wwPDB X-ray Structure Validation Summary Report (i)

Jan 14, 2024 – 06:47 am GMT

PDB ID	:	6T8Y
Title	:	NAD+-dependent fungal formate dehydrogenase from Chaetomium thermophilum: A complex with the reduced form of the cofactor NADH and the substrate formate at a secondary site.
Authors	:	Isupov, M.N.; Yelmazer, B.; De Rose, S.A.; Littlechild, J.A.
Deposited on	:	2019-10-25
Resolution	:	1.26 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

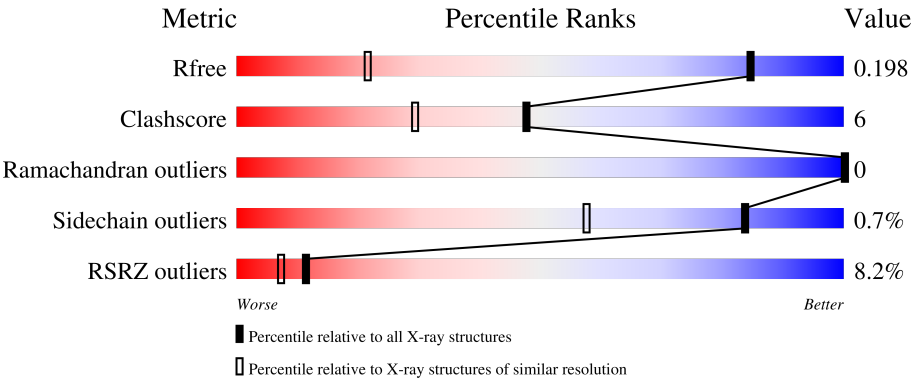
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.26 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	1023 (1.28-1.24)
Clashscore	141614	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)
RSRZ outliers	127900	1004 (1.28-1.24)

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 <=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	AAA	410	3% 84% 7% 9%
1	BBB	410	10% 84% 7% 9%
1	CCC	410	14% 80% 11% 9%
1	DDD	410	3% 84% 7% 9%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 27517 atoms, of which 12972 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 Formate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	372	Total	C	H	N	O	S	118	31	0
			6287	1959	3189	555	573	11			
1	BBB	375	Total	C	H	N	O	S	118	29	0
			6270	1961	3174	547	578	10			
1	CCC	373	Total	C	H	N	O	S	116	36	0
			6355	1981	3233	555	576	10			
1	DDD	374	Total	C	H	N	O	S	121	27	0
			6229	1943	3154	550	572	10			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-33	MET	-	initiating methionine	UNP G0SGU4
AAA	-32	ALA	-	expression tag	UNP G0SGU4
AAA	-31	HIS	-	expression tag	UNP G0SGU4
AAA	-30	HIS	-	expression tag	UNP G0SGU4
AAA	-29	HIS	-	expression tag	UNP G0SGU4
AAA	-28	HIS	-	expression tag	UNP G0SGU4
AAA	-27	HIS	-	expression tag	UNP G0SGU4
AAA	-26	HIS	-	expression tag	UNP G0SGU4
AAA	-25	VAL	-	expression tag	UNP G0SGU4
AAA	-24	GLY	-	expression tag	UNP G0SGU4
AAA	-23	THR	-	expression tag	UNP G0SGU4
AAA	-22	GLY	-	expression tag	UNP G0SGU4
AAA	-21	SER	-	expression tag	UNP G0SGU4
AAA	-20	ASN	-	expression tag	UNP G0SGU4
AAA	-19	ASP	-	expression tag	UNP G0SGU4
AAA	-18	ASP	-	expression tag	UNP G0SGU4
AAA	-17	ASP	-	expression tag	UNP G0SGU4
AAA	-16	ASP	-	expression tag	UNP G0SGU4
AAA	-15	LYS	-	expression tag	UNP G0SGU4
AAA	-14	SER	-	expression tag	UNP G0SGU4
AAA	-13	PRO	-	expression tag	UNP G0SGU4

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-12	ASP	-	expression tag	UNP G0SGU4
AAA	-11	PRO	-	expression tag	UNP G0SGU4
AAA	-10	ASN	-	expression tag	UNP G0SGU4
AAA	-9	TRP	-	expression tag	UNP G0SGU4
AAA	-8	GLU	-	expression tag	UNP G0SGU4
AAA	-7	LEU	-	expression tag	UNP G0SGU4
AAA	-6	VAL	-	expression tag	UNP G0SGU4
AAA	-5	TYR	-	expression tag	UNP G0SGU4
AAA	-4	THR	-	expression tag	UNP G0SGU4
AAA	-3	ALA	-	expression tag	UNP G0SGU4
AAA	-2	ARG	-	expression tag	UNP G0SGU4
AAA	-1	LEU	-	expression tag	UNP G0SGU4
AAA	0	GLN	-	expression tag	UNP G0SGU4
AAA	371	HIS	-	expression tag	UNP G0SGU4
AAA	372	HIS	-	expression tag	UNP G0SGU4
AAA	373	HIS	-	expression tag	UNP G0SGU4
AAA	374	HIS	-	expression tag	UNP G0SGU4
AAA	375	HIS	-	expression tag	UNP G0SGU4
AAA	376	HIS	-	expression tag	UNP G0SGU4
BBB	-33	MET	-	initiating methionine	UNP G0SGU4
BBB	-32	ALA	-	expression tag	UNP G0SGU4
BBB	-31	HIS	-	expression tag	UNP G0SGU4
BBB	-30	HIS	-	expression tag	UNP G0SGU4
BBB	-29	HIS	-	expression tag	UNP G0SGU4
BBB	-28	HIS	-	expression tag	UNP G0SGU4
BBB	-27	HIS	-	expression tag	UNP G0SGU4
BBB	-26	HIS	-	expression tag	UNP G0SGU4
BBB	-25	VAL	-	expression tag	UNP G0SGU4
BBB	-24	GLY	-	expression tag	UNP G0SGU4
BBB	-23	THR	-	expression tag	UNP G0SGU4
BBB	-22	GLY	-	expression tag	UNP G0SGU4
BBB	-21	SER	-	expression tag	UNP G0SGU4
BBB	-20	ASN	-	expression tag	UNP G0SGU4
BBB	-19	ASP	-	expression tag	UNP G0SGU4
BBB	-18	ASP	-	expression tag	UNP G0SGU4
BBB	-17	ASP	-	expression tag	UNP G0SGU4
BBB	-16	ASP	-	expression tag	UNP G0SGU4
BBB	-15	LYS	-	expression tag	UNP G0SGU4
BBB	-14	SER	-	expression tag	UNP G0SGU4
BBB	-13	PRO	-	expression tag	UNP G0SGU4
BBB	-12	ASP	-	expression tag	UNP G0SGU4
BBB	-11	PRO	-	expression tag	UNP G0SGU4

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-10	ASN	-	expression tag	UNP G0SGU4
BBB	-9	TRP	-	expression tag	UNP G0SGU4
BBB	-8	GLU	-	expression tag	UNP G0SGU4
BBB	-7	LEU	-	expression tag	UNP G0SGU4
BBB	-6	VAL	-	expression tag	UNP G0SGU4
BBB	-5	TYR	-	expression tag	UNP G0SGU4
BBB	-4	THR	-	expression tag	UNP G0SGU4
BBB	-3	ALA	-	expression tag	UNP G0SGU4
BBB	-2	ARG	-	expression tag	UNP G0SGU4
BBB	-1	LEU	-	expression tag	UNP G0SGU4
BBB	0	GLN	-	expression tag	UNP G0SGU4
BBB	371	HIS	-	expression tag	UNP G0SGU4
BBB	372	HIS	-	expression tag	UNP G0SGU4
BBB	373	HIS	-	expression tag	UNP G0SGU4
BBB	374	HIS	-	expression tag	UNP G0SGU4
BBB	375	HIS	-	expression tag	UNP G0SGU4
BBB	376	HIS	-	expression tag	UNP G0SGU4
CCC	-33	MET	-	initiating methionine	UNP G0SGU4
CCC	-32	ALA	-	expression tag	UNP G0SGU4
CCC	-31	HIS	-	expression tag	UNP G0SGU4
CCC	-30	HIS	-	expression tag	UNP G0SGU4
CCC	-29	HIS	-	expression tag	UNP G0SGU4
CCC	-28	HIS	-	expression tag	UNP G0SGU4
CCC	-27	HIS	-	expression tag	UNP G0SGU4
CCC	-26	HIS	-	expression tag	UNP G0SGU4
CCC	-25	VAL	-	expression tag	UNP G0SGU4
CCC	-24	GLY	-	expression tag	UNP G0SGU4
CCC	-23	THR	-	expression tag	UNP G0SGU4
CCC	-22	GLY	-	expression tag	UNP G0SGU4
CCC	-21	SER	-	expression tag	UNP G0SGU4
CCC	-20	ASN	-	expression tag	UNP G0SGU4
CCC	-19	ASP	-	expression tag	UNP G0SGU4
CCC	-18	ASP	-	expression tag	UNP G0SGU4
CCC	-17	ASP	-	expression tag	UNP G0SGU4
CCC	-16	ASP	-	expression tag	UNP G0SGU4
CCC	-15	LYS	-	expression tag	UNP G0SGU4
CCC	-14	SER	-	expression tag	UNP G0SGU4
CCC	-13	PRO	-	expression tag	UNP G0SGU4
CCC	-12	ASP	-	expression tag	UNP G0SGU4
CCC	-11	PRO	-	expression tag	UNP G0SGU4
CCC	-10	ASN	-	expression tag	UNP G0SGU4
CCC	-9	TRP	-	expression tag	UNP G0SGU4

