



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 03:15 PM JST

PDB ID : 6A0U  
Title : Homoserine dehydrogenase K195A mutant from *Thermus thermophilus* HB8 complexed with HSE and NADP+  
Authors : Akai, S.; Ikushiro, H.; Sawai, T.; Yano, T.; Kamiya, N.; Miyahara, I.  
Deposited on : 2018-06-06  
Resolution : 1.93 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](mailto: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>.

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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 : 2.36  
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) : 2.36

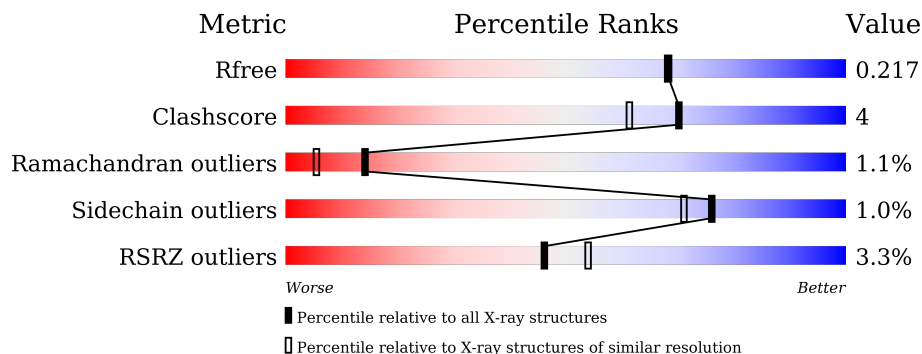
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

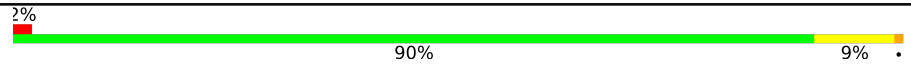
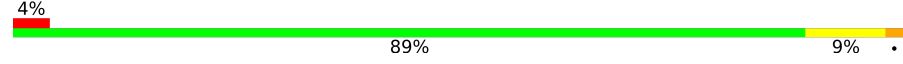
The reported resolution of this entry is 1.93 Å.

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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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  $\geq 3$ , 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	332	 2% 90% 9% .
1	B	332	 4% 89% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	HSE	B	409	-	X	-	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5935 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.

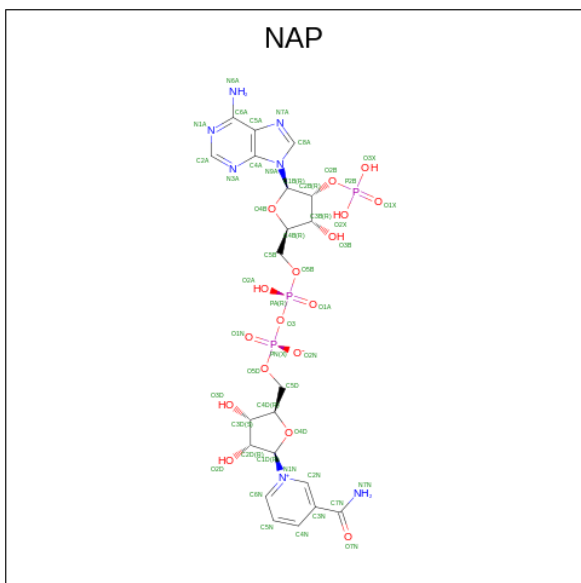
- Molecule 1 is a protein called Homoserine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	331	Total 2596	C 1659	N 454	O 479	S 4	0	15	0
1	A	331	Total 2603	C 1662	N 460	O 477	S 4	0	14	0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

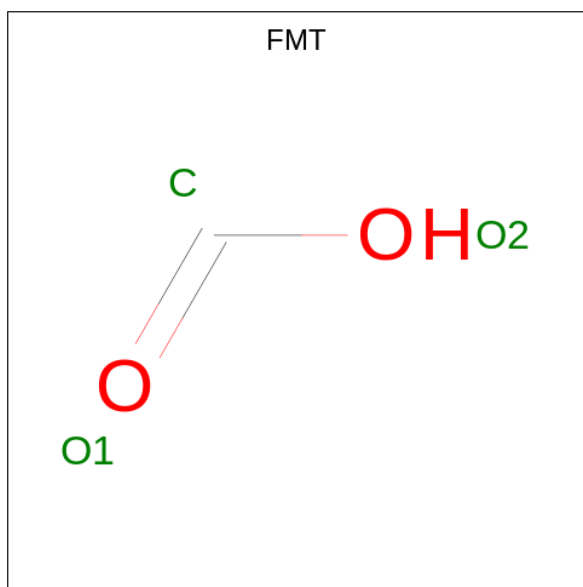
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	B	1	Total 1	Na 1	0	0
2	A	1	Total 1	Na 1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



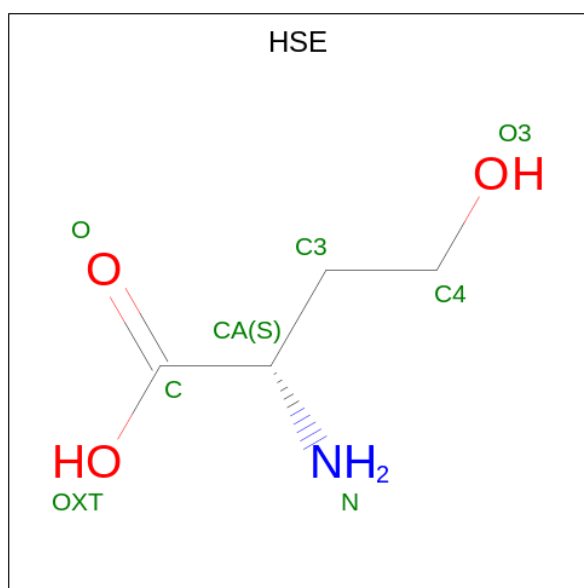
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
4	B	1	3	1 2	0	0
4	B	1	3	1 2	0	0
4	B	1	3	1 2	0	0
4	B	1	3	1 2	0	0
4	B	1	3	1 2	0	0
4	B	1	3	1 2	0	0
4	A	1	3	1 2	0	0
4	A	1	3	1 2	0	0
4	A	1	3	1 2	0	0
4	A	1	3	1 2	0	0

