Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 10:12 PM EST

PDB ID	:	6C7N
Title	:	Monoclinic form of malic enzyme from sorghum at 2 angstroms resolution
Authors	:	Trajtenberg, F.; Alvarez, C.; Buschiazzo, A.
Deposited on	:	2018-01-23
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*
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:

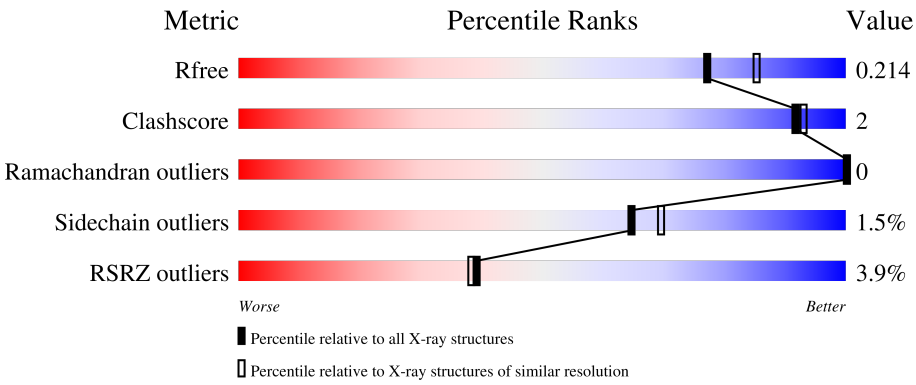
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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	A	613	2% 87% • 10%
1	B	613	% 85% 5% 10%
1	C	613	7% 80% 6% 13%
1	D	613	3% 61% • 37%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18830 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 Malic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	553	4397	2816	741	817	23	0	15	0
1	B	553	4347	2785	729	811	22	0	10	0
1	C	535	4903	3145	813	920	25	0	169	0
1	D	389	3079	1976	516	570	17	0	8	0

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	expression tag	UNP Q84LQ5
A	25	SER	-	expression tag	UNP Q84LQ5
A	26	GLY	-	expression tag	UNP Q84LQ5
A	27	MET	-	expression tag	UNP Q84LQ5
A	28	LYS	-	expression tag	UNP Q84LQ5
A	29	GLU	-	expression tag	UNP Q84LQ5
A	30	THR	-	expression tag	UNP Q84LQ5
A	31	ALA	-	expression tag	UNP Q84LQ5
A	32	ALA	-	expression tag	UNP Q84LQ5
A	33	ALA	-	expression tag	UNP Q84LQ5
A	34	LYS	-	expression tag	UNP Q84LQ5
A	35	PHE	-	expression tag	UNP Q84LQ5
A	36	GLU	-	expression tag	UNP Q84LQ5
A	37	ARG	-	expression tag	UNP Q84LQ5
A	38	GLN	-	expression tag	UNP Q84LQ5
A	39	HIS	-	expression tag	UNP Q84LQ5
A	40	MET	-	expression tag	UNP Q84LQ5
A	41	ASP	-	expression tag	UNP Q84LQ5
A	42	SER	-	expression tag	UNP Q84LQ5
A	43	PRO	-	expression tag	UNP Q84LQ5
A	44	ASP	-	expression tag	UNP Q84LQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	45	LEU	-	expression tag	UNP Q84LQ5
A	46	GLY	-	expression tag	UNP Q84LQ5
A	47	THR	-	expression tag	UNP Q84LQ5
A	48	ASP	-	expression tag	UNP Q84LQ5
A	49	ASP	-	expression tag	UNP Q84LQ5
A	50	ASP	-	expression tag	UNP Q84LQ5
A	51	ASP	-	expression tag	UNP Q84LQ5
A	52	LYS	-	expression tag	UNP Q84LQ5
A	53	ALA	-	expression tag	UNP Q84LQ5
A	54	MET	-	expression tag	UNP Q84LQ5
A	55	ALA	-	expression tag	UNP Q84LQ5
A	56	ASP	-	expression tag	UNP Q84LQ5
A	57	ILE	-	expression tag	UNP Q84LQ5
A	58	GLY	-	expression tag	UNP Q84LQ5
A	59	SER	-	expression tag	UNP Q84LQ5
A	60	GLU	-	expression tag	UNP Q84LQ5
A	61	PHE	-	expression tag	UNP Q84LQ5
A	115	ARG	LYS	conflict	UNP Q84LQ5
B	24	GLY	-	expression tag	UNP Q84LQ5
B	25	SER	-	expression tag	UNP Q84LQ5
B	26	GLY	-	expression tag	UNP Q84LQ5
B	27	MET	-	expression tag	UNP Q84LQ5
B	28	LYS	-	expression tag	UNP Q84LQ5
B	29	GLU	-	expression tag	UNP Q84LQ5
B	30	THR	-	expression tag	UNP Q84LQ5
B	31	ALA	-	expression tag	UNP Q84LQ5
B	32	ALA	-	expression tag	UNP Q84LQ5
B	33	ALA	-	expression tag	UNP Q84LQ5
B	34	LYS	-	expression tag	UNP Q84LQ5
B	35	PHE	-	expression tag	UNP Q84LQ5
B	36	GLU	-	expression tag	UNP Q84LQ5
B	37	ARG	-	expression tag	UNP Q84LQ5
B	38	GLN	-	expression tag	UNP Q84LQ5
B	39	HIS	-	expression tag	UNP Q84LQ5
B	40	MET	-	expression tag	UNP Q84LQ5
B	41	ASP	-	expression tag	UNP Q84LQ5
B	42	SER	-	expression tag	UNP Q84LQ5
B	43	PRO	-	expression tag	UNP Q84LQ5
B	44	ASP	-	expression tag	UNP Q84LQ5
B	45	LEU	-	expression tag	UNP Q84LQ5
B	46	GLY	-	expression tag	UNP Q84LQ5
B	47	THR	-	expression tag	UNP Q84LQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	48	ASP	-	expression tag	UNP Q84LQ5
B	49	ASP	-	expression tag	UNP Q84LQ5
B	50	ASP	-	expression tag	UNP Q84LQ5
B	51	ASP	-	expression tag	UNP Q84LQ5
B	52	LYS	-	expression tag	UNP Q84LQ5
B	53	ALA	-	expression tag	UNP Q84LQ5
B	54	MET	-	expression tag	UNP Q84LQ5
B	55	ALA	-	expression tag	UNP Q84LQ5
B	56	ASP	-	expression tag	UNP Q84LQ5
B	57	ILE	-	expression tag	UNP Q84LQ5
B	58	GLY	-	expression tag	UNP Q84LQ5
B	59	SER	-	expression tag	UNP Q84LQ5
B	60	GLU	-	expression tag	UNP Q84LQ5
B	61	PHE	-	expression tag	UNP Q84LQ5
B	115	ARG	LYS	conflict	UNP Q84LQ5
C	24	GLY	-	expression tag	UNP Q84LQ5
C	25	SER	-	expression tag	UNP Q84LQ5
C	26	GLY	-	expression tag	UNP Q84LQ5
C	27	MET	-	expression tag	UNP Q84LQ5
C	28	LYS	-	expression tag	UNP Q84LQ5
C	29	GLU	-	expression tag	UNP Q84LQ5
C	30	THR	-	expression tag	UNP Q84LQ5
C	31	ALA	-	expression tag	UNP Q84LQ5
C	32	ALA	-	expression tag	UNP Q84LQ5
C	33	ALA	-	expression tag	UNP Q84LQ5
C	34	LYS	-	expression tag	UNP Q84LQ5
C	35	PHE	-	expression tag	UNP Q84LQ5
C	36	GLU	-	expression tag	UNP Q84LQ5
C	37	ARG	-	expression tag	UNP Q84LQ5
C	38	GLN	-	expression tag	UNP Q84LQ5
C	39	HIS	-	expression tag	UNP Q84LQ5
C	40	MET	-	expression tag	UNP Q84LQ5
C	41	ASP	-	expression tag	UNP Q84LQ5
C	42	SER	-	expression tag	UNP Q84LQ5
C	43	PRO	-	expression tag	UNP Q84LQ5
C	44	ASP	-	expression tag	UNP Q84LQ5
C	45	LEU	-	expression tag	UNP Q84LQ5
C	46	GLY	-	expression tag	UNP Q84LQ5
C	47	THR	-	expression tag	UNP Q84LQ5
C	48	ASP	-	expression tag	UNP Q84LQ5
C	49	ASP	-	expression tag	UNP Q84LQ5
C	50	ASP	-	expression tag	UNP Q84LQ5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	51	ASP	-	expression tag	UNP Q84LQ5
C	52	LYS	-	expression tag	UNP Q84LQ5
C	53	ALA	-	expression tag	UNP Q84LQ5
C	54	MET	-	expression tag	UNP Q84LQ5
C	55	ALA	-	expression tag	UNP Q84LQ5
C	56	ASP	-	expression tag	UNP Q84LQ5
C	57	ILE	-	expression tag	UNP Q84LQ5
C	58	GLY	-	expression tag	UNP Q84LQ5
C	59	SER	-	expression tag	UNP Q84LQ5
C	60	GLU	-	expression tag	UNP Q84LQ5
C	61	PHE	-	expression tag	UNP Q84LQ5
C	115	ARG	LYS	conflict	UNP Q84LQ5
D	24	GLY	-	expression tag	UNP Q84LQ5
D	25	SER	-	expression tag	UNP Q84LQ5
D	26	GLY	-	expression tag	UNP Q84LQ5
D	27	MET	-	expression tag	UNP Q84LQ5
D	28	LYS	-	expression tag	UNP Q84LQ5
D	29	GLU	-	expression tag	UNP Q84LQ5
D	30	THR	-	expression tag	UNP Q84LQ5
D	31	ALA	-	expression tag	UNP Q84LQ5
D	32	ALA	-	expression tag	UNP Q84LQ5
D	33	ALA	-	expression tag	UNP Q84LQ5
D	34	LYS	-	expression tag	UNP Q84LQ5
D	35	PHE	-	expression tag	UNP Q84LQ5
D	36	GLU	-	expression tag	UNP Q84LQ5
D	37	ARG	-	expression tag	UNP Q84LQ5
D	38	GLN	-	expression tag	UNP Q84LQ5
D	39	HIS	-	expression tag	UNP Q84LQ5
D	40	MET	-	expression tag	UNP Q84LQ5
D	41	ASP	-	expression tag	UNP Q84LQ5
D	42	SER	-	expression tag	UNP Q84LQ5
D	43	PRO	-	expression tag	UNP Q84LQ5
D	44	ASP	-	expression tag	UNP Q84LQ5
D	45	LEU	-	expression tag	UNP Q84LQ5
D	46	GLY	-	expression tag	UNP Q84LQ5
D	47	THR	-	expression tag	UNP Q84LQ5
D	48	ASP	-	expression tag	UNP Q84LQ5
D	49	ASP	-	expression tag	UNP Q84LQ5
D	50	ASP	-	expression tag	UNP Q84LQ5
D	51	ASP	-	expression tag	UNP Q84LQ5
D	52	LYS	-	expression tag	UNP Q84LQ5
D	53	ALA	-	expression tag	UNP Q84LQ5

