



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2019 – 08:38 AM EST

PDB ID : 6A0S  
Title : Homoserine dehydrogenase from *Thermus thermophilus* HB8 complexed with HSE and NADPH  
Authors : Akai, S.; Ikushiro, H.; Sawai, T.; Yano, T.; Kamiya, N.; Miyahara, I.  
Deposited on : 2018-06-06  
Resolution : 2.00 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.

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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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

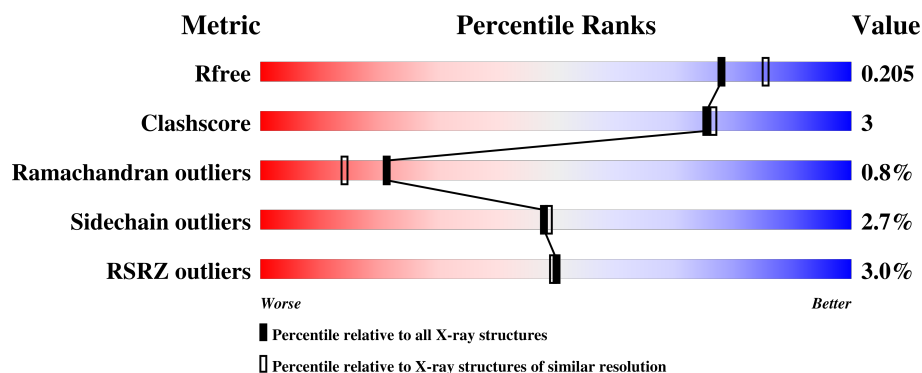
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	 3% 90% 8% •
1	B	332	 3% 87% 12% •

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 5871 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.

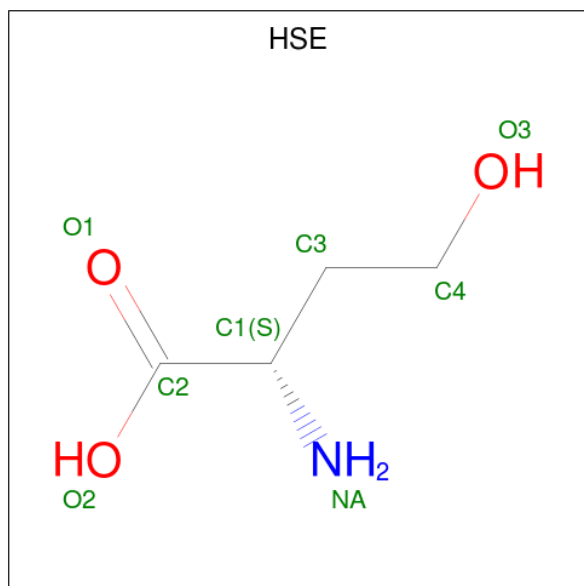
- Molecule 1 is a protein called Homoserine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	331	Total	C	N	O	S	0	13	0
			2578	1653	450	471	4			
1	A	331	Total	C	N	O	S	0	10	0
			2567	1642	454	467	4			

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

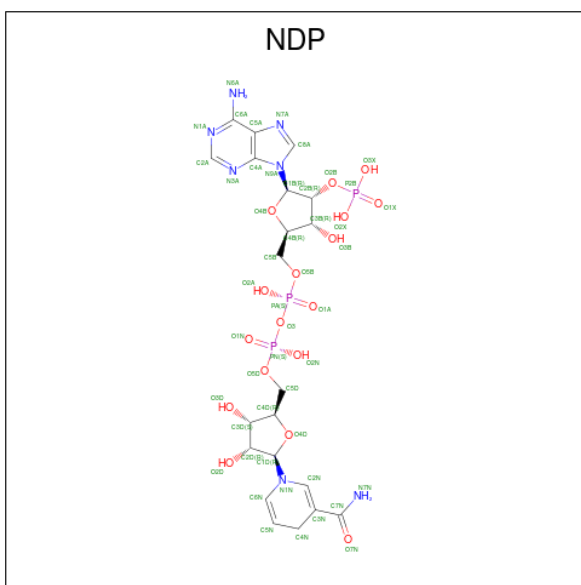
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is L-HOMOSERINE (three-letter code: HSE) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>3</sub>).



