



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:00 PM UTC

PDB ID : 8J1C / pdb_00008j1c
Title : Structure of amino acid dehydrogenase in complex with NADP
Authors : Sakuraba, H.; Ohshima, T.
Deposited on : 2023-04-12
Resolution : 2.20 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

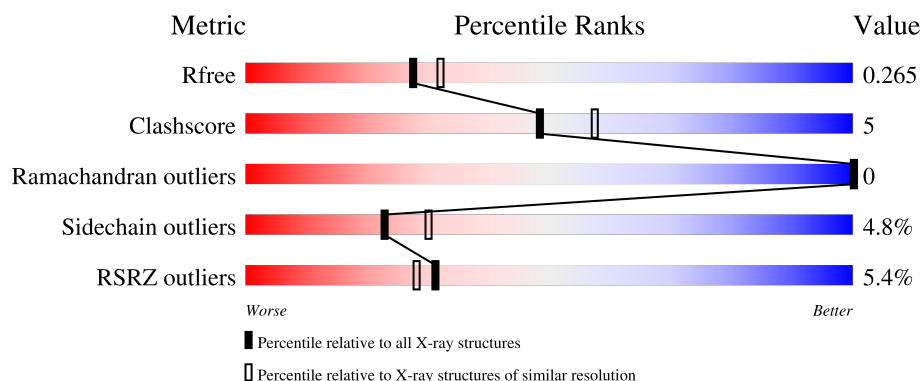
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	336	5% 78% 10% • 11%
1	B	336	5% 74% 13% • 11%
1	C	336	4% 78% 13% • 8%
1	D	336	6% 77% 13% • 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9525 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 Ornithine cyclodeaminase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2262	1437	396	418	11			
1	B	299	Total	C	N	O	S	0	0	0
			2234	1420	387	416	11			
1	C	309	Total	C	N	O	S	0	0	0
			2319	1469	406	433	11			
1	D	306	Total	C	N	O	S	0	0	0
			2304	1460	404	429	11			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	316	ASP	-	expression tag	UNP A0A7Y0ZV07
A	317	PRO	-	expression tag	UNP A0A7Y0ZV07
A	318	ASN	-	expression tag	UNP A0A7Y0ZV07
A	319	SER	-	expression tag	UNP A0A7Y0ZV07
A	320	SER	-	expression tag	UNP A0A7Y0ZV07
A	321	SER	-	expression tag	UNP A0A7Y0ZV07
A	322	VAL	-	expression tag	UNP A0A7Y0ZV07
A	323	ASP	-	expression tag	UNP A0A7Y0ZV07
A	324	LYS	-	expression tag	UNP A0A7Y0ZV07
A	325	LEU	-	expression tag	UNP A0A7Y0ZV07
A	326	ALA	-	expression tag	UNP A0A7Y0ZV07
A	327	ALA	-	expression tag	UNP A0A7Y0ZV07
A	328	ALA	-	expression tag	UNP A0A7Y0ZV07
A	329	LEU	-	expression tag	UNP A0A7Y0ZV07
A	330	GLU	-	expression tag	UNP A0A7Y0ZV07
A	331	HIS	-	expression tag	UNP A0A7Y0ZV07
A	332	HIS	-	expression tag	UNP A0A7Y0ZV07
A	333	HIS	-	expression tag	UNP A0A7Y0ZV07
A	334	HIS	-	expression tag	UNP A0A7Y0ZV07
A	335	HIS	-	expression tag	UNP A0A7Y0ZV07
A	336	HIS	-	expression tag	UNP A0A7Y0ZV07

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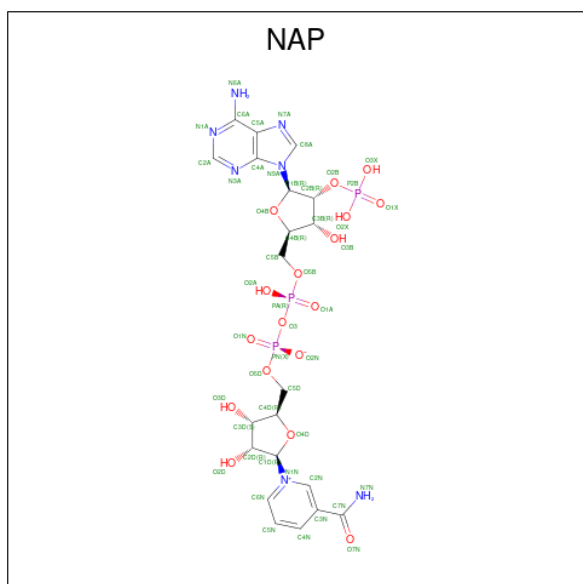
Chain	Residue	Modelled	Actual	Comment	Reference
B	316	ASP	-	expression tag	UNP A0A7Y0ZV07
B	317	PRO	-	expression tag	UNP A0A7Y0ZV07
B	318	ASN	-	expression tag	UNP A0A7Y0ZV07
B	319	SER	-	expression tag	UNP A0A7Y0ZV07
B	320	SER	-	expression tag	UNP A0A7Y0ZV07
B	321	SER	-	expression tag	UNP A0A7Y0ZV07
B	322	VAL	-	expression tag	UNP A0A7Y0ZV07
B	323	ASP	-	expression tag	UNP A0A7Y0ZV07
B	324	LYS	-	expression tag	UNP A0A7Y0ZV07
B	325	LEU	-	expression tag	UNP A0A7Y0ZV07
B	326	ALA	-	expression tag	UNP A0A7Y0ZV07
B	327	ALA	-	expression tag	UNP A0A7Y0ZV07
B	328	ALA	-	expression tag	UNP A0A7Y0ZV07
B	329	LEU	-	expression tag	UNP A0A7Y0ZV07
B	330	GLU	-	expression tag	UNP A0A7Y0ZV07
B	331	HIS	-	expression tag	UNP A0A7Y0ZV07
B	332	HIS	-	expression tag	UNP A0A7Y0ZV07
B	333	HIS	-	expression tag	UNP A0A7Y0ZV07
B	334	HIS	-	expression tag	UNP A0A7Y0ZV07
B	335	HIS	-	expression tag	UNP A0A7Y0ZV07
B	336	HIS	-	expression tag	UNP A0A7Y0ZV07
C	316	ASP	-	expression tag	UNP A0A7Y0ZV07
C	317	PRO	-	expression tag	UNP A0A7Y0ZV07
C	318	ASN	-	expression tag	UNP A0A7Y0ZV07
C	319	SER	-	expression tag	UNP A0A7Y0ZV07
C	320	SER	-	expression tag	UNP A0A7Y0ZV07
C	321	SER	-	expression tag	UNP A0A7Y0ZV07
C	322	VAL	-	expression tag	UNP A0A7Y0ZV07
C	323	ASP	-	expression tag	UNP A0A7Y0ZV07
C	324	LYS	-	expression tag	UNP A0A7Y0ZV07
C	325	LEU	-	expression tag	UNP A0A7Y0ZV07
C	326	ALA	-	expression tag	UNP A0A7Y0ZV07
C	327	ALA	-	expression tag	UNP A0A7Y0ZV07
C	328	ALA	-	expression tag	UNP A0A7Y0ZV07
C	329	LEU	-	expression tag	UNP A0A7Y0ZV07
C	330	GLU	-	expression tag	UNP A0A7Y0ZV07
C	331	HIS	-	expression tag	UNP A0A7Y0ZV07
C	332	HIS	-	expression tag	UNP A0A7Y0ZV07
C	333	HIS	-	expression tag	UNP A0A7Y0ZV07
C	334	HIS	-	expression tag	UNP A0A7Y0ZV07
C	335	HIS	-	expression tag	UNP A0A7Y0ZV07
C	336	HIS	-	expression tag	UNP A0A7Y0ZV07

