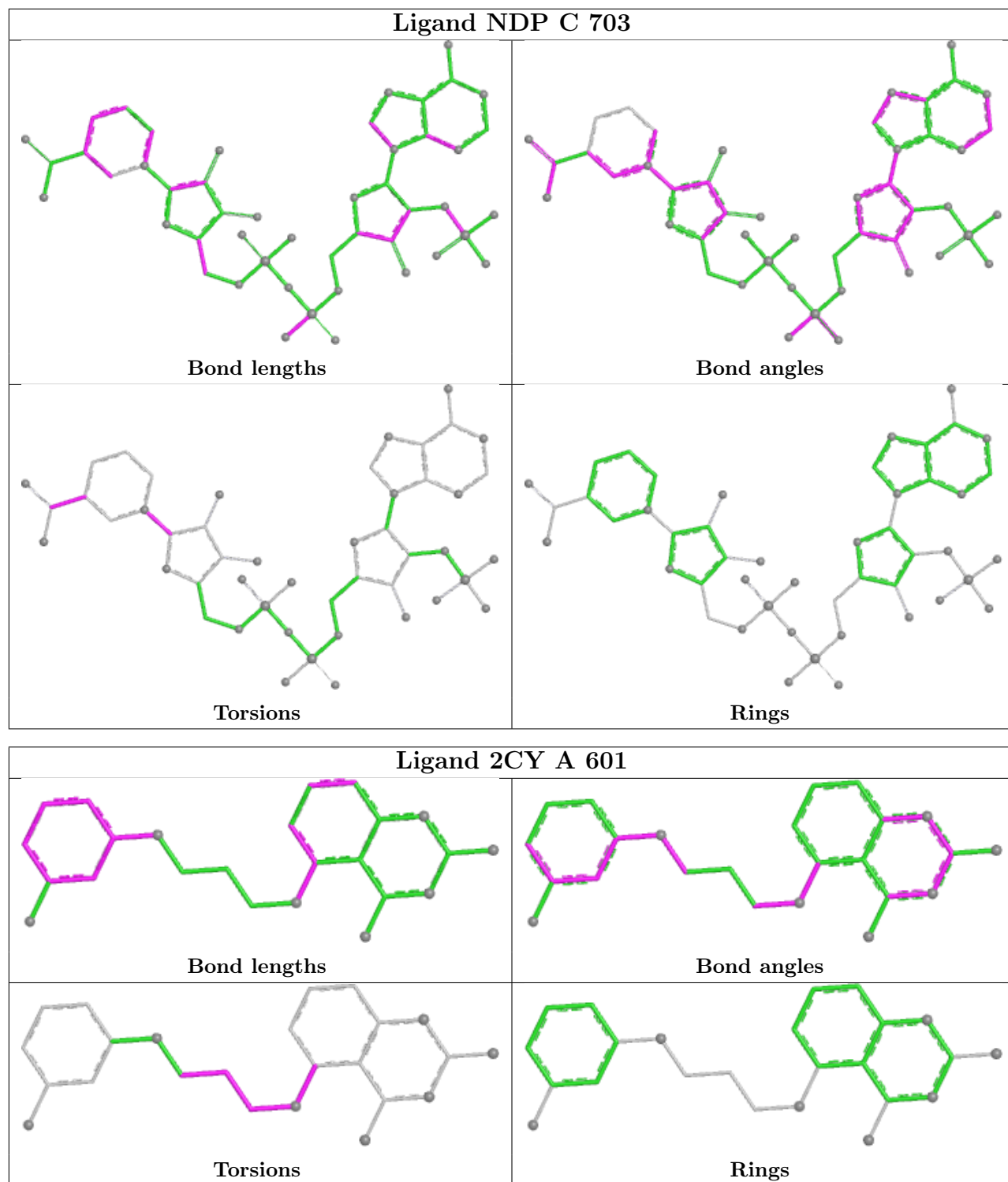
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	PO4	1	0
3	C	703	NDP	4	0
2	A	601	2CY	1	0
3	A	701	NDP	1	0