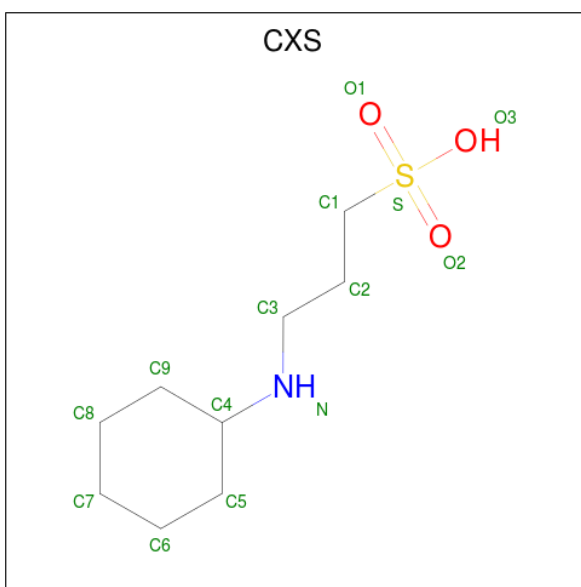
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 8	C 4	N 1	O 3	0	0
3	A	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula:  $C_{21}H_{30}N_7O_{17}P_3$ ).



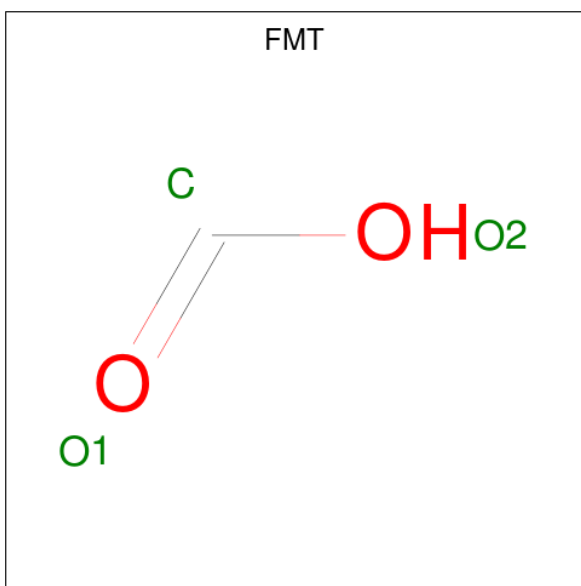
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
4	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

- Molecule 5 is 3-CYCLOHEXYL-1-PROPYLSULFONIC ACID (three-letter code: CXS) (formula:  $\text{C}_9\text{H}_{19}\text{NO}_3\text{S}$ ).



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

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula:  $\text{CH}_2\text{O}_2$ ).



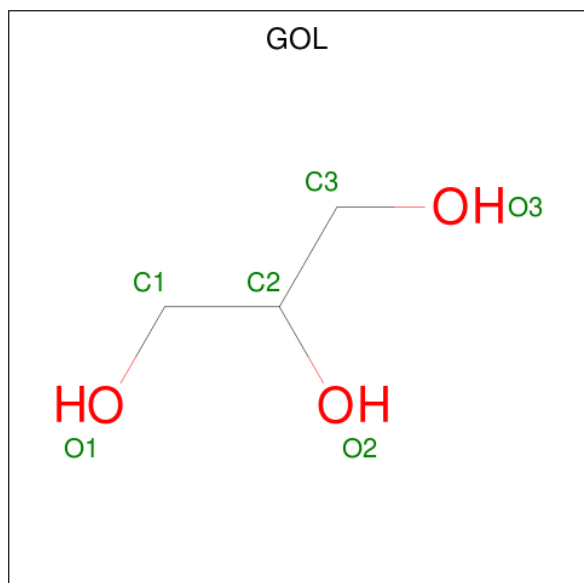
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		
6	B	1	Total	C	O	0	0
			3	1	2		

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

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



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

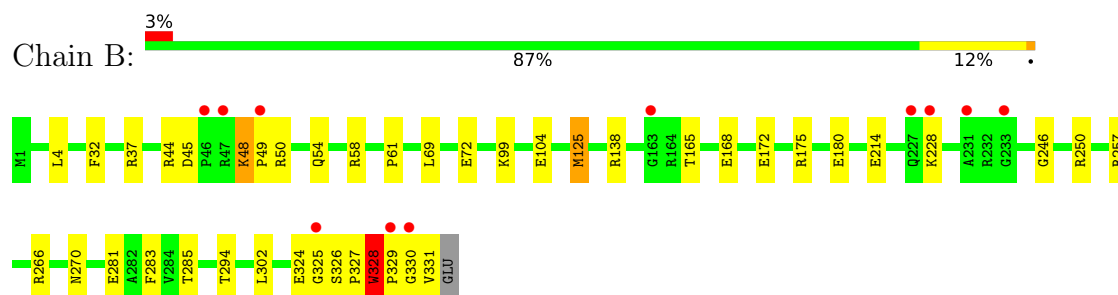
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	272	Total 279	O 279	0	17
8	A	264	Total 274	O 274	0	18