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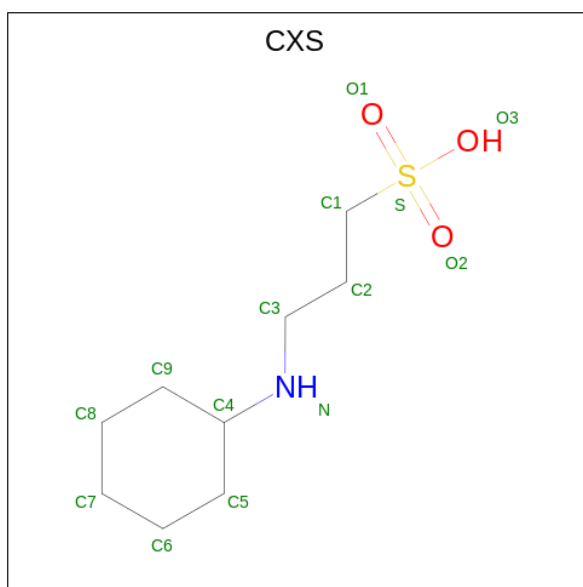
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		
4	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is L-HOMOSERINE (three-letter code: HSE) (formula:  $C_4H_9NO_3$ ).



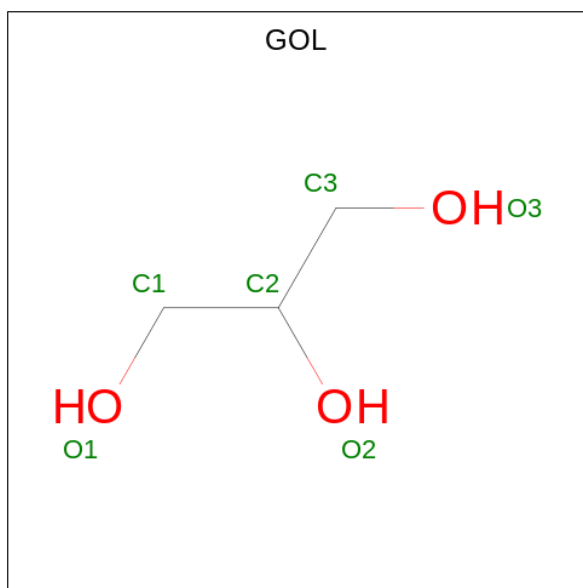
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula:  $C_9H_{19}NO_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	B	1	14	9	1	3	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 8 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	11	2		

- Molecule 9 is water.

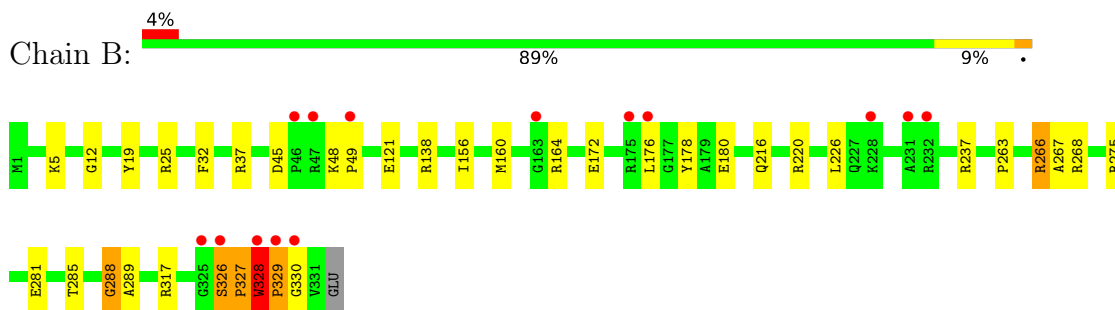
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	249	Total	O	0	12
			254	254		
9	A	276	Total	O	0	15
			284	284		



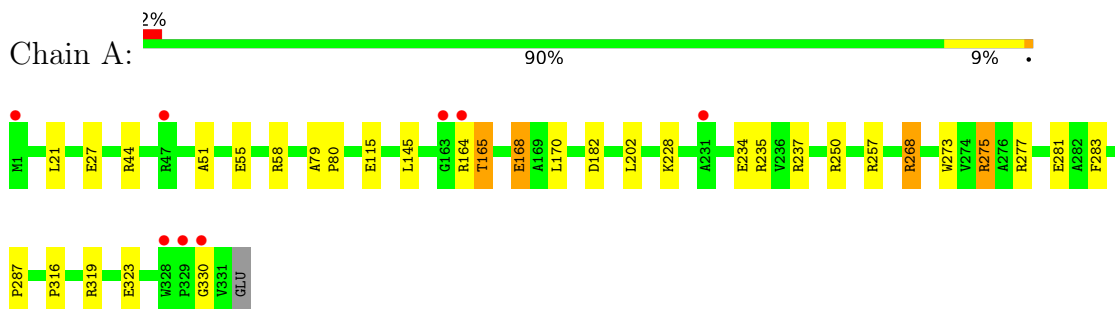
### 3 Residue-property plots [i](#)

