



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:12 AM UTC

PDB ID : 4JQ2 / pdb_00004jq2
Title : AKR1C2 complex with sulindac
Authors : Yosaatmadja, Y.; Flanagan, J.U.; Squire, C.J.
Deposited on : 2013-03-19
Resolution : 1.75 Å(reported)

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

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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

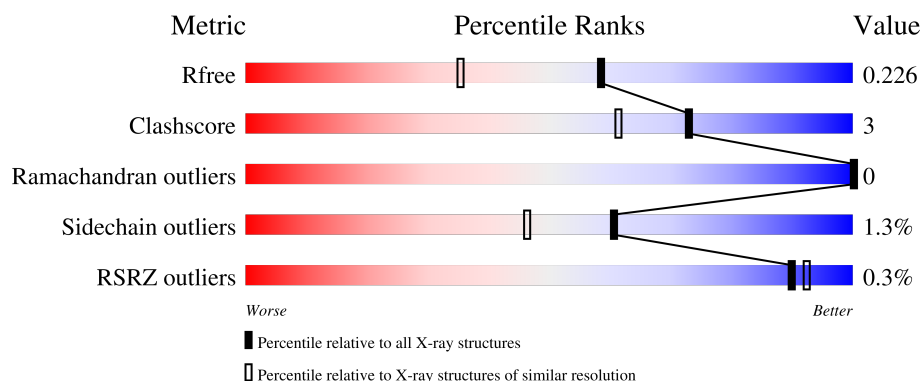
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	331	 89% 6% 5%
1	B	331	 87% 9% . .

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	EDO	B	504	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5630 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.

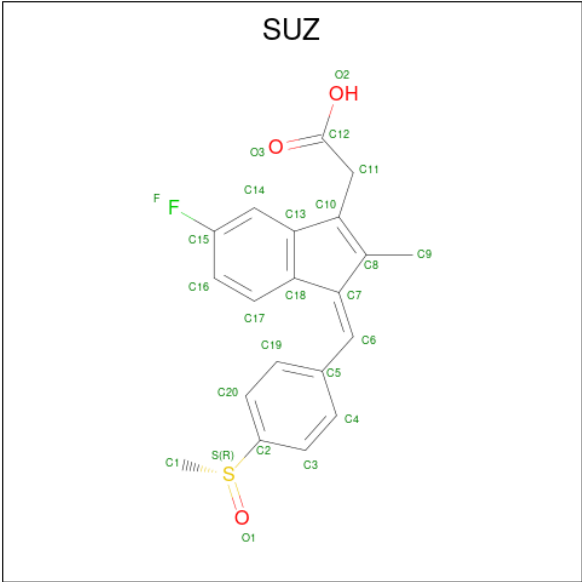
- Molecule 1 is a protein called Aldo-keto reductase family 1 member C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	5	0
			2570	1649	448	462	11			
1	B	318	Total	C	N	O	S	0	5	0
			2572	1646	449	465	12			

There are 16 discrepancies between the modelled and reference sequences:

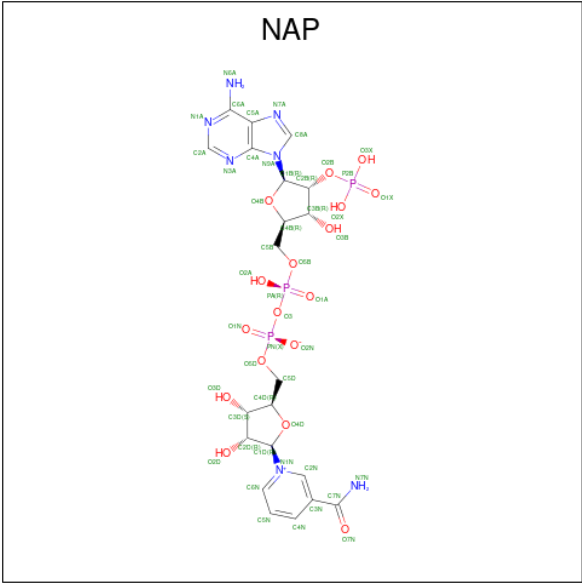
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	LEU	-	expression tag	UNP P52895
A	325	GLU	-	expression tag	UNP P52895
A	326	HIS	-	expression tag	UNP P52895
A	327	HIS	-	expression tag	UNP P52895
A	328	HIS	-	expression tag	UNP P52895
A	329	HIS	-	expression tag	UNP P52895
A	330	HIS	-	expression tag	UNP P52895
A	331	HIS	-	expression tag	UNP P52895
B	324	LEU	-	expression tag	UNP P52895
B	325	GLU	-	expression tag	UNP P52895
B	326	HIS	-	expression tag	UNP P52895
B	327	HIS	-	expression tag	UNP P52895
B	328	HIS	-	expression tag	UNP P52895
B	329	HIS	-	expression tag	UNP P52895
B	330	HIS	-	expression tag	UNP P52895
B	331	HIS	-	expression tag	UNP P52895

- Molecule 2 is [(1Z)-5-fluoro-2-methyl-1-{4-[methylsulfinyl]benzylidene}-1H-inden-3-yl]acetic acid (CCD ID: SUZ) (formula: C₂₀H₁₇FO₃S).