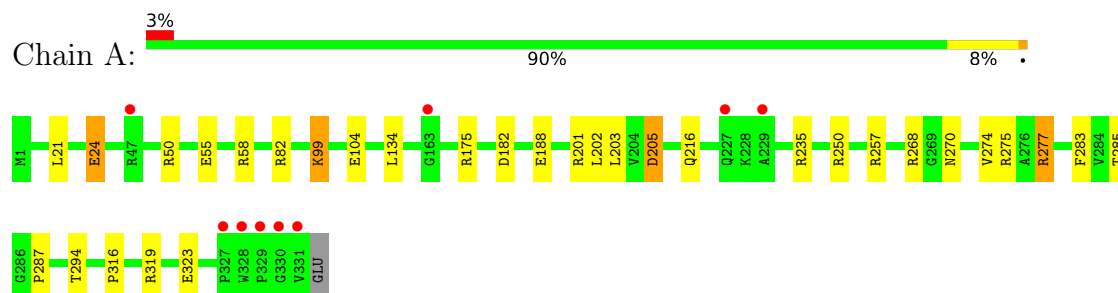
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	119.62Å 119.62Å 144.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 33.58 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.00) 99.8 (33.58-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.75 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.159 , 0.200 0.168 , 0.205	Depositor DCC
$R_{free}$ test set	4061 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.49% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CXS, HSE, NA, FMT, NDP

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	1.24	7/2626 (0.3%)	1.13	10/3575 (0.3%)
1	B	1.26	2/2655 (0.1%)	1.16	12/3615 (0.3%)
All	All	1.25	9/5281 (0.2%)	1.14	22/7190 (0.3%)

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	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	104	GLU	CD-OE2	9.69	1.36	1.25
1	B	104	GLU	CD-OE1	8.58	1.35	1.25
1	A	55	GLU	CD-OE1	6.66	1.32	1.25
1	A	188	GLU	CD-OE2	-6.25	1.18	1.25
1	A	270	ASN	CB-CG	5.95	1.64	1.51
1	A	24	GLU	CB-CG	-5.70	1.41	1.52
1	A	182	ASP	CG-OD1	5.28	1.37	1.25
1	A	182	ASP	CB-CG	5.28	1.62	1.51
1	B	180	GLU	CD-OE2	-5.00	1.20	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	175	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	A	182	ASP	CB-CG-OD2	-7.96	111.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	205	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	50	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	A	82	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	275	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	235	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	B	44	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	B	138	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	328	TRP	C-N-CD	-5.79	107.87	120.60
1	B	58	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	50	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	72	GLU	OE1-CD-OE2	5.66	130.10	123.30
1	B	328	TRP	N-CA-C	5.54	125.95	111.00
1	B	266	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	274	VAL	CG1-CB-CG2	-5.44	102.20	110.90
1	A	275	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	37	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	B	125	MET	CG-SD-CE	5.22	108.56	100.20
1	A	205	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	69	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	328	TRP	Peptide
1	B	329	PRO	Peptide

