



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:55 AM UTC

PDB ID : 5N5S / pdb_00005n5s
Title : Crystal structure of aldehyde dehydrogenase 21 (ALDH21) from
Physcomitrella patens in complex with NADP+
Authors : Kopecny, D.; Vigouroux, A.; Briozzo, P.; Morera, S.
Deposited on : 2017-02-14
Resolution : 2.30 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

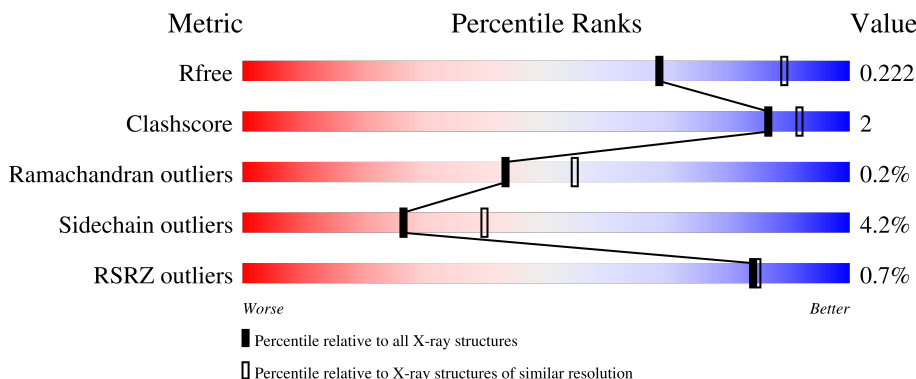
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	515	
1	B	515	
1	C	515	
1	D	515	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15245 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 Aldehyde dehydrogenase 21 (ALDH21).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3713	2374	626	695	18			
1	B	481	Total	C	N	O	S	0	0	0
			3720	2379	627	696	18			
1	C	481	Total	C	N	O	S	0	0	0
			3720	2379	627	696	18			
1	D	480	Total	C	N	O	S	0	0	0
			3713	2374	626	695	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A9SS48
A	-16	GLY	-	expression tag	UNP A9SS48
A	-15	SER	-	expression tag	UNP A9SS48
A	-14	SER	-	expression tag	UNP A9SS48
A	-13	HIS	-	expression tag	UNP A9SS48
A	-12	HIS	-	expression tag	UNP A9SS48
A	-11	HIS	-	expression tag	UNP A9SS48
A	-10	HIS	-	expression tag	UNP A9SS48
A	-9	HIS	-	expression tag	UNP A9SS48
A	-8	HIS	-	expression tag	UNP A9SS48
A	-7	SER	-	expression tag	UNP A9SS48
A	-6	GLN	-	expression tag	UNP A9SS48
A	-5	ASP	-	expression tag	UNP A9SS48
A	-4	PRO	-	expression tag	UNP A9SS48
A	-3	ASN	-	expression tag	UNP A9SS48
A	-2	SER	-	expression tag	UNP A9SS48
A	-1	SER	-	expression tag	UNP A9SS48
A	0	SER	-	expression tag	UNP A9SS48
B	-17	MET	-	initiating methionine	UNP A9SS48
B	-16	GLY	-	expression tag	UNP A9SS48
B	-15	SER	-	expression tag	UNP A9SS48

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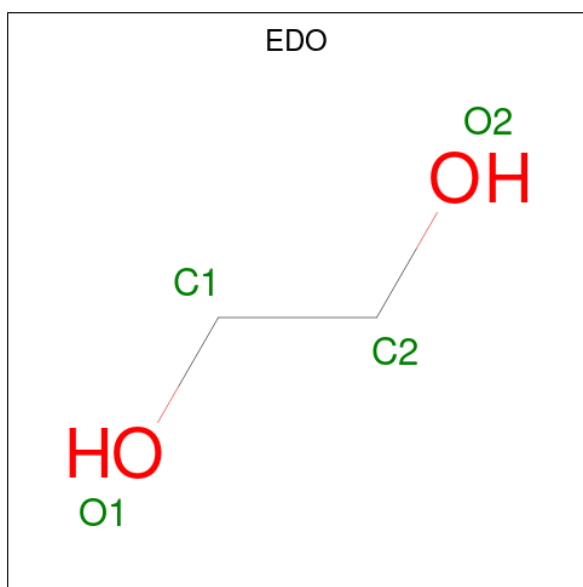
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	SER	-	expression tag	UNP A9SS48
B	-13	HIS	-	expression tag	UNP A9SS48
B	-12	HIS	-	expression tag	UNP A9SS48
B	-11	HIS	-	expression tag	UNP A9SS48
B	-10	HIS	-	expression tag	UNP A9SS48
B	-9	HIS	-	expression tag	UNP A9SS48
B	-8	HIS	-	expression tag	UNP A9SS48
B	-7	SER	-	expression tag	UNP A9SS48
B	-6	GLN	-	expression tag	UNP A9SS48
B	-5	ASP	-	expression tag	UNP A9SS48
B	-4	PRO	-	expression tag	UNP A9SS48
B	-3	ASN	-	expression tag	UNP A9SS48
B	-2	SER	-	expression tag	UNP A9SS48
B	-1	SER	-	expression tag	UNP A9SS48
B	0	SER	-	expression tag	UNP A9SS48
C	-17	MET	-	initiating methionine	UNP A9SS48
C	-16	GLY	-	expression tag	UNP A9SS48
C	-15	SER	-	expression tag	UNP A9SS48
C	-14	SER	-	expression tag	UNP A9SS48
C	-13	HIS	-	expression tag	UNP A9SS48
C	-12	HIS	-	expression tag	UNP A9SS48
C	-11	HIS	-	expression tag	UNP A9SS48
C	-10	HIS	-	expression tag	UNP A9SS48
C	-9	HIS	-	expression tag	UNP A9SS48
C	-8	HIS	-	expression tag	UNP A9SS48
C	-7	SER	-	expression tag	UNP A9SS48
C	-6	GLN	-	expression tag	UNP A9SS48
C	-5	ASP	-	expression tag	UNP A9SS48
C	-4	PRO	-	expression tag	UNP A9SS48
C	-3	ASN	-	expression tag	UNP A9SS48
C	-2	SER	-	expression tag	UNP A9SS48
C	-1	SER	-	expression tag	UNP A9SS48
C	0	SER	-	expression tag	UNP A9SS48
D	-17	MET	-	initiating methionine	UNP A9SS48
D	-16	GLY	-	expression tag	UNP A9SS48
D	-15	SER	-	expression tag	UNP A9SS48
D	-14	SER	-	expression tag	UNP A9SS48
D	-13	HIS	-	expression tag	UNP A9SS48
D	-12	HIS	-	expression tag	UNP A9SS48
D	-11	HIS	-	expression tag	UNP A9SS48
D	-10	HIS	-	expression tag	UNP A9SS48
D	-9	HIS	-	expression tag	UNP A9SS48