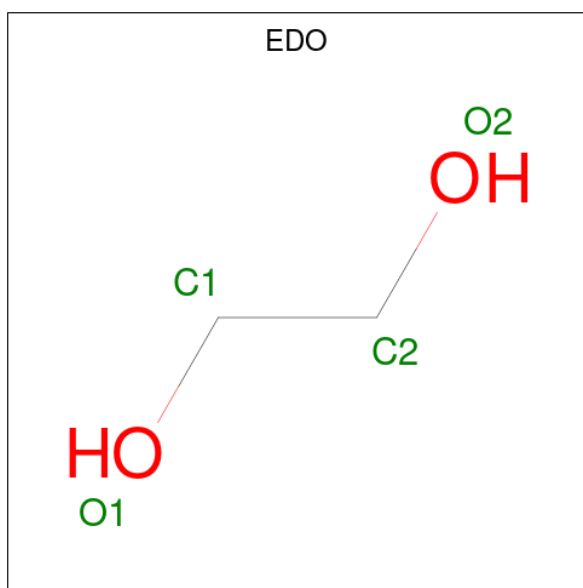
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	O	S	0	0
			25	20	1	3	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



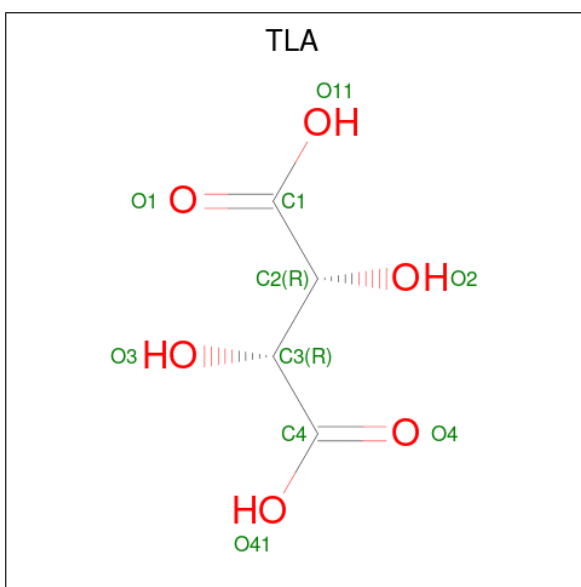
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



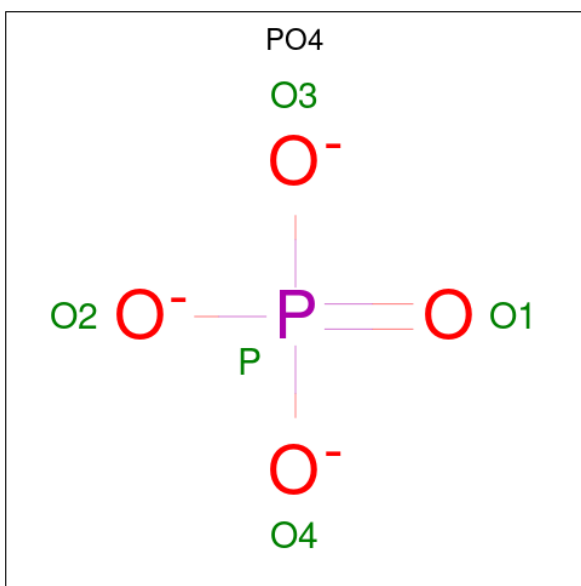
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	164	Total 164	O 164	0	0
7	B	168	Total 168	O 168	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	143.16Å 143.16Å 204.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.79 – 1.75 19.79 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.79-1.75) 98.9 (19.79-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.163 , 0.223 0.172 , 0.226	Depositor DCC
R_{free} test set	4026 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5630	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: PO4, TLA, SUZ, NAP, EDO