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-8	GLU	-	expression tag	UNP G0SGU4
CCC	-7	LEU	-	expression tag	UNP G0SGU4
CCC	-6	VAL	-	expression tag	UNP G0SGU4
CCC	-5	TYR	-	expression tag	UNP G0SGU4
CCC	-4	THR	-	expression tag	UNP G0SGU4
CCC	-3	ALA	-	expression tag	UNP G0SGU4
CCC	-2	ARG	-	expression tag	UNP G0SGU4
CCC	-1	LEU	-	expression tag	UNP G0SGU4
CCC	0	GLN	-	expression tag	UNP G0SGU4
CCC	371	HIS	-	expression tag	UNP G0SGU4
CCC	372	HIS	-	expression tag	UNP G0SGU4
CCC	373	HIS	-	expression tag	UNP G0SGU4
CCC	374	HIS	-	expression tag	UNP G0SGU4
CCC	375	HIS	-	expression tag	UNP G0SGU4
CCC	376	HIS	-	expression tag	UNP G0SGU4
DDD	-33	MET	-	initiating methionine	UNP G0SGU4
DDD	-32	ALA	-	expression tag	UNP G0SGU4
DDD	-31	HIS	-	expression tag	UNP G0SGU4
DDD	-30	HIS	-	expression tag	UNP G0SGU4
DDD	-29	HIS	-	expression tag	UNP G0SGU4
DDD	-28	HIS	-	expression tag	UNP G0SGU4
DDD	-27	HIS	-	expression tag	UNP G0SGU4
DDD	-26	HIS	-	expression tag	UNP G0SGU4
DDD	-25	VAL	-	expression tag	UNP G0SGU4
DDD	-24	GLY	-	expression tag	UNP G0SGU4
DDD	-23	THR	-	expression tag	UNP G0SGU4
DDD	-22	GLY	-	expression tag	UNP G0SGU4
DDD	-21	SER	-	expression tag	UNP G0SGU4
DDD	-20	ASN	-	expression tag	UNP G0SGU4
DDD	-19	ASP	-	expression tag	UNP G0SGU4
DDD	-18	ASP	-	expression tag	UNP G0SGU4
DDD	-17	ASP	-	expression tag	UNP G0SGU4
DDD	-16	ASP	-	expression tag	UNP G0SGU4
DDD	-15	LYS	-	expression tag	UNP G0SGU4
DDD	-14	SER	-	expression tag	UNP G0SGU4
DDD	-13	PRO	-	expression tag	UNP G0SGU4
DDD	-12	ASP	-	expression tag	UNP G0SGU4
DDD	-11	PRO	-	expression tag	UNP G0SGU4
DDD	-10	ASN	-	expression tag	UNP G0SGU4
DDD	-9	TRP	-	expression tag	UNP G0SGU4
DDD	-8	GLU	-	expression tag	UNP G0SGU4
DDD	-7	LEU	-	expression tag	UNP G0SGU4

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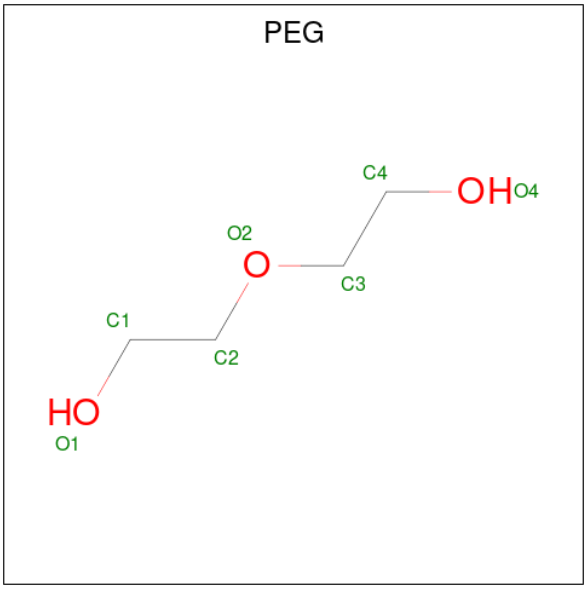
Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-6	VAL	-	expression tag	UNP G0SGU4
DDD	-5	TYR	-	expression tag	UNP G0SGU4
DDD	-4	THR	-	expression tag	UNP G0SGU4
DDD	-3	ALA	-	expression tag	UNP G0SGU4
DDD	-2	ARG	-	expression tag	UNP G0SGU4
DDD	-1	LEU	-	expression tag	UNP G0SGU4
DDD	0	GLN	-	expression tag	UNP G0SGU4
DDD	371	HIS	-	expression tag	UNP G0SGU4
DDD	372	HIS	-	expression tag	UNP G0SGU4
DDD	373	HIS	-	expression tag	UNP G0SGU4
DDD	374	HIS	-	expression tag	UNP G0SGU4
DDD	375	HIS	-	expression tag	UNP G0SGU4
DDD	376	HIS	-	expression tag	UNP G0SGU4

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
2	AAA	1	Total	C	H	O	1	0
			17	4	10	3		
2	BBB	1	Total	C	H	O	1	0
			17	4	10	3		
2	CCC	1	Total	C	H	O	1	0
			17	4	10	3		
2	CCC	1	Total	C	H	O	1	0
			17	4	10	3		

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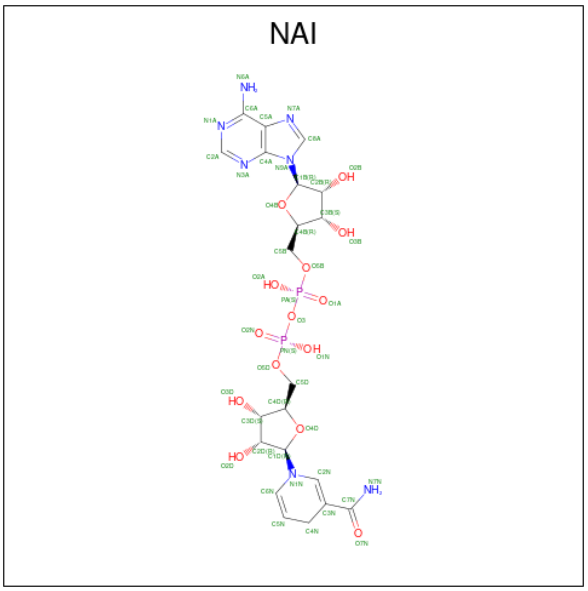
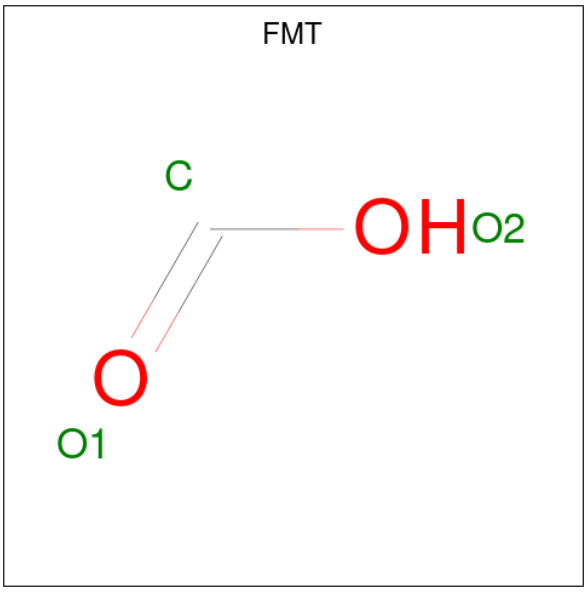
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	DDD	1	Total C H O 17 4 10 3	1	0
2	DDD	1	Total C H O 17 4 10 3	1	0

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



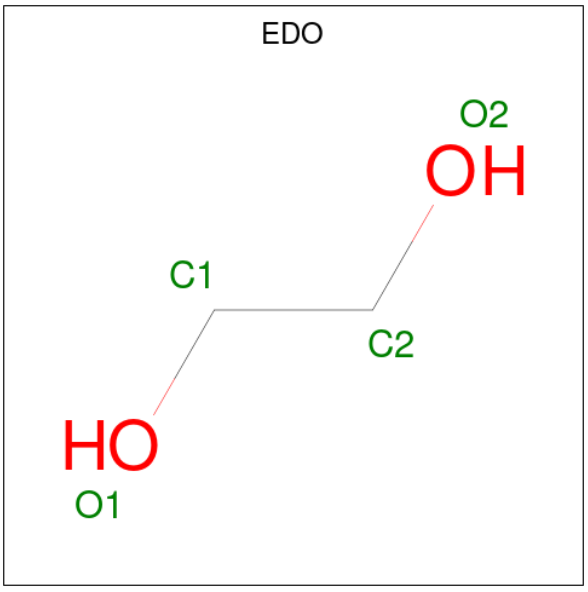
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C H N O P 71 21 27 7 14 2	4	0
3	BBB	1	Total C H N O P 71 21 27 7 14 2	4	0
3	CCC	1	Total C H N O P 71 21 27 7 14 2	4	0
3	DDD	1	Total C H N O P 71 21 27 7 14 2	4	0

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	AAA	1	Total	C	H	O	1	0
			5	1	2	2		
4	BBB	1	Total	C	H	O	1	0
			5	1	2	2		
4	CCC	1	Total	C	H	O	1	0
			5	1	2	2		
4	DDD	1	Total	C	H	O	1	0
			5	1	2	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	AAA	1	Total	C	H	O	1	0
			10	2	6	2		
5	BBB	1	Total	C	H	O	1	0
			10	2	6	2		
5	DDD	1	Total	C	H	O	1	0
			10	2	6	2		

- Molecule 6 is water.

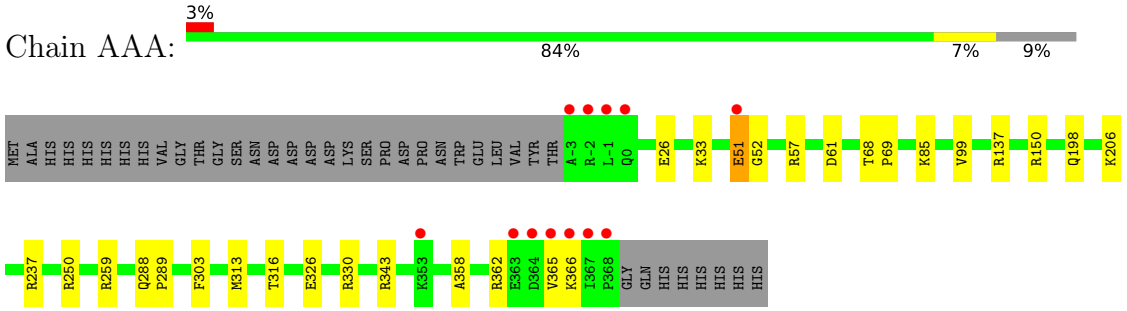
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	501	Total	O	0	0
			501	501		
6	BBB	453	Total	O	0	0
			453	453		
6	CCC	428	Total	O	0	0
			428	428		
6	DDD	511	Total	O	0	0
			511	511		

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.