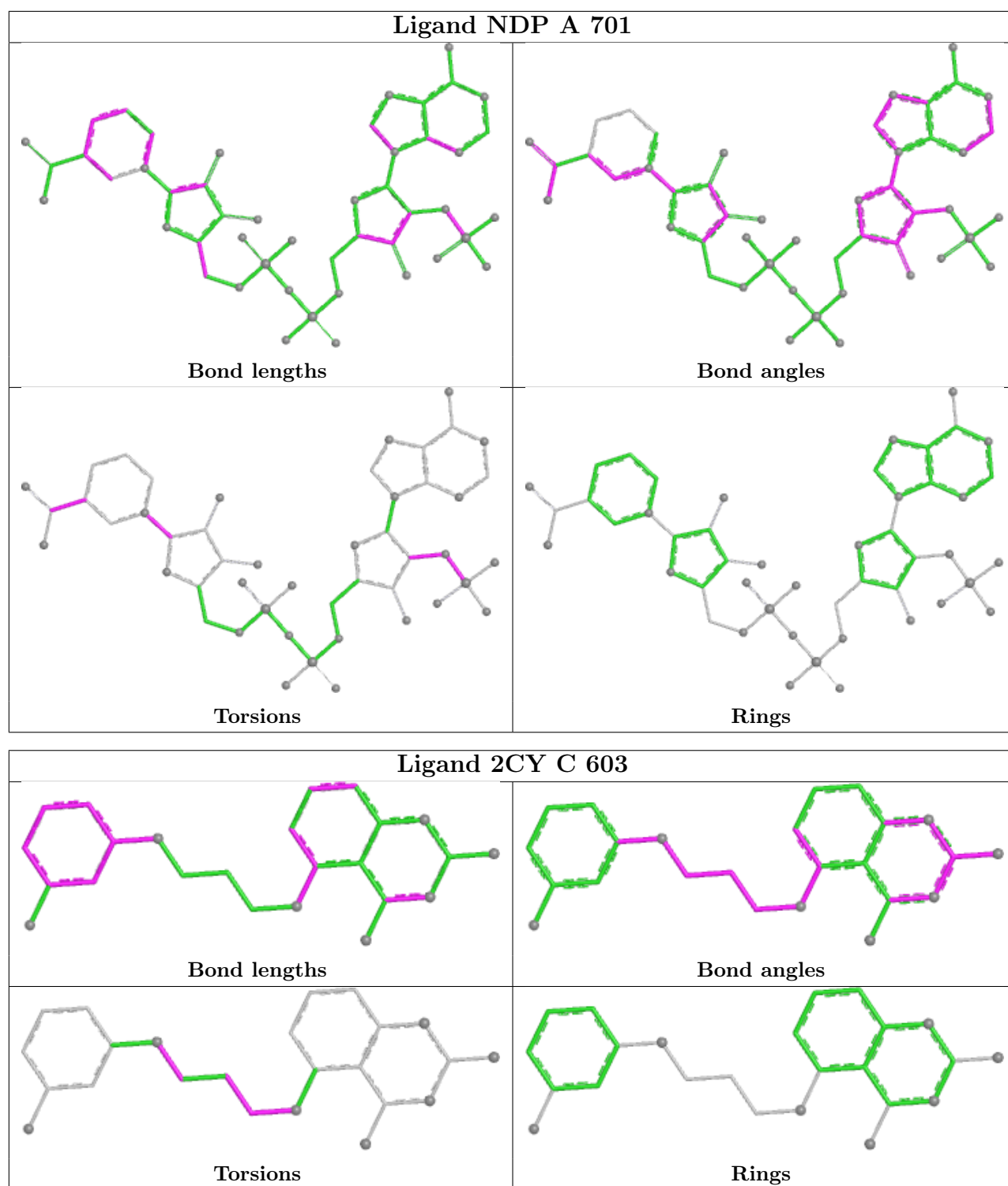
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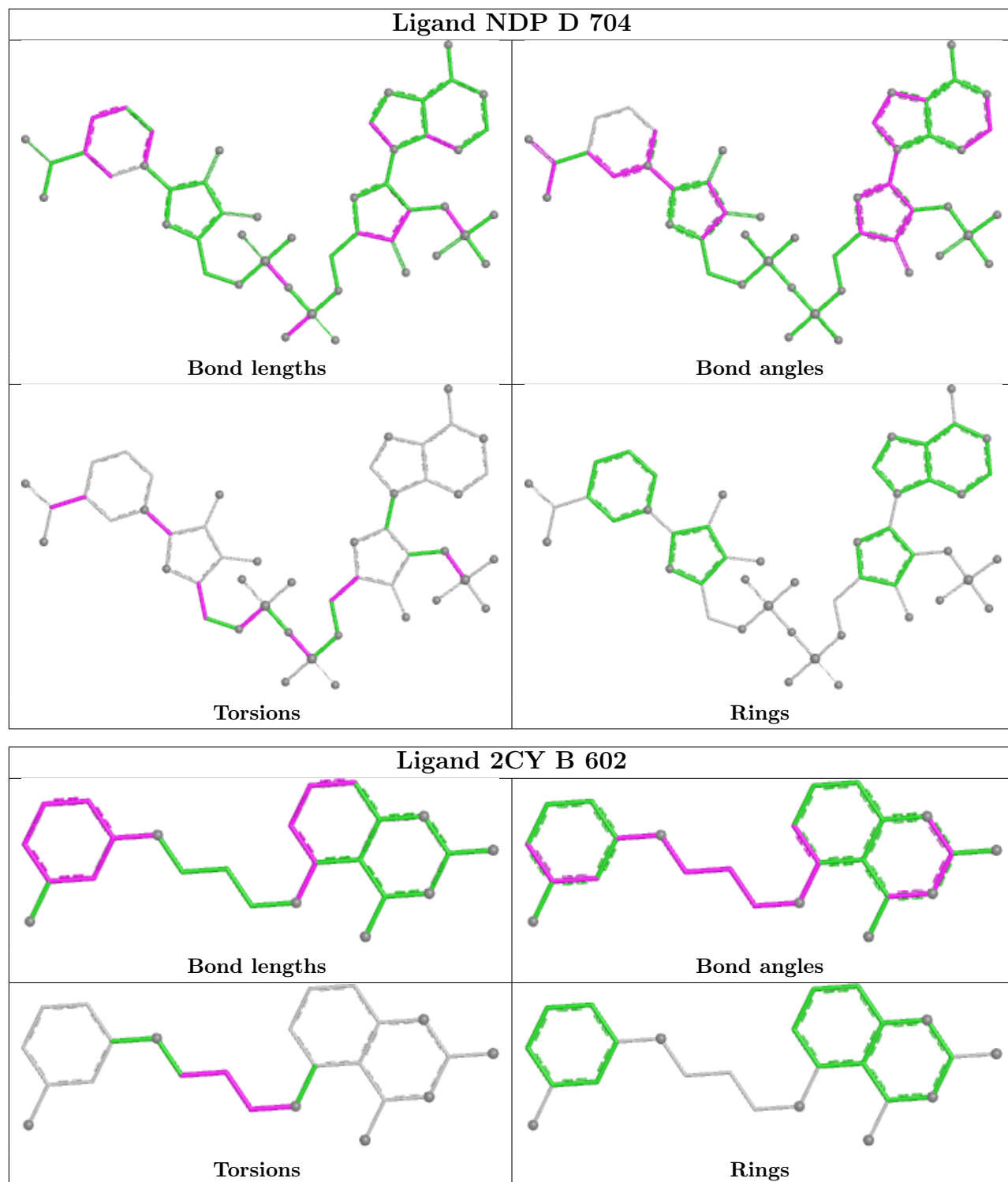
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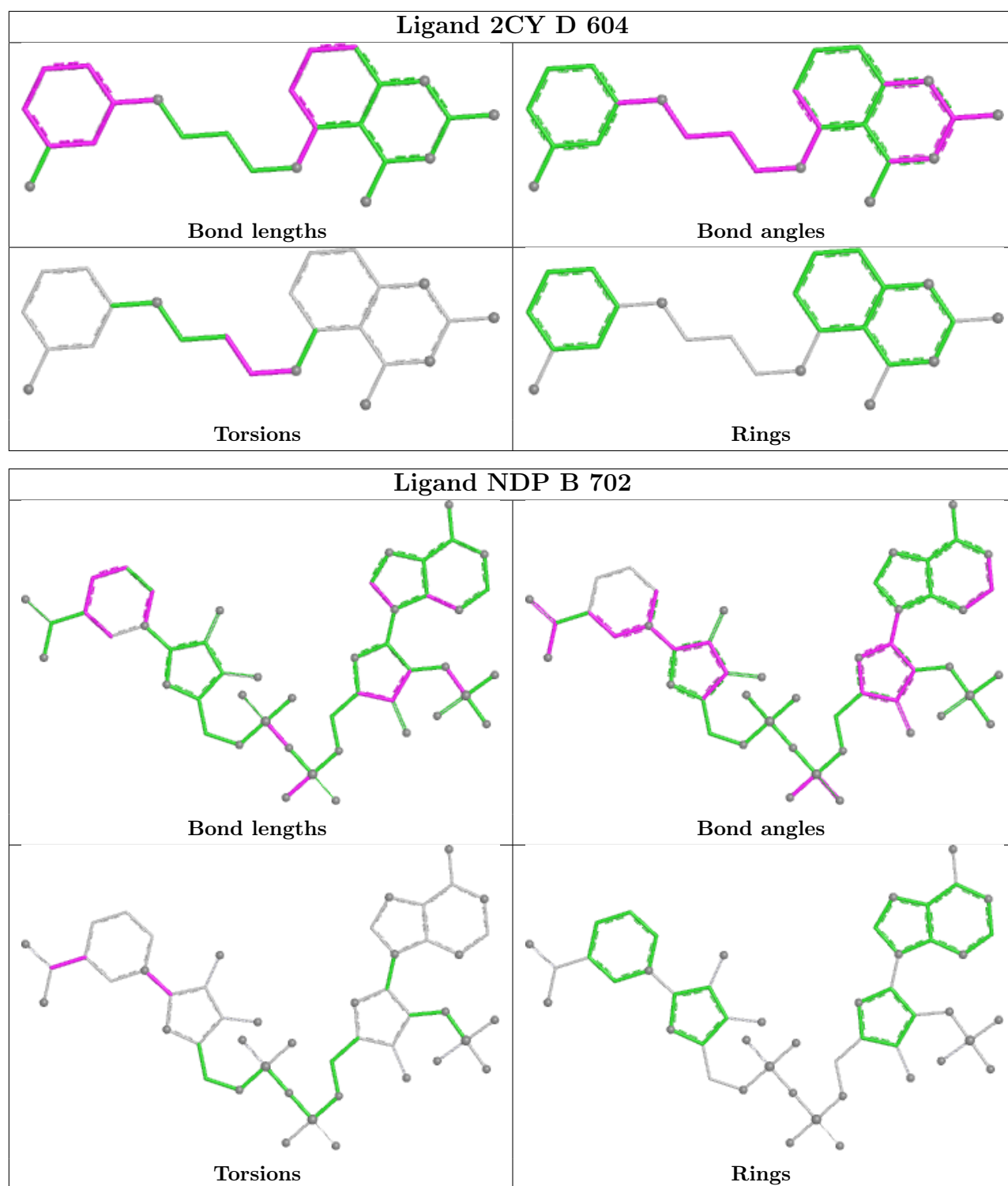
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	804	PO4	1	0
2	C	603	2CY	1	0
3	D	704	NDP	5	0
5	A	809	ACT	2	0
5	D	810	ACT	1	0
2	B	602	2CY	2	0
2	D	604	2CY	3	0
3	B	702	NDP	5	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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	518/521 (99%)	-0.21	11 (2%) 63 54	12, 26, 61, 91	0
1	B	515/521 (98%)	-0.07	16 (3%) 51 41	11, 29, 76, 91	0
1	C	516/521 (99%)	-0.26	7 (1%) 73 64	10, 26, 69, 91	0
1	D	513/521 (98%)	-0.15	13 (2%) 58 48	7, 28, 70, 91	0
All	All	2062/2084 (98%)	-0.17	47 (2%) 61 51	7, 27, 69, 91	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	SER	3.8
1	A	38	GLY	3.4
1	D	38	GLY	3.3
1	B	41	ILE	3.2
1	C	41	ILE	3.2