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: Homoserine dehydrogenase



- Molecule 1: Homoserine dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.67Å 119.67Å 143.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.93 37.40 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-1.93) 99.9 (37.40-1.93)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.79 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.172 , 0.212 0.182 , 0.217	Depositor DCC
$R_{free}$ test set	4475 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtrriage
Anisotropy	0.022	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5935	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CXS, GOL, NAP, HSE, FMT, UNL, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.31	3/2662 (0.1%)	1.19	15/3622 (0.4%)
1	B	1.36	4/2661 (0.2%)	1.23	16/3624 (0.4%)
All	All	1.33	7/5323 (0.1%)	1.21	31/7246 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	GLY	C-O	8.37	1.37	1.23
1	A	165	THR	C-O	7.95	1.38	1.23
1	A	55	GLU	CD-OE1	6.40	1.32	1.25
1	B	178	TYR	CE1-CZ	6.23	1.46	1.38
1	A	168	GLU	C-O	6.09	1.34	1.23
1	B	266	ARG	CD-NE	5.34	1.55	1.46
1	B	19	TYR	CE1-CZ	-5.23	1.31	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	SER	N-CA-C	-9.63	85.01	111.00
1	A	275	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	A	275	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	A	235	ARG	NE-CZ-NH2	7.94	124.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	A	250	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	178	TYR	CB-CG-CD1	6.74	125.04	121.00
1	A	268[A]	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	A	268[B]	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	A	250	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	5	LYS	CD-CE-NZ	-6.48	96.80	111.70
1	B	237	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	37	ARG	NE-CZ-NH2	6.47	123.53	120.30
1	B	275	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	178	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	A	234	GLU	OE1-CD-OE2	-6.37	115.65	123.30
1	B	275	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	25	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	237	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	164	ARG	NE-CZ-NH2	5.79	123.19	120.30
1	B	180	GLU	OE1-CD-OE2	5.60	130.02	123.30
1	A	182	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	257	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	B	164	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	237	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	138	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	58	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	170	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	B	328	TRP	N-CA-C	5.16	124.94	111.00
1	B	237	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	121	GLU	OE1-CD-OE2	5.01	129.31	123.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	266	ARG	Mainchain
1	B	327	PRO	Peptide
1	B	328	TRP	Peptide

## 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	2603	0	2623	20	0
1	B	2596	0	2611	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	48	0	25	2	0
3	B	48	0	25	2	0
4	A	27	0	10	2	0
4	B	18	0	6	0	0
5	A	8	0	3	1	0
5	B	8	0	3	1	0
6	B	14	0	19	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	B	13	0	0	0	0
9	A	284	0	0	4	1
9	B	254	0	0	2	1
All	All	5935	0	5341	39	1

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 4.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HG2	1:A:281[B]:GLU:HG2	1.63	0.81
1:B:327:PRO:O	1:B:328:TRP:HB2	1.90	0.71
1:B:32:PHE:CE1	1:A:316:PRO:HG3	2.31	0.66
1:B:328:TRP:HA	1:B:328:TRP:CE3	2.31	0.65
1:B:48:LYS:HB2	1:B:49:PRO:CD	2.27	0.64
1:A:21[A]:LEU:C	1:A:21[A]:LEU:HD23	2.20	0.61
1:B:327:PRO:O	1:B:328:TRP:CB	2.50	0.59
1:A:165:THR:HG21	4:A:411:FMT:C	2.36	0.56
1:A:165:THR:OG1	1:A:168:GLU:HG3	2.06	0.55
1:A:277[B]:ARG:NH1	9:A:503:HOH:O	2.43	0.52
1:B:328:TRP:HE3	1:B:329:PRO:CD	2.22	0.52
1:B:45[A]:ASP:OD2	1:B:48:LYS:HB3	2.10	0.51
1:B:156:ILE:HG22	1:B:160:MET:HE2	1.93	0.51
1:A:275:ARG:HG2	1:A:281[B]:GLU:CG	2.39	0.49
1:B:220:ARG:CZ	9:B:521:HOH:O	2.60	0.49
1:A:273:TRP:CH2	1:A:275:ARG:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281[A]:GLU:OE1	1:A:268[A]:ARG:NH1	2.42	0.48
1:B:268[A]:ARG:CZ	1:B:268[A]:ARG:HB3	2.43	0.48
1:A:79:ALA:HB3	1:A:80:PRO:CD	2.43	0.48
1:B:328:TRP:HA	1:B:328:TRP:HE3	1.77	0.48
1:B:156:ILE:HG22	1:B:160:MET:CE	2.43	0.47
1:A:228:LYS:HG2	9:A:690:HOH:O	2.14	0.47
1:B:289:ALA:HA	3:B:402:NAP:H4N	1.96	0.46
1:B:48:LYS:CB	1:B:49:PRO:CD	2.93	0.46
1:A:115:GLU:HG3	9:A:749:HOH:O	2.16	0.45
1:B:160:MET:HB2	1:B:226:LEU:HD12	1.99	0.45
1:B:288:GLY:O	5:B:409:HSE:H41	2.16	0.45
1:B:317:ARG:NH1	1:A:27[B]:GLU:OE2	2.50	0.44
1:A:277[B]:ARG:HD3	9:A:667:HOH:O	2.17	0.44
1:B:216[A]:GLN:OE1	1:B:220:ARG:NH2	2.50	0.44
1:B:12:GLY:HA3	3:B:402:NAP:O5B	2.17	0.43
1:A:202:LEU:C	1:A:202:LEU:HD23	2.38	0.43
1:B:220:ARG:NH2	9:B:521:HOH:O	2.52	0.43
1:B:285[B]:THR:OG1	1:A:283[B]:PHE:CE2	2.65	0.43
3:A:402:NAP:C4N	5:A:412:HSE:H42	2.50	0.41
1:A:44:ARG:HG3	3:A:402:NAP:C4A	2.51	0.41
1:B:281[A]:GLU:O	1:A:287:PRO:HD3	2.20	0.41
1:A:145:LEU:C	1:A:145:LEU:HD23	2.42	0.40
1:A:51:ALA:H	4:A:407:FMT:C	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:680:HOH:O	9:A:501:HOH:O[3_455]	2.03	0.17