## 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	2567	0	2591	16	0
1	B	2578	0	2621	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	8	0	8	2	0
4	A	48	0	26	2	0
4	B	48	0	26	2	0
5	B	14	0	19	0	0
6	A	21	0	7	0	0
6	B	18	0	6	0	0
7	B	6	0	8	0	0
8	A	274	0	0	2	0
8	B	279	0	0	1	0
All	All	5871	0	5320	36	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (36) 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)
3:A:402:HSE:H42	4:A:403:NDP:H41N	1.63	0.79
1:A:277[A]:ARG:HH11	1:A:277[A]:ARG:HG3	1.47	0.77
1:A:294:THR:OG1	4:A:403:NDP:H42N	1.86	0.75
1:B:48:LYS:HB2	1:B:49:PRO:CD	2.24	0.68
1:B:327:PRO:O	1:B:328:TRP:HB2	1.96	0.64
1:B:125:MET:HG2	1:B:270[A]:ASN:HD22	1.63	0.63
1:A:99:LYS:H	1:A:99:LYS:HD2	1.65	0.61
1:B:45[A]:ASP:OD1	1:B:48:LYS:HB3	2.01	0.60
1:B:328:TRP:CE3	1:B:328:TRP:HA	2.37	0.59
1:A:277[A]:ARG:HH11	1:A:277[A]:ARG:CG	2.16	0.59
3:B:402:HSE:H42	4:B:403:NDP:H41N	1.84	0.59
1:B:4:LEU:HD21	1:B:302[B]:LEU:HD11	1.86	0.57
1:B:283[A]:PHE:CE2	1:A:285[A]:THR:CG2	2.89	0.56
1:B:32:PHE:CE1	1:A:316:PRO:HG3	2.41	0.55
1:B:294:THR:OG1	4:B:403:NDP:H42N	2.06	0.55
1:B:285[B]:THR:CG2	1:A:283[B]:PHE:CE2	2.93	0.52
1:A:99:LYS:N	1:A:99:LYS:HD2	2.25	0.51
1:B:327:PRO:O	1:B:328:TRP:CB	2.59	0.51
1:B:257:ARG:HG3	1:B:331:VAL:HG22	1.94	0.49
3:B:402:HSE:O1	3:B:402:HSE:H41	2.13	0.48
1:B:48:LYS:CB	1:B:49:PRO:CD	2.91	0.48
1:B:250:ARG:NH2	8:B:519:HOH:O	2.48	0.46
1:A:250:ARG:HG3	8:A:719:HOH:O	2.15	0.45
1:B:214[A]:GLU:OE1	1:B:250:ARG:NE	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268[B]:ARG:CD	8:A:624[B]:HOH:O	2.64	0.45
1:B:281[B]:GLU:O	1:A:287:PRO:HD3	2.16	0.45
1:B:48:LYS:HB2	1:B:49:PRO:HD2	1.97	0.45
1:A:277[A]:ARG:NH1	1:A:277[A]:ARG:CG	2.80	0.45
1:B:165:THR:OG1	1:B:168:GLU:HG3	2.19	0.43
1:B:324:GLU:O	1:B:326:SER:N	2.50	0.43
1:A:201:ARG:HA	1:A:205:ASP:O	2.20	0.42
1:B:48:LYS:HB2	1:B:49:PRO:HD3	2.00	0.42
1:A:202:LEU:HD23	1:A:202:LEU:C	2.41	0.41
1:B:45[A]:ASP:CG	1:B:48:LYS:HB3	2.41	0.41
1:A:134:LEU:HD22	1:A:203:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	339/332 (102%)	327 (96%)	12 (4%)	0	100	100
1	B	342/332 (103%)	326 (95%)	11 (3%)	5 (2%)	11	5
All	All	681/664 (103%)	653 (96%)	23 (3%)	5 (1%)	21	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	325	GLY
1	B	328	TRP
1	B	246	GLY
1	B	330	GLY
1	B	48	LYS

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/248 (102%)	242 (96%)	10 (4%)	34	31
1	B	257/248 (104%)	252 (98%)	5 (2%)	60	64
All	All	509/496 (103%)	494 (97%)	15 (3%)	48	45

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	GLN
1	B	61	PRO
1	B	99	LYS
1	B	172	GLU
1	B	228	LYS
1	A	24	GLU
1	A	99	LYS
1	A	175	ARG
1	A	216[A]	GLN
1	A	216[B]	GLN
1	A	257	ARG
1	A	277[A]	ARG
1	A	277[B]	ARG
1	A	319	ARG
1	A	323	GLU

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

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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
3	HSE	A	402	-	3,7,7	1.65	1 (33%)	1,8,8	0.09	0
4	NDP	A	403	-	45,52,52	1.55	8 (17%)	54,80,80	1.70	15 (27%)
6	FMT	A	404	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	405	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	406	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	407	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	408	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	409	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	A	410	-	0,2,2	0.00	-	0,1,1	0.00	-
3	HSE	B	402	-	3,7,7	1.55	0	1,8,8	0.12	0
4	NDP	B	403	-	45,52,52	1.52	9 (20%)	54,80,80	1.58	12 (22%)
5	CXS	B	404	-	14,14,14	1.84	2 (14%)	18,18,18	1.99	4 (22%)
6	FMT	B	405	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	406	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	407	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	408	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	409	-	0,2,2	0.00	-	0,1,1	0.00	-
6	FMT	B	410	-	0,2,2	0.00	-	0,1,1	0.00	-
7	GOL	B	411[B]	-	5,5,5	0.75	0	5,5,5	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HSE	A	402	-	-	1/3/7/7	-
4	NDP	A	403	-	-	7/30/77/77	0/5/5/5
3	HSE	B	402	-	-	1/3/7/7	-
4	NDP	B	403	-	-	7/30/77/77	0/5/5/5
5	CXS	B	404	-	-	0/8/16/16	0/1/1/1
7	GOL	B	411[B]	-	-	3/4/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	404	CXS	C1-S	-4.69	1.70	1.77
5	B	404	CXS	O3-S	4.61	1.63	1.47
4	B	403	NDP	C2A-N3A	3.75	1.38	1.32
4	B	403	NDP	O4B-C4B	-3.53	1.37	1.45
4	A	403	NDP	O4B-C1B	3.49	1.46	1.41
4	A	403	NDP	C5A-C4A	3.35	1.48	1.40
4	A	403	NDP	C6N-C5N	3.24	1.39	1.33
4	B	403	NDP	O4D-C1D	3.10	1.49	1.42
4	A	403	NDP	C2A-N3A	3.10	1.37	1.32
4	B	403	NDP	C6N-C5N	3.06	1.38	1.33
4	B	403	NDP	C4A-N3A	2.98	1.39	1.35
4	A	403	NDP	P2B-O2B	2.86	1.64	1.59
4	B	403	NDP	C5A-C4A	2.75	1.46	1.40
3	A	402	HSE	C3-C4	2.70	1.61	1.51
4	B	403	NDP	C6A-C5A	2.52	1.53	1.43
4	A	403	NDP	O4B-C4B	-2.32	1.39	1.45
4	A	403	NDP	C4N-C5N	-2.30	1.44	1.49
4	B	403	NDP	C3B-C2B	-2.28	1.47	1.52
4	A	403	NDP	O4D-C1D	2.16	1.47	1.42
4	B	403	NDP	O4B-C1B	2.10	1.44	1.41