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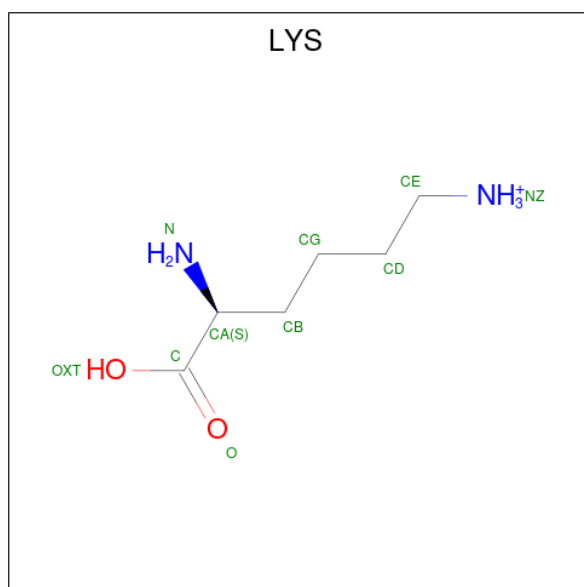
Chain	Residue	Modelled	Actual	Comment	Reference
D	316	ASP	-	expression tag	UNP A0A7Y0ZV07
D	317	PRO	-	expression tag	UNP A0A7Y0ZV07
D	318	ASN	-	expression tag	UNP A0A7Y0ZV07
D	319	SER	-	expression tag	UNP A0A7Y0ZV07
D	320	SER	-	expression tag	UNP A0A7Y0ZV07
D	321	SER	-	expression tag	UNP A0A7Y0ZV07
D	322	VAL	-	expression tag	UNP A0A7Y0ZV07
D	323	ASP	-	expression tag	UNP A0A7Y0ZV07
D	324	LYS	-	expression tag	UNP A0A7Y0ZV07
D	325	LEU	-	expression tag	UNP A0A7Y0ZV07
D	326	ALA	-	expression tag	UNP A0A7Y0ZV07
D	327	ALA	-	expression tag	UNP A0A7Y0ZV07
D	328	ALA	-	expression tag	UNP A0A7Y0ZV07
D	329	LEU	-	expression tag	UNP A0A7Y0ZV07
D	330	GLU	-	expression tag	UNP A0A7Y0ZV07
D	331	HIS	-	expression tag	UNP A0A7Y0ZV07
D	332	HIS	-	expression tag	UNP A0A7Y0ZV07
D	333	HIS	-	expression tag	UNP A0A7Y0ZV07
D	334	HIS	-	expression tag	UNP A0A7Y0ZV07
D	335	HIS	-	expression tag	UNP A0A7Y0ZV07
D	336	HIS	-	expression tag	UNP A0A7Y0ZV07

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



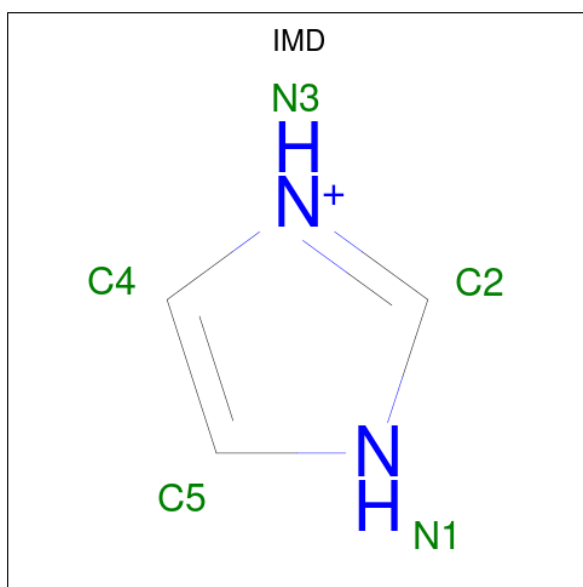
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



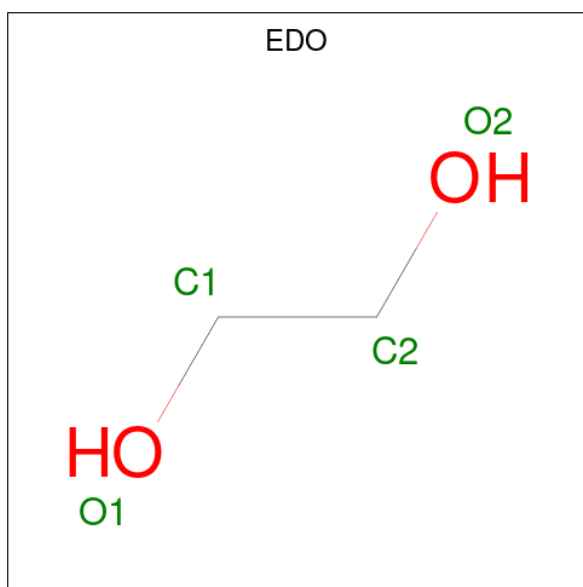
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			5	3	2		
4	C	1	Total	C	N	0	0
			5	3	2		
4	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



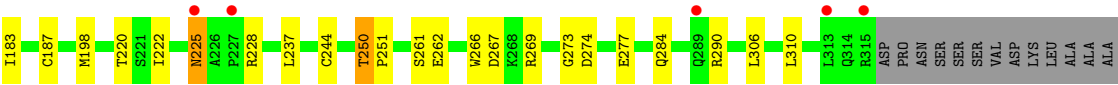
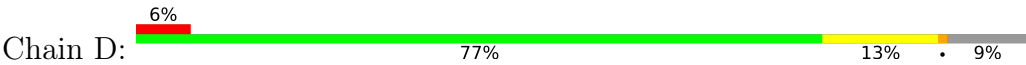
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total 58	O 58	0	0
6	B	53	Total 53	O 53	0	0
6	C	78	Total 78	O 78	0	0
6	D	44	Total 44	O 44	0	0