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	1.11	2/2630 (0.1%)	1.01	1/3563 (0.0%)
1	B	1.19	8/2633 (0.3%)	1.14	8/3569 (0.2%)
All	All	1.15	10/5263 (0.2%)	1.08	9/7132 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	MET	N-CA	5.69	1.53	1.46
1	B	152	GLU	N-CA	-5.59	1.39	1.46
1	A	303	VAL	CA-CB	5.57	1.59	1.53
1	B	141	THR	C-O	-5.43	1.17	1.24
1	B	316	ASN	CG-ND2	-5.37	1.22	1.33
1	B	316	ASN	CG-OD1	5.21	1.33	1.23
1	B	18	VAL	CA-CB	5.17	1.60	1.54
1	A	171	ARG	C-O	5.12	1.29	1.24
1	B	97	PRO	C-O	-5.03	1.17	1.24
1	B	9	LYS	C-O	-5.02	1.18	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	GLY	CA-C-N	-8.71	111.41	120.38
1	B	313	GLY	C-N-CA	-8.71	111.41	120.38
1	B	118	PHE	CA-C-N	-5.84	113.73	120.04
1	B	118	PHE	C-N-CA	-5.84	113.73	120.04
1	B	147	THR	N-CA-C	-5.53	105.33	111.36
1	A	211	ILE	N-CA-C	-5.13	100.99	108.17
1	B	251	THR	CA-C-N	-5.11	113.77	119.19
1	B	251	THR	C-N-CA	-5.11	113.77	119.19
1	B	123	LYS	N-CA-C	5.04	115.40	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2570	0	2588	17	0
1	B	2572	0	2569	15	0
2	A	25	0	16	1	0
3	A	48	0	25	2	0
3	B	48	0	25	3	0
4	A	8	0	12	0	0
4	B	12	0	18	5	0
5	A	10	0	4	0	0
6	B	5	0	0	0	0
7	A	164	0	0	6	0
7	B	168	0	0	1	0
All	All	5630	0	5257	34	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 (34) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG11	7:A:661:HOH:O	1.67	0.90
1:B:142:VAL:H	4:B:504:EDO:H12	1.58	0.68
1:A:4:LYS:N	7:A:584:HOH:O	2.29	0.66
1:B:316:ASN:OD1	4:B:504:EDO:H21	2.01	0.60
1:B:142:VAL:H	4:B:504:EDO:C1	2.16	0.58
1:A:200:ARG:HD2	1:A:204:ASP:OD2	2.04	0.58
1:B:43:GLU:HG2	1:B:68:LYS:HE3	1.86	0.58
4:B:504:EDO:H11	7:B:687:HOH:O	2.08	0.53
1:B:270:LYS:O	3:B:501:NAP:H8A	2.08	0.53
1:A:301:ARG:HG3	1:A:303:VAL:HG23	1.92	0.52
1:A:200:ARG:O	1:A:200:ARG:HD3	2.10	0.51
1:A:8:VAL:CG1	7:A:661:HOH:O	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66[B]:ARG:HD3	1:A:107:GLN:O	2.11	0.50
1:B:270:LYS:HE2	1:B:272:TYR:CD1	2.49	0.48
1:B:39:LYS:HE3	1:B:67:SER:OG	2.16	0.46
1:A:248:HIS:HE1	7:A:611:HOH:O	1.98	0.46
1:A:86:TRP:HA	1:A:86:TRP:CE3	2.50	0.46
1:A:94:LEU:C	1:A:97:PRO:HD2	2.41	0.46
1:B:142:VAL:N	4:B:504:EDO:H12	2.29	0.45
1:B:17:PRO:HB2	1:B:48[A]:HIS:HB2	1.99	0.45
1:A:149:GLU:HG3	1:A:179:LYS:HE3	1.99	0.45
1:B:276:ARG:HD2	3:B:501:NAP:C4A	2.47	0.45
2:A:401:SUZ:C12	3:A:402:NAP:C4N	2.95	0.44
1:A:179:LYS:NZ	7:A:647:HOH:O	2.50	0.44
1:A:133:GLU:HB2	7:A:600:HOH:O	2.17	0.43
1:A:270:LYS:O	3:A:402:NAP:H8A	2.17	0.43
1:B:270:LYS:C	1:B:270:LYS:HD3	2.44	0.43
1:A:8:VAL:HG13	1:A:18:VAL:CG1	2.48	0.43
1:B:71:ASP:OD1	1:B:71:ASP:C	2.61	0.43
1:B:9:LYS:HE2	1:B:13:GLY:HA2	2.00	0.42
1:A:92:PRO:HG3	1:A:146:ALA:HB1	2.01	0.42
1:A:8:VAL:HG13	1:A:18:VAL:HG12	2.01	0.41
1:B:22:GLY:HA3	3:B:501:NAP:H4D	2.02	0.40
1:B:43:GLU:HG2	1:B:68:LYS:CE	2.51	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	319/331 (96%)	311 (98%)	8 (2%)	0	100	100
1	B	321/331 (97%)	312 (97%)	9 (3%)	0	100	100
All	All	640/662 (97%)	623 (97%)	17 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	281/293 (96%)	280 (100%)	1 (0%)	84	80
1	B	281/293 (96%)	275 (98%)	6 (2%)	47	27
All	All	562/586 (96%)	555 (99%)	7 (1%)	61	49

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	B	73	SER
1	B	77	GLU
1	B	222	HIS
1	B	275	GLN
1	B	302	ASN
1	B	320	SER

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

Mol	Chain	Res	Type
1	A	231	ASN
1	B	56	ASN
1	B	167	ASN
1	B	275	GLN
1	B	282	GLN

5.3.3 RNA ⓘ

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](#)