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	404	CXS	O2-S-C1	5.33	113.33	106.92
5	B	404	CXS	C3-N-C4	3.92	121.83	114.14
4	B	403	NDP	PN-O3-PA	-3.76	120.62	132.57
4	A	403	NDP	O2N-PN-O1N	3.54	129.97	112.21
4	A	403	NDP	O7N-C7N-C3N	-3.43	114.43	120.90
4	A	403	NDP	PN-O3-PA	-3.13	122.62	132.57
4	B	403	NDP	C4A-C5A-N7A	-3.11	106.16	109.40
4	B	403	NDP	N3A-C2A-N1A	-3.05	123.76	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403	NDP	C4A-C5A-N7A	-2.96	106.32	109.40
5	B	404	CXS	O3-S-O2	-2.85	104.32	111.27
4	B	403	NDP	C2D-C3D-C4D	2.81	107.99	102.60
4	A	403	NDP	C3D-C2D-C1D	-2.76	96.20	101.44
4	B	403	NDP	O5B-PA-O1A	-2.67	98.64	109.07
4	B	403	NDP	C4B-O4B-C1B	2.63	112.58	109.83
4	A	403	NDP	O5B-C5B-C4B	-2.61	99.97	108.99
4	B	403	NDP	O3D-C3D-C4D	-2.53	103.76	111.07
4	A	403	NDP	O5B-PA-O1A	-2.48	99.38	109.07
4	A	403	NDP	C3N-C2N-N1N	-2.45	119.56	123.09
5	B	404	CXS	O1-S-C1	2.40	109.80	106.92
4	A	403	NDP	C1B-N9A-C4A	-2.38	122.52	126.64
4	B	403	NDP	C3N-C7N-N7N	2.36	121.86	117.67
4	B	403	NDP	C3D-C2D-C1D	-2.33	97.02	101.44
4	A	403	NDP	O2A-PA-O1A	2.31	123.80	112.21
4	A	403	NDP	N3A-C2A-N1A	-2.29	124.98	128.68
4	A	403	NDP	O4B-C1B-C2B	2.29	110.55	106.60
4	B	403	NDP	O2A-PA-O1A	2.24	123.44	112.21
4	A	403	NDP	O3X-P2B-O2X	-2.12	99.33	107.57
4	A	403	NDP	O3X-P2B-O1X	2.10	118.82	110.53
4	B	403	NDP	C1D-N1N-C6N	-2.10	116.31	120.84
4	B	403	NDP	O4B-C1B-C2B	-2.05	103.06	106.60
4	A	403	NDP	C3N-C7N-N7N	2.02	121.26	117.67

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	411[B]	GOL	C1-C2-C3-O3
4	B	403	NDP	C3B-C2B-O2B-P2B
4	B	403	NDP	C1B-C2B-O2B-P2B
4	A	403	NDP	C3B-C2B-O2B-P2B
4	A	403	NDP	C1B-C2B-O2B-P2B
7	B	411[B]	GOL	O2-C2-C3-O3
7	B	411[B]	GOL	O1-C1-C2-O2
4	A	403	NDP	C2D-C1D-N1N-C6N
4	B	403	NDP	C2D-C1D-N1N-C6N
4	A	403	NDP	O4D-C1D-N1N-C6N
4	B	403	NDP	O4D-C1D-N1N-C6N
4	A	403	NDP	O4D-C1D-N1N-C2N
4	B	403	NDP	O4D-C1D-N1N-C2N
4	A	403	NDP	O4B-C4B-C5B-O5B