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	expression tag	UNP A9SS48
D	-7	SER	-	expression tag	UNP A9SS48
D	-6	GLN	-	expression tag	UNP A9SS48
D	-5	ASP	-	expression tag	UNP A9SS48
D	-4	PRO	-	expression tag	UNP A9SS48
D	-3	ASN	-	expression tag	UNP A9SS48
D	-2	SER	-	expression tag	UNP A9SS48
D	-1	SER	-	expression tag	UNP A9SS48
D	0	SER	-	expression tag	UNP A9SS48

- # NAP

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

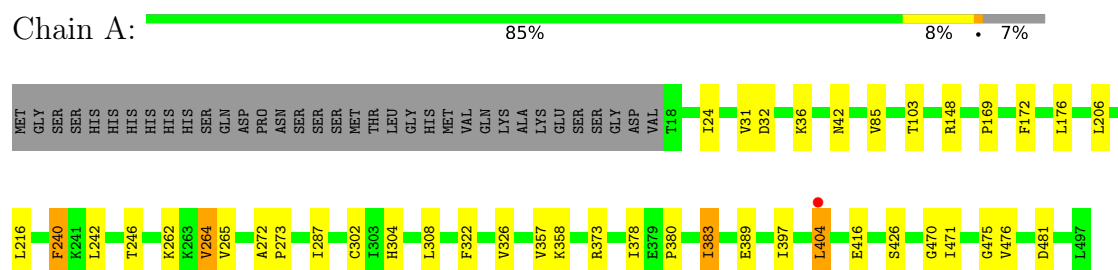
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		
4	B	42	Total	O	0	0
			42	42		
4	C	37	Total	O	0	0
			37	37		
4	D	31	Total	O	0	0
			31	31		

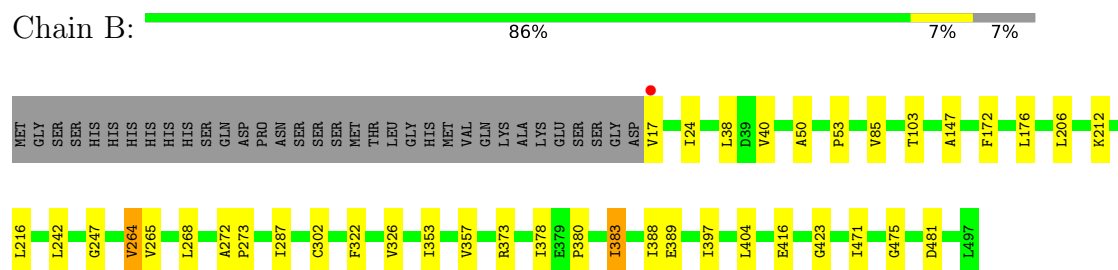
3 Residue-property plots

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.

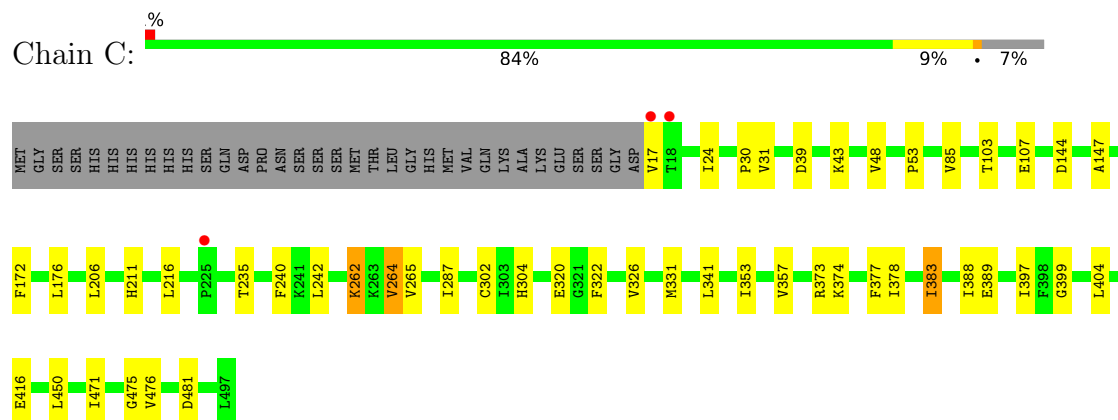
- Molecule 1: Aldehyde dehydrogenase 21 (ALDH21)



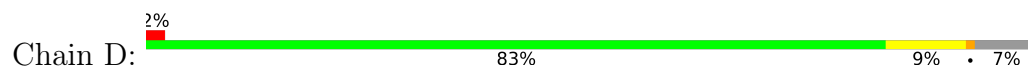
- Molecule 1: Aldehyde dehydrogenase 21 (ALDH21)

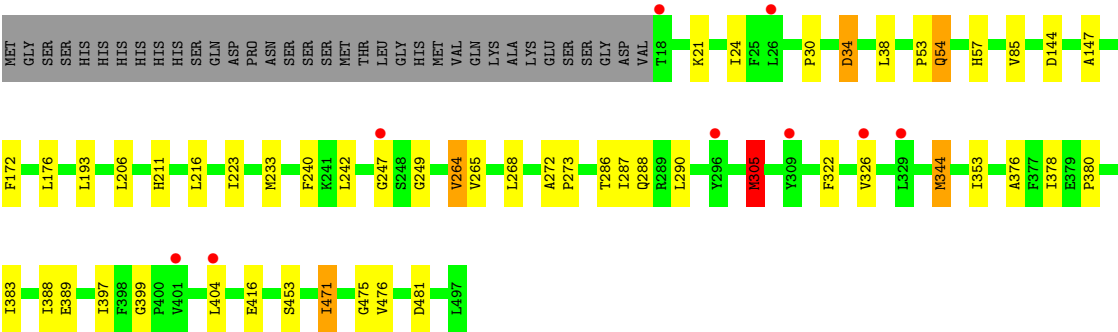


- Molecule 1: Aldehyde dehydrogenase 21 (ALDH21)



- Molecule 1: Aldehyde dehydrogenase 21 (ALDH21)