## 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	343/332 (103%)	330 (96%)	12 (4%)	1 (0%)	41	32
1	B	344/332 (104%)	326 (95%)	11 (3%)	7 (2%)	7	1
All	All	687/664 (104%)	656 (96%)	23 (3%)	8 (1%)	14	4

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	326	SER
1	B	328	TRP
1	B	329	PRO
1	B	176	LEU
1	B	330	GLY
1	A	330	GLY
1	B	267[A]	ALA
1	B	267[B]	ALA

### 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	257/248 (104%)	255 (99%)	2 (1%)	81	78
1	B	257/248 (104%)	254 (99%)	3 (1%)	71	64
All	All	514/496 (104%)	509 (99%)	5 (1%)	76	71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	172	GLU
1	B	263	PRO
1	B	328	TRP
1	A	319	ARG
1	A	323	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 25 ligands modelled in this entry, 2 are monoatomic and 1 is unknown - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FMT	A	403	-	2,2,2	0.60	0	1,1,1	0.63	0
4	FMT	B	405	-	2,2,2	0.76	0	1,1,1	0.65	0
4	FMT	A	404	-	2,2,2	0.45	0	1,1,1	0.82	0
4	FMT	B	406	-	2,2,2	1.09	0	1,1,1	0.68	0
4	FMT	A	410	-	2,2,2	1.05	0	1,1,1	0.52	0
4	FMT	B	403	-	2,2,2	0.29	0	1,1,1	0.19	0
7	GOL	B	411	-	5,5,5	0.76	0	5,5,5	0.89	0
4	FMT	A	409	-	2,2,2	0.45	0	1,1,1	1.23	0
4	FMT	B	408	-	2,2,2	0.96	0	1,1,1	0.81	0
3	NAP	A	402	-	45,52,52	1.56	9 (20%)	56,80,80	1.69	16 (28%)
4	FMT	B	407	-	2,2,2	0.72	0	1,1,1	0.89	0
4	FMT	A	405	-	2,2,2	0.67	0	1,1,1	0.92	0
5	HSE	B	409	-	6,7,7	2.45	4 (66%)	6,8,8	2.06	4 (66%)
4	FMT	A	408	-	2,2,2	0.65	0	1,1,1	0.41	0
4	FMT	A	407	-	2,2,2	0.72	0	1,1,1	0.97	0
4	FMT	A	406	-	2,2,2	0.96	0	1,1,1	0.80	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAP	B	402	-	45,52,52	1.84	11 (24%)	56,80,80	1.76	9 (16%)
7	GOL	A	413	-	5,5,5	1.11	0	5,5,5	1.74	1 (20%)
5	HSE	A	412	-	6,7,7	1.09	1 (16%)	6,8,8	1.97	2 (33%)
4	FMT	B	404	-	2,2,2	0.87	0	1,1,1	0.72	0
6	CXS	B	410	-	14,14,14	2.15	2 (14%)	18,18,18	1.63	4 (22%)
4	FMT	A	411	-	2,2,2	1.50	0	1,1,1	0.33	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	HSE	B	409	-	-	3/7/7/7	-
5	HSE	A	412	-	-	0/7/7/7	-
7	GOL	B	411	-	-	4/4/4/4	-
3	NAP	A	402	-	-	4/31/67/67	0/5/5/5
6	CXS	B	410	-	-	5/8/16/16	0/1/1/1
3	NAP	B	402	-	-	4/31/67/67	0/5/5/5
7	GOL	A	413	-	-	1/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAP	O4D-C1D	6.22	1.49	1.41
6	B	410	CXS	C1-S	-5.94	1.69	1.77
6	B	410	CXS	O3-S	5.02	1.65	1.47
3	B	402	NAP	O4B-C1B	4.76	1.47	1.41
3	A	402	NAP	O4B-C1B	4.66	1.47	1.41
5	B	409	HSE	O-C	3.59	1.33	1.22
3	B	402	NAP	C2A-N3A	3.46	1.37	1.32
3	A	402	NAP	C5A-C4A	3.06	1.49	1.40
5	B	409	HSE	C3-C4	2.97	1.62	1.51
3	A	402	NAP	O4D-C1D	2.88	1.45	1.41
3	A	402	NAP	C2N-C3N	-2.75	1.34	1.39
3	A	402	NAP	C3N-C7N	-2.73	1.46	1.50
3	A	402	NAP	C4N-C3N	2.71	1.43	1.39
3	B	402	NAP	C5A-C4A	2.65	1.47	1.40
5	B	409	HSE	C3-CA	2.64	1.58	1.53
3	B	402	NAP	PN-O2N	-2.47	1.43	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAP	O4B-C4B	-2.41	1.39	1.45
3	B	402	NAP	C5B-C4B	2.36	1.59	1.51
5	B	409	HSE	O3-C4	2.25	1.53	1.42
3	A	402	NAP	C2A-N3A	2.23	1.35	1.32
3	B	402	NAP	C3N-C7N	-2.22	1.47	1.50
3	A	402	NAP	PA-O2A	-2.14	1.45	1.55
5	A	412	HSE	C3-CA	2.13	1.57	1.53
3	B	402	NAP	O4D-C4D	2.09	1.49	1.45
3	B	402	NAP	C4A-N3A	2.08	1.38	1.35
3	B	402	NAP	O5D-C5D	-2.08	1.36	1.44
3	A	402	NAP	C2D-C1D	2.03	1.56	1.53