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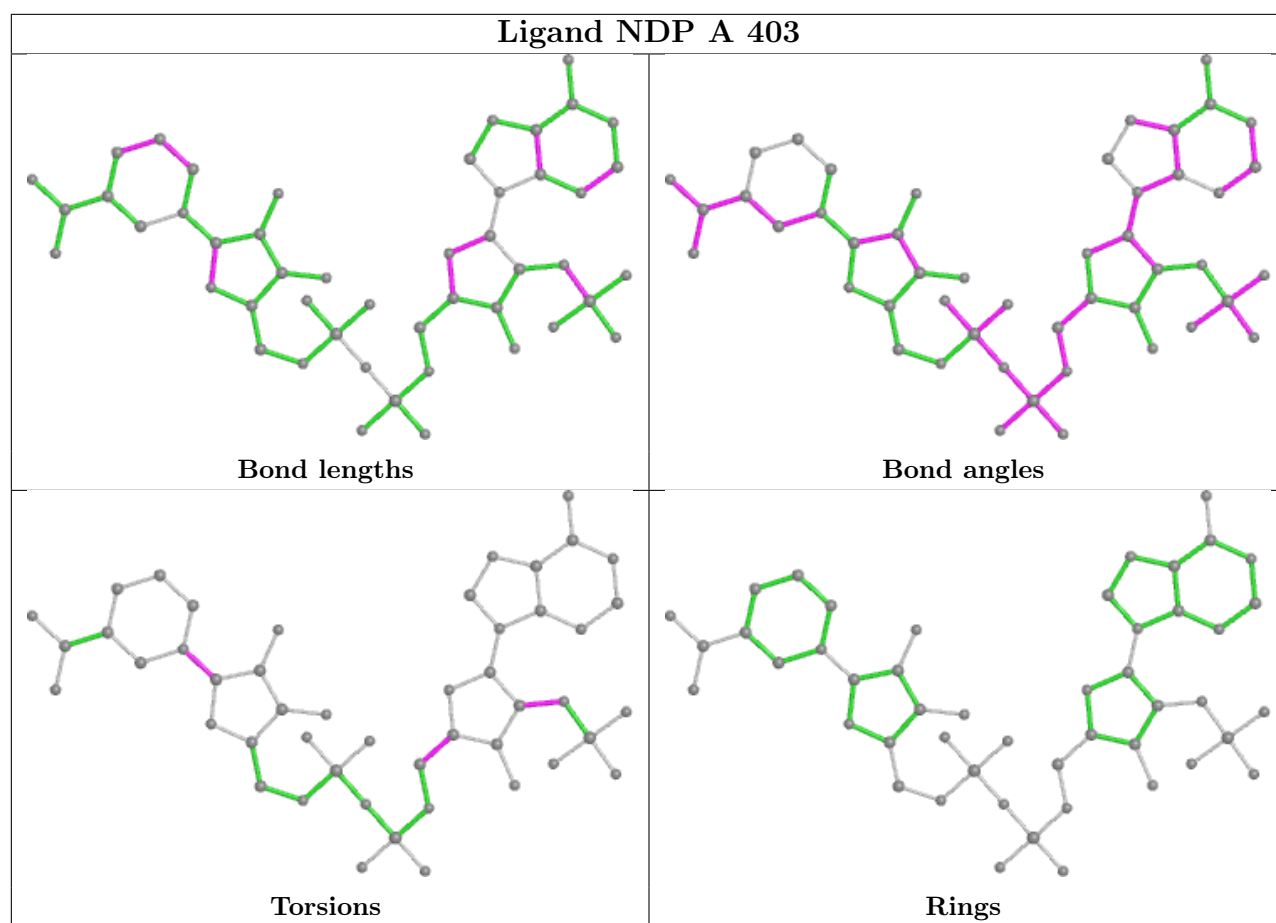
Mol	Chain	Res	Type	Atoms
3	B	402	HSE	C1-C3-C4-O3
3	A	402	HSE	C1-C3-C4-O3
4	B	403	NDP	O4B-C4B-C5B-O5B
4	B	403	NDP	C2D-C1D-N1N-C2N
4	A	403	NDP	C2D-C1D-N1N-C2N