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](#)

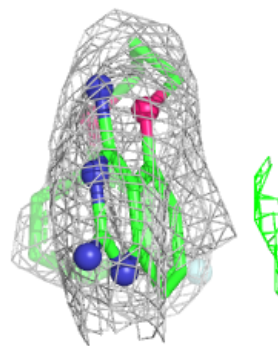
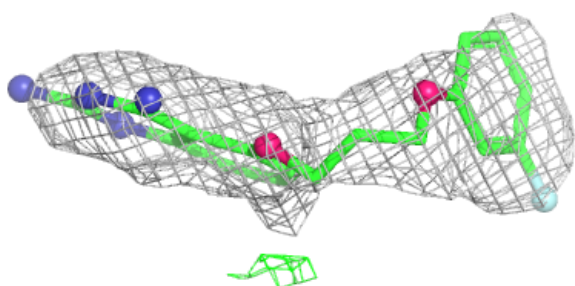
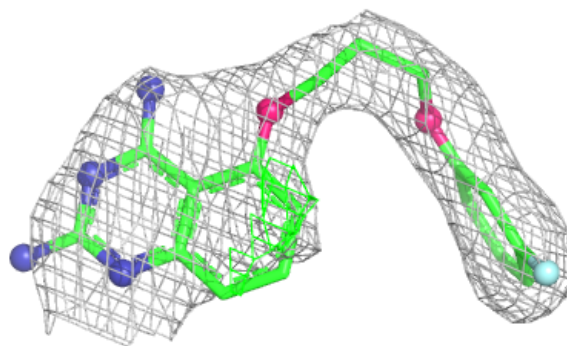
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
5	ACT	B	811	4/4	0.67	0.19	42,45,45,46	0
5	ACT	D	814	4/4	0.73	0.16	31,34,35,37	0
4	PO4	A	802	5/5	0.79	0.14	87,87,88,89	0
4	PO4	C	804	5/5	0.79	0.14	84,84,85,85	0
5	ACT	C	812	4/4	0.80	0.16	32,33,33,35	0
5	ACT	C	813	4/4	0.82	0.19	56,57,57,58	0
4	PO4	C	803	5/5	0.84	0.12	76,76,78,78	0
6	GOL	C	805	6/6	0.84	0.17	42,47,47,48	0
2	2CY	B	602	24/24	0.85	0.16	46,51,55,58	0
5	ACT	D	815	4/4	0.88	0.21	45,45,45,46	0
6	GOL	B	806	6/6	0.88	0.14	40,42,43,44	0
2	2CY	D	604	24/24	0.88	0.16	47,53,58,60	0
2	2CY	A	601	24/24	0.89	0.13	44,49,60,61	0
2	2CY	C	603	24/24	0.90	0.12	44,47,51,52	0
5	ACT	A	808	4/4	0.90	0.11	35,36,36,36	0
3	NDP	B	702	48/48	0.90	0.13	44,52,89,90	0
4	PO4	B	801	5/5	0.91	0.10	64,65,66,67	0
5	ACT	D	816	4/4	0.92	0.12	29,29,30,30	0
5	ACT	A	809	4/4	0.92	0.11	38,39,39,41	0
3	NDP	D	704	48/48	0.92	0.13	41,50,88,90	0
3	NDP	C	703	48/48	0.93	0.11	32,42,80,80	0
3	NDP	A	701	48/48	0.93	0.11	37,45,78,79	0
5	ACT	D	810	4/4	0.93	0.09	32,32,32,33	0
5	ACT	A	807	4/4	0.93	0.14	35,37,37,37	0