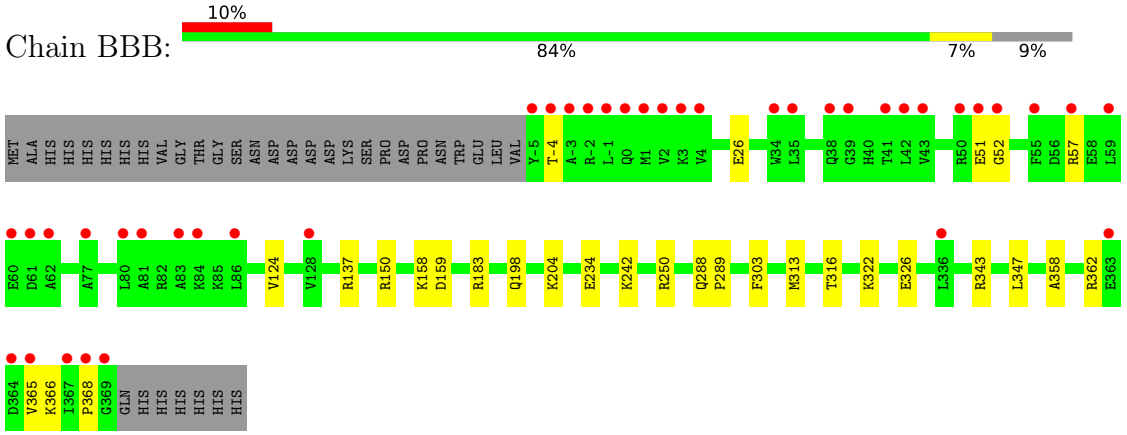
• Molecule 1: Formate dehydrogenase

Chain AAA:



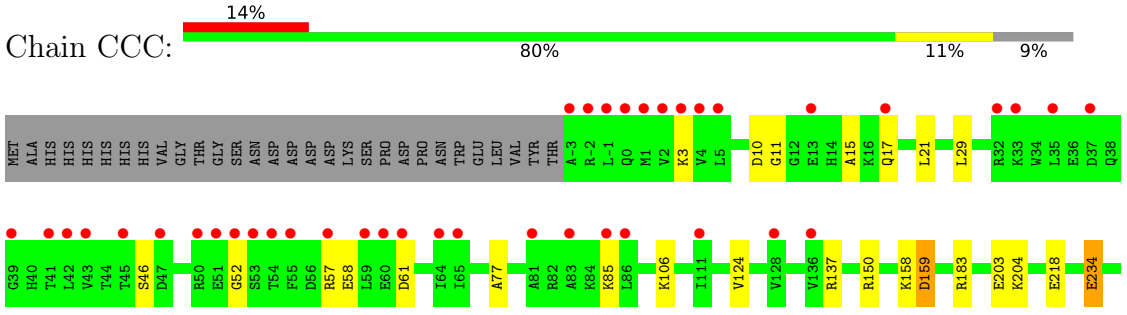
• Molecule 1: Formate dehydrogenase

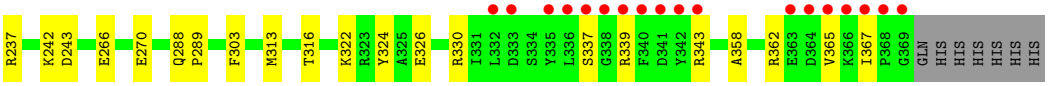
Chain BBB:



• Molecule 1: Formate dehydrogenase

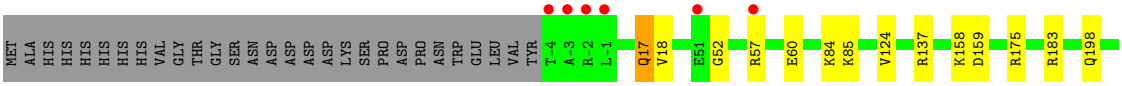
Chain CCC:

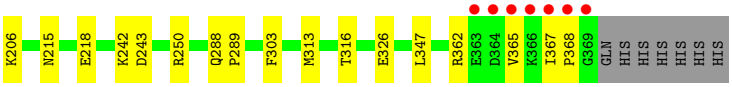




• Molecule 1: Formate dehydrogenase

Chain DDD:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.57Å 94.76Å 94.60Å 85.59° 89.93° 81.61°	Depositor
Resolution (Å)	46.77 – 1.26 46.73 – 1.26	Depositor EDS
% Data completeness (in resolution range)	87.0 (46.77-1.26) 87.0 (46.73-1.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.26Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.169 , 0.193 0.176 , 0.198	Depositor DCC
R_{free} test set	20297 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	16.1	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	27517	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FMT, EDO, PEG, NAI

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	AAA	0.75	2/3229 (0.1%)	0.88	2/4348 (0.0%)
1	BBB	0.75	2/3231 (0.1%)	0.89	4/4355 (0.1%)
1	CCC	0.78	0/3277	0.93	4/4410 (0.1%)
1	DDD	0.77	0/3203	0.89	4/4317 (0.1%)
All	All	0.76	4/12940 (0.0%)	0.90	14/17430 (0.1%)

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	AAA	0	1
1	BBB	0	1
1	CCC	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	26[A]	GLU	CD-OE1	6.38	1.32	1.25
1	BBB	26[B]	GLU	CD-OE1	6.38	1.32	1.25
1	AAA	26[A]	GLU	CD-OE1	6.32	1.32	1.25
1	AAA	26[B]	GLU	CD-OE1	6.32	1.32	1.25

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	150[A]	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	CCC	150[B]	ARG	NE-CZ-NH1	-7.02	116.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DDD	183	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	AAA	250	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	BBB	150[A]	ARG	NE-CZ-NH1	-6.45	117.07	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	137	ARG	Sidechain
1	BBB	137	ARG	Sidechain
1	CCC	137	ARG	Sidechain

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	AAA	3098	3189	3202	28	0
1	BBB	3096	3174	3191	30	0
1	CCC	3122	3233	3257	59	0
1	DDD	3075	3154	3169	39	0
2	AAA	14	20	20	0	0
2	BBB	7	10	10	0	0
2	CCC	14	20	20	0	0
2	DDD	14	20	20	0	0
3	AAA	44	27	27	1	0
3	BBB	44	27	27	2	0
3	CCC	44	27	27	2	0
3	DDD	44	27	27	1	0
4	AAA	3	2	1	0	0
4	BBB	3	2	1	0	0
4	CCC	3	2	1	0	0
4	DDD	3	2	1	0	0
5	AAA	16	24	24	3	0
5	BBB	4	6	6	2	0
5	DDD	4	6	6	0	0
6	AAA	501	0	0	18	0
6	BBB	453	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	CCC	428	0	0	19	0
6	DDD	511	0	0	14	0
All	All	14545	12972	13037	156	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 6.

The worst 5 of 156 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:CCC:204[A]:LYS:HE2	6:CCC:677:HOH:O	1.35	1.24
1:BBB:204[B]:LYS:HE2	6:BBB:1220:HOH:O	1.39	1.19
1:DDD:243[A]:ASP:OD1	6:DDD:504:HOH:O	1.65	1.13
1:BBB:51[B]:GLU:O	1:BBB:51[B]:GLU:OE2	1.67	1.10
1:CCC:203[B]:GLU:OE2	6:CCC:506:HOH:O	1.72	1.06

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	AAA	401/410 (98%)	389 (97%)	12 (3%)	0	100	100
1	BBB	402/410 (98%)	390 (97%)	12 (3%)	0	100	100
1	CCC	407/410 (99%)	395 (97%)	12 (3%)	0	100	100
1	DDD	399/410 (97%)	387 (97%)	12 (3%)	0	100	100
All	All	1609/1640 (98%)	1561 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	336/340 (99%)	333 (99%)	3 (1%)	78 47
1	BBB	336/340 (99%)	334 (99%)	2 (1%)	86 62
1	CCC	341/340 (100%)	336 (98%)	5 (2%)	65 28
1	DDD	333/340 (98%)	331 (99%)	2 (1%)	86 62
All	All	1346/1360 (99%)	1334 (99%)	12 (1%)	84 47

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CCC	159[B]	ASP
1	CCC	234[A]	GLU
1	DDD	17[B]	GLN
1	CCC	234[B]	GLU
1	BBB	-4	THR

