



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 06:21 PM JST

PDB ID : 8J1C
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

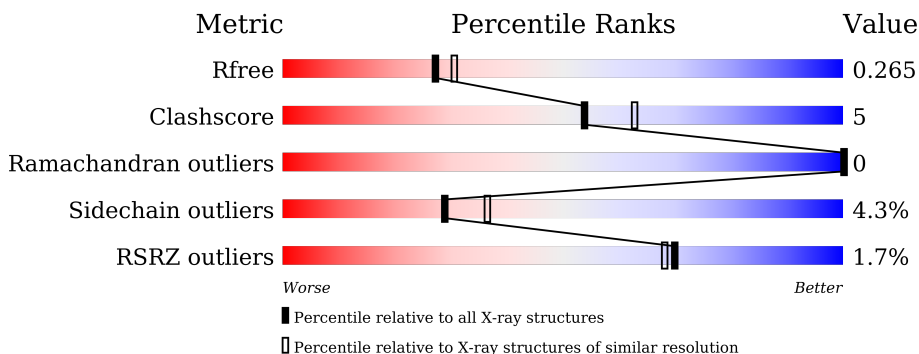
1 Overall quality at a glance

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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	 2% 79% 9% • 11%
1	B	336	 2% 74% 13% • 11%
1	C	336	 % 80% 12% • 8%
1	D	336	 2% 78% 12% • 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LYS	B	402	-	-	-	X

2 Entry composition i

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

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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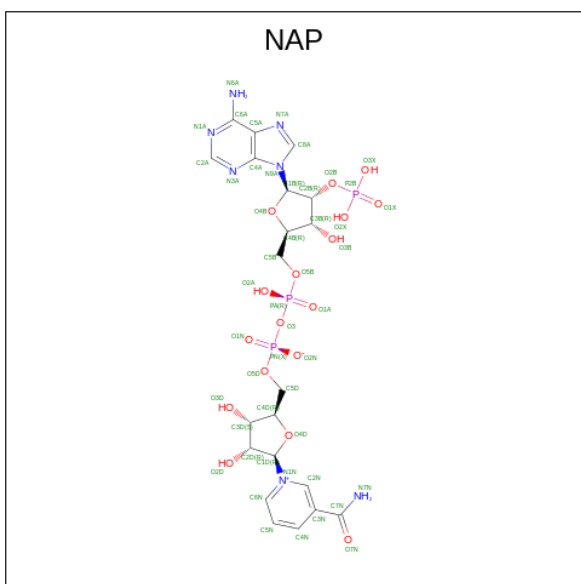
Chain	Residue	Modelled	Actual	Comment	Reference
B	316	ASP	-	expression tag	UNP A0A7Y0ZV07
B	317	PRO	-	expression tag	UNP A0A7Y0ZV07
B	318	ASN	-	expression tag	UNP A0A7Y0ZV07
B	319	SER	-	expression tag	UNP A0A7Y0ZV07
B	320	SER	-	expression tag	UNP A0A7Y0ZV07
B	321	SER	-	expression tag	UNP A0A7Y0ZV07
B	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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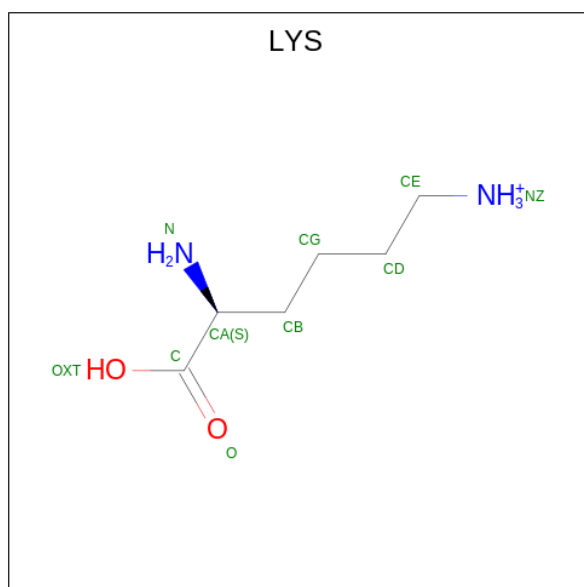
Chain	Residue	Modelled	Actual	Comment	Reference
D	316	ASP	-	expression tag	UNP A0A7Y0ZV07
D	317	PRO	-	expression tag	UNP A0A7Y0ZV07
D	318	ASN	-	expression tag	UNP A0A7Y0ZV07
D	319	SER	-	expression tag	UNP A0A7Y0ZV07
D	320	SER	-	expression tag	UNP A0A7Y0ZV07
D	321	SER	-	expression tag	UNP A0A7Y0ZV07
D	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 (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



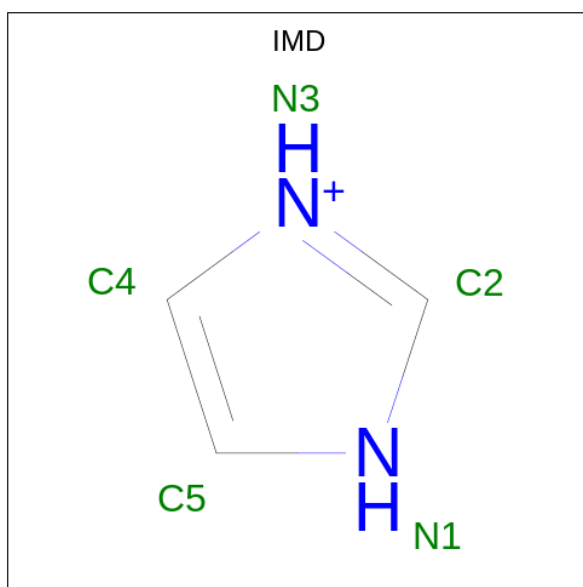
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
2	B	1	48	21	7	17	3	0	0
2	D	1	48	21	7	17	3	0	0