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAP	C3N-C7N-N7N	5.08	123.85	117.75
3	B	402	NAP	PN-O3-PA	-4.73	116.59	132.83
3	B	402	NAP	N3A-C2A-N1A	-4.09	122.29	128.68
3	A	402	NAP	O3D-C3D-C4D	-3.92	99.72	111.05
3	B	402	NAP	O5B-PA-O1A	-3.80	94.21	109.07
6	B	410	CXS	O1-S-C1	3.55	111.19	106.92
3	A	402	NAP	C4A-C5A-N7A	-3.36	105.90	109.40
3	A	402	NAP	C3D-C2D-C1D	-3.32	95.98	100.98
3	B	402	NAP	O7N-C7N-C3N	-3.30	115.69	119.63
6	B	410	CXS	C8-C7-C6	-3.15	101.50	111.18
6	B	410	CXS	C3-N-C4	3.09	120.20	114.14
3	A	402	NAP	C1B-N9A-C4A	-3.08	121.23	126.64
3	A	402	NAP	O2X-P2B-O1X	-3.00	98.93	110.68
3	A	402	NAP	N3A-C2A-N1A	-3.00	123.99	128.68
3	A	402	NAP	PN-O3-PA	-2.96	122.66	132.83
3	B	402	NAP	O3B-C3B-C2B	-2.93	102.85	111.17
5	A	412	HSE	OXT-C-CA	2.84	123.04	113.38
3	A	402	NAP	O2X-P2B-O2B	2.82	118.61	105.99
5	B	409	HSE	C3-CA-N	2.82	117.55	110.17
3	B	402	NAP	O3B-C3B-C4B	2.80	119.16	111.05
3	B	402	NAP	C6N-N1N-C2N	-2.54	119.66	121.97
3	A	402	NAP	C5N-C4N-C3N	-2.47	117.42	120.34
5	B	409	HSE	OXT-C-O	-2.46	118.51	124.09
3	A	402	NAP	C2N-C3N-C4N	2.43	121.01	118.26
5	B	409	HSE	O3-C4-C3	2.39	119.70	111.31
3	B	402	NAP	C3N-C2N-N1N	2.36	122.73	120.43
3	A	402	NAP	C2D-C3D-C4D	2.32	107.16	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	409	HSE	OXT-C-CA	2.31	121.24	113.38
3	A	402	NAP	O3X-P2B-O2X	2.27	116.31	107.64
5	A	412	HSE	C3-CA-N	2.20	115.94	110.17
6	B	410	CXS	O3-S-O2	-2.19	105.92	111.27
3	A	402	NAP	O3X-P2B-O2B	-2.17	96.27	105.99
3	A	402	NAP	C5A-C6A-N6A	2.16	123.64	120.35
7	A	413	GOL	O1-C1-C2	2.16	120.56	110.20
3	A	402	NAP	O7N-C7N-C3N	-2.07	117.15	119.63
3	A	402	NAP	O2A-PA-O1A	2.06	122.44	112.24

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	NAP	O4D-C1D-N1N-C2N
3	A	402	NAP	O4D-C1D-N1N-C2N
5	B	409	HSE	CA-C3-C4-O3
6	B	410	CXS	C2-C1-S-O2
7	B	411	GOL	O1-C1-C2-C3
7	B	411	GOL	C1-C2-C3-O3
7	B	411	GOL	O2-C2-C3-O3
3	B	402	NAP	C3B-C2B-O2B-P2B
3	A	402	NAP	C3B-C2B-O2B-P2B
6	B	410	CXS	C2-C1-S-O3
3	B	402	NAP	C1B-C2B-O2B-P2B
3	A	402	NAP	C1B-C2B-O2B-P2B
7	B	411	GOL	O1-C1-C2-O2
6	B	410	CXS	C9-C4-N-C3
6	B	410	CXS	C2-C1-S-O1
5	B	409	HSE	OXT-C-CA-C3
5	B	409	HSE	O-C-CA-N
6	B	410	CXS	C5-C4-N-C3
7	A	413	GOL	O1-C1-C2-O2
3	B	402	NAP	O4B-C4B-C5B-O5B
3	A	402	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

6 monomers are involved in 7 short contacts:

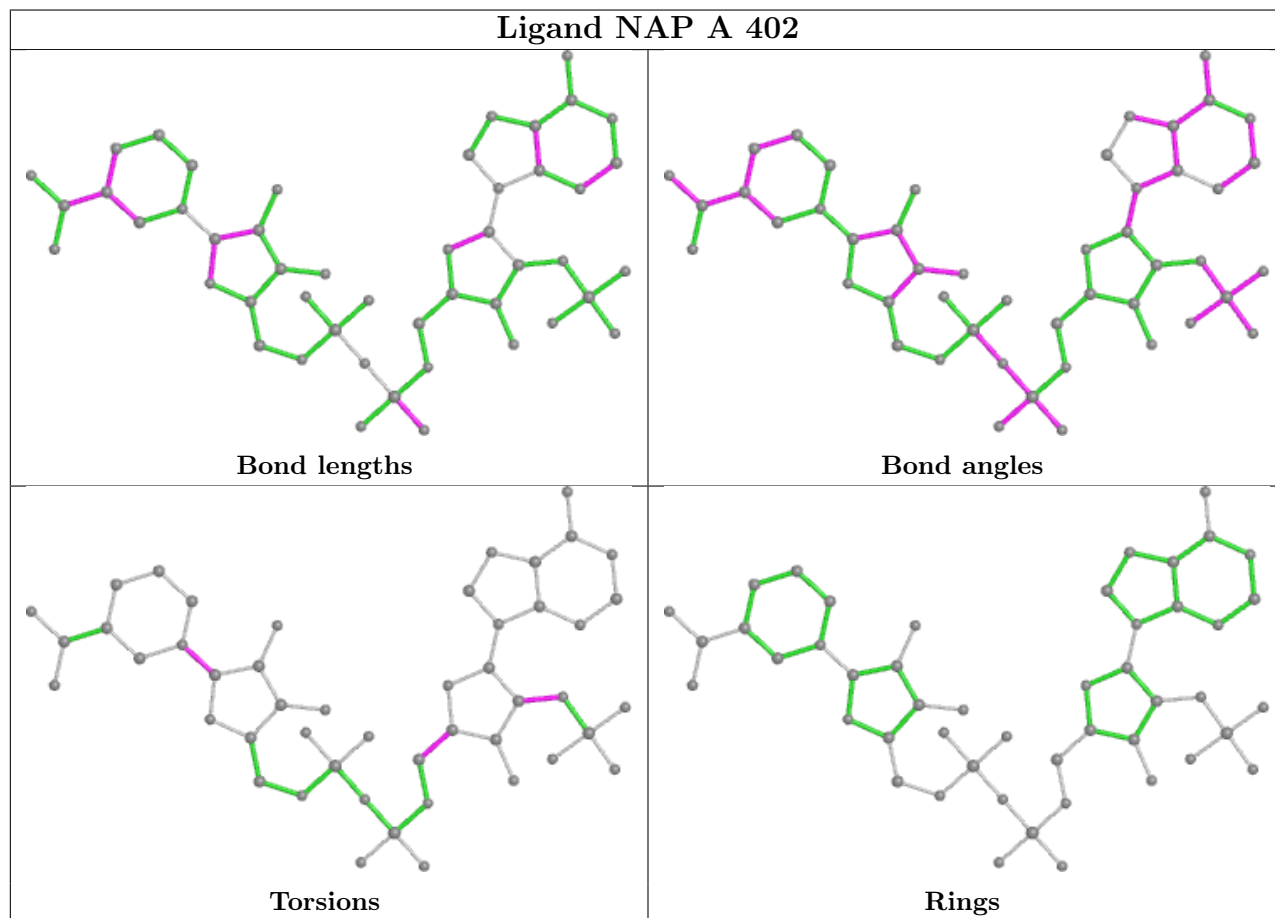
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	NAP	2	0

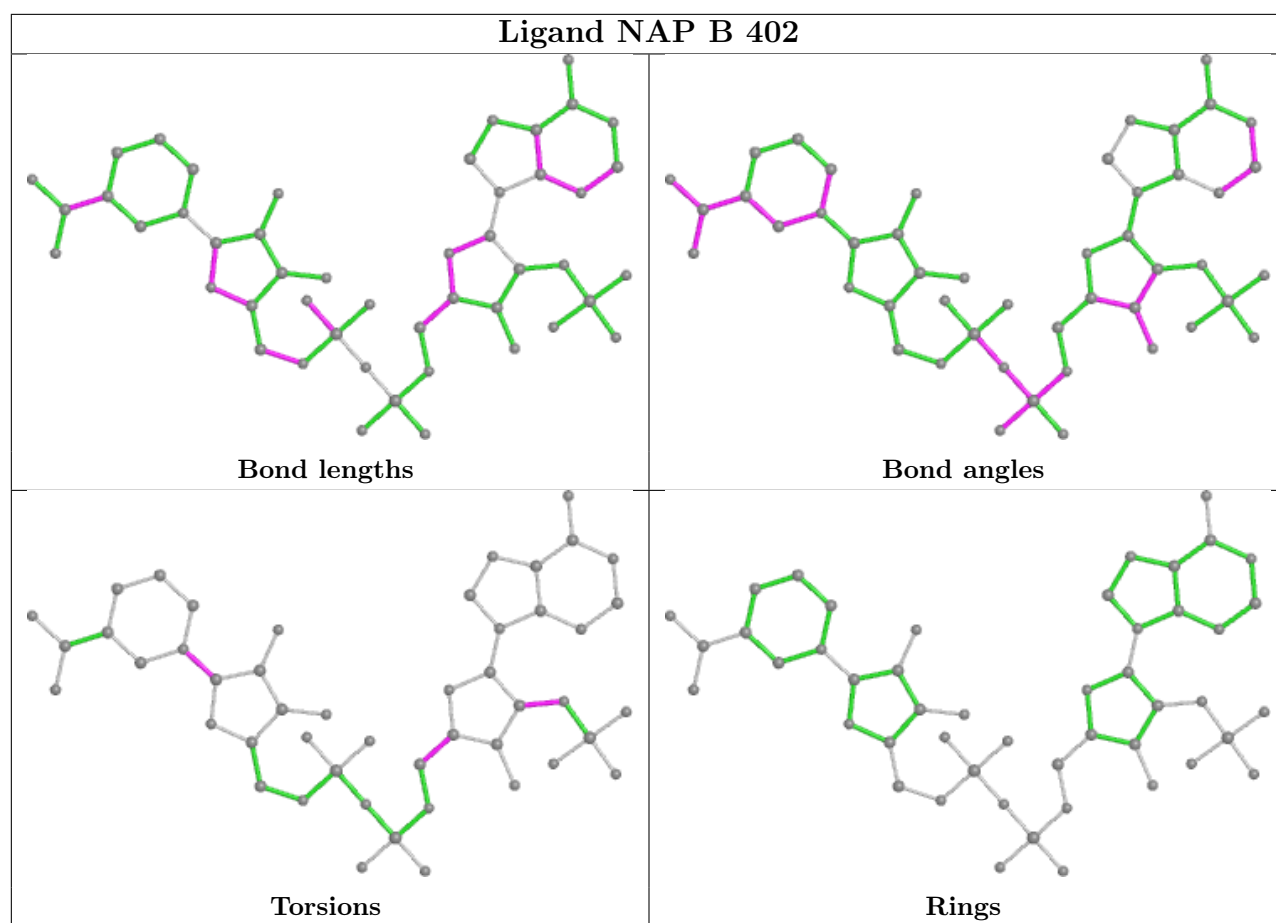
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	409	HSE	1	0
4	A	407	FMT	1	0
3	B	402	NAP	2	0
5	A	412	HSE	1	0
4	A	411	FMT	1	0