Sometimes 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

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

21 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	$\#\|Z\| > 2$
2	PEG	AAA	502	-	6,6,6	0.16	0	5,5,5	0.20	0
3	NAI	AAA	503	-	42,48,48	1.15	5 (11%)	47,73,73	1.36	5 (10%)
2	PEG	AAA	501	-	6,6,6	0.27	0	5,5,5	0.22	0
4	FMT	CCC	404	-	2,2,2	0.39	0	1,1,1	0.16	0
5	EDO	AAA	508	-	3,3,3	0.28	0	2,2,2	0.60	0
4	FMT	AAA	504	-	2,2,2	0.28	0	1,1,1	0.05	0
2	PEG	CCC	403	-	6,6,6	0.23	0	5,5,5	0.13	0
5	EDO	AAA	506	-	3,3,3	0.17	0	2,2,2	0.43	0
3	NAI	DDD	403	-	42,48,48	1.04	3 (7%)	47,73,73	1.18	4 (8%)
4	FMT	DDD	404	-	2,2,2	0.58	0	1,1,1	0.08	0
2	PEG	DDD	401	-	6,6,6	0.25	0	5,5,5	0.21	0
5	EDO	AAA	507	-	3,3,3	0.38	0	2,2,2	0.98	0
2	PEG	DDD	402	-	6,6,6	0.27	0	5,5,5	0.12	0
5	EDO	BBB	904	-	3,3,3	0.16	0	2,2,2	0.48	0
3	NAI	BBB	901	-	42,48,48	1.18	4 (9%)	47,73,73	1.24	4 (8%)
3	NAI	CCC	402	-	42,48,48	1.37	4 (9%)	47,73,73	1.47	6 (12%)
4	FMT	BBB	903	-	2,2,2	0.63	0	1,1,1	0.07	0
5	EDO	DDD	405	-	3,3,3	0.16	0	2,2,2	0.41	0
5	EDO	AAA	505	-	3,3,3	0.38	0	2,2,2	0.62	0
2	PEG	BBB	902	-	6,6,6	0.21	0	5,5,5	0.21	0
2	PEG	CCC	401	-	6,6,6	0.42	0	5,5,5	0.13	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	NAI	DDD	403	-	-	2/25/72/72	0/5/5/5
5	EDO	DDD	405	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	AAA	502	-	-	2/4/4/4	-
3	NAI	AAA	503	-	-	2/25/72/72	0/5/5/5
2	PEG	AAA	501	-	-	1/4/4/4	-
5	EDO	AAA	505	-	-	0/1/1/1	-
2	PEG	BBB	902	-	-	0/4/4/4	-
5	EDO	AAA	508	-	-	1/1/1/1	-
2	PEG	DDD	401	-	-	0/4/4/4	-
5	EDO	AAA	507	-	-	1/1/1/1	-
2	PEG	DDD	402	-	-	0/4/4/4	-
5	EDO	BBB	904	-	-	1/1/1/1	-
5	EDO	AAA	506	-	-	1/1/1/1	-
2	PEG	CCC	403	-	-	2/4/4/4	-
3	NAI	BBB	901	-	-	2/25/72/72	0/5/5/5
3	NAI	CCC	402	-	-	2/25/72/72	0/5/5/5
2	PEG	CCC	401	-	-	0/4/4/4	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	CCC	402	NAI	C4N-C5N	-3.78	1.39	1.48
3	AAA	503	NAI	C2A-N1A	2.94	1.39	1.33
3	AAA	503	NAI	C4N-C5N	-2.72	1.41	1.48
3	DDD	403	NAI	C6N-C5N	2.69	1.38	1.33
3	CCC	402	NAI	C6N-C5N	2.56	1.37	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	AAA	503	NAI	N3A-C2A-N1A	-6.18	119.02	128.68
3	CCC	402	NAI	C4A-C5A-N7A	-4.42	104.79	109.40
3	BBB	901	NAI	O4B-C1B-C2B	-4.22	100.76	106.93
3	CCC	402	NAI	C1B-N9A-C4A	-3.83	119.92	126.64
3	CCC	402	NAI	N3A-C2A-N1A	-3.81	122.72	128.68

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	501	PEG	O1-C1-C2-O2
2	CCC	403	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	AAA	506	EDO	O1-C1-C2-O2
5	DDD	405	EDO	O1-C1-C2-O2
5	AAA	507	EDO	O1-C1-C2-O2

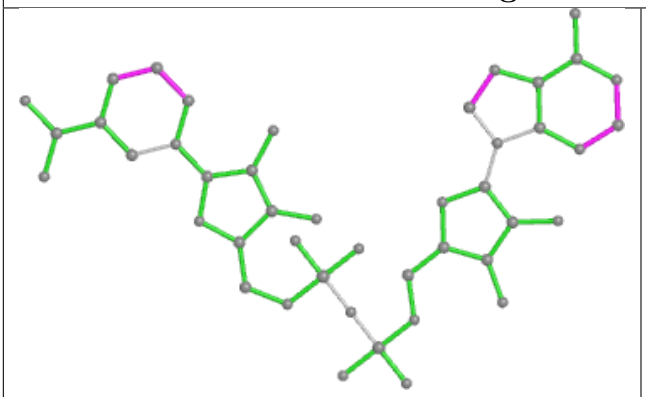
There are no ring outliers.

7 monomers are involved in 11 short contacts:

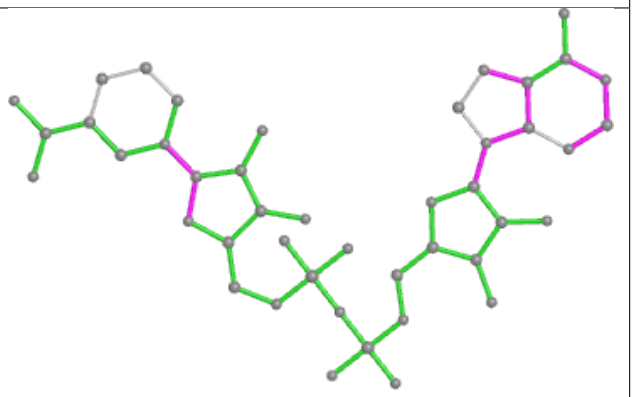
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AAA	503	NAI	1	0
3	DDD	403	NAI	1	0
5	AAA	507	EDO	2	0
5	BBB	904	EDO	2	0
3	BBB	901	NAI	2	0
3	CCC	402	NAI	2	0
5	AAA	505	EDO	1	0

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 then 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.

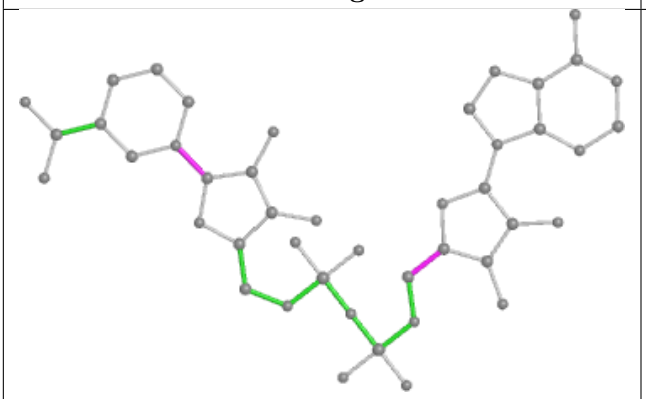
Ligand NAI AAA 503



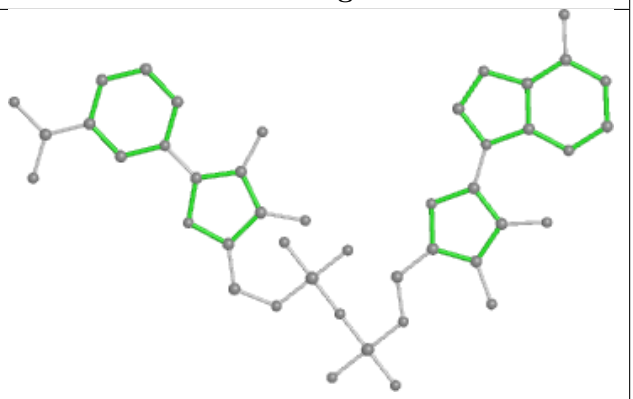
Bond lengths



Bond angles

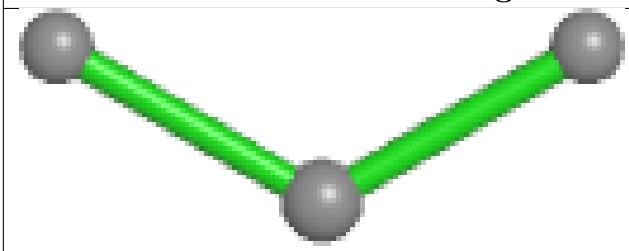


Torsions



Rings

Ligand FMT CCC 404



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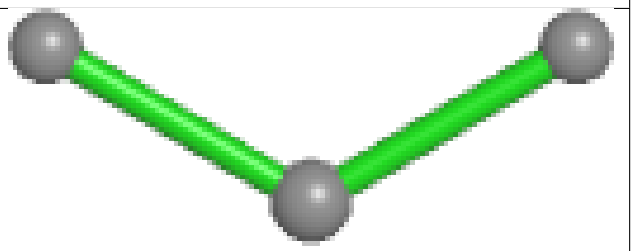

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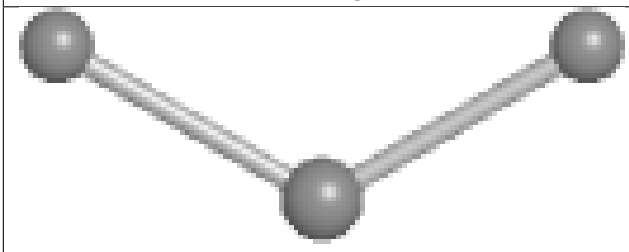

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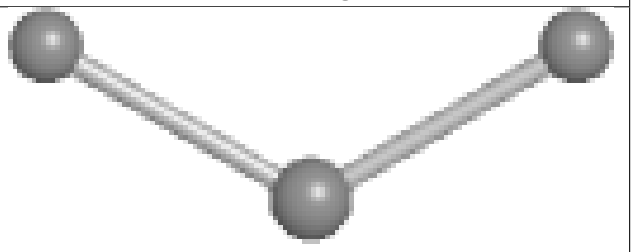
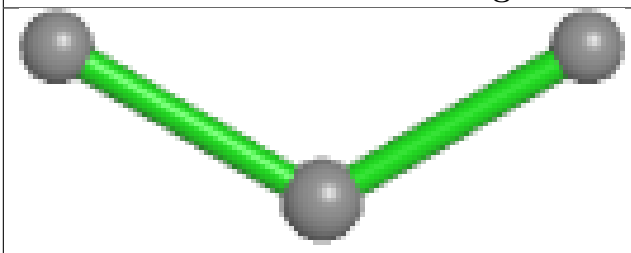
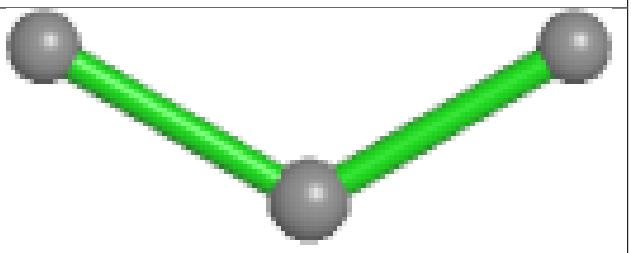