HIS

● Molecule 1: Ornithine cyclodeaminase family protein



LEU
GLU
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.97Å 92.62Å 162.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.80 – 2.20 46.80 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.80-2.20) 100.0 (46.80-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.213 , 0.260 0.219 , 0.265	Depositor DCC
R_{free} test set	3563 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9525	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, IMD, 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	0.58	0/2307	0.98	1/3147 (0.0%)
1	B	0.57	0/2278	0.98	2/3108 (0.1%)
1	C	0.57	0/2367	0.97	2/3233 (0.1%)
1	D	0.58	0/2350	0.99	3/3207 (0.1%)
All	All	0.58	0/9302	0.98	8/12695 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	LEU	N-CA-C	-7.18	103.46	111.71
1	D	176	GLY	N-CA-C	-7.11	103.81	113.27
1	B	169	ALA	N-CA-C	-5.85	105.46	113.30
1	D	72	THR	CB-CA-C	5.54	118.89	109.75
1	A	54	ASP	CA-CB-CG	5.45	118.05	112.60
1	C	109	THR	CA-CB-OG1	-5.44	101.44	109.60
1	C	225	ASN	CB-CA-C	-5.29	104.68	111.50
1	D	250	THR	CA-CB-OG1	-5.14	101.88	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	2262	0	2285	21	0
1	B	2234	0	2254	31	0
1	C	2319	0	2332	22	0
1	D	2304	0	2317	29	0
2	A	48	0	25	2	0
2	B	48	0	25	7	0
2	D	48	0	25	2	0
3	B	10	0	12	2	0
4	B	5	0	5	0	0
4	C	5	0	5	1	0
4	D	5	0	5	0	0
5	B	4	0	6	0	0
6	A	58	0	0	3	0
6	B	53	0	0	3	0
6	C	78	0	0	1	0
6	D	44	0	0	2	0
All	All	9525	0	9296	102	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 5.

All (102) 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:D:187:CYS:SG	6:D:543:HOH:O	2.21	0.98
1:B:108:THR:HG22	2:B:401:NAP:H4N	1.51	0.89
1:A:226:ALA:HB3	1:A:229:ALA:HB2	1.56	0.87
1:B:108:THR:HG21	3:B:402:LYS:HG2	1.67	0.77
1:D:174:LEU:HD11	1:D:183:ILE:HD11	1.68	0.75
1:D:8:ILE:HG12	1:D:100:LEU:HD11	1.77	0.66
1:D:171:LEU:HA	1:D:174:LEU:HB2	1.77	0.65
1:B:106:GLU:HG2	6:B:526:HOH:O	1.97	0.63
1:B:177:LEU:C	6:B:509:HOH:O	2.41	0.63
1:C:244:CYS:O	1:C:274:ASP:HA	2.01	0.60
1:C:311:TYR:O	1:C:315:ARG:HD3	2.02	0.60
1:B:244:CYS:O	1:B:274:ASP:HA	2.03	0.57
1:C:235:HIS:HD2	6:C:573:HOH:O	1.88	0.57
1:B:108:THR:HG22	2:B:401:NAP:C4N	2.30	0.57
1:B:145:ARG:NH2	1:B:173:GLN:OE1	2.38	0.57
1:B:41:PRO:HG2	1:B:59:LEU:HB2	1.87	0.56
1:A:20:ILE:HG23	1:A:25:ILE:CD1	2.36	0.56
1:A:108:THR:O	1:A:111:ARG:HG3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLY:HA2	2:B:401:NAP:H1B	1.88	0.55
1:B:163:LEU:O	1:B:164:ALA:C	2.50	0.54
1:D:144:LEU:HG	1:D:177:LEU:HD13	1.91	0.52
1:B:106:GLU:CG	6:B:526:HOH:O	2.57	0.52
1:A:170:THR:HG23	1:A:171:LEU:HD12	1.92	0.51
1:A:222:ILE:O	2:A:401:NAP:H2N	2.10	0.51
1:A:135:GLY:HA2	2:A:401:NAP:H1B	1.92	0.51
1:B:272:MET:O	1:B:284:GLN:HG3	2.11	0.51
1:D:222:ILE:O	2:D:401:NAP:H2N	2.11	0.51
1:B:144:LEU:HD23	1:B:173:GLN:HG3	1.92	0.51
1:D:267:ASP:OD2	1:D:269:ARG:NH1	2.45	0.50
1:A:185:ASP:OD1	1:A:185:ASP:N	2.44	0.50
1:A:244:CYS:O	1:A:274:ASP:HA	2.11	0.50
1:C:39:VAL:HB	1:C:61:VAL:HB	1.94	0.50
1:B:241:GLN:HB3	1:B:272:MET:SD	2.52	0.50
1:B:148:GLN:HB2	1:B:177:LEU:HD13	1.95	0.49
1:D:141:GLN:HG2	1:D:173:GLN:HB2	1.95	0.49
1:D:244:CYS:O	1:D:274:ASP:HA	2.13	0.49
1:D:170:THR:O	1:D:174:LEU:N	2.46	0.49
1:B:202:SER:HA	2:B:401:NAP:H4D	1.96	0.48
1:C:119:ALA:O	1:C:123:LEU:HB2	2.14	0.48
1:C:267:ASP:OD1	1:C:269:ARG:HD3	2.14	0.48
1:C:226:ALA:HB3	1:C:229:ALA:HB2	1.95	0.47
1:C:45:LEU:C	1:C:45:LEU:HD23	2.39	0.47
1:D:133:ILE:HD12	1:D:144:LEU:HD13	1.95	0.47
1:D:228:ARG:HH22	1:D:262:GLU:CD	2.23	0.47
1:C:131:LEU:HD11	1:C:198:MET:HE2	1.97	0.47
1:D:108:THR:O	1:D:111:ARG:HG3	2.15	0.47
1:B:116:THR:O	1:B:120:VAL:HG23	2.15	0.46
1:A:22:VAL:HG13	1:A:306:LEU:HD21	1.97	0.46
1:A:143:HIS:O	1:A:147:VAL:HG13	2.16	0.46
1:B:170:THR:O	1:B:174:LEU:N	2.42	0.46
1:D:225:ASN:HD22	1:D:225:ASN:H	1.64	0.46
1:D:127:ALA:O	1:D:129:ARG:HG2	2.15	0.46
1:D:148:GLN:HB3	1:D:177:LEU:HD11	1.98	0.46
1:A:184:ALA:HB2	6:A:519:HOH:O	2.16	0.46
1:B:136:SER:HB3	1:B:158:LEU:HD21	1.98	0.46
1:C:130:ARG:HD3	1:C:193:ASP:O	2.15	0.46
1:D:273:GLY:HA2	1:D:277:GLU:OE1	2.16	0.45
1:A:238:ASN:ND2	6:A:501:HOH:O	2.36	0.45
1:D:175:THR:C	1:D:177:LEU:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:SER:HB3	2:B:401:NAP:H52N	1.99	0.45
1:B:308:ASN:O	1:B:312:GLN:HG2	2.16	0.44
1:D:175:THR:O	1:D:178:ASP:N	2.51	0.44
1:B:62:LEU:HD11	1:B:305:ALA:HA	2.00	0.44
1:A:314:GLN:HA	1:A:314:GLN:HE21	1.82	0.44
1:D:144:LEU:CD1	1:D:177:LEU:HD13	2.47	0.44
1:A:48:PHE:CD1	1:B:93:MET:HE3	2.53	0.43
1:A:181:LEU:C	1:A:181:LEU:HD23	2.43	0.43
1:D:43:GLN:HG2	6:D:535:HOH:O	2.18	0.43
1:D:45:LEU:C	1:D:45:LEU:HD23	2.43	0.43
1:C:4:THR:HB	1:C:5:PRO:HA	2.01	0.43
1:C:33:LEU:HD23	1:C:276:PRO:HG3	2.00	0.43
1:C:174:LEU:O	1:C:181:LEU:HD23	2.18	0.43
2:B:401:NAP:H2D	3:B:402:LYS:OXT	2.19	0.43
1:C:224:THR:O	4:C:401:IMD:H4	2.19	0.42
1:D:228:ARG:NH2	1:D:262:GLU:OE2	2.46	0.42
1:D:198:MET:HA	1:D:220:THR:OG1	2.19	0.42
1:A:276:PRO:O	1:A:280:SER:OG	2.35	0.42
1:C:314:GLN:H	1:C:314:GLN:HG3	1.64	0.42
1:A:14:ARG:NH1	1:A:106:GLU:OE1	2.52	0.42
1:C:230:HIS:HB2	1:C:256:GLU:HB3	2.01	0.42
1:B:201:THR:O	2:B:401:NAP:H4D	2.20	0.42
1:C:147:VAL:HA	1:C:150:LEU:HG	2.01	0.42
1:D:135:GLY:HA2	2:D:401:NAP:H1B	2.01	0.42
1:B:92:SER:HB3	1:B:95:ASN:ND2	2.35	0.42
1:D:8:ILE:CG1	1:D:100:LEU:HD11	2.47	0.42
1:D:250:THR:N	1:D:251:PRO:CD	2.82	0.42
1:C:314:GLN:C	1:C:315:ARG:HG3	2.45	0.41
1:A:127:ALA:O	1:A:129:ARG:HG2	2.21	0.41
1:C:261:SER:HA	1:C:266:TRP:O	2.20	0.41
1:D:144:LEU:HG	1:D:177:LEU:CD1	2.50	0.41
1:B:300:GLY:O	1:B:304:ILE:HG12	2.19	0.41
1:B:156:ILE:HD12	1:B:177:LEU:HD21	2.02	0.41
1:B:199:LEU:HD21	1:B:208:LEU:HD22	2.03	0.41
1:D:261:SER:HA	1:D:266:TRP:O	2.21	0.41
1:C:129:ARG:HE	1:C:154:GLN:HG3	1.86	0.40
1:A:20:ILE:HG23	1:A:25:ILE:HD11	2.02	0.40
1:A:28:LYS:NZ	6:A:512:HOH:O	2.54	0.40
1:A:76:ILE:HG21	1:B:93:MET:O	2.21	0.40
1:B:45:LEU:HD12	1:B:56:ILE:HD11	2.03	0.40
1:C:92:SER:HB3	1:C:95:ASN:OD1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LEU:O	1:B:151:ARG:NH1	2.50	0.40
1:C:133:ILE:O	1:C:158:LEU:HA	2.22	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	292/336 (87%)	279 (96%)	13 (4%)	0	100	100
1	B	291/336 (87%)	280 (96%)	11 (4%)	0	100	100
1	C	305/336 (91%)	294 (96%)	11 (4%)	0	100	100
1	D	300/336 (89%)	295 (98%)	5 (2%)	0	100	100
All	All	1188/1344 (88%)	1148 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/267 (89%)	225 (94%)	13 (6%)	19	24
1	B	234/267 (88%)	222 (95%)	12 (5%)	21	27
1	C	243/267 (91%)	234 (96%)	9 (4%)	30	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	241/267 (90%)	229 (95%)	12 (5%)	22	28
All	All	956/1068 (90%)	910 (95%)	46 (5%)	23	30