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



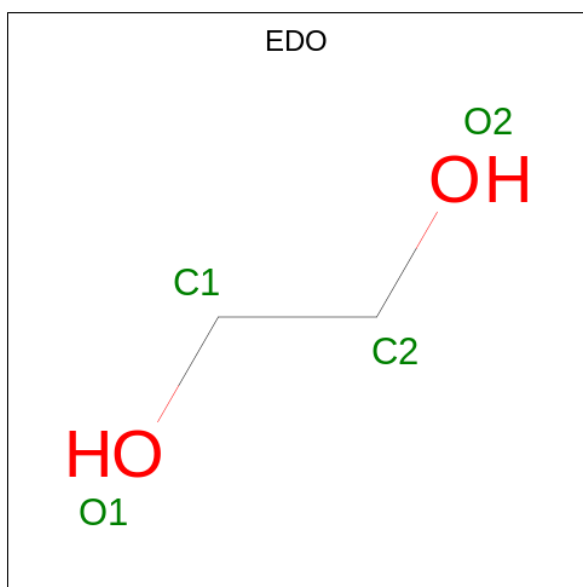
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	10	6	2	2	0	0

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

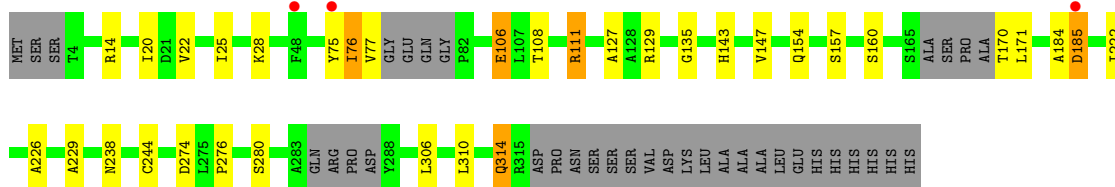
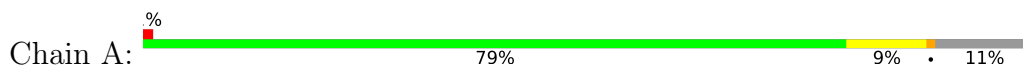
- Molecule 6 is water.

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

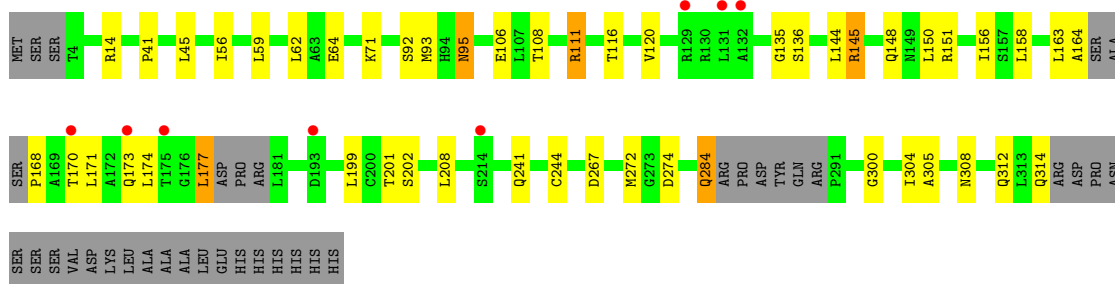
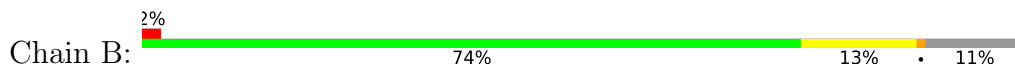
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

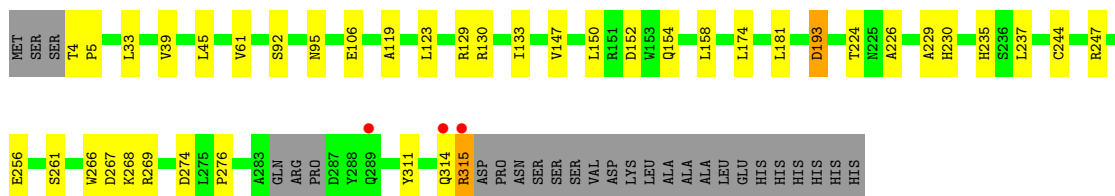
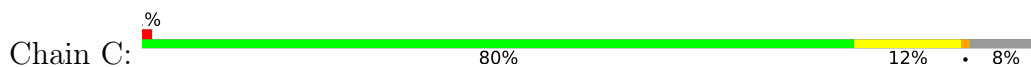
- Molecule 1: Ornithine cyclodeaminase family protein



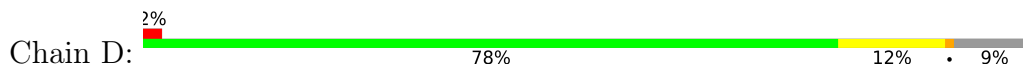
- Molecule 1: Ornithine cyclodeaminase family protein