Rings

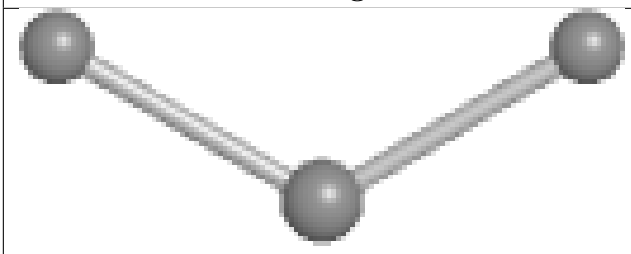
Ligand FMT AAA 504



Bond lengths



Bond angles



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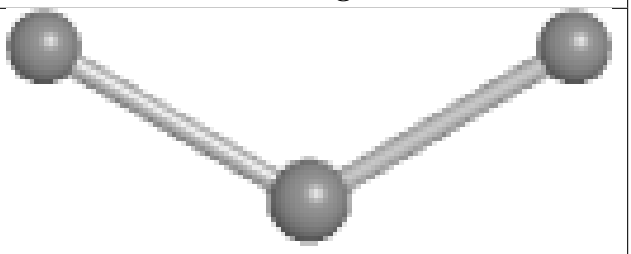
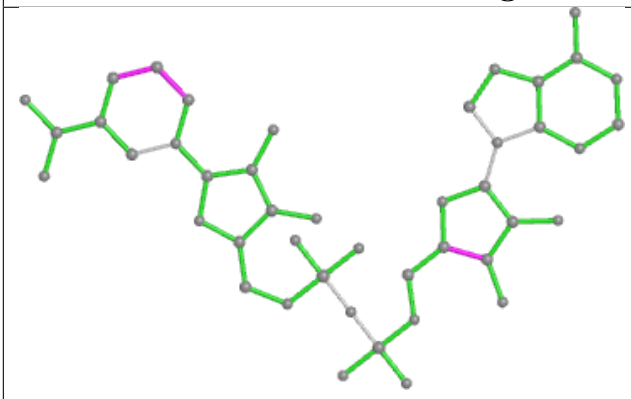
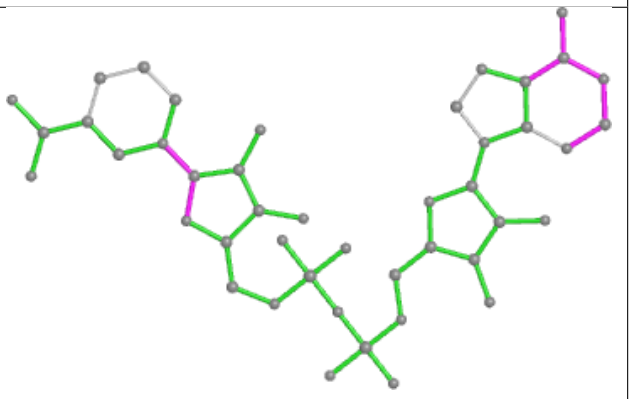