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ILE
1	A	77	VAL
1	A	83	LEU
1	A	106	GLU
1	A	111	ARG
1	A	147	VAL
1	A	154	GLN
1	A	160	SER
1	A	185	ASP
1	A	191	VAL
1	A	228	ARG
1	A	306	LEU
1	A	310	LEU
1	B	14	ARG
1	B	64	GLU
1	B	95	ASN
1	B	106	GLU
1	B	145	ARG
1	B	147	VAL
1	B	168	PRO
1	B	171	LEU
1	B	177	LEU
1	B	267	ASP
1	B	284	GLN
1	B	314	GLN
1	C	106	GLU
1	C	147	VAL
1	C	152	ASP
1	C	193	ASP
1	C	202	SER
1	C	237	LEU
1	C	247	ARG
1	C	268	LYS
1	C	315	ARG
1	D	77	VAL
1	D	79	GLU

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Mol	Chain	Res	Type
1	D	111	ARG
1	D	151	ARG
1	D	170	THR
1	D	177	LEU
1	D	225	ASN
1	D	237	LEU
1	D	284	GLN
1	D	290	ARG
1	D	306	LEU
1	D	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	27	HIS
1	A	57	ASN
1	A	154	GLN
1	A	235	HIS
1	A	241	GLN
1	A	314	GLN
1	B	43	GLN
1	B	95	ASN
1	B	105	HIS
1	B	155	HIS
1	B	308	ASN
1	B	312	GLN
1	C	6	HIS
1	C	24	GLN
1	C	235	HIS
1	C	248	GLN
1	D	6	HIS
1	D	57	ASN
1	D	97	GLN
1	D	141	GLN
1	D	155	HIS
1	D	173	GLN
1	D	225	ASN
1	D	235	HIS
1	D	284	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LYS	B	402	-	8,9,9	0.85	1 (12%)	7,10,10	1.16	1 (14%)
2	NAP	A	401	-	50,52,52	0.79	2 (4%)	71,80,80	1.10	7 (9%)
2	NAP	B	401	-	50,52,52	0.79	2 (4%)	71,80,80	1.21	5 (7%)
4	IMD	C	401	-	5,5,5	0.36	0	5,5,5	0.50	0
4	IMD	B	403	-	5,5,5	0.19	0	5,5,5	0.64	0
4	IMD	D	402	-	5,5,5	0.34	0	5,5,5	0.54	0
5	EDO	B	404	-	3,3,3	1.23	0	2,2,2	0.58	0
2	NAP	D	401	-	50,52,52	0.90	3 (6%)	71,80,80	1.24	7 (9%)