10 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$
3	NAP	B	501	-	50,52,52	2.64	18 (36%)	71,80,80	2.54	19 (26%)
3	NAP	A	402	-	50,52,52	2.62	13 (26%)	71,80,80	2.24	22 (30%)
2	SUZ	A	401	-	25,27,27	2.15	6 (24%)	36,39,39	2.01	8 (22%)
4	EDO	B	503	-	3,3,3	0.78	0	2,2,2	0.22	0
6	PO4	B	505	-	4,4,4	0.77	0	6,6,6	0.80	0
4	EDO	A	404	-	3,3,3	0.70	0	2,2,2	0.29	0
4	EDO	B	504	-	3,3,3	0.44	0	2,2,2	0.29	0
4	EDO	B	502	-	3,3,3	0.60	0	2,2,2	0.34	0
5	TLA	A	405	-	9,9,9	1.35	2 (22%)	12,12,12	1.51	4 (33%)
4	EDO	A	403	-	3,3,3	0.79	0	2,2,2	0.49	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
3	NAP	B	501	-	-	8/35/67/67	0/5/5/5
3	NAP	A	402	-	-	5/35/67/67	0/5/5/5
2	SUZ	A	401	-	-	6/12/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	A	404	-	-	0/1/1/1	-
4	EDO	B	504	-	-	1/1/1/1	-
4	EDO	B	502	-	-	0/1/1/1	-
5	TLA	A	405	-	-	0/12/12/12	-
4	EDO	A	403	-	-	0/1/1/1	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NAP	PN-O3	9.66	1.69	1.59
3	B	501	NAP	PA-O3	9.06	1.69	1.59
3	A	402	NAP	C3N-C7N	-6.46	1.41	1.50
3	B	501	NAP	C3N-C7N	-6.10	1.41	1.50
3	B	501	NAP	O4D-C1D	5.65	1.48	1.40
2	A	401	SUZ	C13-C10	-5.24	1.34	1.44
3	A	402	NAP	PA-O3	5.02	1.64	1.59
3	A	402	NAP	C2A-N3A	4.90	1.42	1.33
3	B	501	NAP	PN-O3	4.89	1.64	1.59
3	A	402	NAP	P2B-O2B	4.68	1.67	1.59
2	A	401	SUZ	C11-C12	4.67	1.58	1.51
3	A	402	NAP	C2A-N1A	4.60	1.42	1.33
3	B	501	NAP	C2A-N1A	4.45	1.41	1.33
3	B	501	NAP	PA-O5B	4.07	1.75	1.59
3	B	501	NAP	C6N-N1N	3.95	1.44	1.35
3	A	402	NAP	O4D-C1D	3.93	1.46	1.40
2	A	401	SUZ	C18-C7	-3.89	1.38	1.45
3	A	402	NAP	C6N-N1N	3.81	1.44	1.35
2	A	401	SUZ	C5-C6	-3.77	1.39	1.46
3	B	501	NAP	C7N-N7N	3.54	1.39	1.33
3	B	501	NAP	C2N-N1N	3.36	1.38	1.35
3	B	501	NAP	C5A-N7A	-3.33	1.33	1.39
3	B	501	NAP	C2A-N3A	3.24	1.39	1.33
3	A	402	NAP	C2N-N1N	3.05	1.38	1.35
3	B	501	NAP	PN-O5D	3.02	1.71	1.59
3	A	402	NAP	C4N-C3N	2.82	1.43	1.39
2	A	401	SUZ	F-C15	-2.73	1.29	1.36
3	B	501	NAP	C1B-N9A	2.62	1.53	1.46
2	A	401	SUZ	C17-C18	-2.59	1.36	1.39
3	B	501	NAP	C5B-C4B	2.58	1.59	1.51
3	A	402	NAP	PA-O5B	2.56	1.69	1.59
3	A	402	NAP	P2B-O2X	-2.55	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	TLA	O1-C1	2.53	1.29	1.22
3	B	501	NAP	C5A-C6A	-2.42	1.34	1.41
5	A	405	TLA	O4-C4	2.19	1.28	1.22
3	B	501	NAP	C8A-N9A	-2.13	1.33	1.37
3	A	402	NAP	C2D-C3D	2.08	1.59	1.53
3	B	501	NAP	C4N-C3N	2.06	1.42	1.39