Rings

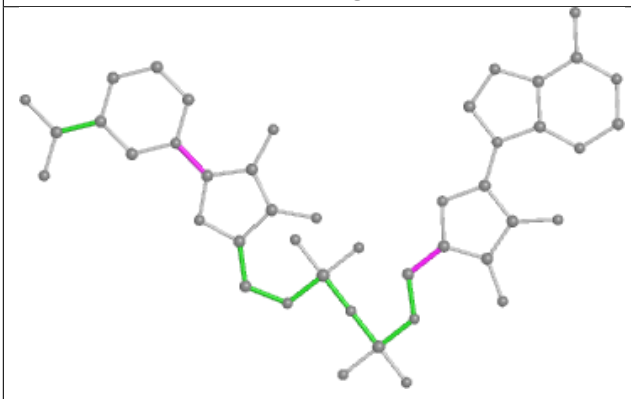
Ligand NAI DDD 403



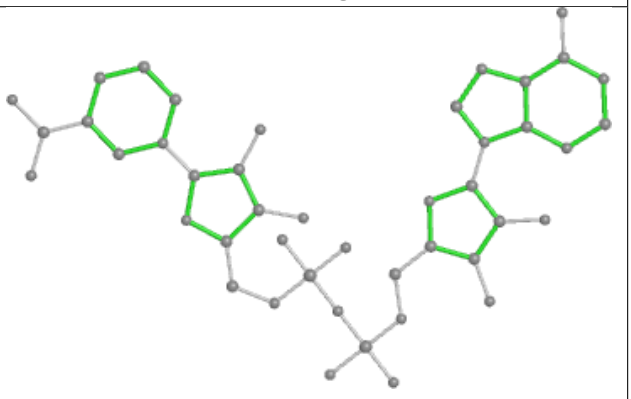
Bond lengths



Bond angles

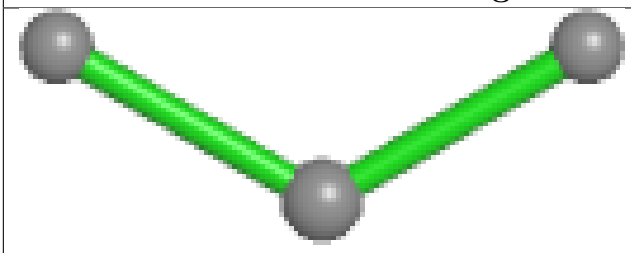


Torsions

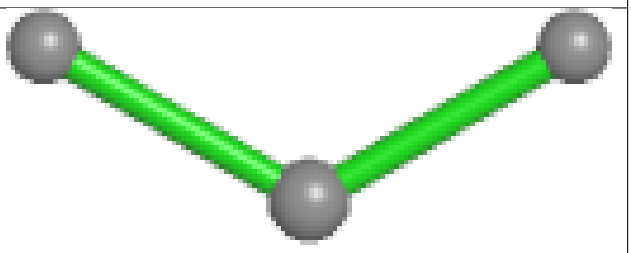


Rings

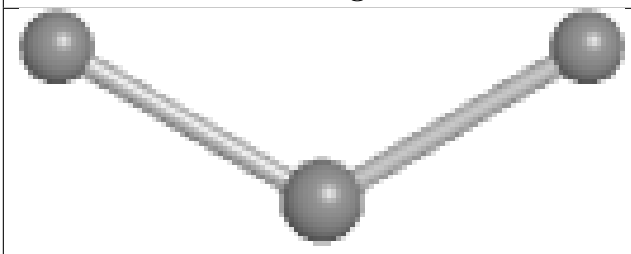
Ligand FMT DDD 404



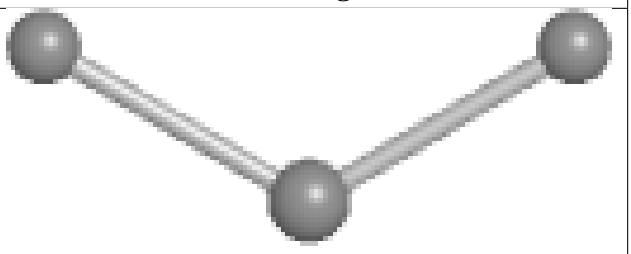
Bond lengths



Bond angles

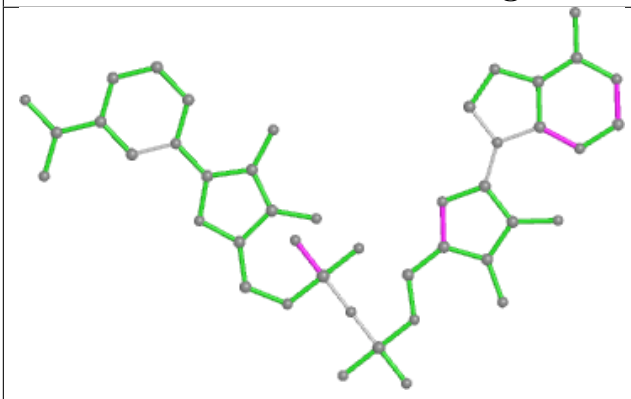


Torsions

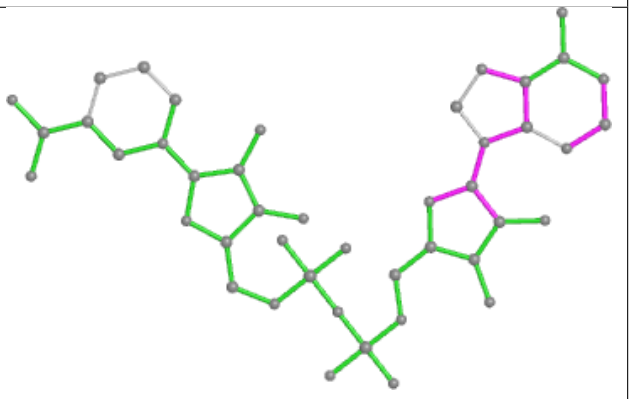


Rings

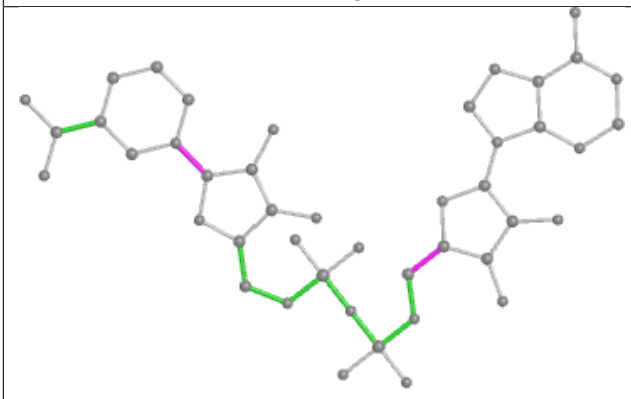
Ligand NAI BBB 901



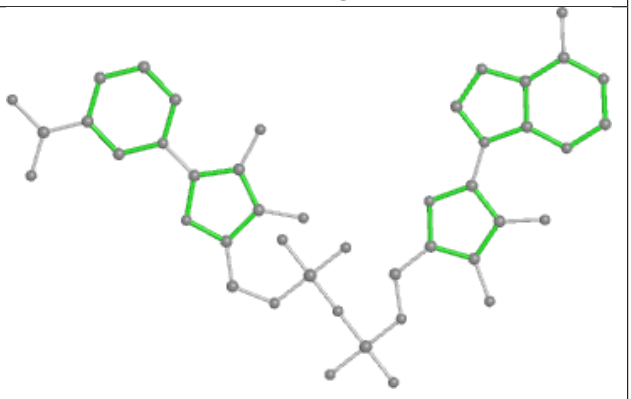
Bond lengths



Bond angles

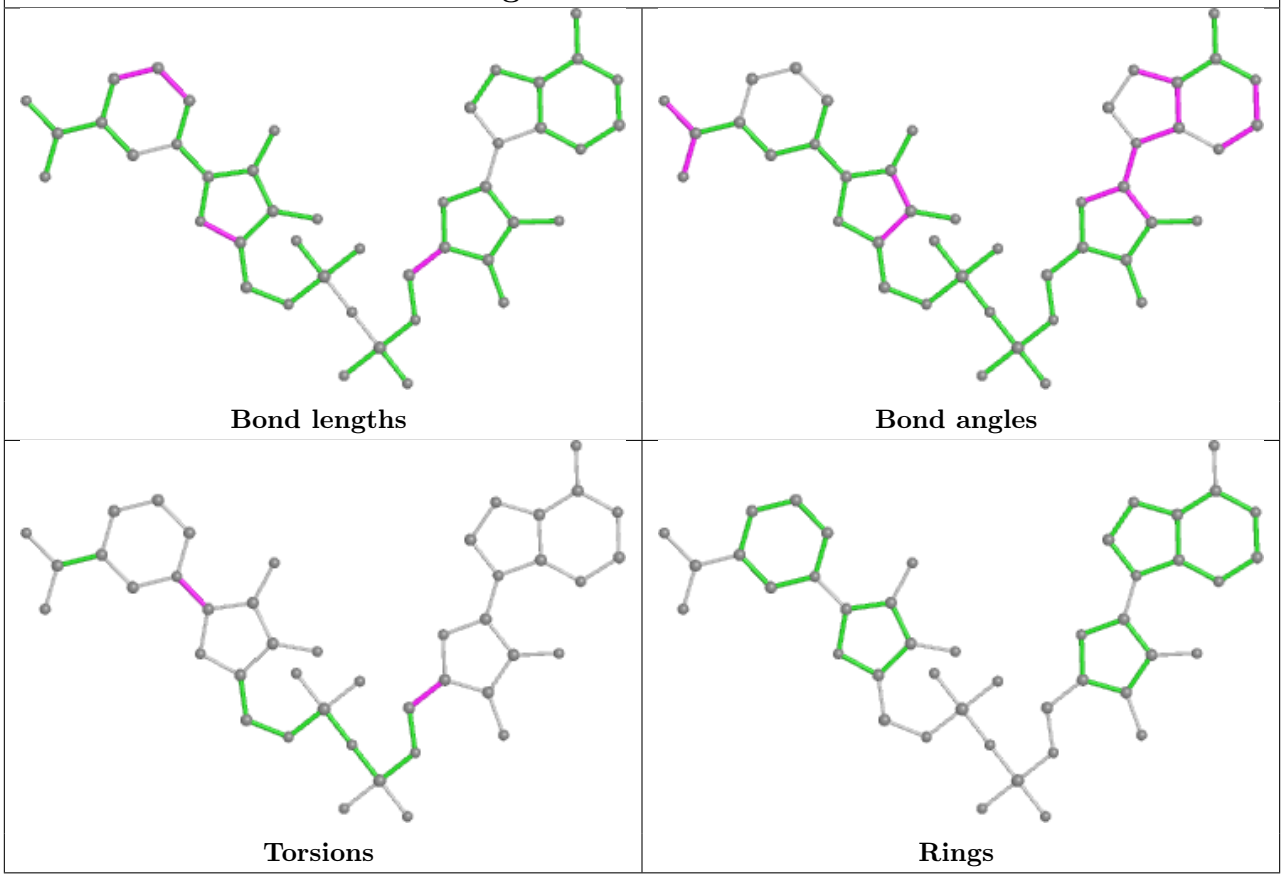


Torsions

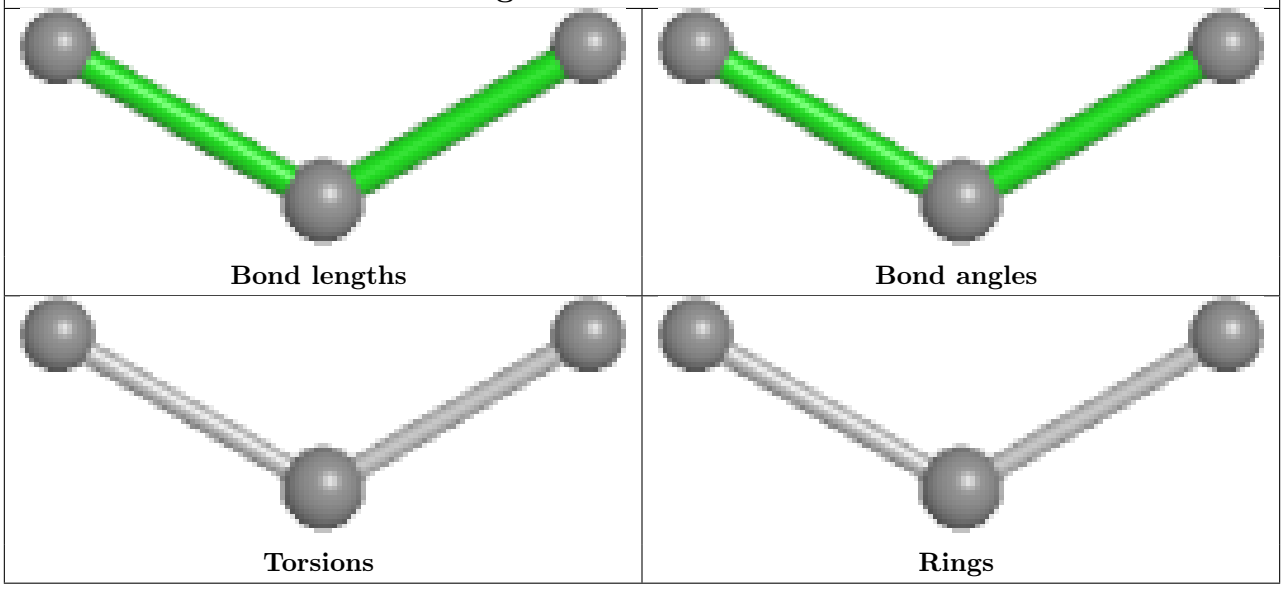


Rings

Ligand NAI CCC 402



Ligand FMT BBB 903



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^{th} 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	AAA	372/410 (90%)	-0.12	12 (3%) 47 39	11, 19, 38, 91	0
1	BBB	375/410 (91%)	0.31	40 (10%) 6 3	11, 20, 50, 102	0
1	CCC	373/410 (90%)	0.68	58 (15%) 2 1	10, 21, 53, 115	1 (0%)
1	DDD	374/410 (91%)	-0.10	13 (3%) 44 36	11, 19, 39, 86	0
All	All	1494/1640 (91%)	0.19	123 (8%) 11 7	10, 20, 48, 115	1 (0%)

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	369	GLY	11.6
1	BBB	-5	TYR	9.3
1	DDD	-4	THR	8.6
1	AAA	367	ILE	8.6
1	AAA	365	VAL	7.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

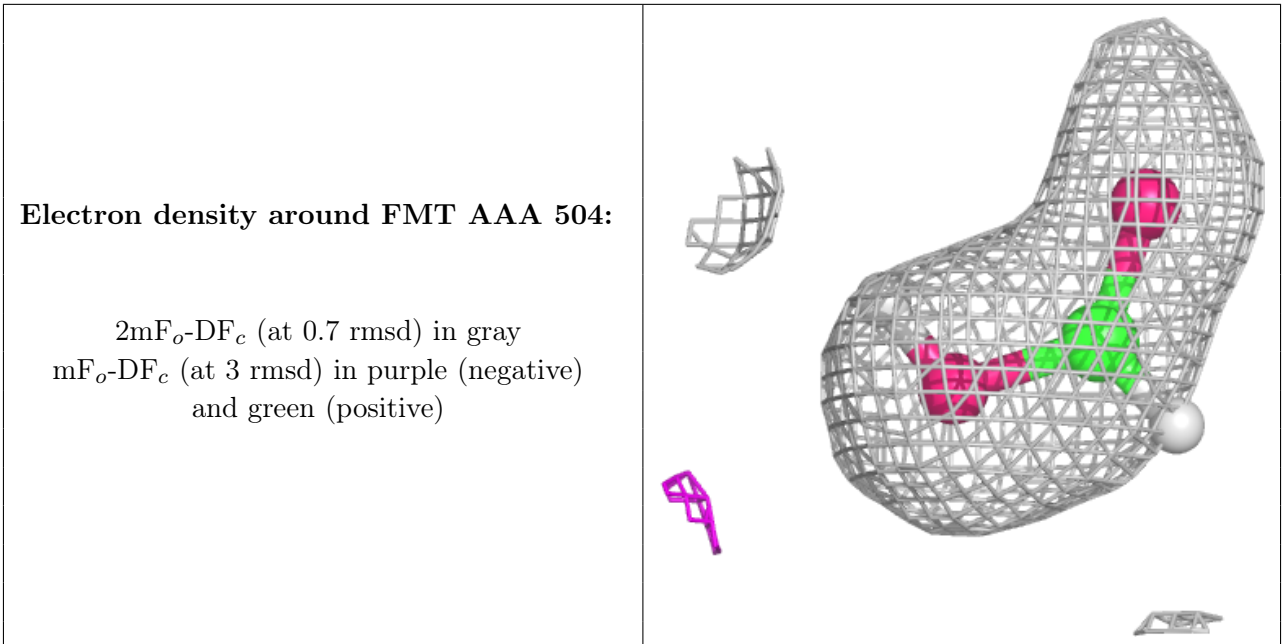
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