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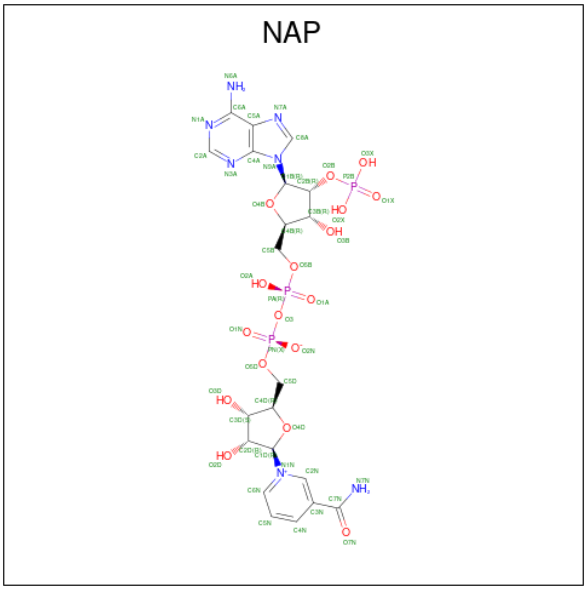
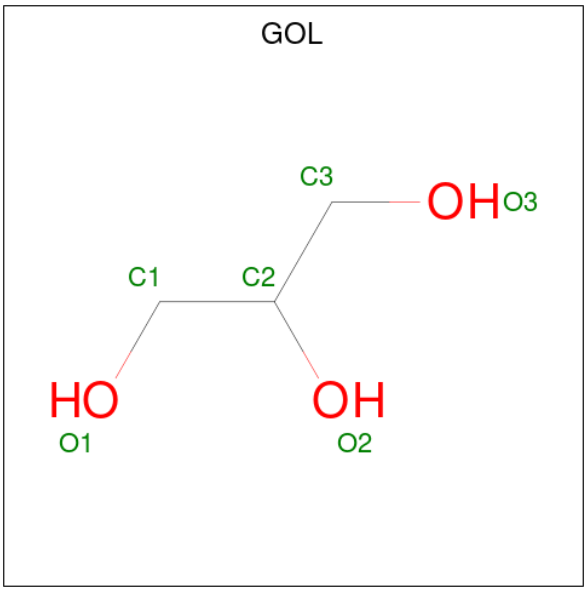
Chain	Residue	Modelled	Actual	Comment	Reference
D	54	MET	-	expression tag	UNP Q84LQ5
D	55	ALA	-	expression tag	UNP Q84LQ5
D	56	ASP	-	expression tag	UNP Q84LQ5
D	57	ILE	-	expression tag	UNP Q84LQ5
D	58	GLY	-	expression tag	UNP Q84LQ5
D	59	SER	-	expression tag	UNP Q84LQ5
D	60	GLU	-	expression tag	UNP Q84LQ5
D	61	PHE	-	expression tag	UNP Q84LQ5
D	115	ARG	LYS	conflict	UNP Q84LQ5

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	C	1	96	42	14	34	6	0	1
			Total	C	N	O	P		
2	D	1	52	22	4	22	4	0	1

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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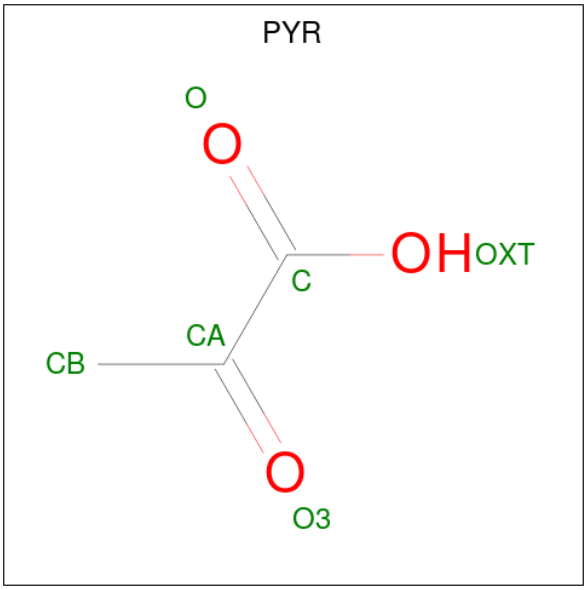
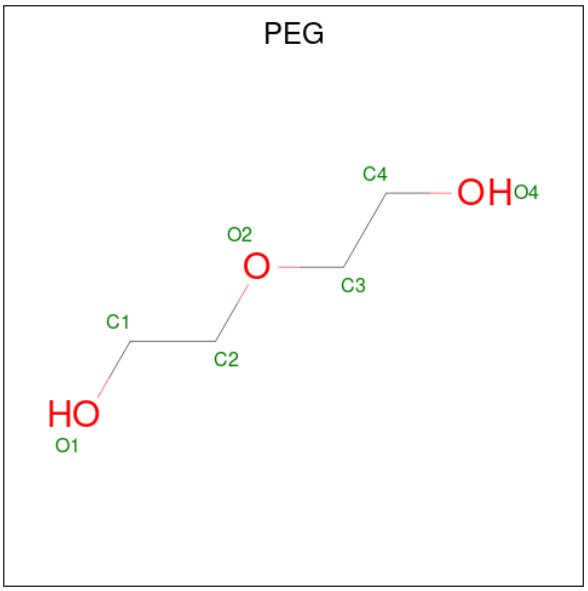
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0
			Total	C	O		
3	D	1	6	3	3	0	0

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	12	6	6	0	1
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	C	1	6	3	3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	7	4	3	0	0

- Molecule 6 is water.

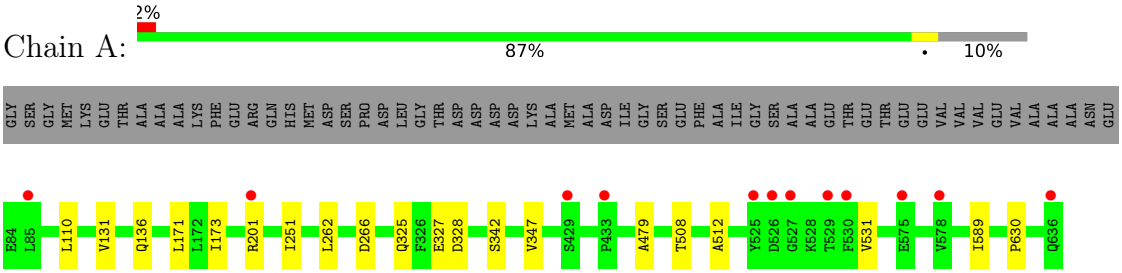
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	563	565	565	0	6
			Total	O		
6	B	610	615	615	0	6
			Total	O		
6	C	278	281	281	0	8
			Total	O		
6	D	264	266	266	0	3

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.