3	B	501	NAP	P2B-O2X	-2.03	1.47	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAP	O2N-PN-O3	-10.71	78.33	107.27
3	A	402	NAP	O2N-PN-O3	-8.54	84.20	107.27
3	B	501	NAP	N3A-C2A-N1A	-7.80	116.77	128.58
2	A	401	SUZ	C1-S-C2	6.45	115.44	97.82
3	A	402	NAP	O3-PN-O1N	-6.33	91.67	110.70
3	B	501	NAP	O2A-PA-O5B	-5.92	80.72	107.57
3	B	501	NAP	C4D-O4D-C1D	-5.36	105.02	109.92
3	A	402	NAP	N3A-C2A-N1A	-5.14	120.80	128.58
2	A	401	SUZ	C18-C13-C10	-4.87	105.50	109.07
2	A	401	SUZ	C5-C6-C7	-4.83	120.16	129.68
3	B	501	NAP	O2A-PA-O3	4.81	120.27	107.27
3	A	402	NAP	C5A-C4A-N3A	-4.31	120.78	126.72
3	A	402	NAP	O2A-PA-O5B	-4.17	88.67	107.57
3	A	402	NAP	O2A-PA-O3	4.01	118.10	107.27
3	B	501	NAP	C5A-C4A-N3A	-3.89	121.36	126.72
3	B	501	NAP	O5B-PA-O1A	-3.81	93.85	108.94
3	B	501	NAP	O3-PN-O1N	-3.78	99.32	110.70
3	B	501	NAP	O2N-PN-O5D	3.78	124.69	107.57
3	A	402	NAP	C4A-C5A-N7A	-3.48	106.61	110.58
3	B	501	NAP	O2N-PN-O1N	3.35	128.03	112.44
3	B	501	NAP	O2A-PA-O1A	3.31	127.85	112.44
3	A	402	NAP	O2N-PN-O1N	3.19	127.27	112.44
3	A	402	NAP	N9A-C8A-N7A	-3.09	109.56	113.94
3	B	501	NAP	C2A-N3A-C4A	3.06	119.31	111.83
3	B	501	NAP	C2D-C3D-C4D	-3.00	96.80	102.61
2	A	401	SUZ	C16-C15-C14	-3.00	119.27	123.23
3	A	402	NAP	C5A-N7A-C8A	2.99	108.15	103.45
3	A	402	NAP	C6A-C5A-C4A	2.97	121.23	117.18
3	B	501	NAP	C6A-C5A-C4A	2.97	121.23	117.18
3	B	501	NAP	N9A-C8A-N7A	-2.93	109.78	113.94
3	A	402	NAP	O4B-C1B-N9A	-2.81	102.68	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	NAP	C5A-N7A-C8A	2.75	107.77	103.45
3	A	402	NAP	C2A-N3A-C4A	2.75	118.54	111.83
3	A	402	NAP	O2A-PA-O1A	2.74	125.20	112.44
3	B	501	NAP	C4A-C5A-N7A	-2.62	107.58	110.58
2	A	401	SUZ	O1-S-C1	2.55	110.07	105.52
3	B	501	NAP	C5A-C4A-N9A	2.53	108.57	105.81
5	A	405	TLA	O41-C4-C3	2.52	120.33	113.31
3	A	402	NAP	C2B-C1B-N9A	2.50	117.86	113.75
2	A	401	SUZ	C13-C10-C8	2.48	110.97	109.22
3	A	402	NAP	C2B-C3B-C4B	2.41	107.17	101.99
3	A	402	NAP	C2D-C3D-C4D	-2.38	98.00	102.61
3	A	402	NAP	O5B-PA-O1A	-2.38	99.51	108.94
3	A	402	NAP	O2N-PN-O5D	2.31	118.05	107.57
3	A	402	NAP	C5A-C4A-N9A	2.31	108.33	105.81
2	A	401	SUZ	C18-C7-C8	2.30	108.19	106.07
3	A	402	NAP	N3A-C4A-N9A	2.19	130.89	127.17
3	B	501	NAP	C2B-C3B-C4B	2.13	106.57	101.99
5	A	405	TLA	O4-C4-C3	-2.13	115.95	121.62
3	A	402	NAP	C5A-C6A-N6A	-2.12	118.04	123.29
5	A	405	TLA	O3-C3-C2	-2.09	105.91	110.17
2	A	401	SUZ	C11-C10-C8	-2.06	125.43	128.04
5	A	405	TLA	O2-C2-C1	-2.04	106.34	110.69