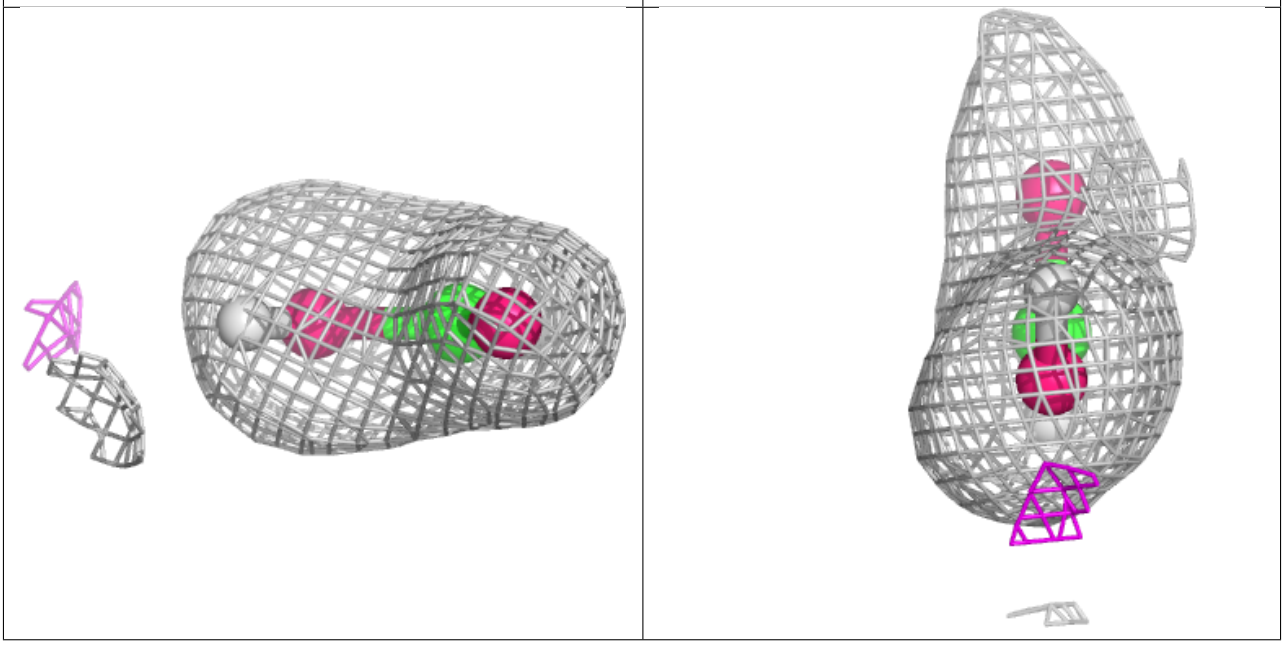
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	AAA	507	4/4	0.83	0.14	31,38,54,54	1
5	EDO	DDD	405	4/4	0.83	0.18	46,54,60,60	1
2	PEG	CCC	403	7/7	0.85	0.09	47,59,70,70	1
5	EDO	AAA	506	4/4	0.86	0.13	44,52,56,56	1
5	EDO	BBB	904	4/4	0.87	0.09	51,52,54,54	1
4	FMT	AAA	504	3/3	0.88	0.12	25,25,30,36	1
4	FMT	CCC	404	3/3	0.93	0.06	25,25,27,35	1
4	FMT	DDD	404	3/3	0.93	0.07	24,27,32,32	1
5	EDO	AAA	505	4/4	0.94	0.12	30,31,39,39	1
5	EDO	AAA	508	4/4	0.94	0.36	32,35,45,45	1
2	PEG	DDD	402	7/7	0.95	0.07	33,37,51,51	1
4	FMT	BBB	903	3/3	0.95	0.06	25,32,38,38	1
2	PEG	AAA	501	7/7	0.97	0.06	23,25,87,87	1
2	PEG	AAA	502	7/7	0.97	0.06	31,35,65,65	1
2	PEG	BBB	902	7/7	0.97	0.07	24,25,59,59	1
2	PEG	CCC	401	7/7	0.97	0.07	22,25,52,52	1
2	PEG	DDD	401	7/7	0.98	0.06	22,26,63,63	1
3	NAI	CCC	402	44/44	0.99	0.06	12,15,18,20	4
3	NAI	DDD	403	44/44	0.99	0.07	11,13,16,17	4
3	NAI	AAA	503	44/44	0.99	0.06	12,14,16,19	4
3	NAI	BBB	901	44/44	0.99	0.07	13,16,17,18	4

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 FMT AAA 504:

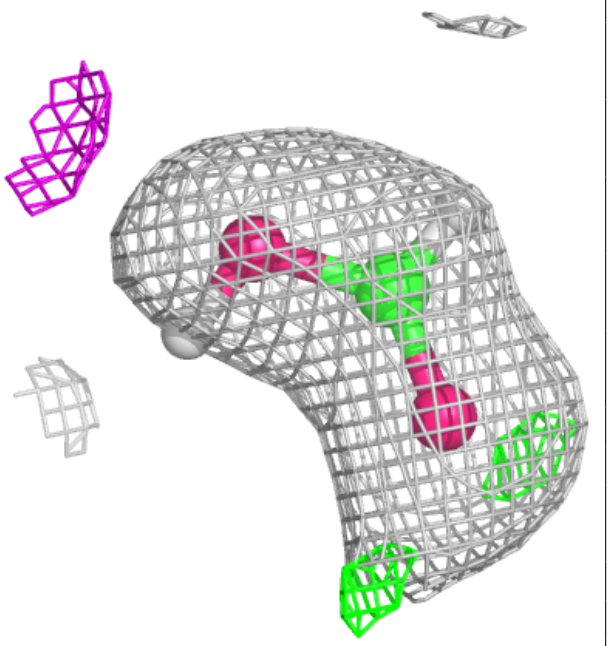
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

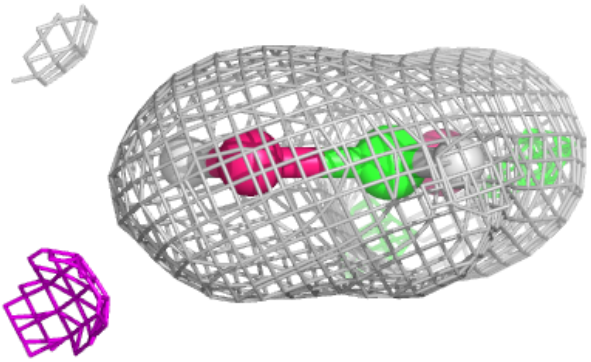


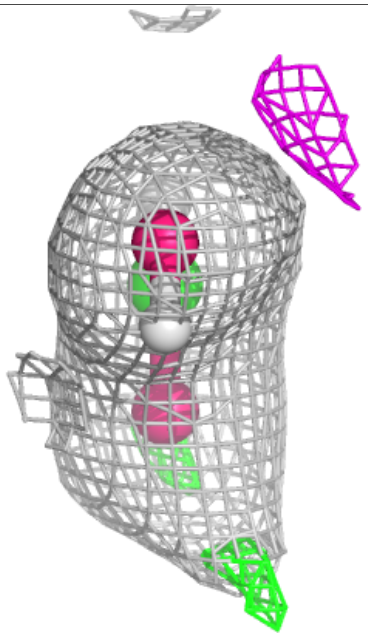


Electron density around FMT CCC 404:

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

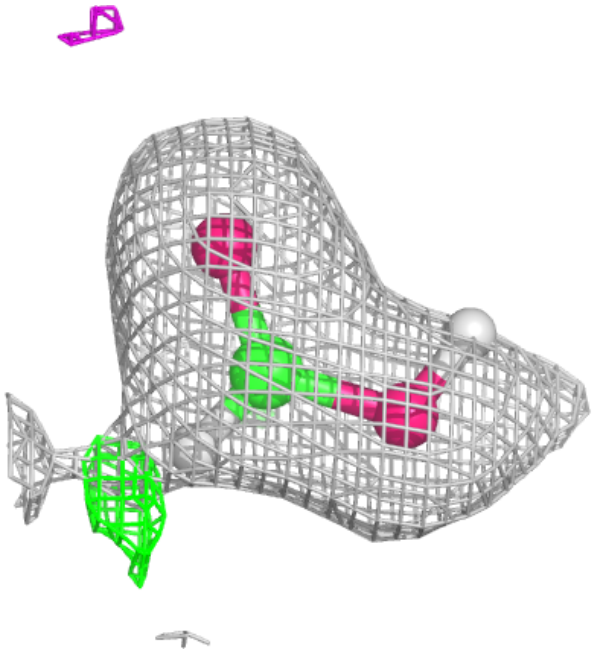


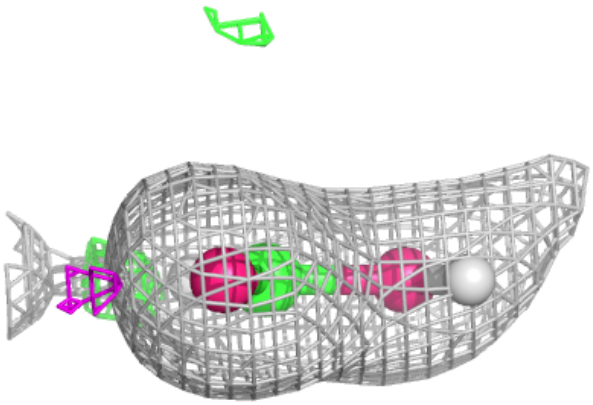


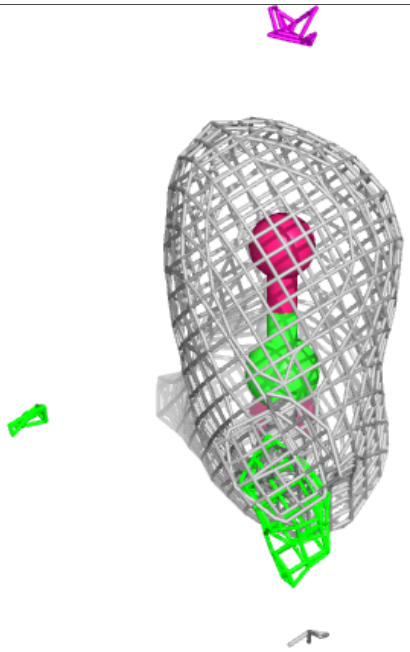


Electron density around FMT DDD 404:

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

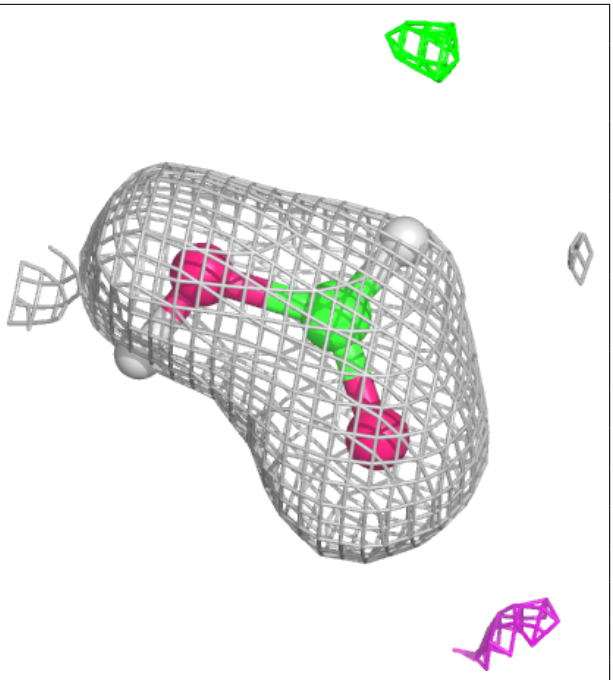


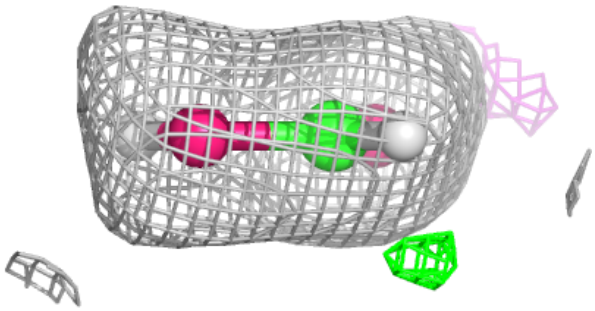


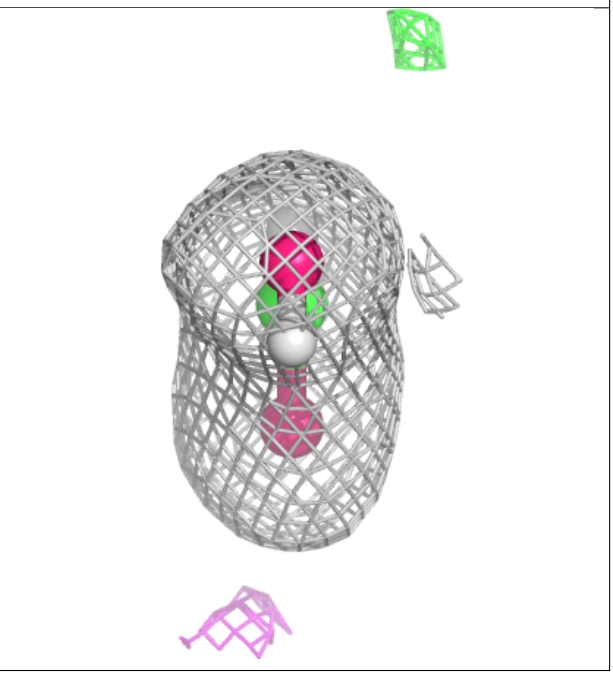


Electron density around FMT BBB 903:

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

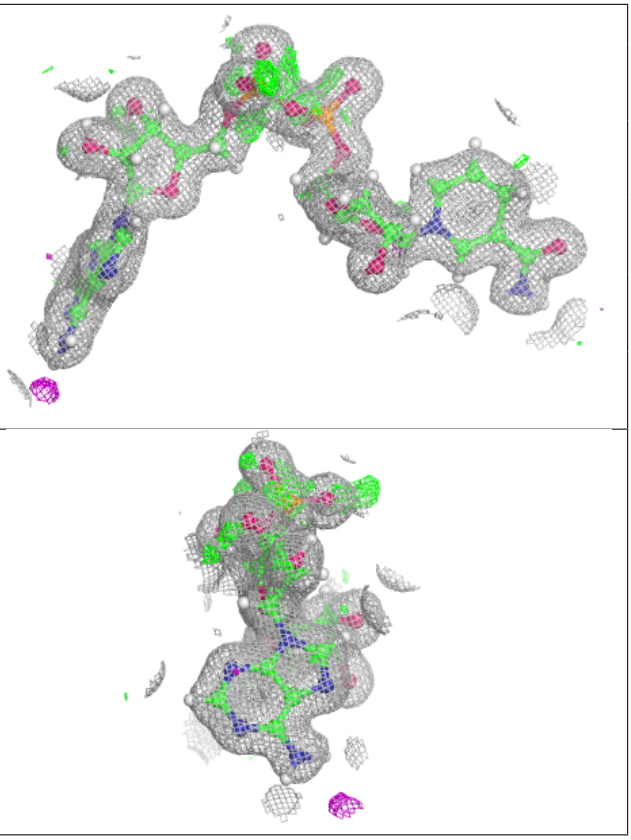






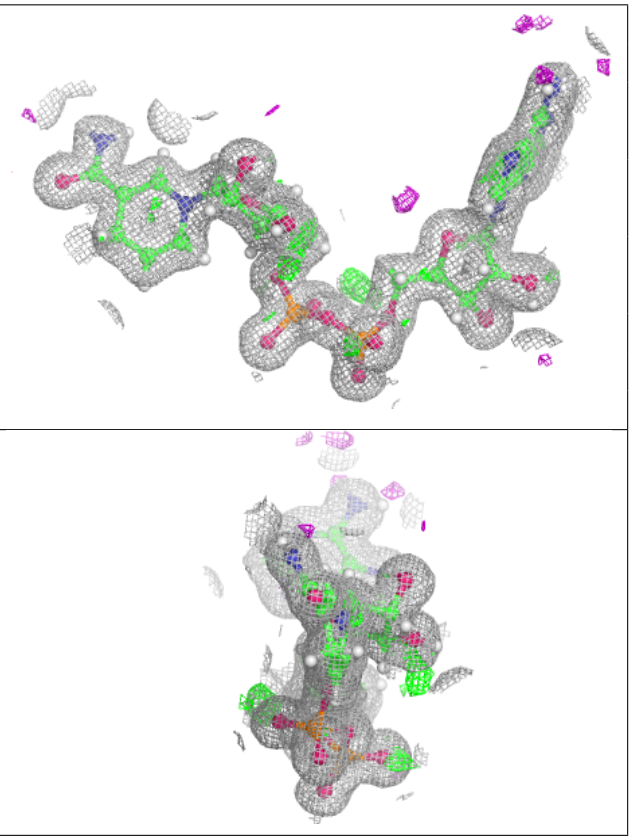
Electron density around NAI CCC 402:

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



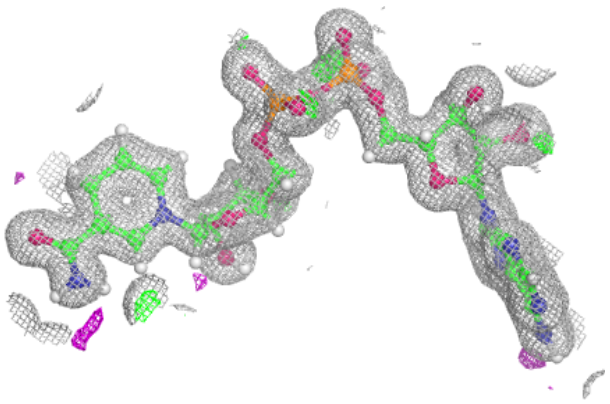
Electron density around NAI DDD 403:

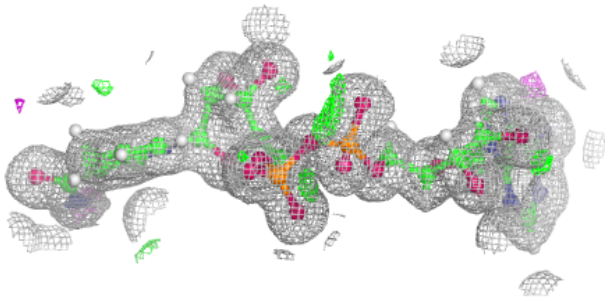
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

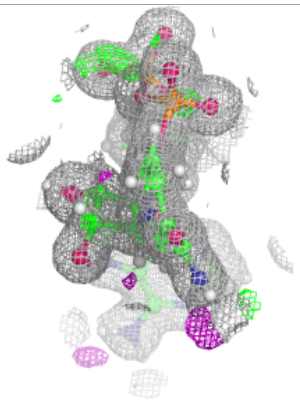


Electron density around NAI AAA 503:

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

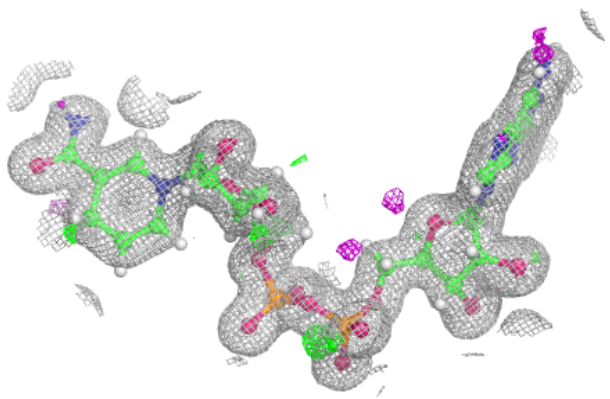


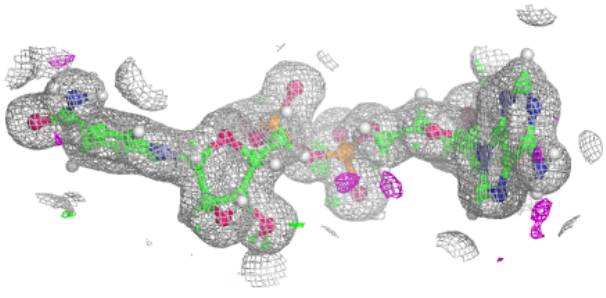


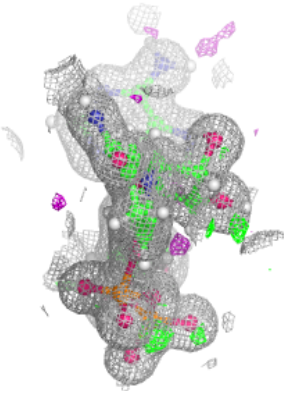


Electron density around NAI BBB 901:

$2mF_o$-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.