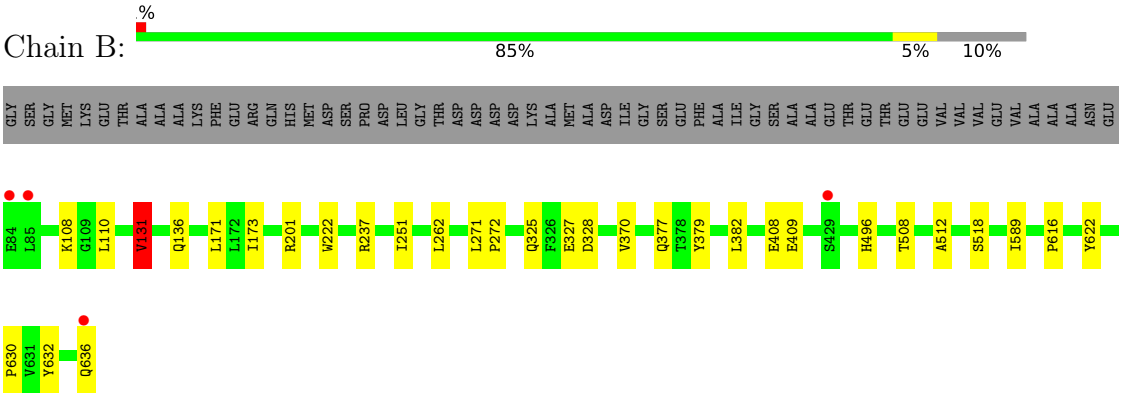
• Molecule 1: Malic enzyme

Chain A:



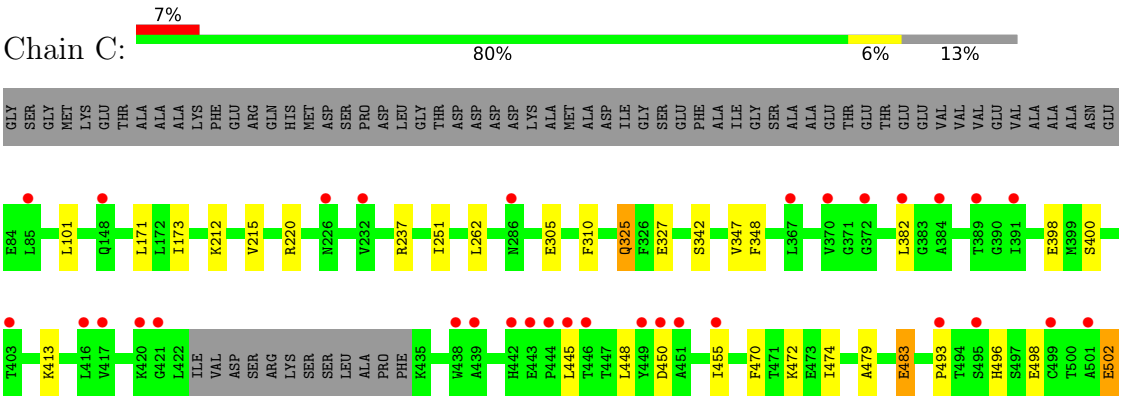
• Molecule 1: Malic enzyme

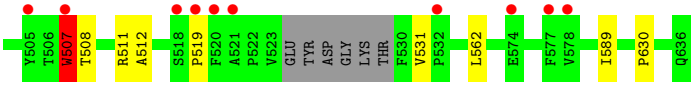
Chain B:



• Molecule 1: Malic enzyme

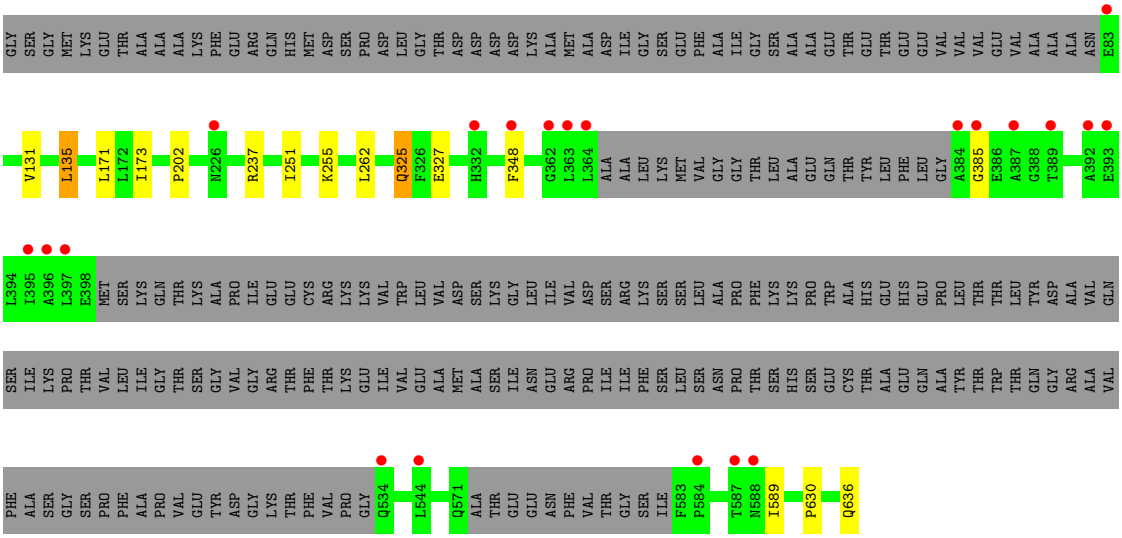
Chain C:





- Molecule 1: Malic enzyme

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.10Å 64.26Å 202.72Å 90.00° 93.65° 90.00°	Depositor
Resolution (Å)	29.28 – 2.00 29.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.28-2.00) 100.0 (29.22-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.180 , 0.210 0.180 , 0.214	Depositor DCC
R_{free} test set	1819 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 65.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18830	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, PYR, GOL, PEG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.54	0/4496	0.62	0/6104
1	B	0.57	0/4452	0.63	2/6045 (0.0%)
1	C	6.85	11/5011 (0.2%)	1.64	26/6791 (0.4%)
1	D	0.49	0/3145	0.59	0/4267
All	All	3.73	11/17104 (0.1%)	1.03	28/23207 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	507[A]	TRP	CB-CG	264.15	6.25	1.50
1	C	507[B]	TRP	CB-CG	264.15	6.25	1.50
1	C	502[A]	GLU	CB-CG	156.20	4.49	1.52
1	C	502[B]	GLU	CB-CG	156.20	4.49	1.52
1	C	483[A]	GLU	CB-CG	147.96	4.33	1.52
1	C	483[B]	GLU	CB-CG	147.96	4.33	1.52
1	C	531[B]	VAL	C-N	25.94	1.83	1.34
1	C	519[A]	PRO	C-N	19.11	1.78	1.34
1	C	519[B]	PRO	C-N	19.11	1.78	1.34
1	C	400[A]	SER	C-N	10.34	1.57	1.34
1	C	400[B]	SER	C-N	10.34	1.57	1.34

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	483[A]	GLU	CA-CB-CG	-42.27	20.40	113.40
1	C	483[B]	GLU	CA-CB-CG	-42.27	20.40	113.40
1	C	531[B]	VAL	O-C-N	-38.19	48.55	121.10
1	C	519[A]	PRO	O-C-N	-31.84	71.76	122.70
1	C	519[B]	PRO	O-C-N	-31.84	71.76	122.70
1	C	400[A]	SER	O-C-N	29.84	170.45	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	400[B]	SER	O-C-N	29.84	170.45	122.70
1	C	519[A]	PRO	C-N-CA	-26.01	56.68	121.70
1	C	519[B]	PRO	C-N-CA	-26.01	56.68	121.70
1	C	531[B]	VAL	C-N-CD	-24.78	66.09	120.60
1	C	519[A]	PRO	CA-C-N	-23.32	65.89	117.20
1	C	519[B]	PRO	CA-C-N	-23.32	65.89	117.20
1	C	400[A]	SER	C-N-CA	-23.27	63.54	121.70
1	C	400[B]	SER	C-N-CA	-23.27	63.54	121.70
1	C	400[A]	SER	CA-C-N	-23.11	66.36	117.20
1	C	400[B]	SER	CA-C-N	-23.11	66.36	117.20
1	C	502[A]	GLU	CB-CG-CD	-20.33	59.31	114.20
1	C	502[B]	GLU	CB-CG-CD	-20.33	59.31	114.20
1	C	507[A]	TRP	CB-CG-CD2	12.67	143.07	126.60
1	C	507[B]	TRP	CB-CG-CD2	12.67	143.07	126.60
1	C	507[A]	TRP	CB-CG-CD1	-12.54	110.70	127.00
1	C	507[B]	TRP	CB-CG-CD1	-12.54	110.70	127.00
1	C	507[A]	TRP	CA-CB-CG	10.92	134.45	113.70
1	C	507[B]	TRP	CA-CB-CG	10.92	134.45	113.70
1	C	502[A]	GLU	CA-CB-CG	6.56	127.84	113.40
1	C	502[B]	GLU	CA-CB-CG	6.56	127.84	113.40
1	B	131	VAL	CA-CB-CG2	5.70	119.45	110.90
1	B	131	VAL	CA-CB-CG1	5.57	119.25	110.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4397	0	4384	11	0
1	B	4347	0	4343	16	0
1	C	4903	0	4843	23	0
1	D	3079	0	3056	7	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	96	0	50	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	52	0	28	1	0
3	A	42	0	56	1	0
3	B	30	0	40	2	0
3	C	12	0	16	0	0
3	D	18	0	24	0	0
4	B	18	0	0	0	0
4	C	6	0	0	0	0
5	B	7	0	10	1	0
6	A	565	0	0	0	0
6	B	615	0	0	2	0
6	C	281	0	0	1	0
6	D	266	0	0	0	0
All	All	18830	0	16900	55	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 2.