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	LYS	B	402	-	-	4/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	401	-	-	6/35/67/67	0/5/5/5
2	NAP	B	401	-	-	3/35/67/67	0/5/5/5
4	IMD	C	401	-	-	-	0/1/1/1
4	IMD	B	403	-	-	-	0/1/1/1
4	IMD	D	402	-	-	-	0/1/1/1
5	EDO	B	404	-	-	1/1/1/1	-
2	NAP	D	401	-	-	6/35/67/67	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	NAP	C2N-N1N	3.21	1.38	1.35
2	B	401	NAP	P2B-O2B	3.04	1.64	1.59
2	A	401	NAP	C2N-N1N	2.87	1.38	1.35
2	D	401	NAP	P2B-O2B	2.85	1.64	1.59
2	B	401	NAP	C2N-N1N	2.69	1.37	1.35
2	D	401	NAP	PA-O3	2.57	1.62	1.59
2	A	401	NAP	P2B-O2B	2.47	1.63	1.59
3	B	402	LYS	OXT-C	-2.25	1.23	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NAP	C4D-O4D-C1D	-4.99	105.36	109.92
2	B	401	NAP	O4B-C1B-N9A	4.06	115.88	108.09
2	D	401	NAP	O4B-C1B-N9A	4.01	115.80	108.09
2	B	401	NAP	C3B-C2B-C1B	-3.99	95.18	102.81
2	B	401	NAP	O4B-C1B-C2B	-3.97	99.75	106.59
2	A	401	NAP	C4D-O4D-C1D	-3.46	106.76	109.92
2	A	401	NAP	O4B-C1B-C2B	-3.45	100.64	106.59
2	D	401	NAP	C3B-C2B-C1B	-3.37	96.35	102.81
2	A	401	NAP	P2B-O2B-C2B	-3.25	114.75	123.43
2	A	401	NAP	O4B-C1B-N9A	3.23	114.30	108.09
2	B	401	NAP	C4B-O4B-C1B	-3.10	102.63	109.47
2	D	401	NAP	O4B-C1B-C2B	-2.97	101.48	106.59
3	B	402	LYS	OXT-C-O	-2.97	117.35	124.08
2	A	401	NAP	C3B-C2B-C1B	-2.93	97.19	102.81
2	D	401	NAP	C6N-N1N-C2N	-2.68	119.60	121.88
2	D	401	NAP	C4B-O4B-C1B	-2.41	104.14	109.47
2	A	401	NAP	C6N-N1N-C2N	-2.27	119.95	121.88
2	D	401	NAP	P2B-O2B-C2B	-2.25	117.42	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	C4B-O4B-C1B	-2.16	104.69	109.47
2	B	401	NAP	O2A-PA-O1A	2.03	121.91	112.44

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	O4D-C1D-N1N-C6N
2	A	401	NAP	C2D-C1D-N1N-C2N
2	A	401	NAP	C2D-C1D-N1N-C6N
2	D	401	NAP	O4D-C1D-N1N-C2N
2	D	401	NAP	O4D-C1D-N1N-C6N
2	D	401	NAP	C2D-C1D-N1N-C2N
2	D	401	NAP	C2D-C1D-N1N-C6N
2	B	401	NAP	C3B-C2B-O2B-P2B
2	D	401	NAP	C3B-C2B-O2B-P2B
2	A	401	NAP	C3B-C2B-O2B-P2B
2	A	401	NAP	C1B-C2B-O2B-P2B
3	B	402	LYS	CE-CD-CG-CB
3	B	402	LYS	O-C-CA-CB
3	B	402	LYS	OXT-C-CA-CB
5	B	404	EDO	O1-C1-C2-O2
2	B	401	NAP	C2B-O2B-P2B-O2X
2	D	401	NAP	C2B-O2B-P2B-O2X
2	B	401	NAP	O4D-C1D-N1N-C2N
3	B	402	LYS	CA-CB-CG-CD

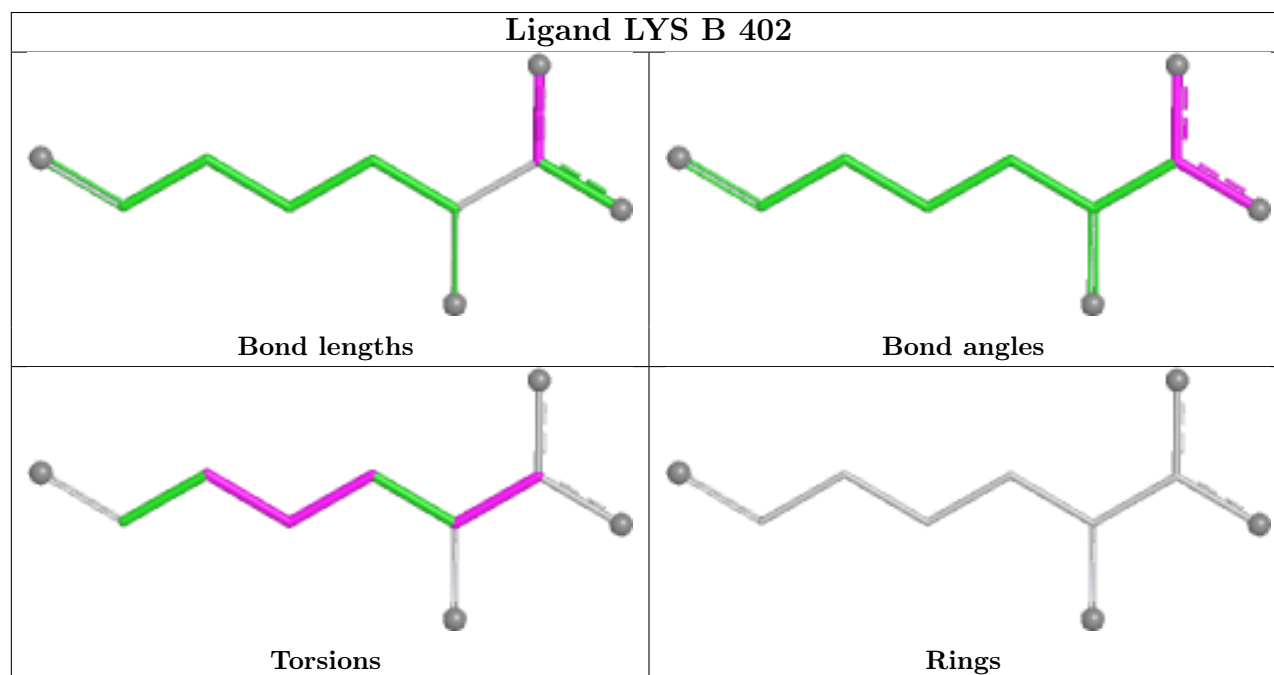
There are no ring outliers.