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	89.38Å 165.28Å 138.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.13 – 2.30 46.13 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.13-2.30) 99.9 (46.13-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.183 , 0.207 0.201 , 0.222	Depositor DCC
R_{free} test set	4579 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.2	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	0.96	EDS
Total number of atoms	15245	wwPDB-VP
Average B, all atoms (Å ²)	83.0	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 32.17 % 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 9.8245e-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: EDO, NAP

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	0.78	0/3789	1.33	8/5123 (0.2%)
1	B	0.78	0/3796	1.34	5/5133 (0.1%)
1	C	0.77	0/3796	1.35	9/5133 (0.2%)
1	D	0.77	1/3789 (0.0%)	1.34	6/5123 (0.1%)
All	All	0.78	1/15170 (0.0%)	1.34	28/20512 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	305	MET	SD-CE	-5.40	1.66	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	34	ASP	CA-CB-CG	7.43	120.03	112.60
1	B	475	GLY	N-CA-C	-6.09	98.75	113.18
1	D	475	GLY	N-CA-C	-6.09	98.76	113.18
1	C	475	GLY	N-CA-C	-5.80	99.42	113.18
1	A	42	ASN	N-CA-C	-5.78	100.41	109.25
1	A	475	GLY	N-CA-C	-5.63	99.83	113.18
1	A	103	THR	CA-C-N	5.46	127.54	120.44
1	A	103	THR	C-N-CA	5.46	127.54	120.44
1	B	147	ALA	CA-C-N	5.45	127.59	120.28
1	B	147	ALA	C-N-CA	5.45	127.59	120.28
1	D	144	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	240	PHE	CA-CB-CG	5.42	119.22	113.80
1	D	240	PHE	CA-CB-CG	5.36	119.16	113.80
1	C	144	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	147	ALA	CA-C-N	5.29	127.36	120.28
1	C	147	ALA	C-N-CA	5.29	127.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	THR	CA-C-N	5.25	127.27	120.44
1	B	103	THR	C-N-CA	5.25	127.27	120.44
1	D	147	ALA	CA-C-N	5.21	127.26	120.28
1	D	147	ALA	C-N-CA	5.21	127.26	120.28
1	A	470	GLY	CA-C-N	5.20	129.71	122.23
1	A	470	GLY	C-N-CA	5.20	129.71	122.23
1	C	103	THR	CA-C-N	5.14	127.12	120.44
1	C	103	THR	C-N-CA	5.14	127.12	120.44
1	A	32	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	240	PHE	CA-CB-CG	5.09	118.89	113.80
1	C	450	LEU	CA-C-N	5.06	129.74	122.35
1	C	450	LEU	C-N-CA	5.06	129.74	122.35

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	3713	0	3756	13	0
1	B	3720	0	3765	12	0
1	C	3720	0	3765	18	0
1	D	3713	0	3756	19	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
3	B	4	0	6	0	0
3	D	8	0	12	0	0
4	A	65	0	0	0	0
4	B	42	0	0	0	0
4	C	37	0	0	0	0
4	D	31	0	0	0	0
All	All	15245	0	15160	62	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 2.

All (62) 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:302:CYS:SG	2:C:501:NAP:C4N	2.85	0.65
1:A:302:CYS:SG	2:A:600:NAP:C4N	2.90	0.60
1:D:264:VAL:HG12	1:D:471:ILE:HD11	1.84	0.58
1:C:331:MET:HE2	1:C:377:PHE:HD1	1.70	0.57
1:D:38:LEU:HB2	1:D:54:GLN:HG2	1.87	0.57
1:B:302:CYS:SG	2:B:502:NAP:C4N	2.93	0.57
1:C:172:PHE:HB2	1:C:176:LEU:HD12	1.92	0.51
1:C:235:THR:O	1:C:262:LYS:HE2	2.11	0.51
1:A:242:LEU:HD11	1:A:265:VAL:HG23	1.92	0.50
1:D:24:ILE:HG23	1:D:53:PRO:HD2	1.94	0.50
1:B:172:PHE:HB2	1:B:176:LEU:HD12	1.94	0.49
1:B:242:LEU:HD11	1:B:265:VAL:HG23	1.93	0.49
1:C:242:LEU:HD11	1:C:265:VAL:HG23	1.94	0.49
1:D:172:PHE:HB2	1:D:176:LEU:HD12	1.94	0.48
1:D:193:LEU:HD23	1:D:223:ILE:HG12	1.94	0.48
1:D:242:LEU:HD11	1:D:265:VAL:HG23	1.94	0.48
1:D:344:MET:HE1	1:D:399:GLY:HA2	1.96	0.48
1:A:172:PHE:HB2	1:A:176:LEU:HD12	1.94	0.47
1:D:286:THR:O	1:D:290:LEU:HG	2.15	0.46
1:C:264:VAL:HG12	1:C:471:ILE:HD11	1.98	0.46
1:B:264:VAL:HG12	1:B:471:ILE:HD11	1.98	0.46
1:C:331:MET:HE3	1:C:341:LEU:HD12	1.98	0.46
1:D:85:VAL:HG11	1:D:216:LEU:HD13	1.98	0.45
1:D:305:MET:HE3	1:D:453:SER:HB2	1.99	0.45
1:A:264:VAL:HG12	1:A:471:ILE:HD11	1.98	0.45
1:C:24:ILE:HG23	1:C:53:PRO:HD2	1.98	0.44
1:B:247:GLY:O	1:B:268:LEU:HA	2.16	0.44
1:C:30:PRO:HD3	1:C:211:HIS:CD2	2.51	0.44
1:C:85:VAL:HG11	1:C:216:LEU:HD13	1.99	0.44
1:C:322:PHE:O	1:C:326:VAL:HG23	2.18	0.44
1:D:322:PHE:O	1:D:326:VAL:HG23	2.18	0.43
1:A:85:VAL:HG11	1:A:216:LEU:HD13	1.99	0.43
1:A:322:PHE:O	1:A:326:VAL:HG23	2.18	0.43
1:C:43:LYS:HD3	1:C:107:GLU:O	2.18	0.43
1:B:322:PHE:O	1:B:326:VAL:HG23	2.19	0.43
1:A:326:VAL:HG13	1:A:380:PRO:HB2	2.01	0.43
1:A:357:VAL:HG22	1:A:383:ILE:HD11	2.02	0.42
1:B:272:ALA:HA	1:B:273:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ILE:HG23	1:B:53:PRO:HD2	2.01	0.42
1:B:85:VAL:HG11	1:B:216:LEU:HD13	2.01	0.42
1:C:24:ILE:HG13	1:C:31:VAL:HG23	2.02	0.42
1:D:344:MET:HB2	1:D:376:ALA:O	2.20	0.42
1:D:30:PRO:HD3	1:D:211:HIS:CE1	2.55	0.41
1:A:272:ALA:HA	1:A:273:PRO:HD3	1.96	0.41
1:D:326:VAL:HG13	1:D:380:PRO:HB2	2.03	0.41
1:D:247:GLY:O	1:D:268:LEU:HA	2.20	0.41
1:B:326:VAL:HG13	1:B:380:PRO:HB2	2.02	0.41
1:B:357:VAL:HG22	1:B:383:ILE:HD11	2.03	0.41
1:A:24:ILE:HG13	1:A:31:VAL:HG23	2.01	0.41
1:C:353:ILE:HG12	1:C:399:GLY:HA3	2.03	0.41
1:D:249:GLY:HA2	1:D:268:LEU:HD13	2.03	0.41
1:D:272:ALA:HA	1:D:273:PRO:HD3	2.00	0.41
1:D:290:LEU:HA	1:D:305:MET:HE1	2.03	0.41
1:D:57:HIS:NE2	1:D:233:MET:HE2	2.37	0.40
1:A:169:PRO:HG3	1:A:246:THR:HG22	2.03	0.40
1:C:357:VAL:HG22	1:C:383:ILE:HD11	2.03	0.40
1:C:374:LYS:HG3	1:C:377:PHE:HB2	2.02	0.40
1:C:39:ASP:HB3	1:C:48:VAL:HG12	2.04	0.40
1:C:172:PHE:HB2	1:C:176:LEU:CD1	2.51	0.40
1:A:240:PHE:HB2	1:A:262:LYS:HE3	2.03	0.40
1:A:308:LEU:HD23	1:A:404:LEU:CD1	2.50	0.40
1:B:40:VAL:HB	1:B:50:ALA:HB3	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	478/515 (93%)	458 (96%)	19 (4%)	1 (0%)	43 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	479/515 (93%)	458 (96%)	20 (4%)	1 (0%)	43	55
1	C	479/515 (93%)	460 (96%)	18 (4%)	1 (0%)	43	55
1	D	478/515 (93%)	459 (96%)	18 (4%)	1 (0%)	43	55
All	All	1914/2060 (93%)	1835 (96%)	75 (4%)	4 (0%)	43	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	476	VAL
1	A	476	VAL
1	D	476	VAL
1	B	423	GLY