All (55) 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:C:508[A]:THR:HG21	1:C:512[A]:ALA:HB2	1.77	0.64
1:C:508[B]:THR:HG21	1:C:512[B]:ALA:HB2	1.81	0.63
1:A:251:ILE:HG22	1:A:327[A]:GLU:OE1	2.00	0.61
1:C:479[A]:ALA:HB2	1:C:508[A]:THR:HG22	1.83	0.60
1:B:251:ILE:HG22	1:B:327[A]:GLU:OE1	2.05	0.56
1:B:518[A]:SER:HB3	6:B:1356[A]:HOH:O	2.05	0.56
1:D:262:LEU:HD22	1:D:589:ILE:HG21	1.88	0.55
1:C:262:LEU:HD22	1:C:589:ILE:HG21	1.87	0.55
1:A:110:LEU:HB3	1:A:131:VAL:HG13	1.89	0.54
1:B:382:LEU:HD11	5:B:1009:PEG:H22	1.89	0.53
1:A:508:THR:HG21	1:A:512:ALA:HB2	1.90	0.53
1:D:173:ILE:HD12	1:D:630:PRO:HG3	1.91	0.53
1:B:110:LEU:HB3	1:B:131:VAL:HG13	1.92	0.52
1:A:262:LEU:HD22	1:A:589:ILE:HG21	1.90	0.52
1:C:445[B]:LEU:HD22	1:C:450[B]:ASP:HB3	1.91	0.52
1:A:173:ILE:HD12	1:A:630:PRO:HG3	1.92	0.51
1:D:251:ILE:HG22	1:D:327[A]:GLU:OE1	2.09	0.51
1:A:342[B]:SER:HA	1:A:347[B]:VAL:HG22	1.93	0.51
1:C:251:ILE:HG22	1:C:327[A]:GLU:OE1	2.11	0.51
1:C:325:GLN:HG3	1:C:348[A]:PHE:HD2	1.76	0.51
1:B:496:HIS:HA	3:B:1008:GOL:H12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HD22	1:B:589:ILE:HG21	1.95	0.49
1:B:508:THR:HG21	1:B:512:ALA:HB2	1.95	0.49
1:B:173:ILE:HD12	1:B:630:PRO:HG3	1.94	0.48
1:A:251:ILE:HG21	1:A:328:ASP:OD2	2.13	0.48
1:C:398[A]:GLU:HB2	1:C:562:LEU:HD22	1.95	0.48
1:C:212:LYS:HE2	1:C:305:GLU:HB3	1.95	0.48
1:D:131:VAL:HG13	1:D:135:LEU:HD22	1.95	0.47
1:C:173:ILE:HD12	1:C:630:PRO:HG3	1.95	0.47
1:C:448[A]:LEU:HD23	1:C:474[A]:ILE:HD13	1.96	0.47
1:D:385:GLY:HA3	2:D:1001[B]:NAP:O1A	2.15	0.47
1:C:470[A]:PHE:CG	1:C:498[A]:GLU:HB3	2.50	0.46
1:C:382[B]:LEU:HD13	1:C:448[B]:LEU:HD22	1.98	0.46
1:B:131:VAL:HG22	1:B:136:GLN:HG3	1.99	0.45
1:C:342:SER:HA	1:C:347[A]:VAL:HG22	1.99	0.44
1:A:479:ALA:HB2	1:A:508:THR:HG22	2.00	0.44
1:D:325:GLN:HG3	1:D:348[A]:PHE:HD2	1.83	0.44
1:C:483[B]:GLU:HA	1:C:511[B]:ARG:HH21	1.83	0.43
1:C:220[B]:ARG:HD3	6:C:1221:HOH:O	2.18	0.43
1:A:201[C]:ARG:HH22	1:B:201:ARG:HD2	1.84	0.43
1:A:266:ASP:HB2	3:A:1008:GOL:H31	2.01	0.42
1:C:472[B]:LYS:HG3	1:C:507[B]:TRP:CD1	2.54	0.42
1:C:479[B]:ALA:HB2	1:C:508[B]:THR:HG22	2.01	0.42
1:C:101:LEU:HD13	1:D:202[B]:PRO:HG2	2.01	0.42
1:B:616:PRO:HG2	1:B:622:TYR:CG	2.55	0.42
1:C:493[B]:PRO:HD2	1:C:496[B]:HIS:CD2	2.55	0.42
1:C:215:VAL:HG11	1:C:310:PHE:HA	2.02	0.41
1:A:131:VAL:HG22	1:A:136:GLN:HG3	2.01	0.41
1:B:108:LYS:HE3	1:B:632:TYR:HB3	2.01	0.41
1:B:377:GLN:HB2	1:B:379:TYR:CZ	2.55	0.41
1:B:222:TRP:CE2	1:B:271:LEU:HD13	2.55	0.41
1:C:325:GLN:HA	1:C:348[A]:PHE:O	2.21	0.41
1:C:470[B]:PHE:CG	1:C:498[B]:GLU:HB3	2.56	0.40
1:B:272:PRO:HD3	3:B:1006:GOL:H31	2.03	0.40
1:B:408:GLU:HB2	6:B:1504:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	565/613 (92%)	555 (98%)	10 (2%)	0	100	100
1	B	559/613 (91%)	550 (98%)	9 (2%)	0	100	100
1	C	637/613 (104%)	627 (98%)	10 (2%)	0	100	100
1	D	389/613 (64%)	382 (98%)	7 (2%)	0	100	100
All	All	2150/2452 (88%)	2114 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	466/501 (93%)	463 (99%)	3 (1%)	86	90
1	B	463/501 (92%)	454 (98%)	9 (2%)	57	61
1	C	514/501 (103%)	504 (98%)	10 (2%)	57	61
1	D	322/501 (64%)	316 (98%)	6 (2%)	57	61
All	All	1765/2004 (88%)	1737 (98%)	28 (2%)	65	67