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/332 (99%)	-0.10	8 (2%) 59 66	18, 26, 51, 68	0
1	B	331/332 (99%)	-0.10	14 (4%) 36 43	18, 26, 55, 75	0
All	All	662/664 (99%)	-0.10	22 (3%) 46 54	18, 26, 53, 75	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	PRO	4.6
1	B	326	SER	4.1
1	A	47	ARG	3.8
1	B	330	GLY	3.6
1	B	328	TRP	3.5
1	B	176	LEU	3.5
1	A	329	PRO	3.4
1	B	163	GLY	3.2
1	A	163	GLY	2.7
1	B	46	PRO	2.7
1	B	231	ALA	2.7
1	A	328	TRP	2.7
1	B	49	PRO	2.6
1	A	231	ALA	2.5
1	B	325	GLY	2.5
1	B	47	ARG	2.5
1	A	164	ARG	2.3
1	A	330	GLY	2.1
1	B	232	ARG	2.1
1	A	1	MET	2.1
1	B	228	LYS	2.0
1	B	175	ARG	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.

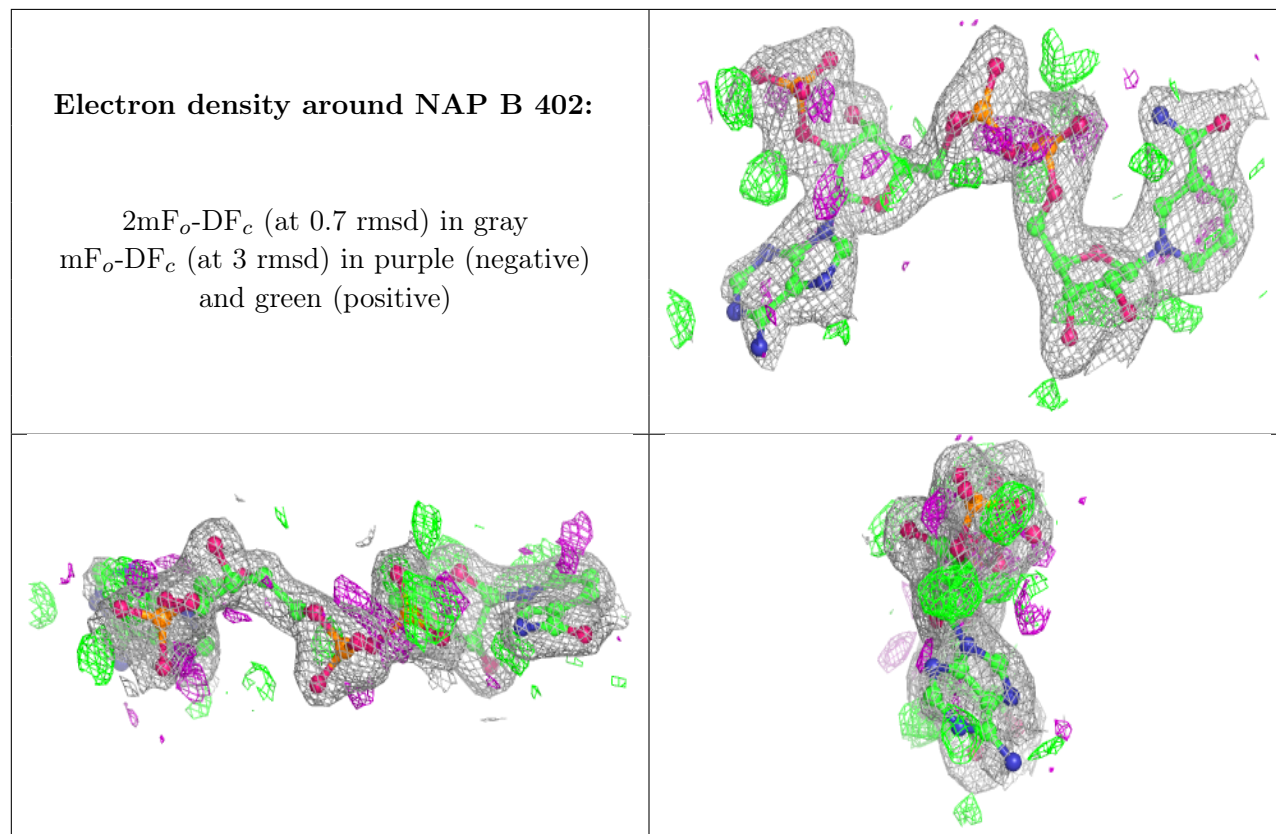
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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.