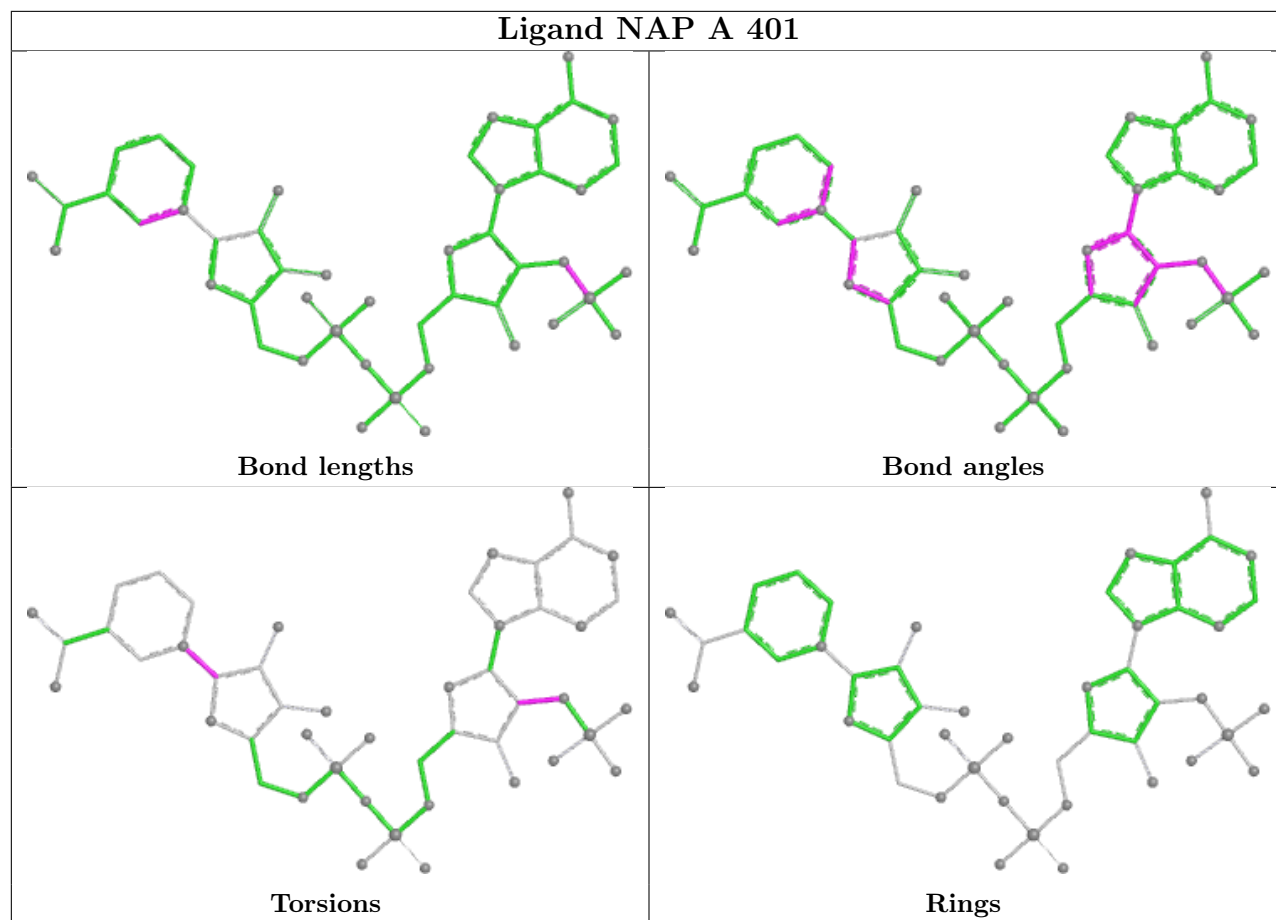
5 monomers are involved in 13 short contacts:

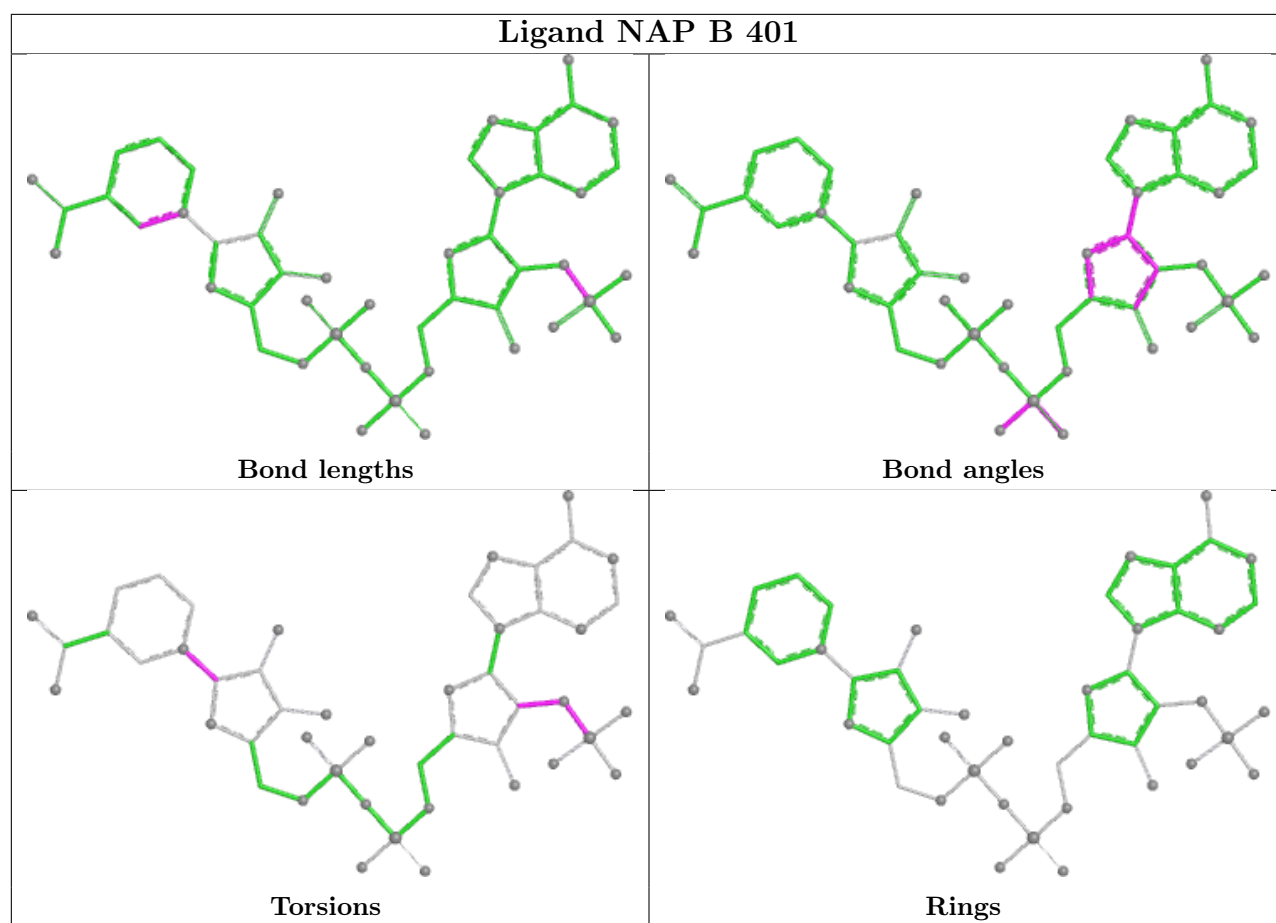
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	LYS	2	0
2	A	401	NAP	2	0
2	B	401	NAP	7	0
4	C	401	IMD	1	0
2	D	401	NAP	2	0