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LEU
1	A	325	GLN

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Mol	Chain	Res	Type
1	A	531	VAL
1	B	131	VAL
1	B	171	LEU
1	B	237	ARG
1	B	325	GLN
1	B	328	ASP
1	B	370	VAL
1	B	409	GLU
1	B	636[A]	GLN
1	B	636[B]	GLN
1	C	171	LEU
1	C	237	ARG
1	C	325	GLN
1	C	413[B]	LYS
1	C	455[A]	ILE
1	C	455[B]	ILE
1	C	502[A]	GLU
1	C	502[B]	GLU
1	C	507[A]	TRP
1	C	507[B]	TRP
1	D	135	LEU
1	D	171	LEU
1	D	237	ARG
1	D	255	LYS
1	D	325	GLN
1	D	636	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	325	GLN
1	B	325	GLN
1	C	325	GLN
1	D	136	GLN
1	D	325	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	1002	-	5,5,5	0.12	0	5,5,5	0.38	0
4	PYR	B	1003	-	5,5,5	1.70	2 (40%)	3,6,6	2.73	1 (33%)
2	NAP	D	1001[B]	-	24,27,52	0.73	1 (4%)	34,41,80	0.58	0
4	PYR	B	1002[B]	-	5,5,5	1.84	2 (40%)	3,6,6	2.24	1 (33%)
3	GOL	C	1004	-	5,5,5	0.08	0	5,5,5	0.37	0
3	GOL	A	1005	-	5,5,5	0.07	0	5,5,5	0.23	0
3	GOL	A	1003	-	5,5,5	0.11	0	5,5,5	0.37	0
4	PYR	B	1002[A]	-	5,5,5	2.15	2 (40%)	3,6,6	1.62	1 (33%)
2	NAP	D	1001[A]	-	24,27,52	0.74	1 (4%)	34,41,80	0.58	0
3	GOL	A	1008	-	5,5,5	0.08	0	5,5,5	0.41	0
4	PYR	C	1002	-	5,5,5	0.26	0	3,6,6	0.77	0
3	GOL	A	1004	-	5,5,5	0.08	0	5,5,5	0.23	0
3	GOL	C	1003	-	5,5,5	0.06	0	5,5,5	0.23	0
2	NAP	C	1001[B]	-	45,52,52	0.61	0	56,80,80	0.68	2 (3%)
3	GOL	D	1002	-	5,5,5	0.07	0	5,5,5	0.23	0
3	GOL	B	1004	-	5,5,5	0.17	0	5,5,5	0.49	0
3	GOL	A	1006	-	5,5,5	0.05	0	5,5,5	0.20	0
2	NAP	B	1001	-	45,52,52	0.63	0	56,80,80	0.76	1 (1%)
2	NAP	C	1001[A]	-	45,52,52	0.60	0	56,80,80	0.63	1 (1%)
3	GOL	D	1003	-	5,5,5	0.08	0	5,5,5	0.16	0
3	GOL	A	1007	-	5,5,5	0.12	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	B	1007	-	5,5,5	0.15	0	5,5,5	0.29	0
3	GOL	D	1004	-	5,5,5	0.06	0	5,5,5	0.53	0
5	PEG	B	1009	-	6,6,6	0.19	0	5,5,5	0.16	0
3	GOL	B	1005	-	5,5,5	0.08	0	5,5,5	0.24	0
2	NAP	A	1001	-	45,52,52	0.62	0	56,80,80	0.75	2 (3%)
3	GOL	B	1006	-	5,5,5	0.12	0	5,5,5	0.16	0
3	GOL	B	1008	-	5,5,5	0.15	0	5,5,5	0.31	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	GOL	A	1002	-	-	2/4/4/4	-
4	PYR	B	1003	-	-	2/4/4/4	-
2	NAP	D	1001[B]	-	-	2/20/36/67	0/2/2/5
4	PYR	B	1002[B]	-	-	1/4/4/4	-
3	GOL	C	1004	-	-	2/4/4/4	-
3	GOL	A	1005	-	-	2/4/4/4	-
3	GOL	A	1003	-	-	0/4/4/4	-
4	PYR	B	1002[A]	-	-	0/4/4/4	-
2	NAP	D	1001[A]	-	-	1/20/36/67	0/2/2/5
3	GOL	A	1008	-	-	2/4/4/4	-
4	PYR	C	1002	-	-	4/4/4/4	-
3	GOL	A	1004	-	-	0/4/4/4	-
3	GOL	C	1003	-	-	0/4/4/4	-
2	NAP	C	1001[B]	-	-	4/31/67/67	0/5/5/5
3	GOL	D	1002	-	-	0/4/4/4	-
3	GOL	B	1004	-	-	0/4/4/4	-
3	GOL	A	1006	-	-	2/4/4/4	-
2	NAP	B	1001	-	-	4/31/67/67	0/5/5/5
2	NAP	C	1001[A]	-	-	8/31/67/67	0/5/5/5
3	GOL	D	1003	-	-	0/4/4/4	-
3	GOL	A	1007	-	-	0/4/4/4	-
3	GOL	B	1007	-	-	0/4/4/4	-
3	GOL	D	1004	-	-	1/4/4/4	-
5	PEG	B	1009	-	-	3/4/4/4	-
3	GOL	B	1005	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	1001	-	-	5/31/67/67	0/5/5/5
3	GOL	B	1006	-	-	2/4/4/4	-
3	GOL	B	1008	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1002[A]	PYR	O-C	3.68	1.32	1.22
2	D	1001[A]	NAP	PA-O5B	3.13	1.66	1.54
4	B	1002[A]	PYR	OXT-C	-2.99	1.21	1.30
4	B	1002[B]	PYR	O-C	2.96	1.30	1.22
2	D	1001[B]	NAP	PA-O5B	2.86	1.65	1.54
4	B	1002[B]	PYR	OXT-C	-2.83	1.22	1.30
4	B	1003	PYR	O-C	2.67	1.29	1.22
4	B	1003	PYR	OXT-C	-2.57	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1003	PYR	OXT-C-CA	4.72	126.87	113.97
4	B	1002[B]	PYR	OXT-C-CA	3.85	124.50	113.97
4	B	1002[A]	PYR	OXT-C-CA	2.76	121.53	113.97
2	B	1001	NAP	C5A-C6A-N6A	2.33	123.89	120.35
2	C	1001[A]	NAP	C5A-C6A-N6A	2.30	123.85	120.35
2	C	1001[B]	NAP	C5A-C6A-N6A	2.26	123.78	120.35
2	A	1001	NAP	C5A-C6A-N6A	2.13	123.59	120.35
2	C	1001[B]	NAP	C2N-N1N-C1D	-2.10	114.46	119.14
2	A	1001	NAP	C3B-C2B-C1B	-2.00	99.13	102.89

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	NAP	O4D-C1D-N1N-C6N
2	B	1001	NAP	O4D-C1D-N1N-C6N
2	C	1001[A]	NAP	C2B-O2B-P2B-O3X
2	C	1001[A]	NAP	O4D-C1D-N1N-C6N
2	C	1001[A]	NAP	C2D-C1D-N1N-C6N
2	C	1001[B]	NAP	C2B-O2B-P2B-O3X
2	D	1001[A]	NAP	O4D-C1D-N1N-C6N
3	A	1005	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1005	GOL	O2-C2-C3-O3
3	A	1006	GOL	C1-C2-C3-O3
3	A	1006	GOL	O2-C2-C3-O3
3	A	1008	GOL	C1-C2-C3-O3
3	B	1005	GOL	O1-C1-C2-O2
3	B	1005	GOL	O1-C1-C2-C3
4	B	1003	PYR	O-C-CA-CB
4	B	1003	PYR	OXT-C-CA-CB
4	C	1002	PYR	O-C-CA-O3
4	C	1002	PYR	O-C-CA-CB
4	C	1002	PYR	OXT-C-CA-O3
4	C	1002	PYR	OXT-C-CA-CB
2	A	1001	NAP	C3B-C2B-O2B-P2B
2	B	1001	NAP	C3B-C2B-O2B-P2B
2	C	1001[B]	NAP	C3B-C2B-O2B-P2B
5	B	1009	PEG	O1-C1-C2-O2
2	C	1001[A]	NAP	C3B-C2B-O2B-P2B
3	A	1002	GOL	C1-C2-C3-O3
3	C	1004	GOL	O1-C1-C2-C3
2	C	1001[B]	NAP	C1B-C2B-O2B-P2B
3	A	1008	GOL	O2-C2-C3-O3
2	D	1001[B]	NAP	C3D-C4D-C5D-O5D
2	A	1001	NAP	C1B-C2B-O2B-P2B
2	B	1001	NAP	C1B-C2B-O2B-P2B
2	C	1001[A]	NAP	C1B-C2B-O2B-P2B
2	D	1001[B]	NAP	O4D-C4D-C5D-O5D
2	C	1001[A]	NAP	C2B-O2B-P2B-O1X
5	B	1009	PEG	C1-C2-O2-C3
5	B	1009	PEG	C4-C3-O2-C2
3	A	1002	GOL	O2-C2-C3-O3
3	B	1006	GOL	O1-C1-C2-O2
3	C	1004	GOL	O1-C1-C2-O2
4	B	1002[B]	PYR	OXT-C-CA-CB
2	C	1001[A]	NAP	O4B-C4B-C5B-O5B
2	C	1001[B]	NAP	O4B-C4B-C5B-O5B
3	B	1006	GOL	O1-C1-C2-C3
3	D	1004	GOL	O1-C1-C2-C3
2	A	1001	NAP	C2D-C1D-N1N-C6N
2	C	1001[A]	NAP	C2D-C1D-N1N-C2N
2	A	1001	NAP	O4B-C4B-C5B-O5B
2	B	1001	NAP	O4B-C4B-C5B-O5B

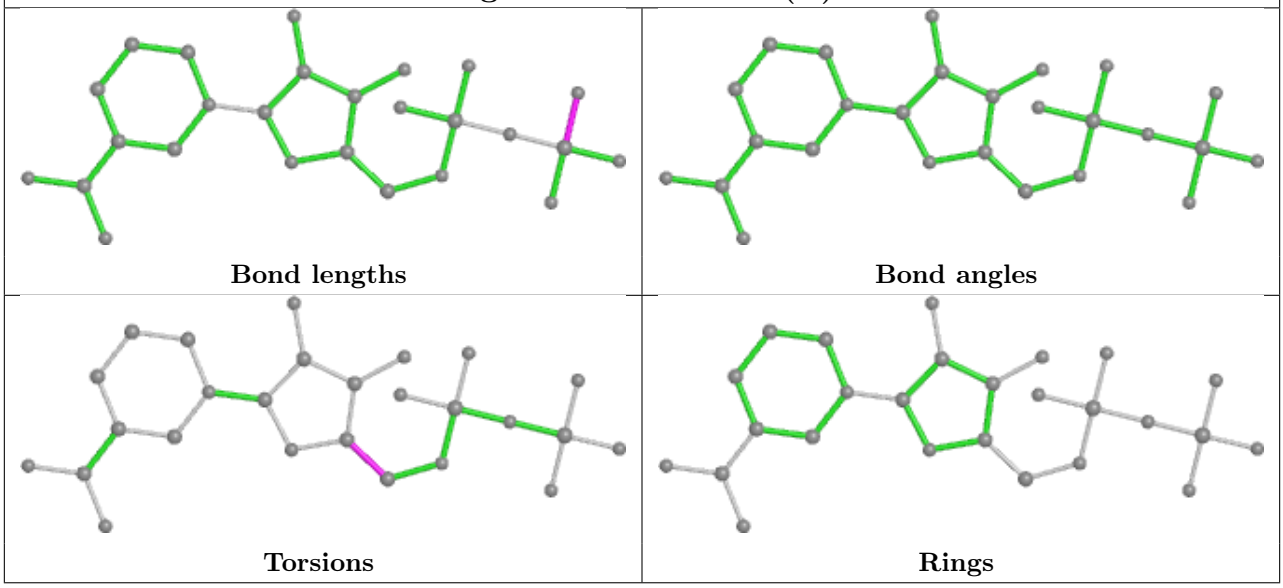
There are no ring outliers.