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SUZ	C20-C2-S-O1
2	A	401	SUZ	C20-C2-S-C1
2	A	401	SUZ	C3-C2-S-O1
2	A	401	SUZ	C3-C2-S-C1
3	B	501	NAP	PA-O3-PN-O5D
3	B	501	NAP	C5D-O5D-PN-O3
3	B	501	NAP	O4D-C4D-C5D-O5D
2	A	401	SUZ	C4-C5-C6-C7
2	A	401	SUZ	C19-C5-C6-C7
4	B	504	EDO	O1-C1-C2-O2
3	A	402	NAP	O4B-C4B-C5B-O5B
3	B	501	NAP	C3D-C4D-C5D-O5D
3	A	402	NAP	PA-O3-PN-O5D
3	B	501	NAP	C5D-O5D-PN-O1N
3	A	402	NAP	C4D-C5D-O5D-PN

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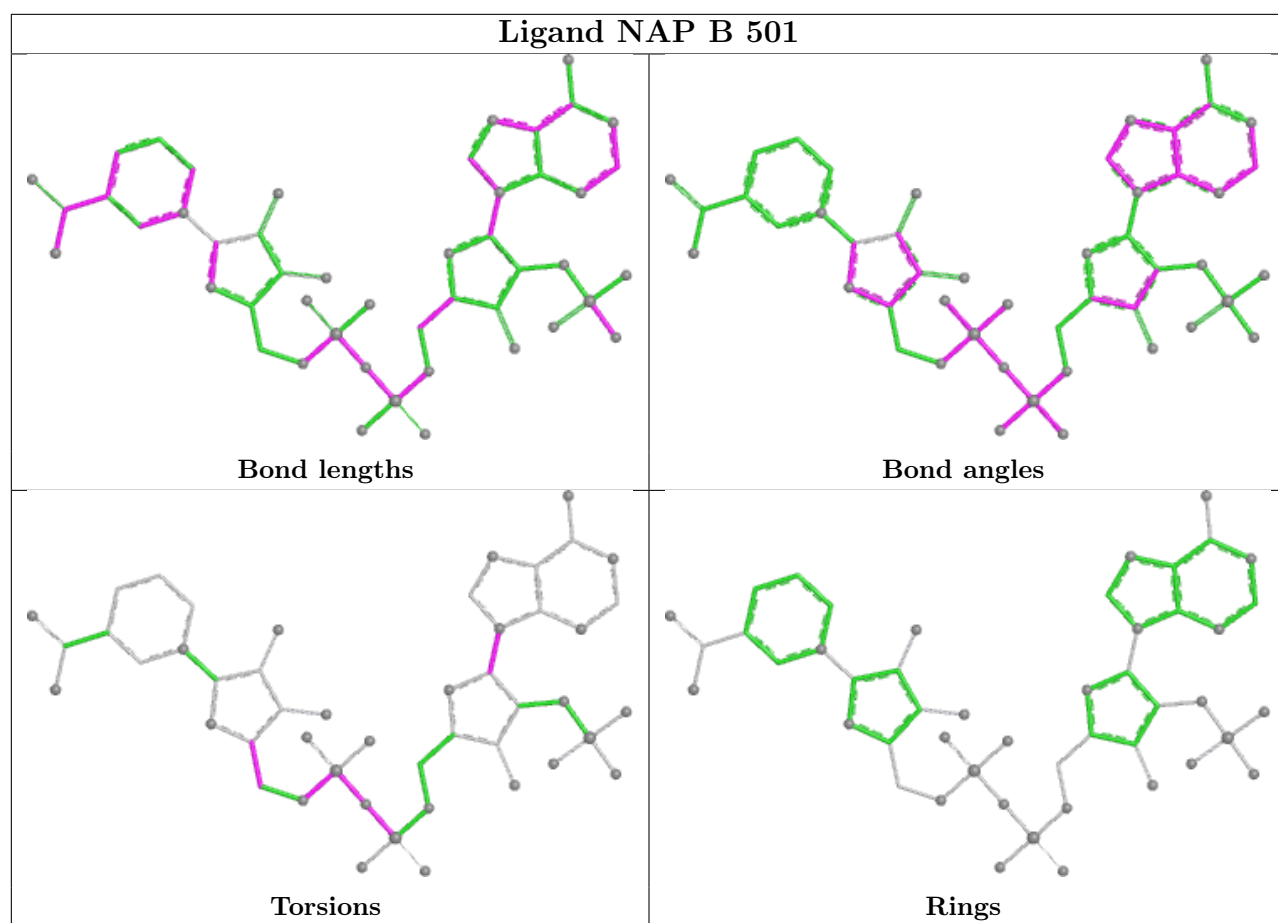
Mol	Chain	Res	Type	Atoms
3	B	501	NAP	C2B-C1B-N9A-C8A
3	B	501	NAP	O4B-C1B-N9A-C8A
3	A	402	NAP	PA-O3-PN-O2N
3	B	501	NAP	PN-O3-PA-O2A
3	A	402	NAP	C3B-C4B-C5B-O5B