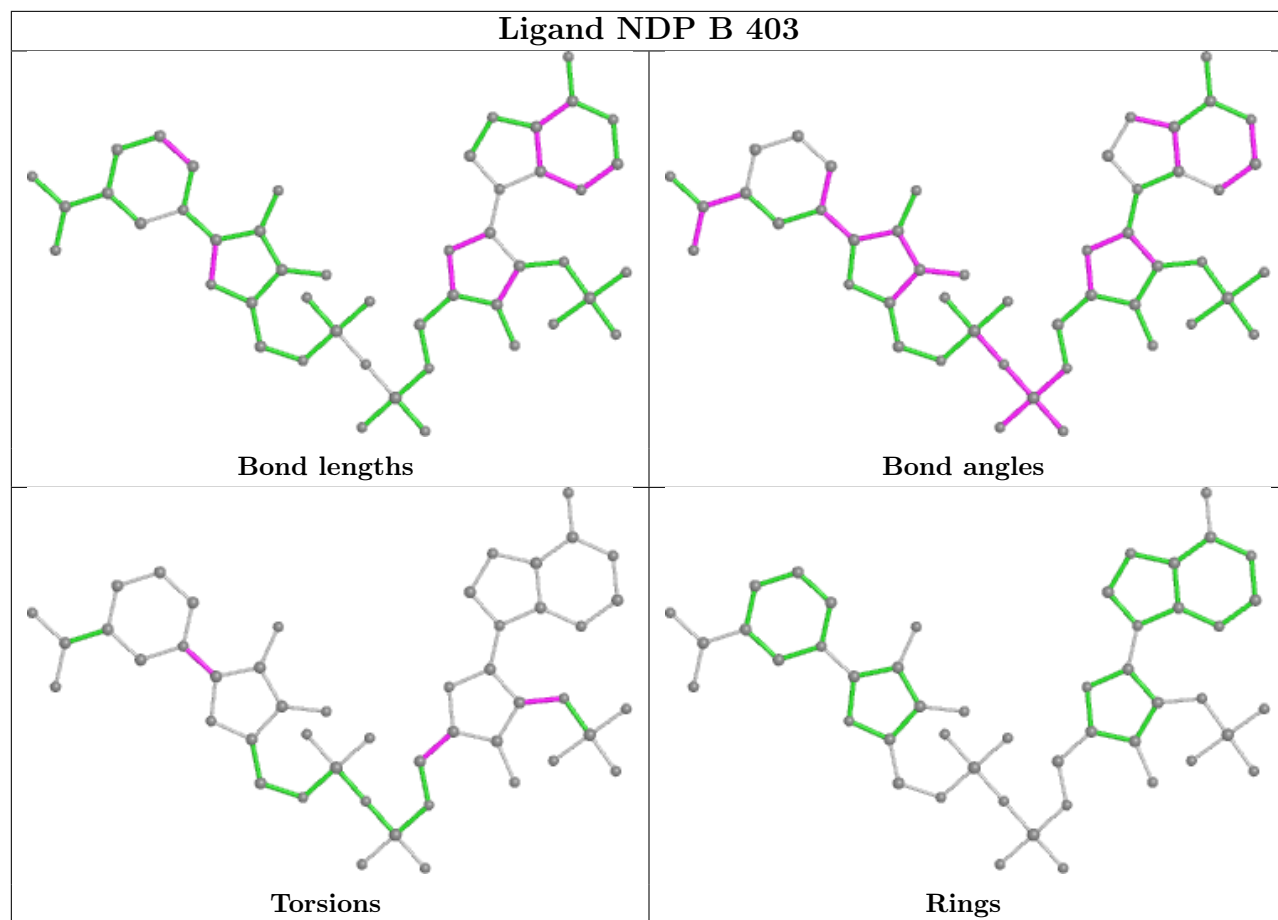
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	HSE	1	0
4	A	403	NDP	2	0
3	B	402	HSE	2	0
4	B	403	NDP	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, 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%)	-0.29	9 (2%) 54 53	23, 34, 63, 83	0
1	B	331/332 (99%)	-0.28	11 (3%) 46 46	23, 33, 68, 94	0
All	All	662/664 (99%)	-0.28	20 (3%) 50 49	23, 33, 65, 94	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	329	PRO	6.6
1	A	328	TRP	4.5
1	B	325	GLY	4.3
1	A	329	PRO	4.2
1	A	47	ARG	4.1
1	B	46	PRO	3.4
1	A	163	GLY	3.1
1	B	163	GLY	3.1
1	B	231	ALA	2.8
1	B	330	GLY	2.7
1	A	227	GLN	2.6
1	B	49	PRO	2.5
1	A	331	VAL	2.5
1	A	327	PRO	2.4
1	A	330	GLY	2.4
1	B	227	GLN	2.3
1	B	228	LYS	2.2
1	B	47	ARG	2.2
1	B	233	GLY	2.1
1	A	229	ALA	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