5 monomers are involved in 5 short contacts:

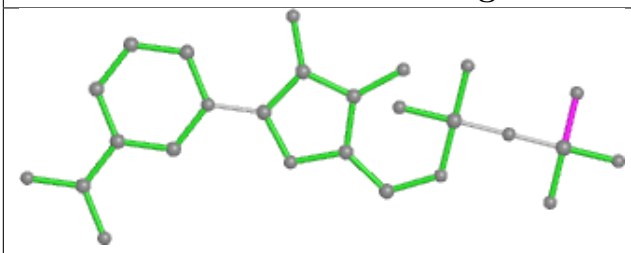
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1001[B]	NAP	1	0
3	A	1008	GOL	1	0
5	B	1009	PEG	1	0
3	B	1006	GOL	1	0
3	B	1008	GOL	1	0

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.

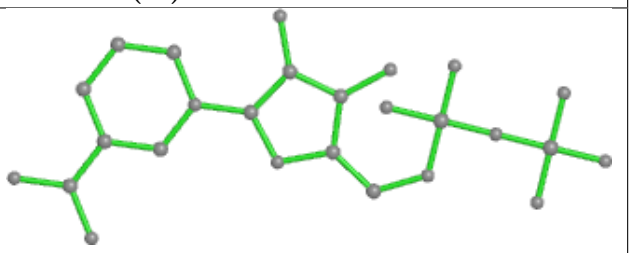
Ligand NAP D 1001 (B)



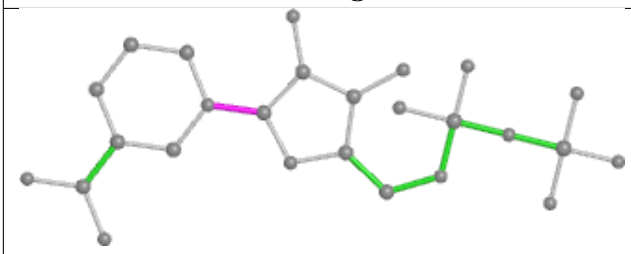
Ligand NAP D 1001 (A)



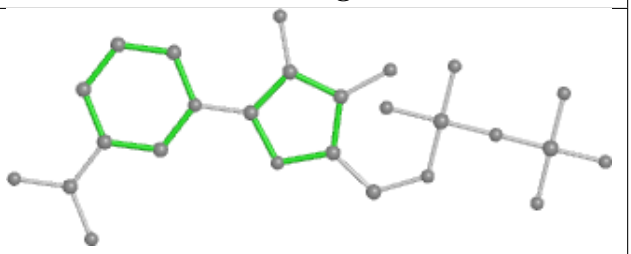
Bond lengths



Bond angles

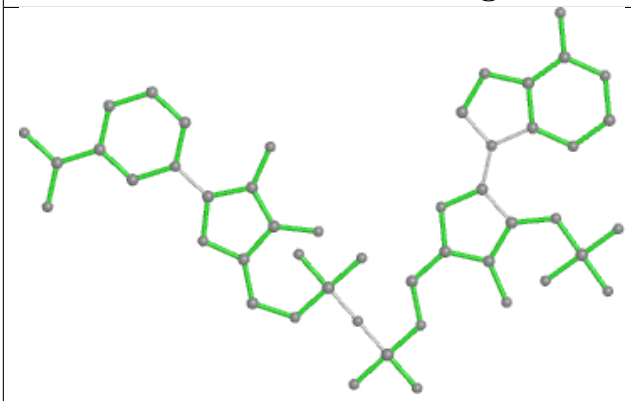


Torsions

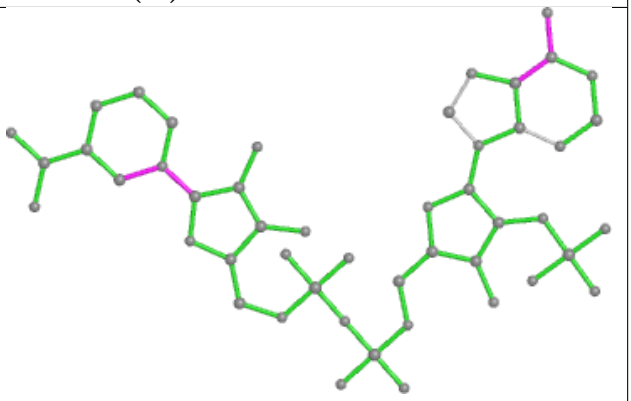


Rings

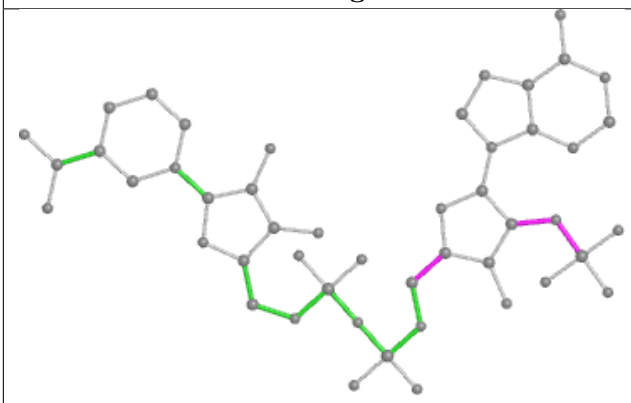
Ligand NAP C 1001 (B)