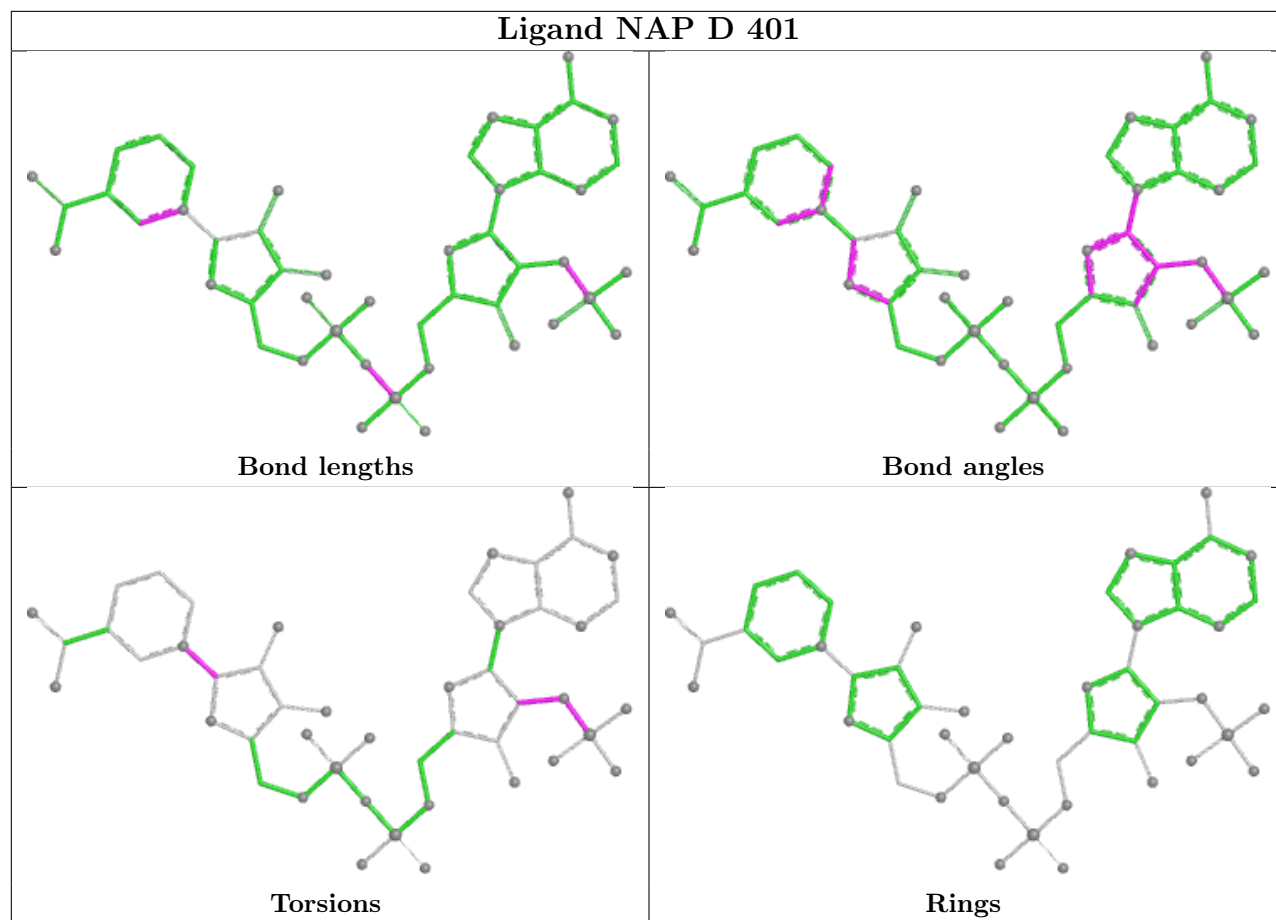
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	300/336 (89%)	0.46	16 (5%) 32 29	31, 49, 80, 99	0
1	B	299/336 (88%)	0.50	18 (6%) 27 24	30, 53, 83, 120	0
1	C	309/336 (91%)	0.16	12 (3%) 43 40	29, 44, 77, 105	0
1	D	306/336 (91%)	0.33	20 (6%) 25 22	32, 45, 73, 106	0
All	All	1214/1344 (90%)	0.36	66 (5%) 31 28	29, 47, 79, 120	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	171	LEU	6.8
1	B	173	GLN	6.0
1	B	174	LEU	5.7
1	D	164	ALA	5.5
1	A	170	THR	5.3
1	D	169	ALA	5.3
1	D	170	THR	5.2
1	D	174	LEU	4.5
1	B	171	LEU	4.4
1	D	177	LEU	4.4
1	B	170	THR	4.3
1	A	77	VAL	4.2
1	A	82	PRO	4.0
1	C	315	ARG	4.0
1	B	169	ALA	4.0
1	B	168	PRO	3.9
1	D	181	LEU	3.8
1	B	164	ALA	3.8
1	B	181	LEU	3.6
1	A	288	TYR	3.5
1	B	172	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	75	TYR	3.5
1	D	173	GLN	3.4
1	C	314	GLN	3.4
1	C	288	TYR	3.2
1	A	171	LEU	3.2
1	A	83	LEU	3.1
1	C	283	ALA	3.0
1	D	163	LEU	3.0
1	D	175	THR	2.8
1	A	155	HIS	2.8
1	B	291	PRO	2.8
1	B	175	THR	2.8
1	D	176	GLY	2.8
1	B	177	LEU	2.8
1	A	283	ALA	2.8
1	C	4	THR	2.7
1	A	164	ALA	2.7
1	D	4	THR	2.6
1	C	313	LEU	2.5
1	D	315	ARG	2.5
1	C	179	PRO	2.5
1	D	289	GLN	2.4
1	B	131	LEU	2.3
1	A	157	SER	2.3
1	D	162	SER	2.3
1	B	37	LEU	2.2
1	D	227	PRO	2.2
1	C	282	MET	2.2
1	C	6	HIS	2.2
1	A	48	PHE	2.2
1	B	281	ASP	2.2
1	A	314	GLN	2.1
1	D	129	ARG	2.1
1	B	132	ALA	2.1
1	A	163	LEU	2.1
1	B	144	LEU	2.1
1	D	313	LEU	2.1
1	A	173	GLN	2.1
1	C	168	PRO	2.1
1	D	172	ALA	2.1
1	C	78	GLY	2.1
1	A	128	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	225	ASN	2.0
1	D	225	ASN	2.0
1	B	193	ASP	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](#)