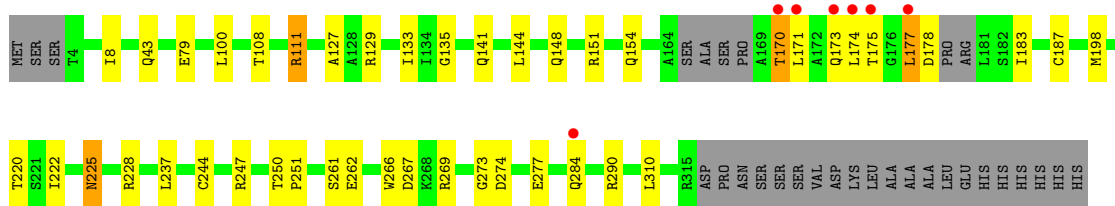


- Molecule 1: Ornithine cyclodeaminase family protein



- Molecule 1: Ornithine cyclodeaminase family protein





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 46.75 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.80-2.20) 100.0 (46.75-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.20Å)	Xtrriage
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 (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtrriage
Anisotropy	0.405	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for k,h,-l	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/2307	0.68	0/3147
1	B	0.35	0/2278	0.68	0/3108
1	C	0.37	0/2367	0.69	0/3233
1	D	0.36	0/2350	0.71	0/3207
All	All	0.36	0/9302	0.69	0/12695

There are no bond length outliers.

There are no bond angle outliers.

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	2262	0	2285	19	0
1	B	2234	0	2254	32	0
1	C	2319	0	2332	20	0
1	D	2304	0	2317	28	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	4	0
4	B	5	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	99	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 (99) 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: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:177:LEU:C	6:B:509:HOH:O	2.41	0.58
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
1:B:135:GLY:HA2	2:B:401:NAP:H1B	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:163:LEU:O	1:B:164:ALA:C	2.50	0.49
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:D:133:ILE:HD12	1:D:144:LEU:HD13	1.95	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: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:D:43:GLN:HG2	6:D:535:HOH:O	2.18	0.43
1:B:111:ARG:HH22	3:B:402:LYS:HZ1	1.66	0.43
1:C:4:THR:HB	1:C:5:PRO:HA	2.01	0.43
1:B:71:LYS:HZ1	3:B:402:LYS:HE3	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:LEU:C	1:C:45:LEU:HD23	2.39	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:D:228:ARG:HH22	1:D:262:GLU:CD	2.23	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: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
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
1:D:175:THR:C	1:D:177:LEU:N	2.73	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%)	227 (95%)	11 (5%)	27	34
1	B	234/267 (88%)	223 (95%)	11 (5%)	26	33
1	C	243/267 (91%)	236 (97%)	7 (3%)	42	54
1	D	241/267 (90%)	229 (95%)	12 (5%)	24	30
All	All	956/1068 (90%)	915 (96%)	41 (4%)	29	36

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	TYR
1	A	76	ILE
1	A	77	VAL
1	A	106	GLU
1	A	111	ARG
1	A	154	GLN
1	A	157	SER
1	A	160	SER

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Mol	Chain	Res	Type
1	A	185	ASP
1	A	310	LEU
1	A	314	GLN
1	B	14	ARG
1	B	64	GLU
1	B	95	ASN
1	B	111	ARG
1	B	145	ARG
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	152	ASP
1	C	193	ASP
1	C	237	LEU
1	C	247	ARG
1	C	268	LYS
1	C	315	ARG
1	D	79	GLU
1	D	111	ARG
1	D	151	ARG
1	D	154	GLN
1	D	170	THR
1	D	177	LEU
1	D	225	ASN
1	D	237	LEU
1	D	247	ARG
1	D	284	GLN
1	D	290	ARG
1	D	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	154	GLN
1	A	314	GLN
1	B	43	GLN
1	B	95	ASN