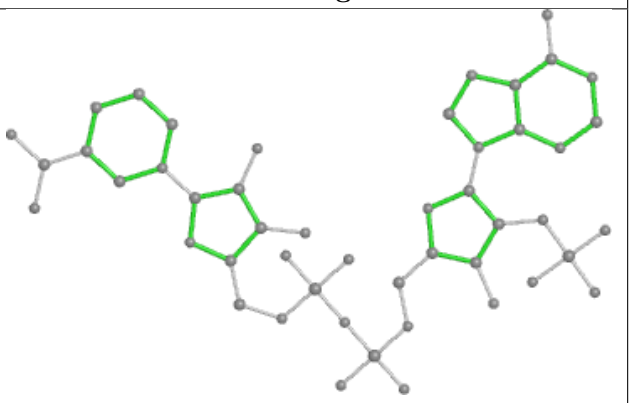
Bond lengths



Bond angles

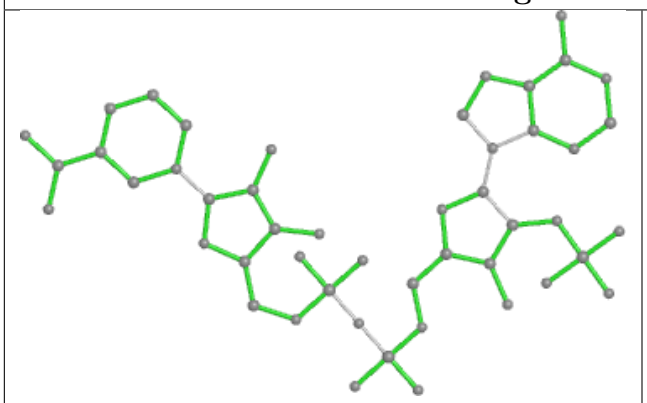


Torsions

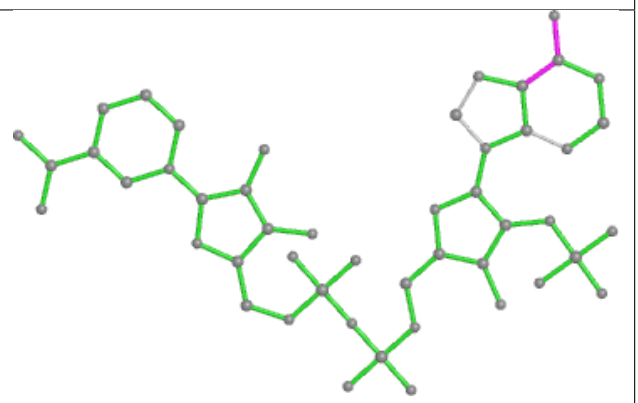


Rings

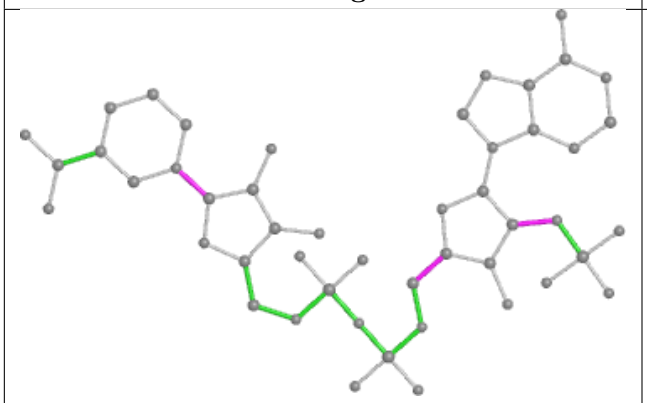
Ligand NAP B 1001



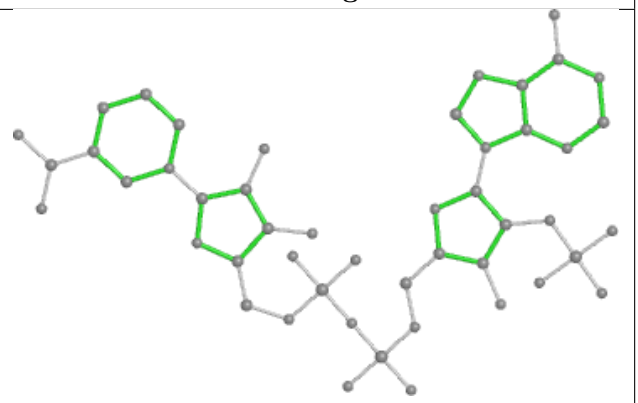
Bond lengths



Bond angles

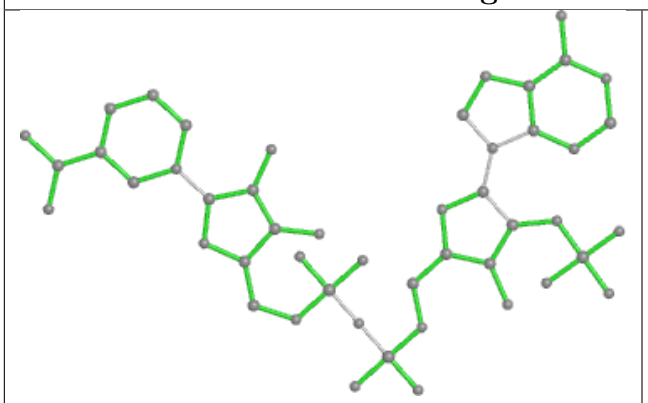


Torsions

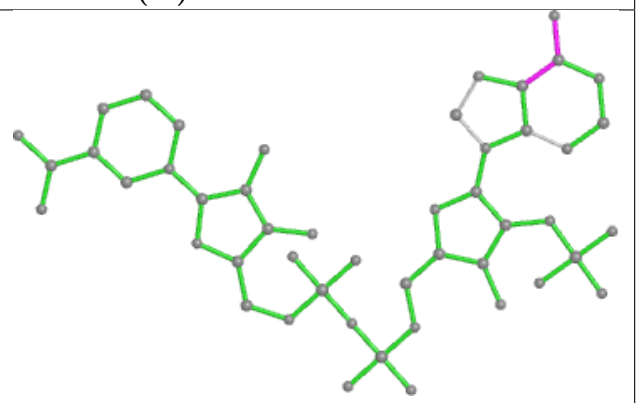


Rings

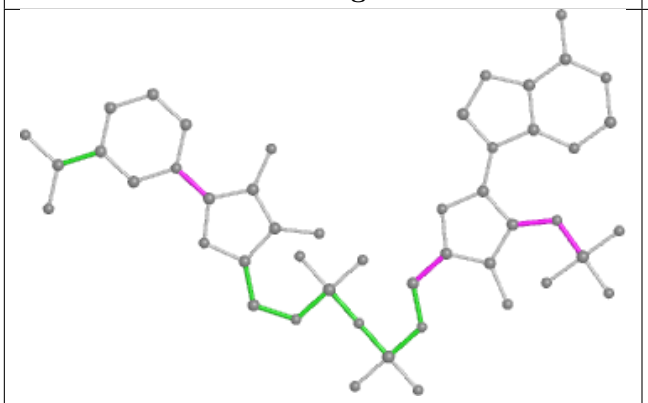
Ligand NAP C 1001 (A)