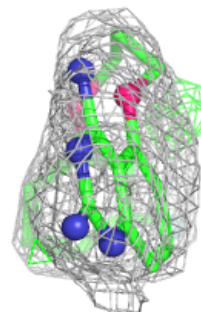
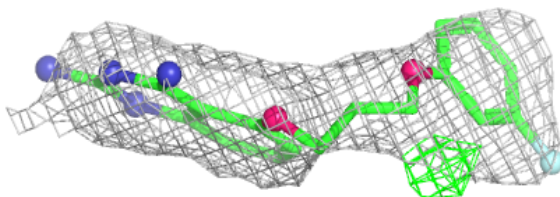
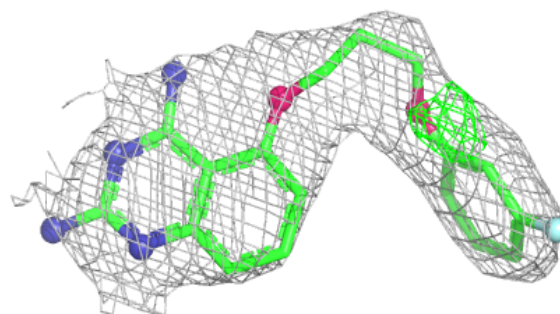
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2CY B 602:

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

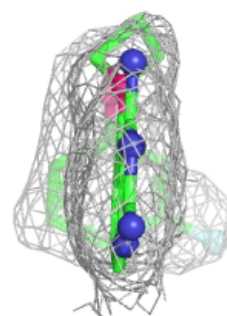
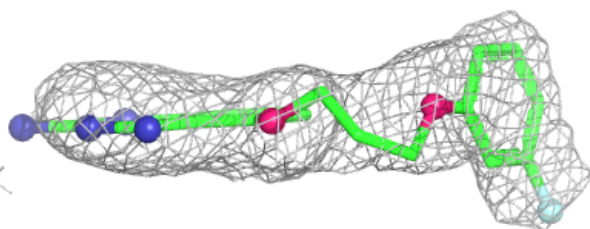
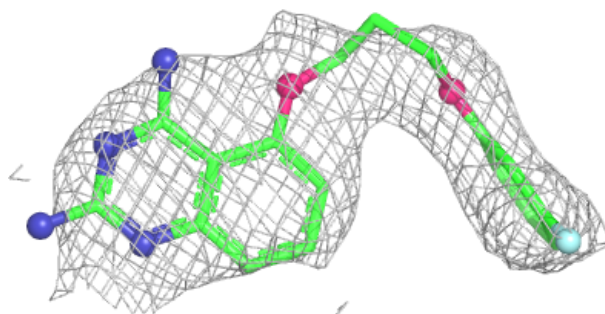
**Electron density around 2CY D 604:**

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

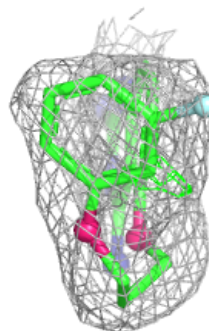
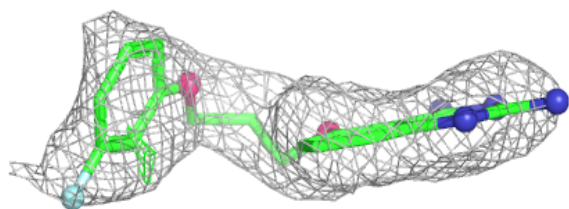
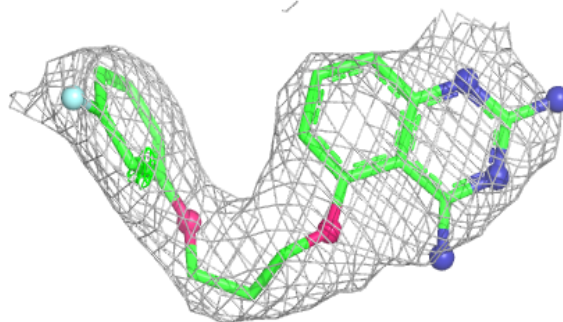


Electron density around 2CY A 601:

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

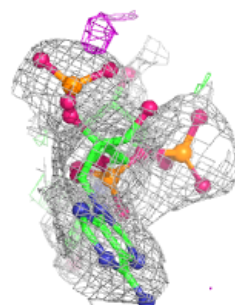
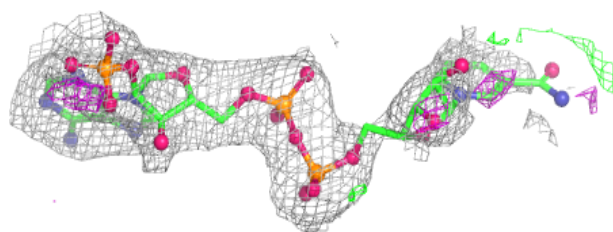
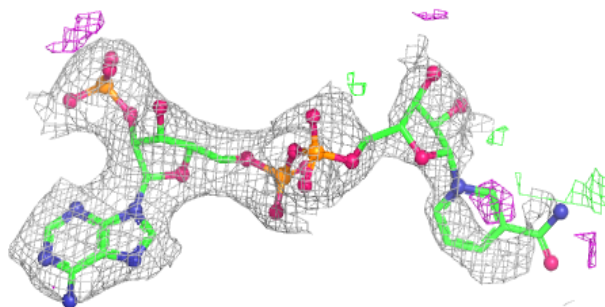
**Electron density around 2CY C 603:**

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and green (positive)