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Mol	Chain	Res	Type
1	B	97	GLN
1	B	238	ASN
1	C	24	GLN
1	C	43	GLN
1	C	148	GLN
1	C	225	ASN
1	C	238	ASN
1	C	248	GLN
1	D	97	GLN
1	D	155	HIS
1	D	173	GLN
1	D	241	GLN
1	D	284	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	EDO	B	404	-	3,3,3	1.22	0	2,2,2	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	A	401	-	45,52,52	0.78	2 (4%)	56,80,80	1.01	4 (7%)
4	IMD	B	403	-	3,5,5	0.26	0	4,5,5	0.75	0
2	NAP	D	401	-	45,52,52	0.83	2 (4%)	56,80,80	1.07	4 (7%)
3	LYS	B	402	-	8,9,9	0.82	1 (12%)	9,10,10	1.26	2 (22%)
2	NAP	B	401	-	45,52,52	0.82	2 (4%)	56,80,80	1.22	3 (5%)
4	IMD	C	401	-	3,5,5	0.23	0	4,5,5	0.61	0
4	IMD	D	402	-	3,5,5	0.24	0	4,5,5	0.66	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
5	EDO	B	404	-	-	1/1/1/1	-
2	NAP	A	401	-	-	7/31/67/67	0/5/5/5
2	NAP	D	401	-	-	7/31/67/67	0/5/5/5
4	IMD	B	403	-	-	-	0/1/1/1
3	LYS	B	402	-	-	4/9/9/9	-
2	NAP	B	401	-	-	3/31/67/67	0/5/5/5
4	IMD	C	401	-	-	-	0/1/1/1
4	IMD	D	402	-	-	-	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	P2B-O2B	2.94	1.64	1.59
2	D	401	NAP	C2N-N1N	2.91	1.38	1.35
2	D	401	NAP	P2B-O2B	2.76	1.64	1.59
2	A	401	NAP	C2N-N1N	2.61	1.38	1.35
2	B	401	NAP	C2N-N1N	2.44	1.37	1.35
2	A	401	NAP	P2B-O2B	2.41	1.63	1.59
3	B	402	LYS	OXT-C	-2.16	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NAP	C3B-C2B-C1B	-4.10	95.18	102.89
2	B	401	NAP	O4B-C1B-C2B	-3.94	99.75	106.59
2	D	401	NAP	C3B-C2B-C1B	-3.48	96.35	102.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	O4B-C1B-C2B	-3.43	100.64	106.59
2	A	401	NAP	C3B-C2B-C1B	-3.03	97.19	102.89
3	B	402	LYS	OXT-C-O	-2.97	117.35	124.09
2	D	401	NAP	O4B-C1B-C2B	-2.94	101.48	106.59
2	D	401	NAP	C6N-N1N-C2N	-2.61	119.60	121.97
2	B	401	NAP	C5A-C6A-N6A	2.30	123.85	120.35
2	A	401	NAP	C6N-N1N-C2N	-2.22	119.95	121.97
3	B	402	LYS	OXT-C-CA	2.22	120.94	113.38
2	D	401	NAP	C4A-C5A-N7A	2.13	111.62	109.40
2	A	401	NAP	C5A-C6A-N6A	2.02	123.42	120.35

There are no chirality outliers.

All (22) torsion outliers are listed below:

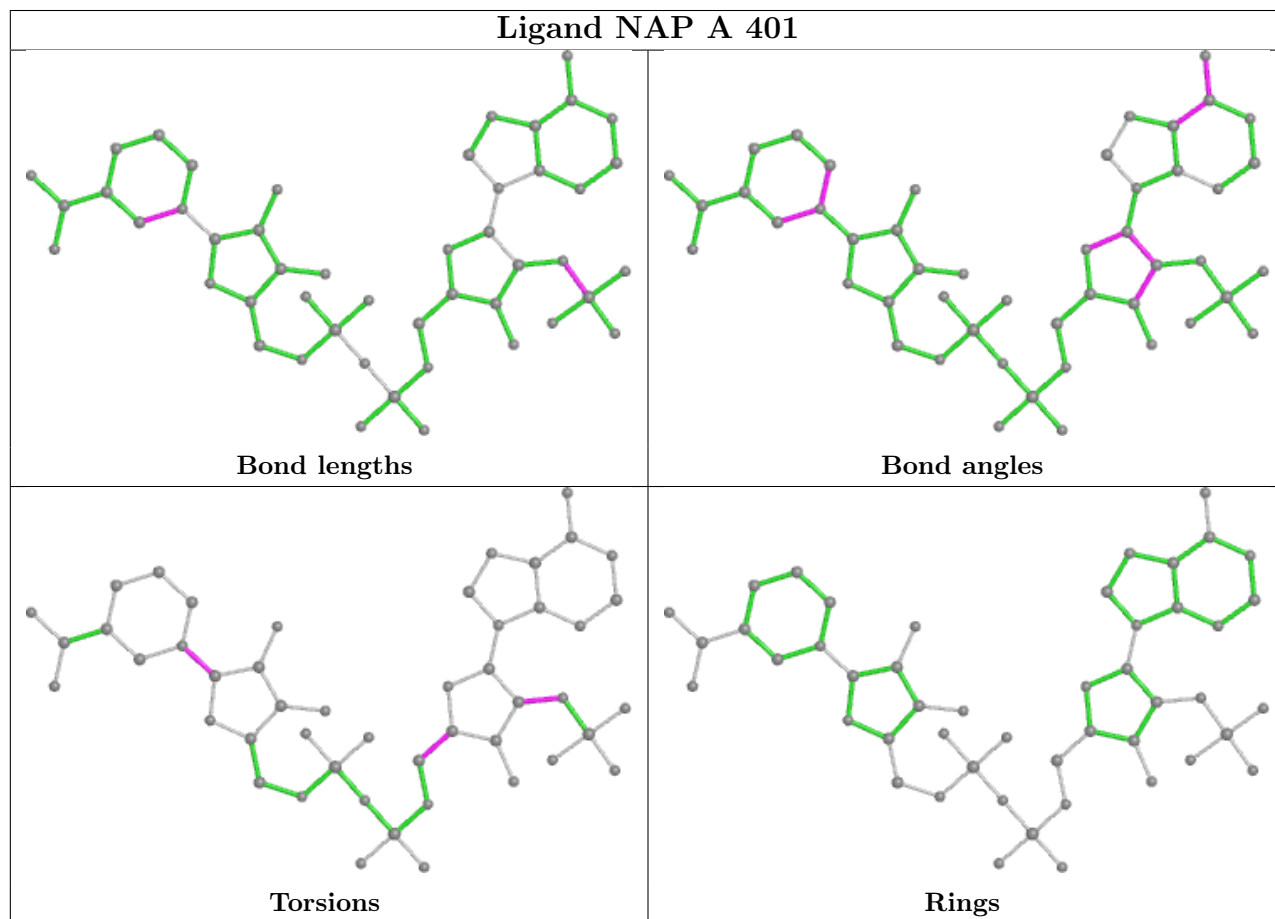
Mol	Chain	Res	Type	Atoms
2	A	401	NAP	O4D-C1D-N1N-C2N
2	A	401	NAP	O4D-C1D-N1N-C6N
2	A	401	NAP	C2D-C1D-N1N-C2N
2	A	401	NAP	C2D-C1D-N1N-C6N
2	D	401	NAP	C2B-O2B-P2B-O2X
2	D	401	NAP	O4D-C1D-N1N-C2N
2	D	401	NAP	O4D-C1D-N1N-C6N
2	D	401	NAP	C2D-C1D-N1N-C2N
2	D	401	NAP	C2D-C1D-N1N-C6N
2	B	401	NAP	C3B-C2B-O2B-P2B
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
5	B	404	EDO	O1-C1-C2-O2
3	B	402	LYS	OXT-C-CA-CB
2	B	401	NAP	C2B-O2B-P2B-O2X
3	B	402	LYS	O-C-CA-CB
3	B	402	LYS	CA-CB-CG-CD
2	A	401	NAP	O4B-C4B-C5B-O5B
2	B	401	NAP	O4B-C4B-C5B-O5B
2	D	401	NAP	O4B-C4B-C5B-O5B