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	394/425 (93%)	378 (96%)	16 (4%)	27	41
1	B	395/425 (93%)	379 (96%)	16 (4%)	27	41
1	C	395/425 (93%)	379 (96%)	16 (4%)	27	41
1	D	394/425 (93%)	375 (95%)	19 (5%)	23	35
All	All	1578/1700 (93%)	1511 (96%)	67 (4%)	26	40

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	148	ARG
1	A	206	LEU
1	A	264	VAL
1	A	287	ILE
1	A	304	HIS
1	A	358	LYS

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Mol	Chain	Res	Type
1	A	373	ARG
1	A	378	ILE
1	A	383	ILE
1	A	389	GLU
1	A	397	ILE
1	A	404	LEU
1	A	416	GLU
1	A	426	SER
1	A	481	ASP
1	B	17	VAL
1	B	38	LEU
1	B	206	LEU
1	B	212	LYS
1	B	264	VAL
1	B	287	ILE
1	B	353	ILE
1	B	373	ARG
1	B	378	ILE
1	B	383	ILE
1	B	388	ILE
1	B	389	GLU
1	B	397	ILE
1	B	404	LEU
1	B	416	GLU
1	B	481	ASP
1	C	17	VAL
1	C	206	LEU
1	C	262	LYS
1	C	264	VAL
1	C	287	ILE
1	C	304	HIS
1	C	320	GLU
1	C	373	ARG
1	C	378	ILE
1	C	383	ILE
1	C	388	ILE
1	C	389	GLU
1	C	397	ILE
1	C	404	LEU
1	C	416	GLU
1	C	481	ASP
1	D	21	LYS

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Mol	Chain	Res	Type
1	D	34	ASP
1	D	54	GLN
1	D	206	LEU
1	D	264	VAL
1	D	287	ILE
1	D	288	GLN
1	D	305	MET
1	D	344	MET
1	D	353	ILE
1	D	378	ILE
1	D	383	ILE
1	D	388	ILE
1	D	389	GLU
1	D	397	ILE
1	D	404	LEU
1	D	416	GLU
1	D	471	ILE
1	D	481	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	54	GLN
1	A	304	HIS
1	A	472	GLN
1	B	23	ASN
1	B	175	ASN
1	B	304	HIS
1	B	372	ASN
1	B	421	HIS
1	C	23	ASN
1	C	57	HIS
1	C	271	ASN
1	C	421	HIS
1	C	472	GLN
1	D	175	ASN
1	D	211	HIS
1	D	472	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 ⓘ

7 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	EDO	B	501	-	3,3,3	0.67	0	2,2,2	0.12	0
2	NAP	D	503	-	50,52,52	1.04	1 (2%)	71,80,80	0.88	3 (4%)
2	NAP	C	501	-	50,52,52	0.98	1 (2%)	71,80,80	0.77	3 (4%)
3	EDO	D	501	-	3,3,3	0.70	0	2,2,2	0.22	0
3	EDO	D	502	-	3,3,3	0.64	0	2,2,2	0.24	0
2	NAP	A	600	-	50,52,52	0.96	1 (2%)	71,80,80	0.84	3 (4%)
2	NAP	B	502	-	50,52,52	0.96	1 (2%)	71,80,80	0.94	2 (2%)