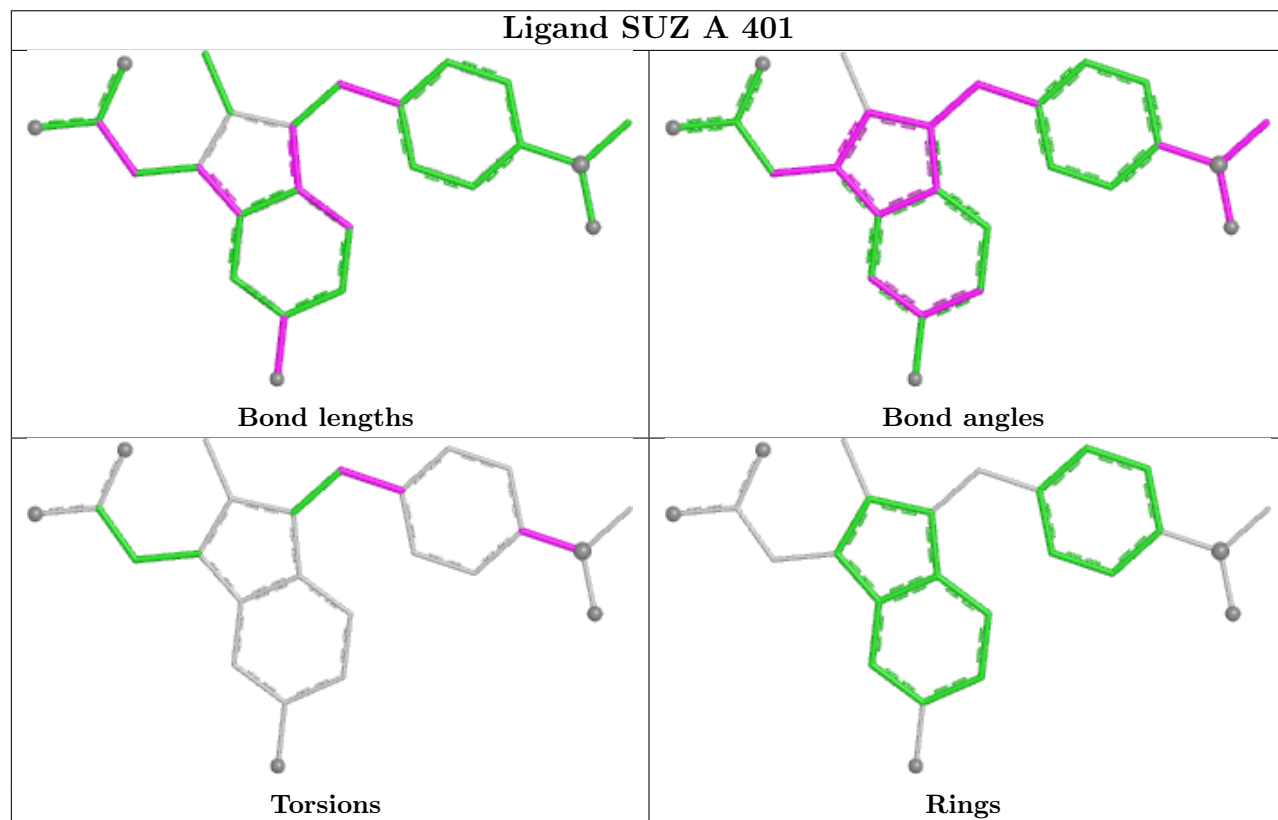
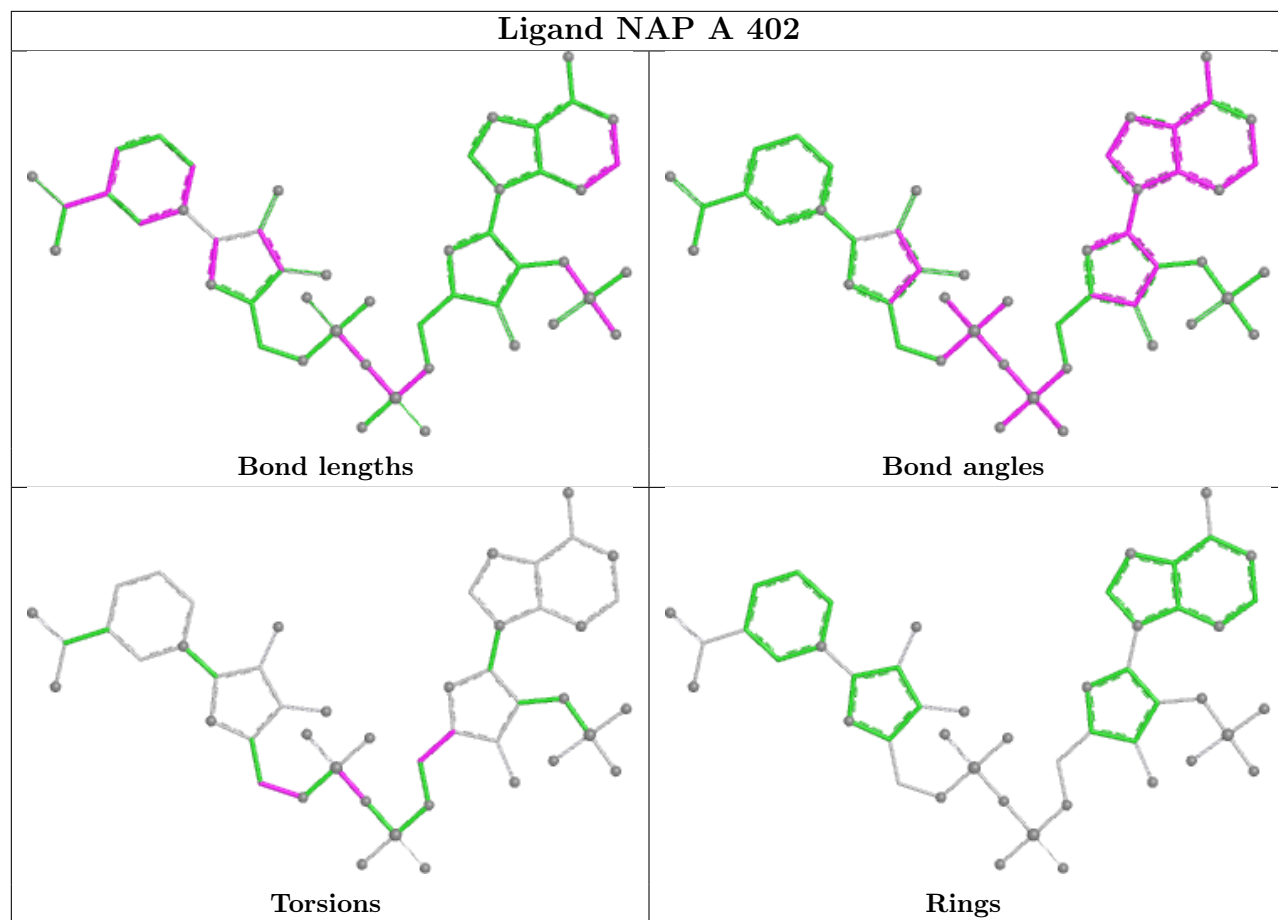
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	NAP	3	0
3	A	402	NAP	2	0
2	A	401	SUZ	1	0
4	B	504	EDO	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 [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	316/331 (95%)	-0.40	0	100 100	12, 32, 50, 71	18 (5%)
1	B	318/331 (96%)	-0.26	2 (0%)	85 89	11, 31, 67, 88	13 (4%)
All	All	634/662 (95%)	-0.33	2 (0%)	90 92	11, 31, 60, 88	31 (4%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	HIS	2.4
1	B	228	VAL	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(Å ²)	Q < 0.9
4	EDO	A	404	4/4	0.81	0.18	54,56,66,73	0
2	SUZ	A	401	25/25	0.90	0.10	28,39,61,65	25
5	TLA	A	405	10/10	0.90	0.09	43,51,57,67	0