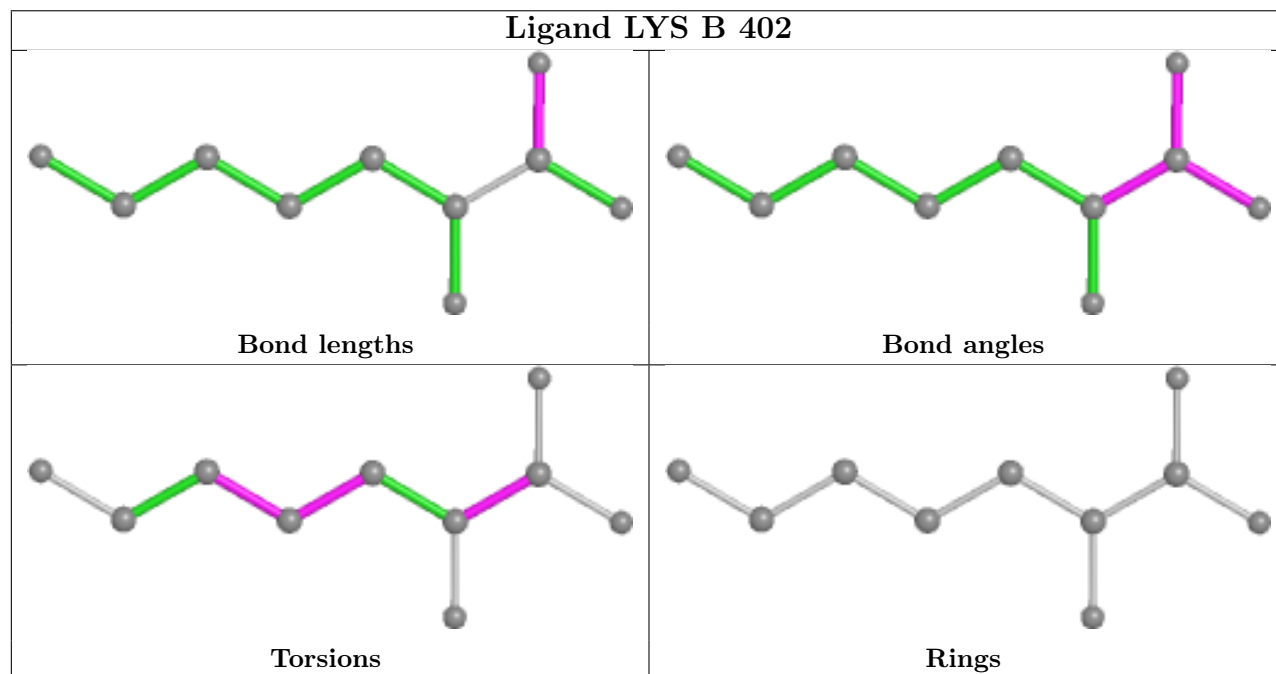
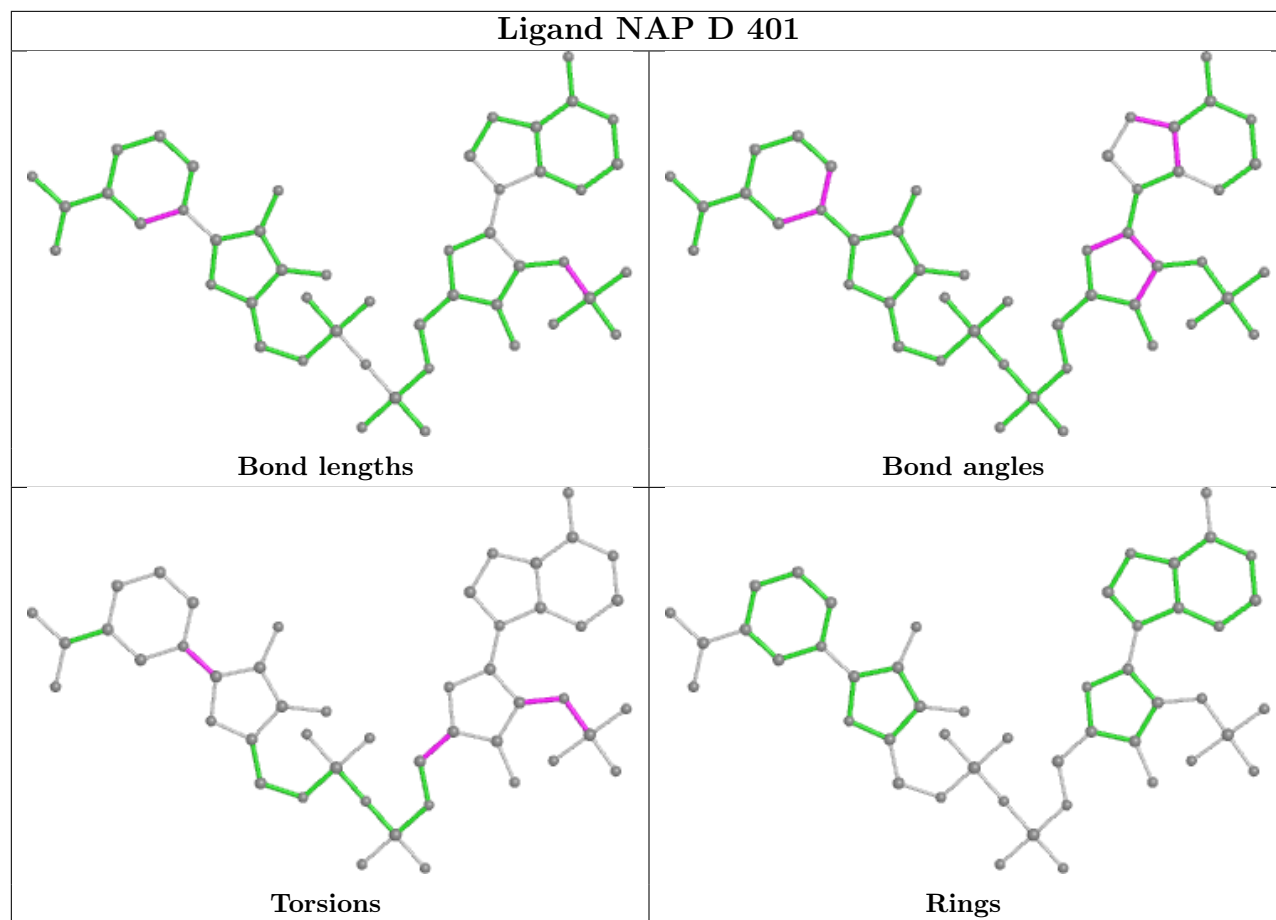
There are no ring outliers.