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	EDO	B	501	-	-	0/1/1/1	-
2	NAP	D	503	-	-	5/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	C	501	-	-	3/35/67/67	0/5/5/5
3	EDO	D	501	-	-	0/1/1/1	-
3	EDO	D	502	-	-	0/1/1/1	-
2	NAP	A	600	-	-	1/35/67/67	0/5/5/5
2	NAP	B	502	-	-	2/35/67/67	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	503	NAP	C2N-N1N	6.55	1.42	1.35
2	C	501	NAP	C2N-N1N	6.38	1.42	1.35
2	B	502	NAP	C2N-N1N	6.03	1.41	1.35
2	A	600	NAP	C2N-N1N	6.00	1.41	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	NAP	C2B-C1B-N9A	4.58	121.29	113.75
2	D	503	NAP	C2B-C1B-N9A	4.17	120.62	113.75
2	A	600	NAP	C2B-C1B-N9A	3.51	119.52	113.75
2	B	502	NAP	O3-PA-O1A	2.91	119.45	110.70
2	A	600	NAP	O3-PA-O1A	2.70	118.81	110.70
2	D	503	NAP	O3-PA-O1A	2.54	118.35	110.70
2	C	501	NAP	O3-PA-O1A	2.31	117.64	110.70
2	D	503	NAP	O2B-P2B-O1X	2.15	117.00	109.33
2	C	501	NAP	O2B-P2B-O1X	2.15	117.00	109.33
2	A	600	NAP	C4D-O4D-C1D	2.07	111.82	109.92
2	C	501	NAP	O2X-P2B-O2B	-2.06	97.82	105.85

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	503	NAP	C5B-O5B-PA-O1A
2	D	503	NAP	C5D-O5D-PN-O1N
2	D	503	NAP	C3B-C2B-O2B-P2B
2	A	600	NAP	C4D-C5D-O5D-PN
2	C	501	NAP	C4D-C5D-O5D-PN
2	B	502	NAP	C5B-O5B-PA-O1A
2	D	503	NAP	C4D-C5D-O5D-PN
2	B	502	NAP	C4D-C5D-O5D-PN

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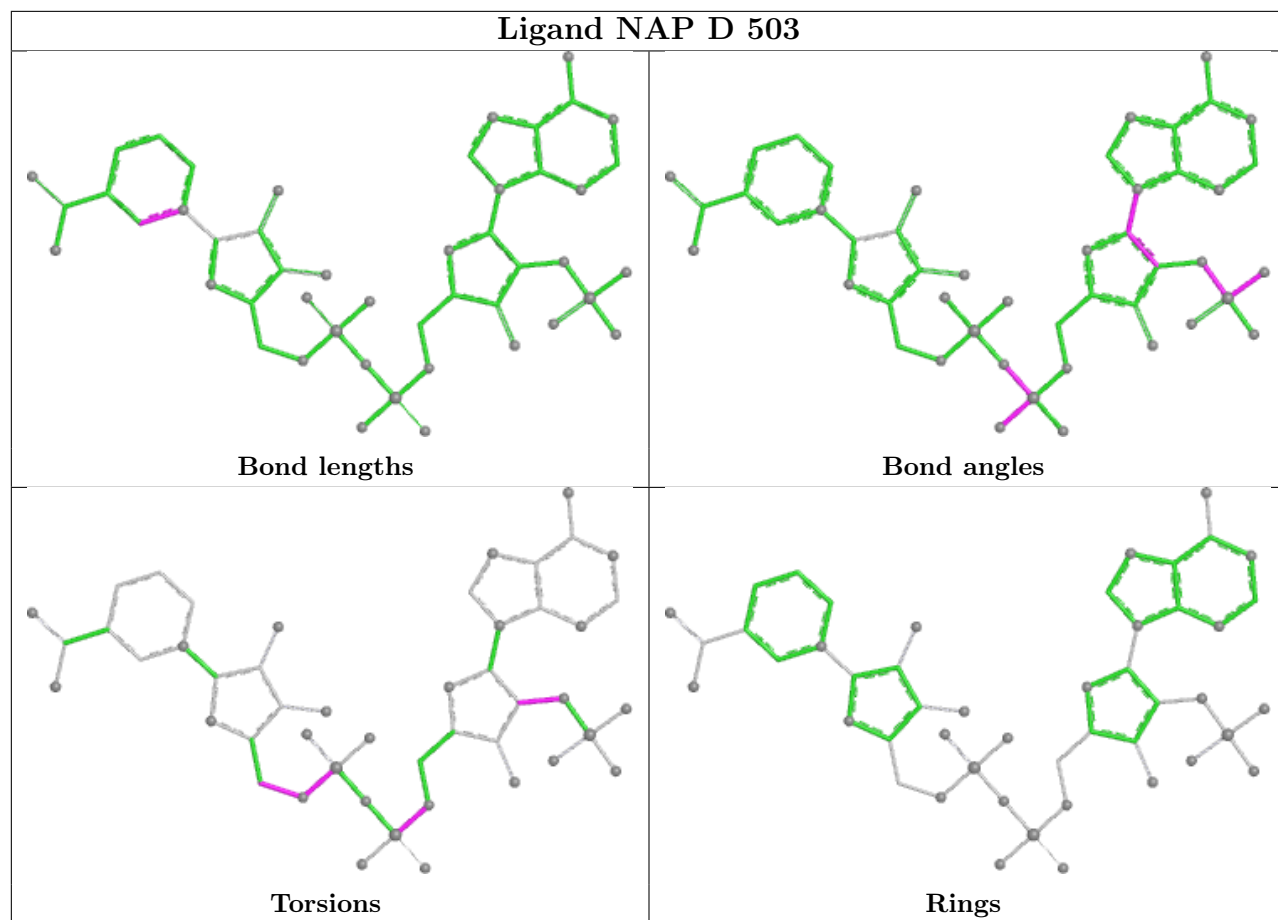
Mol	Chain	Res	Type	Atoms
2	C	501	NAP	C3B-C2B-O2B-P2B
2	D	503	NAP	C1B-C2B-O2B-P2B
2	C	501	NAP	C1B-C2B-O2B-P2B