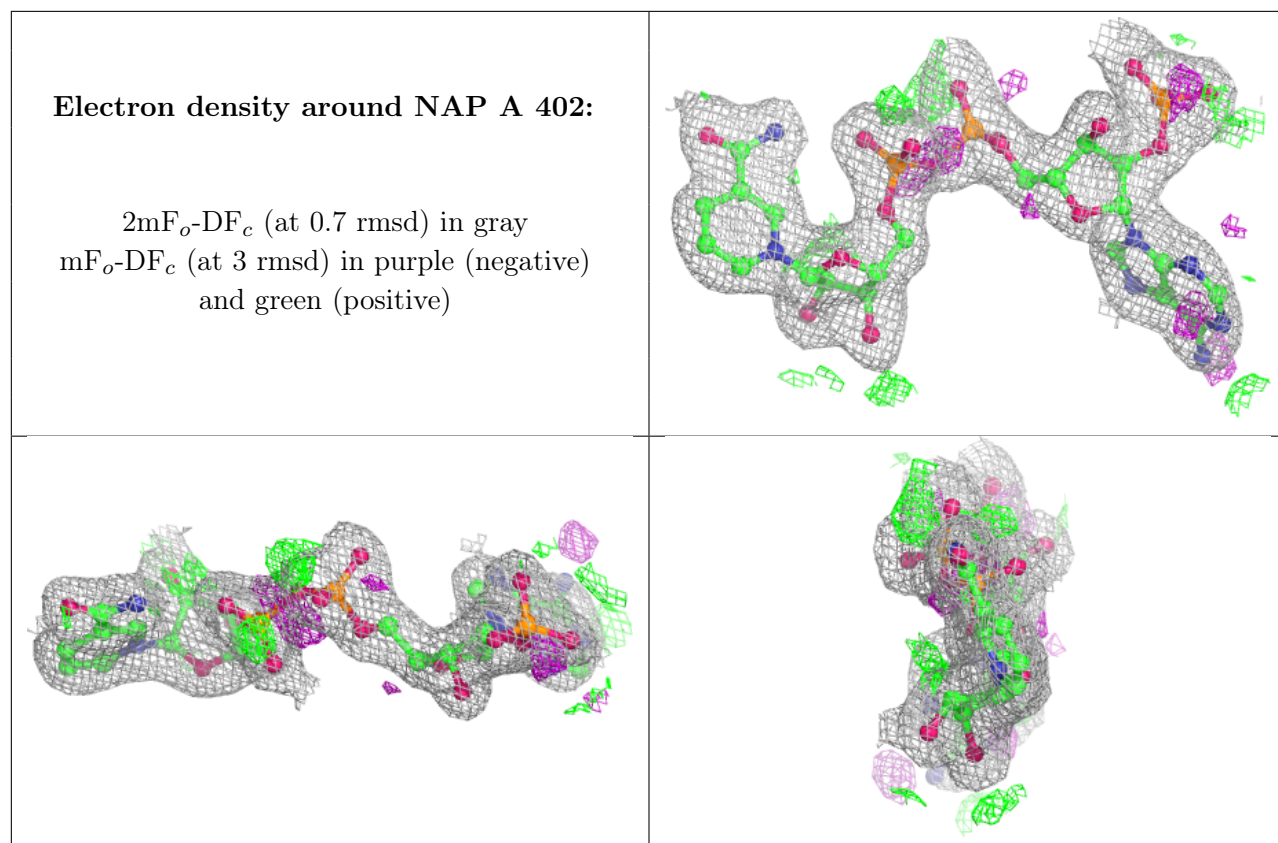
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	CXS	B	410	14/14	0.78	0.18	39,42,78,83	14
4	FMT	A	411	3/3	0.87	0.18	41,41,43,45	0
5	HSE	B	409	8/8	0.90	0.13	28,31,43,54	0
8	UNL	B	412	13/-	0.90	0.14	31,37,59,60	0
3	NAP	B	402	48/48	0.91	0.13	24,38,60,69	0
4	FMT	B	407	3/3	0.91	0.14	55,55,56,57	0
7	GOL	B	411	6/6	0.92	0.10	42,46,50,52	0
7	GOL	A	413	6/6	0.93	0.11	30,38,45,48	0
4	FMT	B	406	3/3	0.93	0.20	45,45,48,53	0
3	NAP	A	402	48/48	0.94	0.10	23,31,49,58	0
4	FMT	B	408	3/3	0.94	0.25	43,43,53,54	0
4	FMT	A	409	3/3	0.94	0.14	46,46,49,52	0
5	HSE	A	412	8/8	0.95	0.08	25,31,33,34	0
4	FMT	B	405	3/3	0.95	0.12	45,45,54,56	0
4	FMT	A	410	3/3	0.95	0.19	49,49,53,57	0
4	FMT	A	404	3/3	0.95	0.09	36,36,40,51	0
4	FMT	A	407	3/3	0.95	0.16	28,28,29,42	0
4	FMT	B	403	3/3	0.96	0.12	27,27,32,34	0
4	FMT	A	406	3/3	0.96	0.12	38,38,38,41	0
4	FMT	A	405	3/3	0.97	0.25	36,36,52,53	0
4	FMT	A	403	3/3	0.97	0.08	27,27,28,30	0
4	FMT	B	404	3/3	0.97	0.11	34,34,39,42	0
4	FMT	A	408	3/3	0.98	0.18	32,32,45,50	0
2	NA	A	401	1/1	0.99	0.10	18,18,18,18	0
2	NA	B	401	1/1	0.99	0.12	19,19,19,19	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.







## 6.5 Other polymers [i](#)

There are no such residues in this entry.