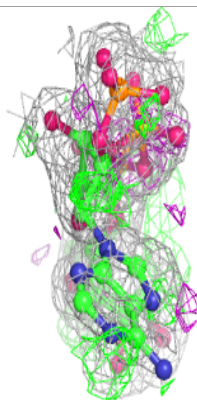
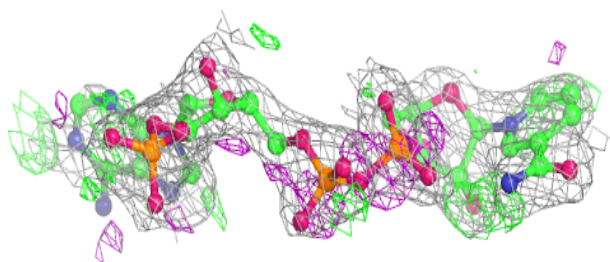
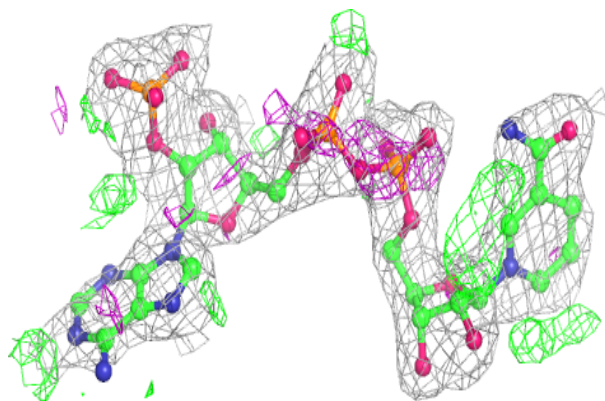
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	B	411[B]	6/6	0.78	0.37	38,53,58,58	6
6	FMT	A	409	3/3	0.80	0.26	59,59,69,70	0
6	FMT	A	410	3/3	0.82	0.17	56,56,61,62	3
5	CXS	B	404	14/14	0.89	0.15	41,47,68,74	14
6	FMT	A	407	3/3	0.90	0.14	47,47,49,53	3
6	FMT	B	408	3/3	0.91	0.13	45,45,46,47	3
4	NDP	B	403	48/48	0.92	0.14	30,42,59,65	48
6	FMT	B	410	3/3	0.92	0.17	47,47,55,56	0
4	NDP	A	403	48/48	0.93	0.13	29,39,58,72	48
6	FMT	B	406	3/3	0.94	0.26	41,41,61,65	0
6	FMT	B	409	3/3	0.95	0.18	47,47,49,62	0
6	FMT	B	407	3/3	0.95	0.22	28,28,30,42	3
6	FMT	A	406	3/3	0.95	0.11	46,46,54,55	0
3	HSE	B	402	8/8	0.96	0.09	30,36,38,41	0
3	HSE	A	402	8/8	0.97	0.10	32,37,39,41	0
6	FMT	A	408	3/3	0.97	0.26	35,35,42,55	0
6	FMT	A	405	3/3	0.98	0.15	31,31,41,47	0
6	FMT	B	405	3/3	0.98	0.09	40,40,49,50	0
6	FMT	A	404	3/3	0.98	0.30	46,46,55,55	0
2	NA	A	401	1/1	0.99	0.07	23,23,23,23	0
2	NA	B	401	1/1	0.99	0.17	24,24,24,24	0

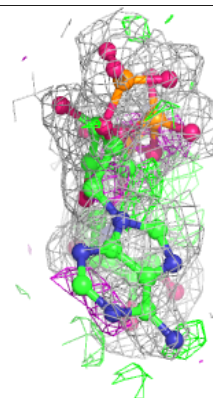
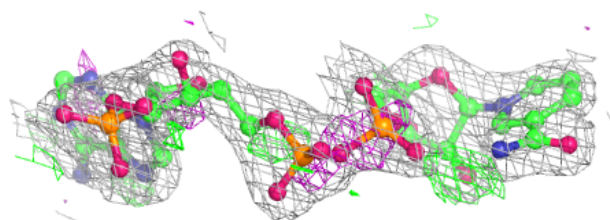
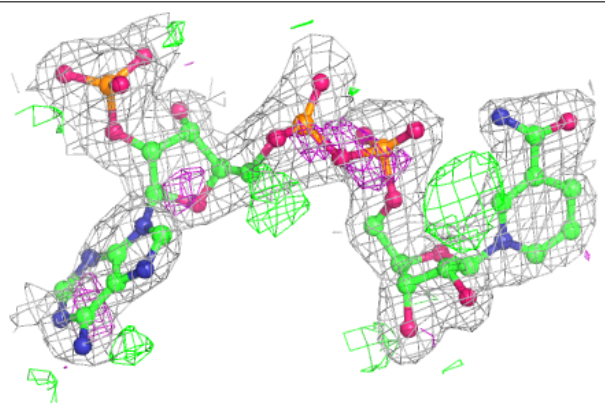
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around NDP B 403:**

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

**Electron density around NDP A 403:**

$2mF_o-DF_c$  (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.