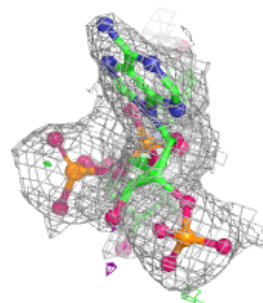
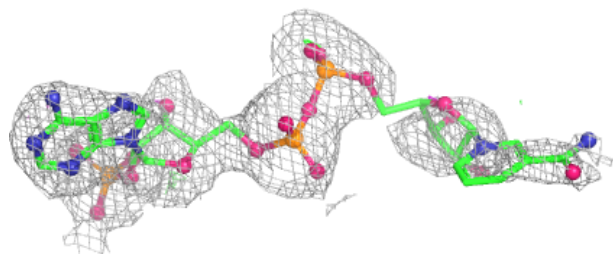
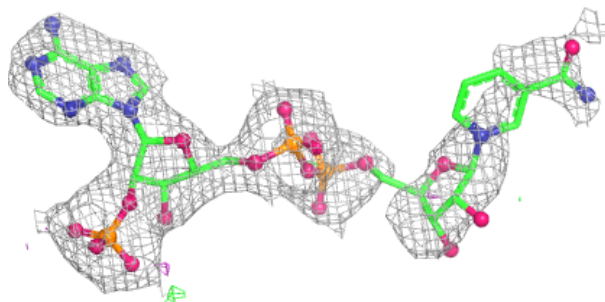


Electron density around NDP B 702:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

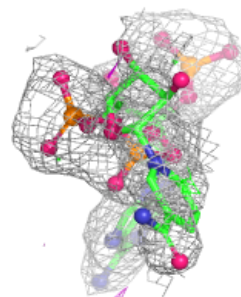
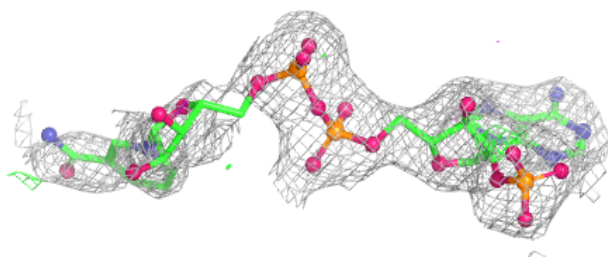
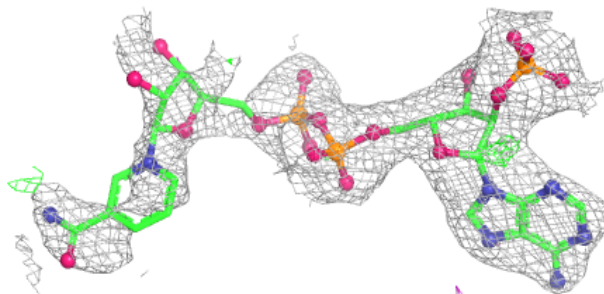
**Electron density around NDP D 704:**

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and green (positive)

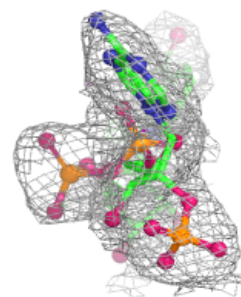
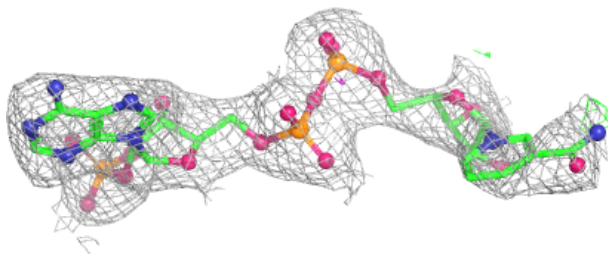
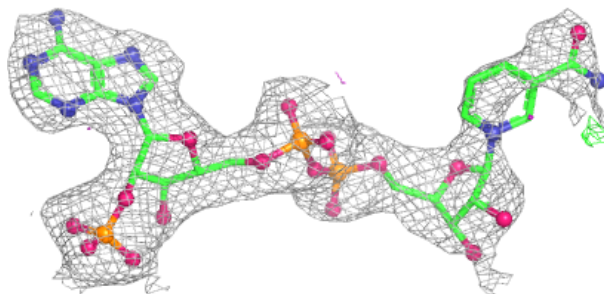


Electron density around NDP C 703:

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

**Electron density around NDP A 701:**

$2mF_o-DF_c$ (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.