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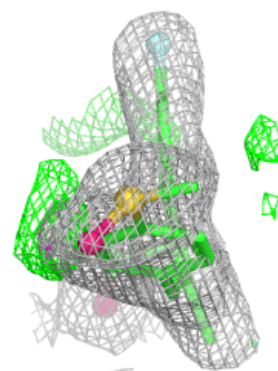
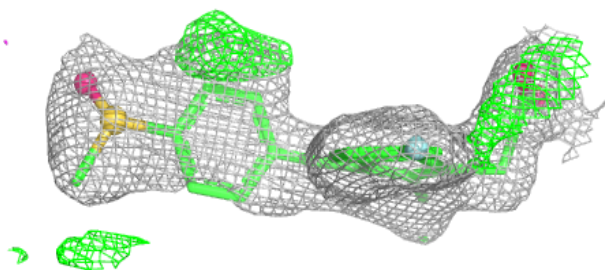
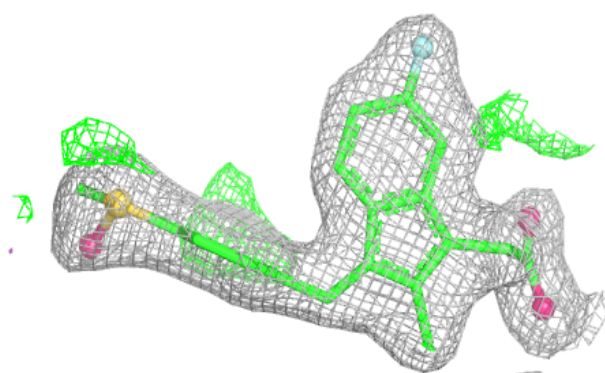
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	503	4/4	0.91	0.11	38,45,47,50	0
6	PO4	B	505	5/5	0.91	0.07	55,57,65,75	5
3	NAP	B	501	48/48	0.94	0.07	28,59,76,82	0
4	EDO	B	504	4/4	0.94	0.18	29,37,39,40	0
4	EDO	B	502	4/4	0.95	0.08	34,36,36,40	0
3	NAP	A	402	48/48	0.98	0.05	25,35,43,58	0
4	EDO	A	403	4/4	0.98	0.06	23,25,29,30	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.

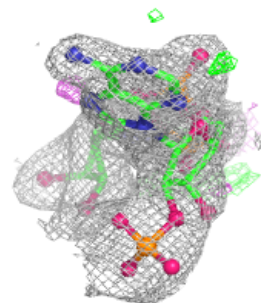
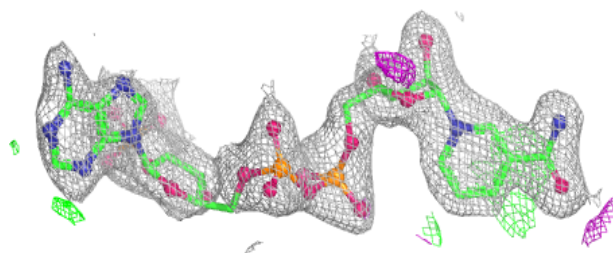
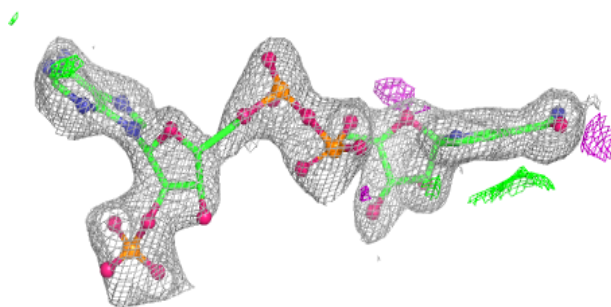
Electron density around SUZ A 401:

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

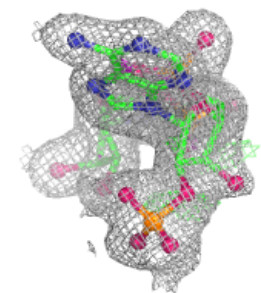
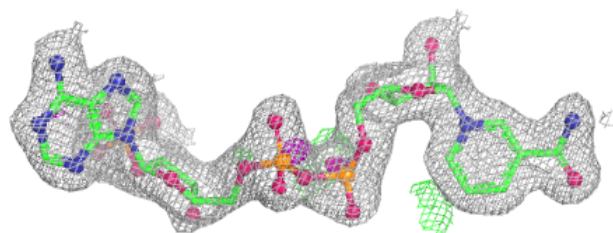
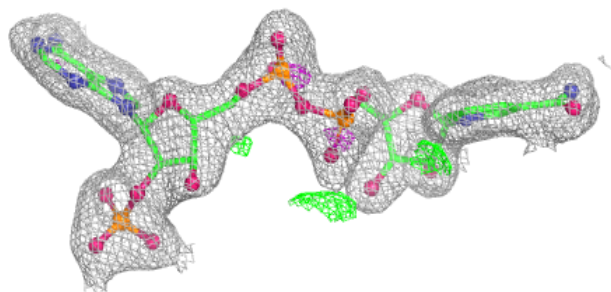


Electron density around NAP B 501:

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

**Electron density around NAP A 402:**

$2mF_o-DF_c$ (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.