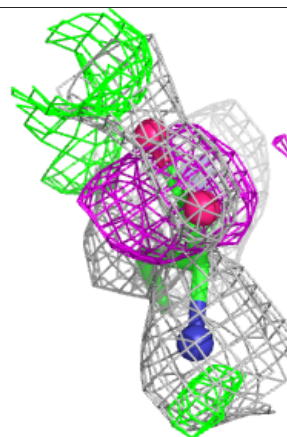
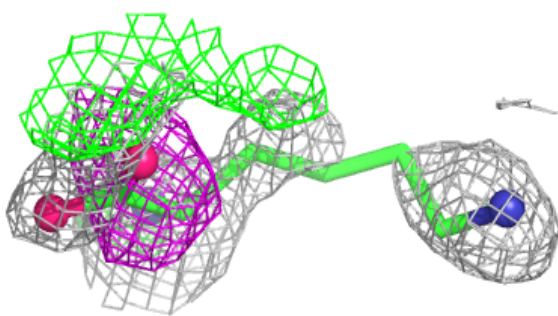
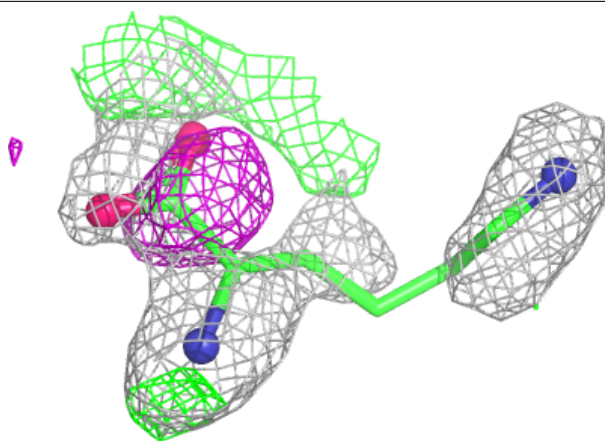
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	LYS	B	402	10/10	0.52	0.28	57,67,71,74	0
5	EDO	B	404	4/4	0.80	0.19	49,51,54,55	0
2	NAP	A	401	48/48	0.91	0.10	46,65,82,88	0
2	NAP	B	401	48/48	0.92	0.11	41,58,96,99	0
2	NAP	D	401	48/48	0.92	0.11	39,51,78,89	0
4	IMD	D	402	5/5	0.93	0.11	51,52,52,54	0
4	IMD	B	403	5/5	0.96	0.07	33,37,38,38	0
4	IMD	C	401	5/5	0.97	0.06	37,40,41,44	0

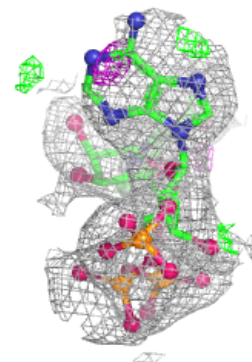
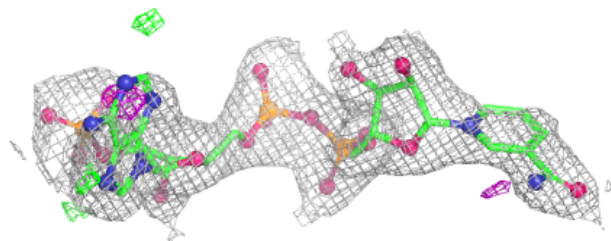
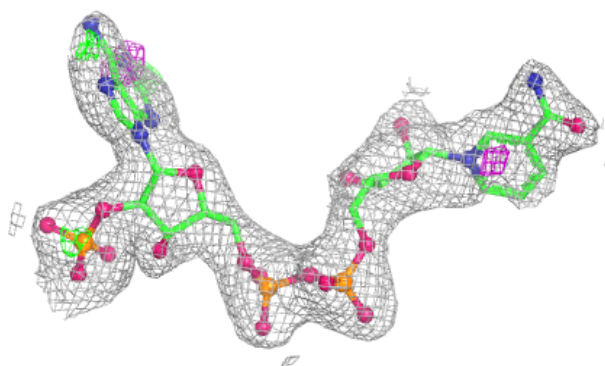
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LYS B 402:

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

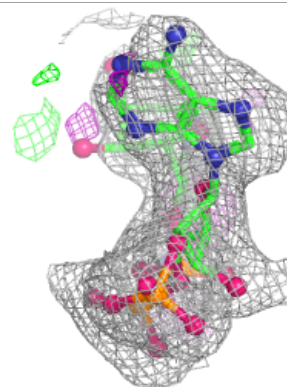
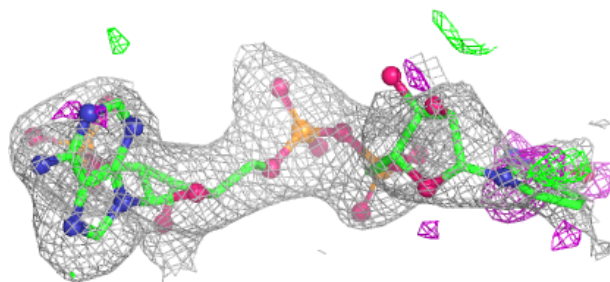
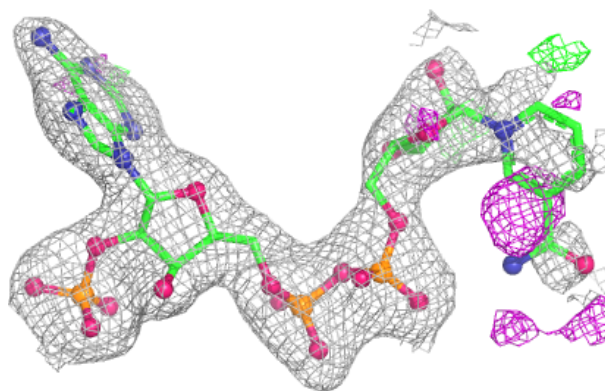
**Electron density around NAP A 401:**

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

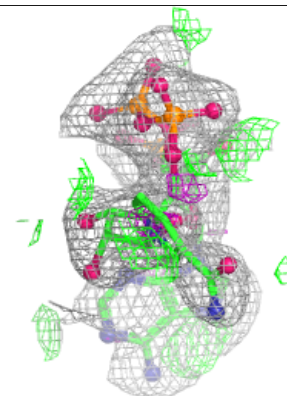
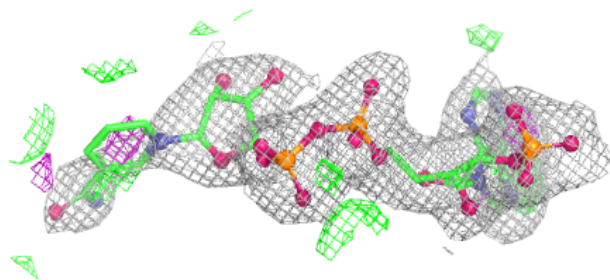
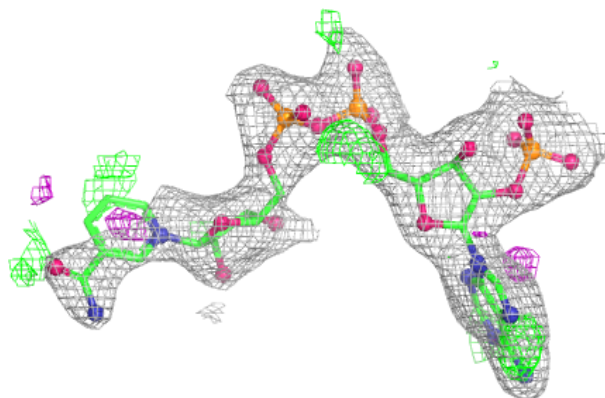


Electron density around NAP B 401:

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

**Electron density around NAP D 401:**

$2mF_o-DF_c$ (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.