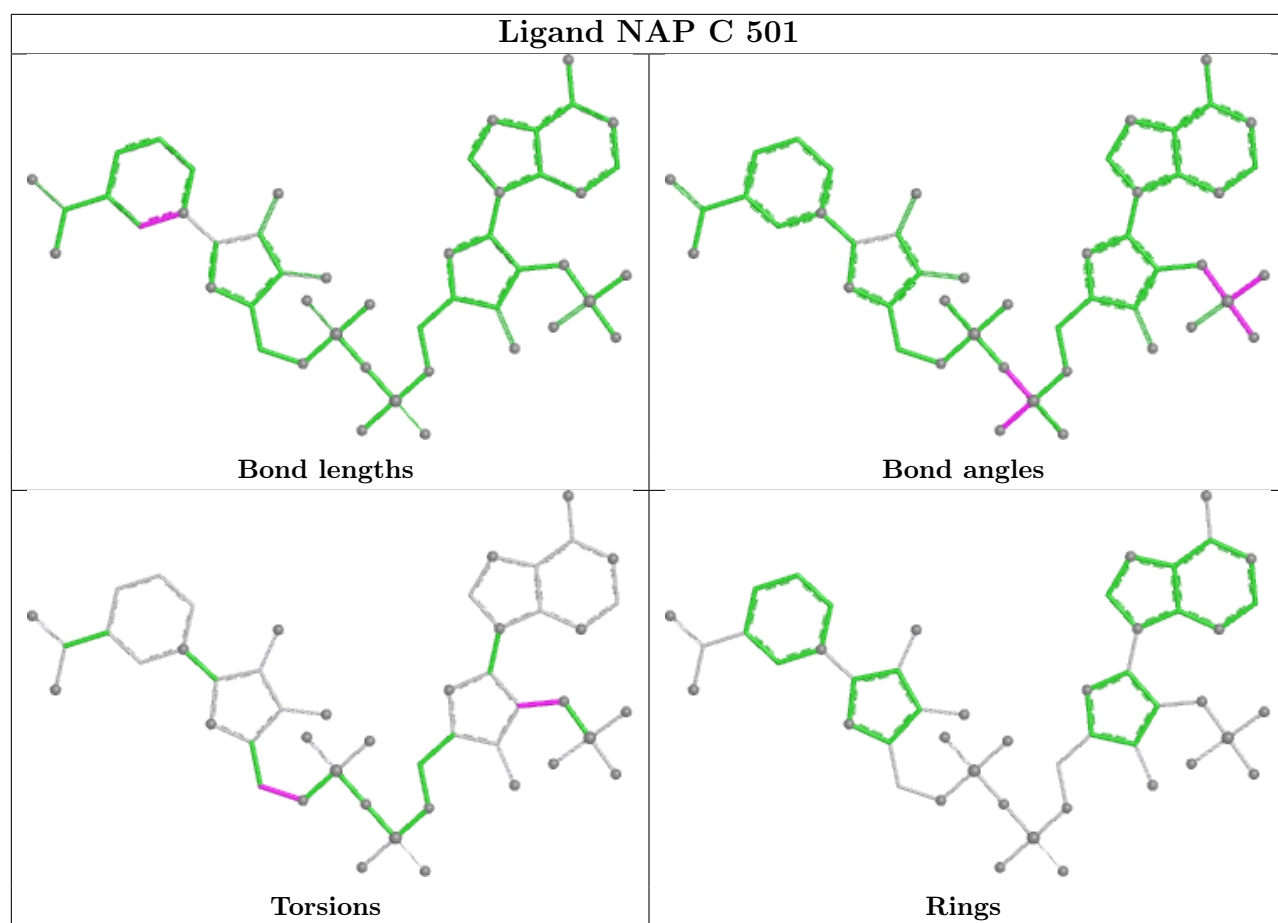
There are no ring outliers.

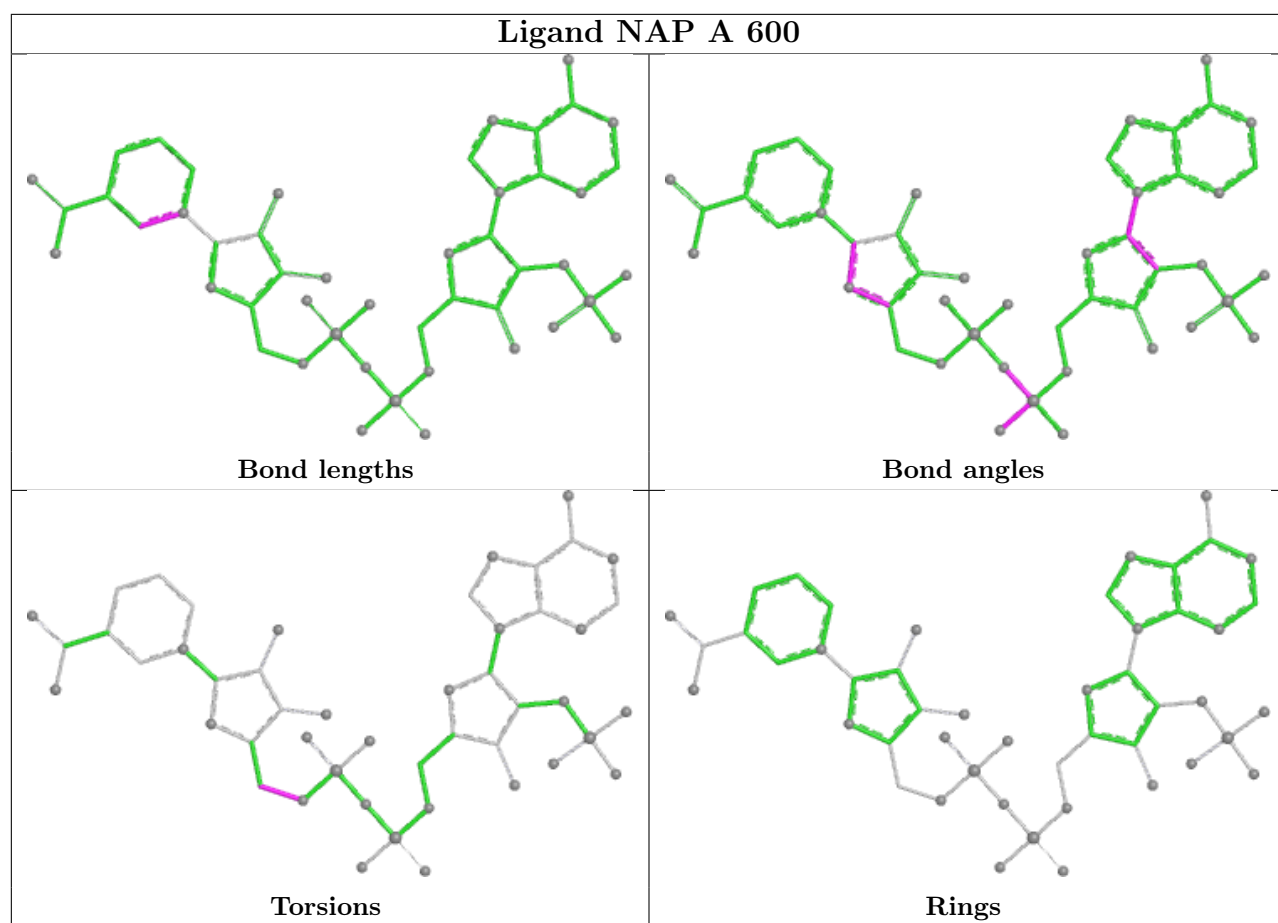
3 monomers are involved in 3 short contacts:

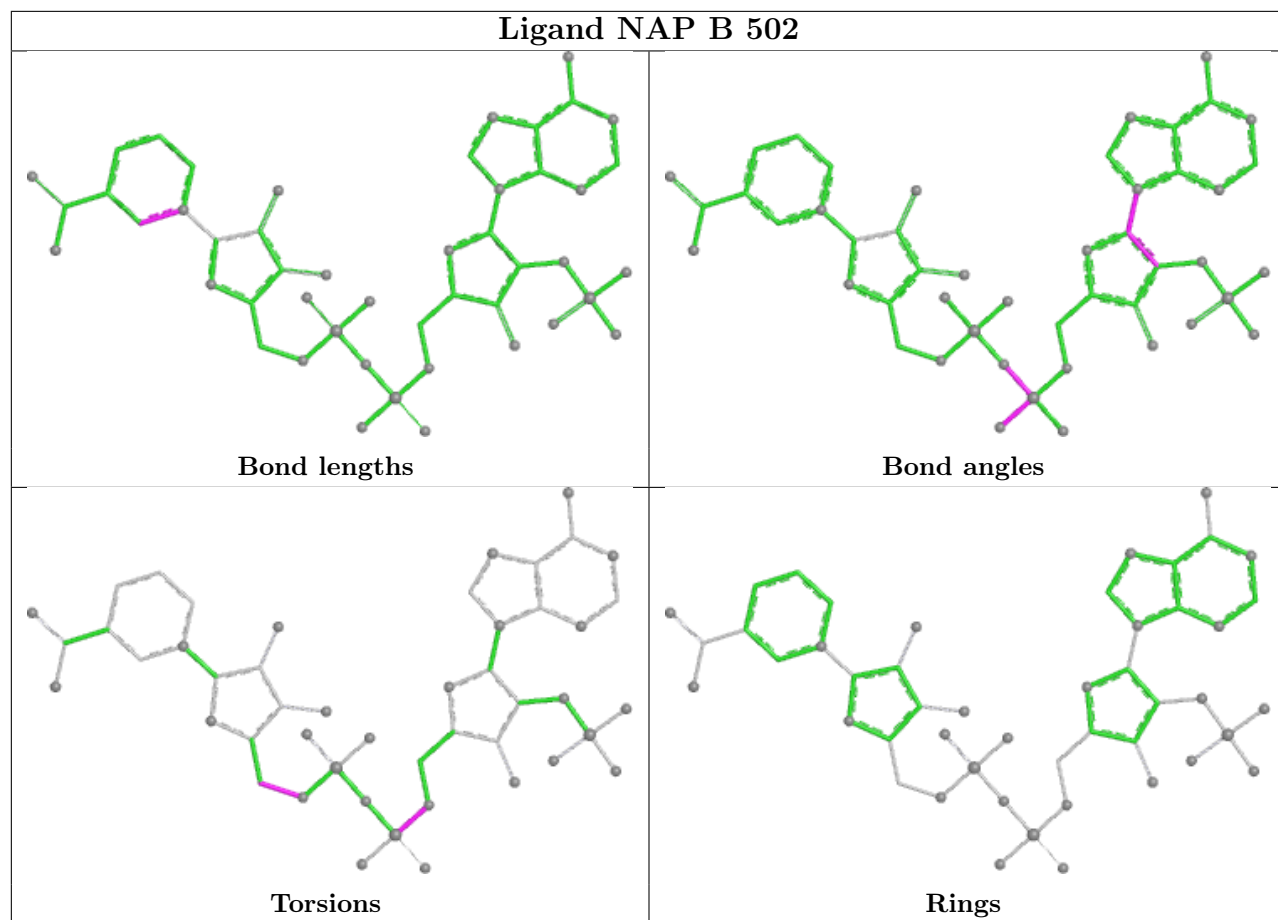
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NAP	1	0
2	A	600	NAP	1	0
2	B	502	NAP	1	0

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	480/515 (93%)	-0.10	1 (0%) 91 91	51, 71, 102, 129	0
1	B	481/515 (93%)	-0.02	1 (0%) 91 91	52, 76, 113, 144	0
1	C	481/515 (93%)	0.03	3 (0%) 85 86	50, 78, 115, 144	0
1	D	480/515 (93%)	0.22	9 (1%) 66 68	46, 93, 151, 173	0
All	All	1922/2060 (93%)	0.03	14 (0%) 84 85	46, 79, 126, 173	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	404	LEU	3.2
1	A	404	LEU	2.9
1	C	17	VAL	2.8
1	C	225	PRO	2.5
1	D	401	VAL	2.4
1	D	18	THR	2.4
1	D	26	LEU	2.2
1	D	309	TYR	2.2
1	D	329	LEU	2.1
1	B	17	VAL	2.1
1	C	18	THR	2.1
1	D	296	TYR	2.1
1	D	247	GLY	2.1
1	D	326	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](#)

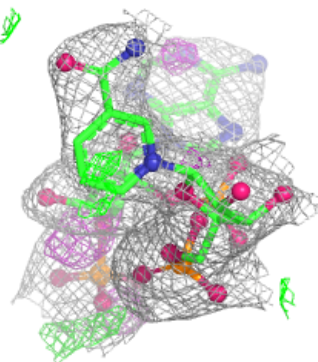
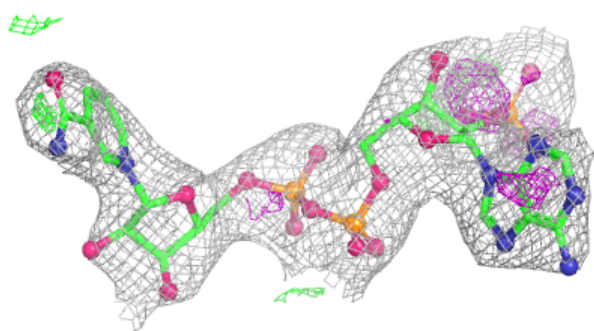
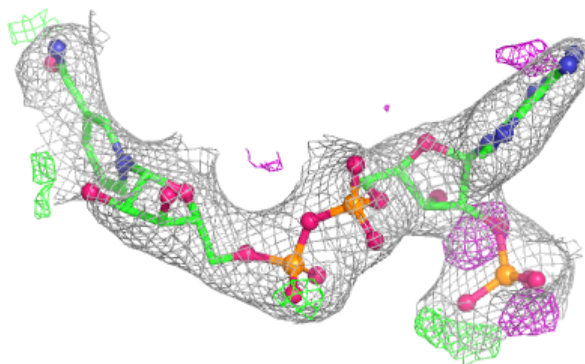
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	D	502	4/4	0.79	0.15	71,74,75,77	0
3	EDO	B	501	4/4	0.82	0.11	73,77,80,80	0
3	EDO	D	501	4/4	0.86	0.17	68,74,75,76	0
2	NAP	D	503	48/48	0.90	0.10	86,96,103,104	0
2	NAP	B	502	48/48	0.93	0.08	52,81,92,93	0
2	NAP	C	501	48/48	0.94	0.07	61,74,78,80	0
2	NAP	A	600	48/48	0.95	0.07	61,70,90,91	0