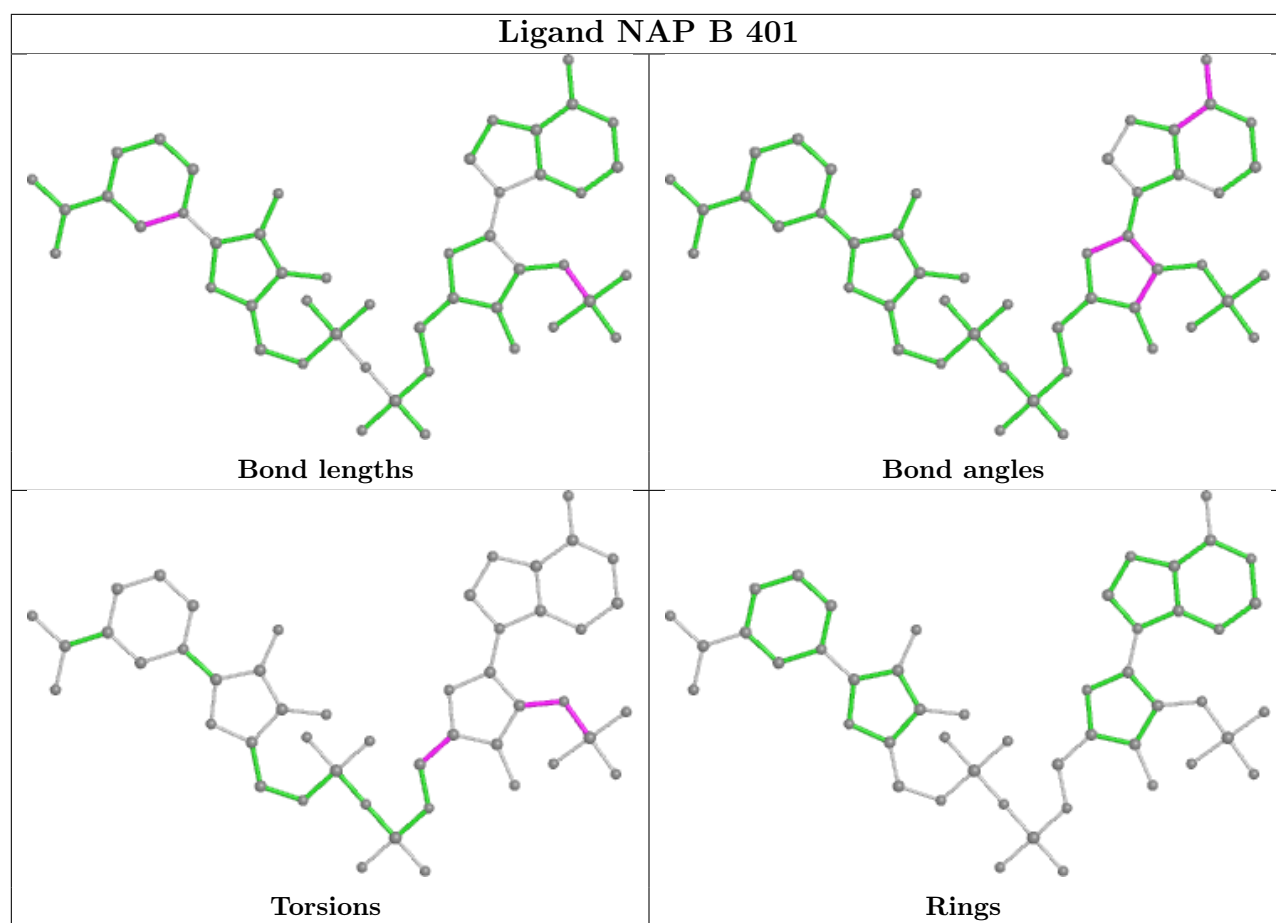
5 monomers are involved in 15 short contacts:

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

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%)	-0.03	3 (1%) 82 81	31, 49, 80, 99	0
1	B	299/336 (88%)	-0.01	8 (2%) 54 52	30, 53, 83, 120	0
1	C	309/336 (91%)	-0.23	3 (0%) 82 81	29, 44, 77, 105	0
1	D	306/336 (91%)	-0.14	7 (2%) 60 58	32, 45, 73, 106	0
All	All	1214/1344 (90%)	-0.10	21 (1%) 70 68	29, 47, 79, 120	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	170	THR	5.7
1	B	173	GLN	4.4
1	B	170	THR	4.3
1	D	171	LEU	4.2
1	D	177	LEU	3.9
1	D	173	GLN	3.6
1	A	75	TYR	3.1
1	B	129	ARG	3.1
1	C	314	GLN	2.9
1	C	315	ARG	2.8
1	D	174	LEU	2.7
1	B	193	ASP	2.7
1	A	185	ASP	2.7
1	D	284	GLN	2.6
1	B	132	ALA	2.6
1	D	175	THR	2.6
1	B	131	LEU	2.6
1	B	175	THR	2.5
1	C	289	GLN	2.2
1	B	214	SER	2.0
1	A	48	PHE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

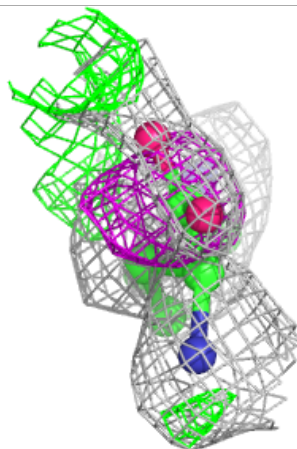
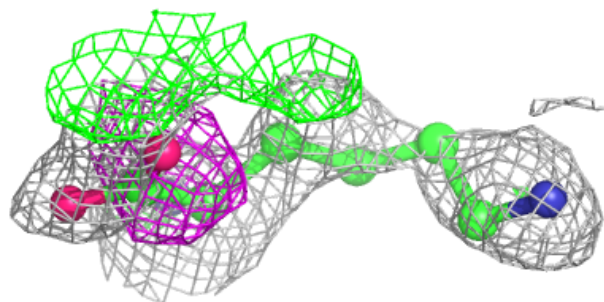
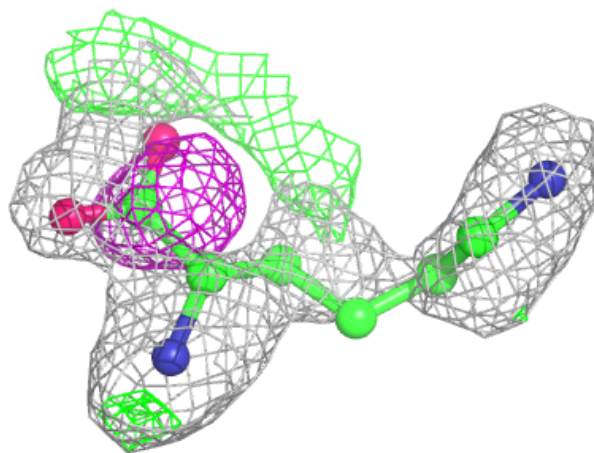
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LYS	B	402	10/10	0.33	0.41	57,67,71,74	0
5	EDO	B	404	4/4	0.80	0.20	49,51,54,55	0
2	NAP	A	401	48/48	0.91	0.17	46,65,82,88	0
2	NAP	B	401	48/48	0.94	0.17	41,58,96,99	0
2	NAP	D	401	48/48	0.95	0.14	39,51,78,89	0
4	IMD	D	402	5/5	0.97	0.14	51,52,52,54	0
4	IMD	B	403	5/5	0.98	0.15	33,37,38,38	0
4	IMD	C	401	5/5	0.98	0.12	37,40,41,44	0

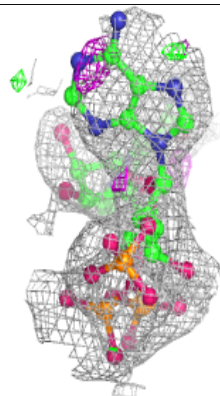
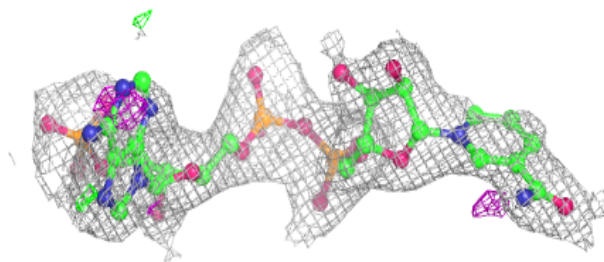
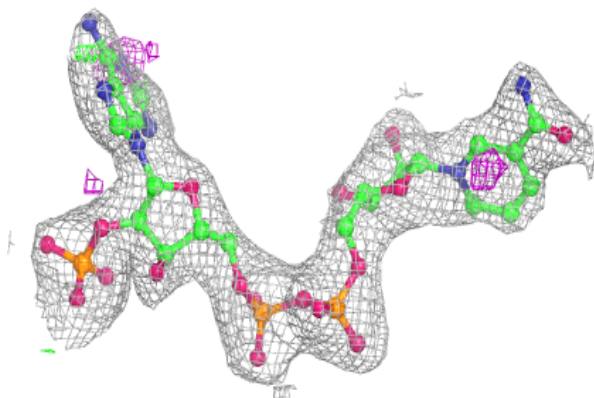
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

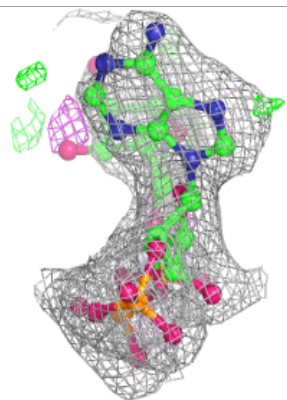
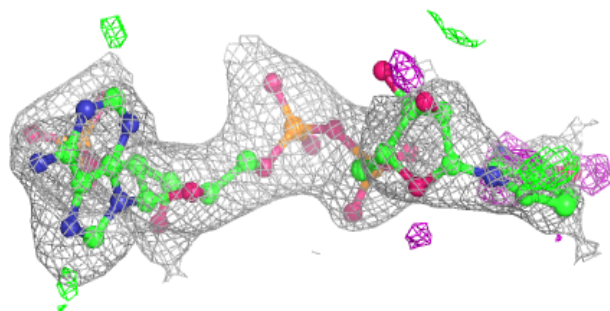
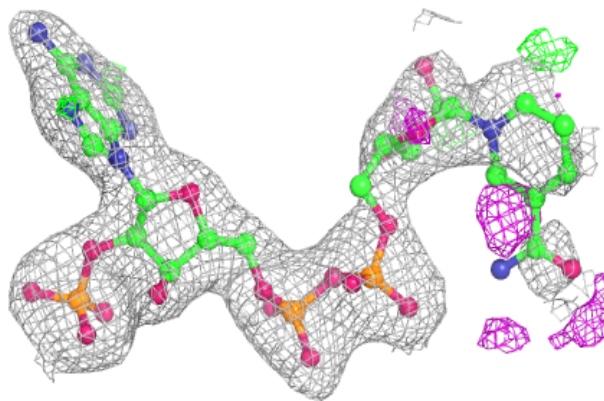
**Electron density around NAP A 401:**

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

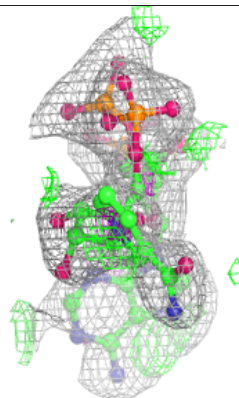
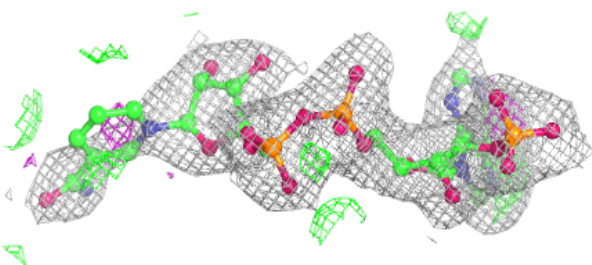
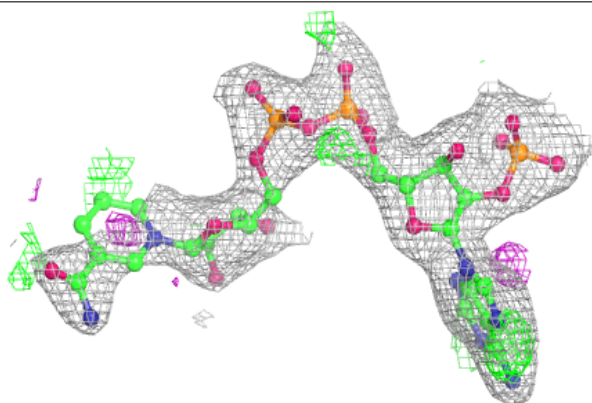


Electron density around NAP B 401:

$2mF_o-DF_c$ (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.