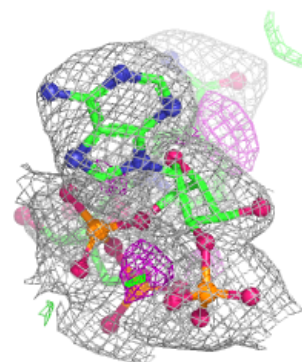
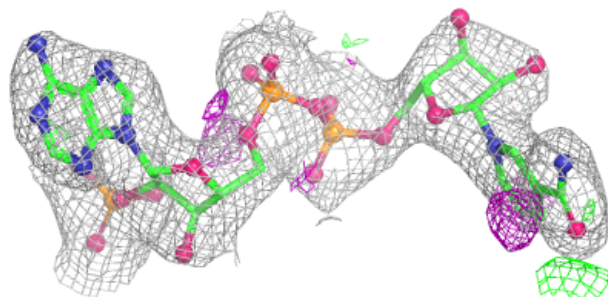
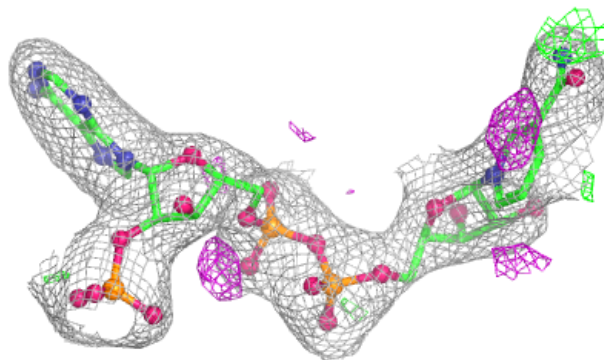
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 503:

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

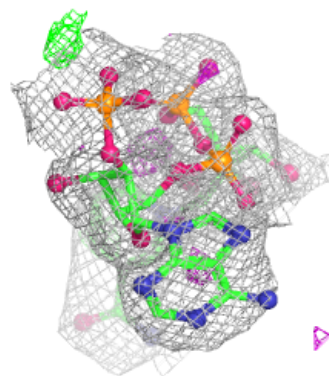
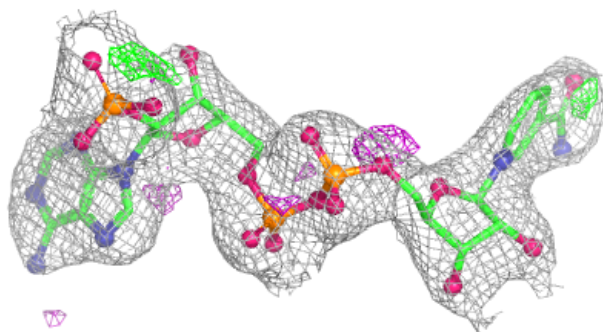
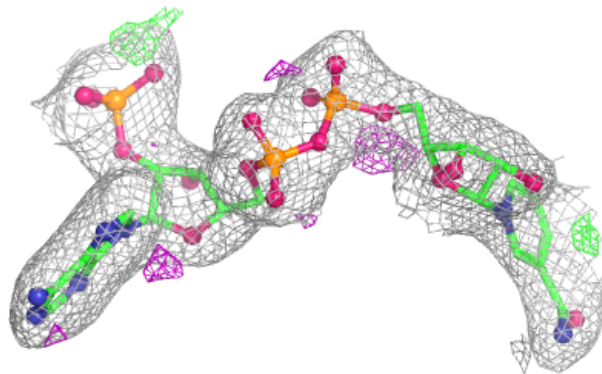
**Electron density around NAP B 502:**

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

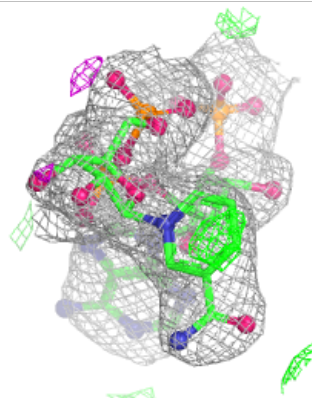
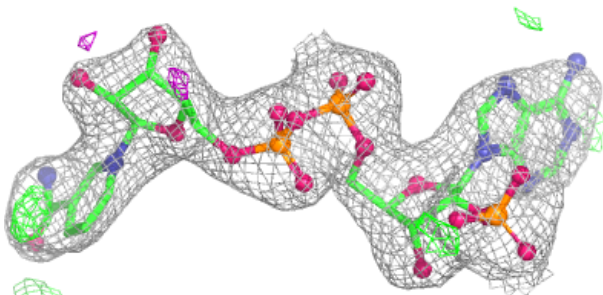
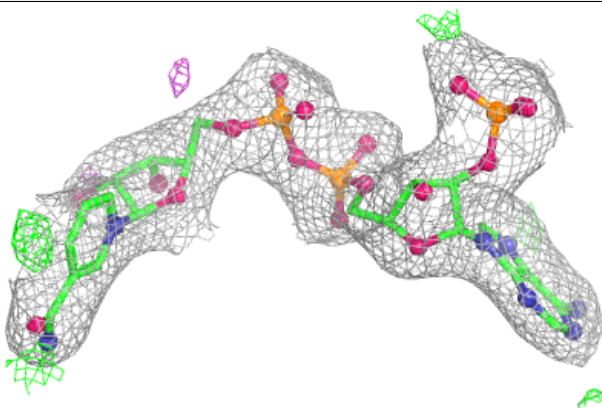


Electron density around NAP C 501:

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

**Electron density around NAP A 600:**

$2mF_o-DF_c$ (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.