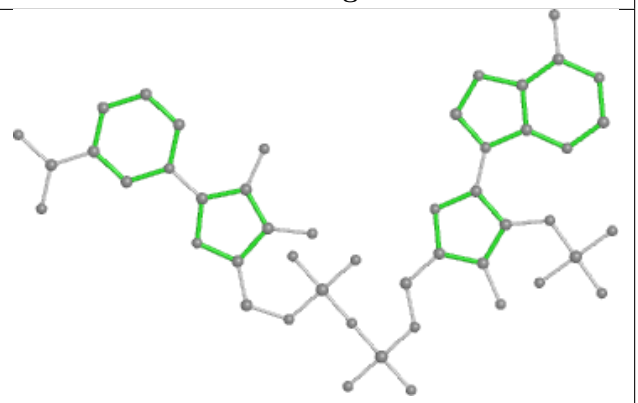
Bond lengths



Bond angles

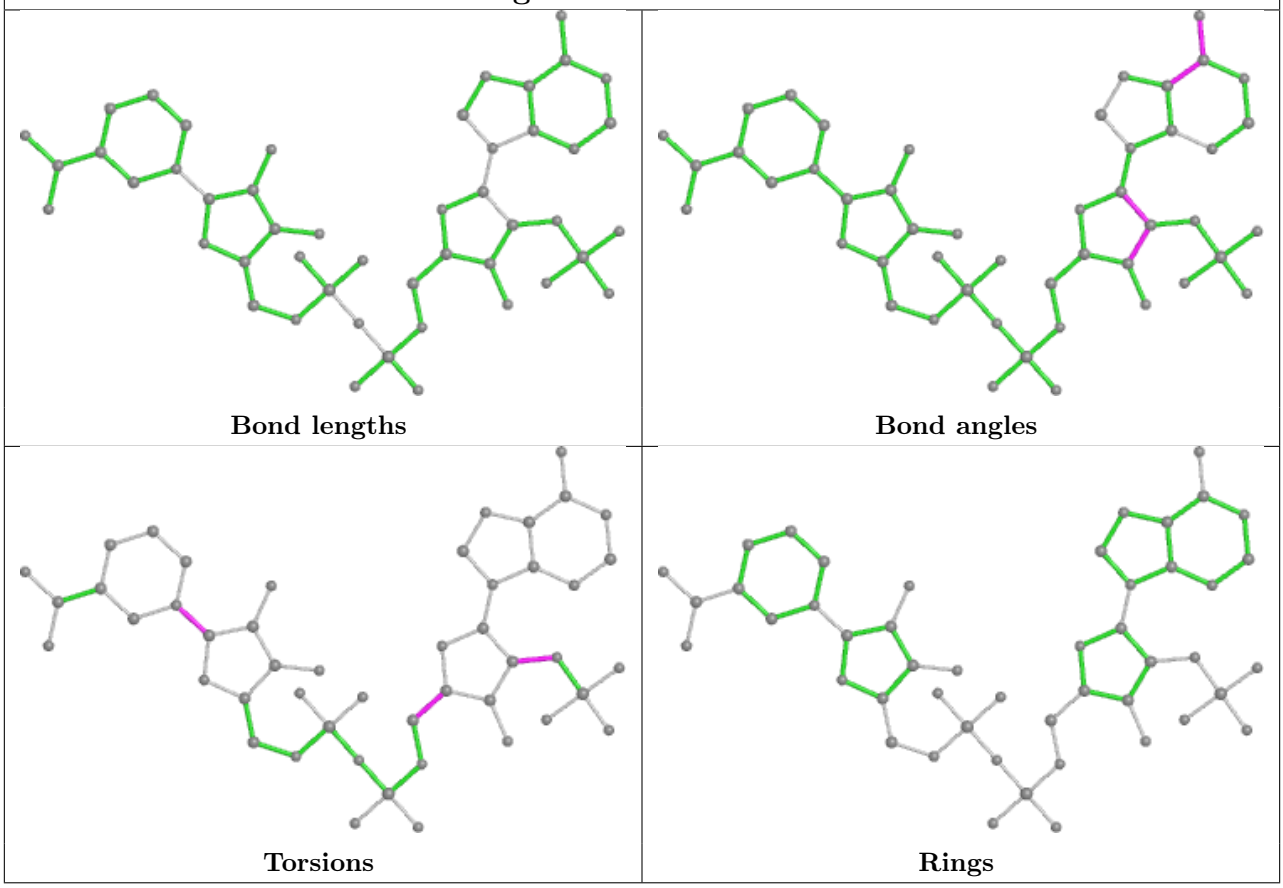


Torsions



Rings

Ligand NAP A 1001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	553/613 (90%)	-0.26	12 (2%)	62	60	15, 25, 50, 80	0
1	B	553/613 (90%)	-0.35	4 (0%)	87	87	15, 22, 38, 57	1 (0%)
1	C	535/613 (87%)	0.31	42 (7%)	12	11	21, 37, 55, 67	61 (11%)
1	D	389/613 (63%)	-0.00	21 (5%)	25	24	21, 34, 70, 85	0
All	All	2030/2452 (82%)	-0.09	79 (3%)	39	38	15, 29, 53, 85	62 (3%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	384	ALA	8.3
1	D	389	THR	8.1
1	C	446[B]	THR	5.4
1	D	396	ALA	5.1
1	D	587	THR	4.5
1	C	370[B]	VAL	4.5
1	D	395	ILE	4.4
1	C	420[B]	LYS	4.3
1	A	527	GLY	4.3
1	D	363	LEU	4.2
1	C	443[B]	GLU	4.2
1	A	85	LEU	3.9
1	D	385	GLY	3.8
1	C	444[B]	PRO	3.7
1	C	495[B]	SER	3.6
1	C	507[A]	TRP	3.5
1	A	529	THR	3.5
1	A	530	PHE	3.5
1	C	455[A]	ILE	3.4
1	B	429	SER	3.4
1	C	574[B]	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	387	ALA	3.3
1	C	449[A]	TYR	3.2
1	D	332	HIS	3.1
1	D	392	ALA	3.1
1	C	501[A]	ALA	3.1
1	C	505[A]	TYR	3.1
1	D	348[A]	PHE	3.1
1	D	534	GLN	3.0
1	C	578[B]	VAL	3.0
1	C	442[B]	HIS	3.0
1	C	439[A]	ALA	3.0
1	A	525	TYR	2.9
1	C	438[A]	TRP	2.9
1	C	499[A]	CYS	2.9
1	C	372[B]	GLY	2.8
1	C	521[B]	ALA	2.8
1	C	417[A]	VAL	2.8
1	D	362	GLY	2.8
1	C	389[A]	THR	2.8
1	C	493[B]	PRO	2.7
1	C	532[A]	PRO	2.7
1	C	519[A]	PRO	2.7
1	D	393	GLU	2.7
1	D	397	LEU	2.6
1	C	577[B]	PHE	2.6
1	C	445[B]	LEU	2.6
1	C	148	GLN	2.6
1	A	429	SER	2.6
1	D	83	GLU	2.6
1	B	636[A]	GLN	2.6
1	C	451[A]	ALA	2.5
1	C	403[B]	THR	2.5
1	A	636[A]	GLN	2.5
1	B	85	LEU	2.5
1	D	544	LEU	2.5
1	C	384[A]	ALA	2.5
1	A	578	VAL	2.4
1	C	518[A]	SER	2.4
1	C	520[B]	PHE	2.3
1	D	364	LEU	2.3
1	A	201[A]	ARG	2.3
1	C	421[B]	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	575	GLU	2.3
1	C	450[A]	ASP	2.3
1	A	526	ASP	2.2
1	C	232	VAL	2.2
1	D	588	ASN	2.2
1	B	84	GLU	2.2
1	C	391[A]	ILE	2.2
1	C	85	LEU	2.1
1	D	226	ASN	2.1
1	D	584	PRO	2.1
1	C	367	LEU	2.1
1	C	286	ASN	2.0
1	A	433	PRO	2.0
1	C	382[A]	LEU	2.0
1	C	226	ASN	2.0
1	C	416[A]	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1007	6/6	0.69	0.23	53,59,61,62	0
3	GOL	A	1005	6/6	0.75	0.21	40,44,48,49	0
4	PYR	C	1002	6/6	0.78	0.26	53,55,56,56	0
3	GOL	B	1005	6/6	0.79	0.21	36,41,46,48	0
3	GOL	A	1008	6/6	0.80	0.27	34,48,50,52	0
3	GOL	D	1002	6/6	0.81	0.18	53,56,57,58	0
3	GOL	B	1007	6/6	0.82	0.22	27,42,45,50	0

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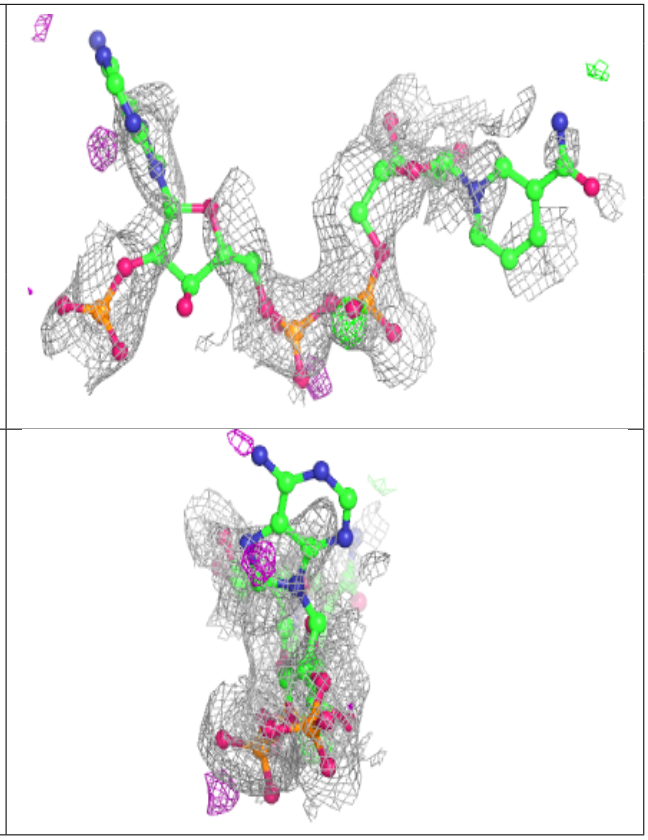
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1006	6/6	0.82	0.26	54,62,62,67	0
3	GOL	A	1003	6/6	0.82	0.21	43,49,55,59	0
2	NAP	C	1001[A]	48/48	0.83	0.25	32,48,57,58	48
2	NAP	C	1001[B]	48/48	0.83	0.25	30,36,41,42	48
3	GOL	B	1006	6/6	0.83	0.20	35,49,53,55	0
3	GOL	C	1003	6/6	0.84	0.23	54,61,61,63	0
2	NAP	D	1001[A]	26/48	0.84	0.27	44,48,63,65	26
3	GOL	D	1004	6/6	0.84	0.18	44,59,61,63	0
2	NAP	D	1001[B]	26/48	0.84	0.27	31,48,53,53	26
4	PYR	B	1002[A]	6/6	0.85	0.27	3,5,6,6	6
4	PYR	B	1002[B]	6/6	0.85	0.27	45,49,49,50	6
4	PYR	B	1003	6/6	0.85	0.26	35,38,39,43	6
3	GOL	A	1004	6/6	0.85	0.15	46,50,51,55	0
5	PEG	B	1009	7/7	0.85	0.18	39,49,51,52	0
3	GOL	C	1004	6/6	0.87	0.25	54,61,63,66	0
3	GOL	D	1003	6/6	0.89	0.25	52,60,61,63	0
3	GOL	B	1004	6/6	0.90	0.17	49,52,53,55	0
3	GOL	B	1008	6/6	0.91	0.39	39,47,50,53	0
3	GOL	A	1002	6/6	0.92	0.12	45,46,47,50	0
2	NAP	A	1001	48/48	0.97	0.08	22,27,33,35	0
2	NAP	B	1001	48/48	0.97	0.08	16,21,24,27	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.

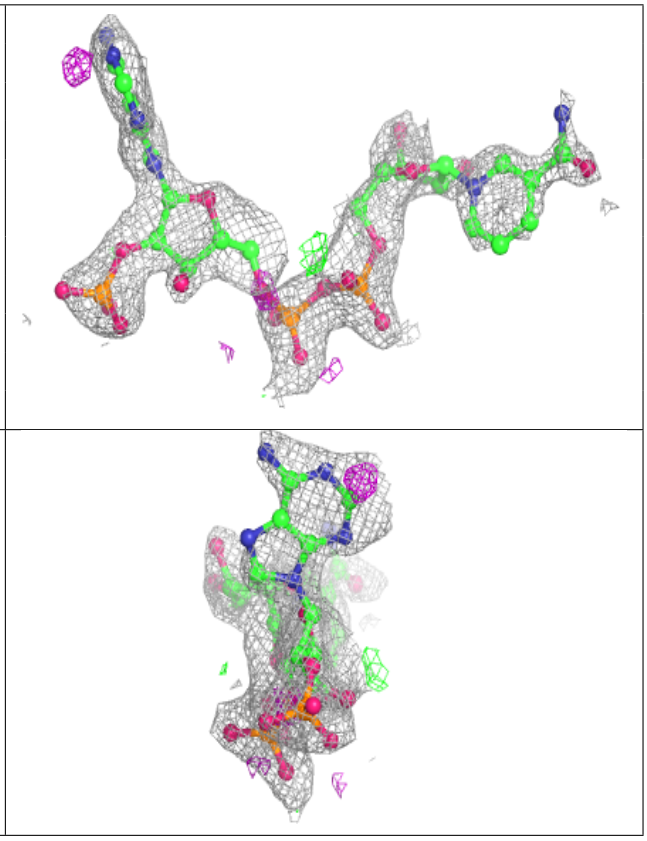
Electron density around NAP C 1001 (A):

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



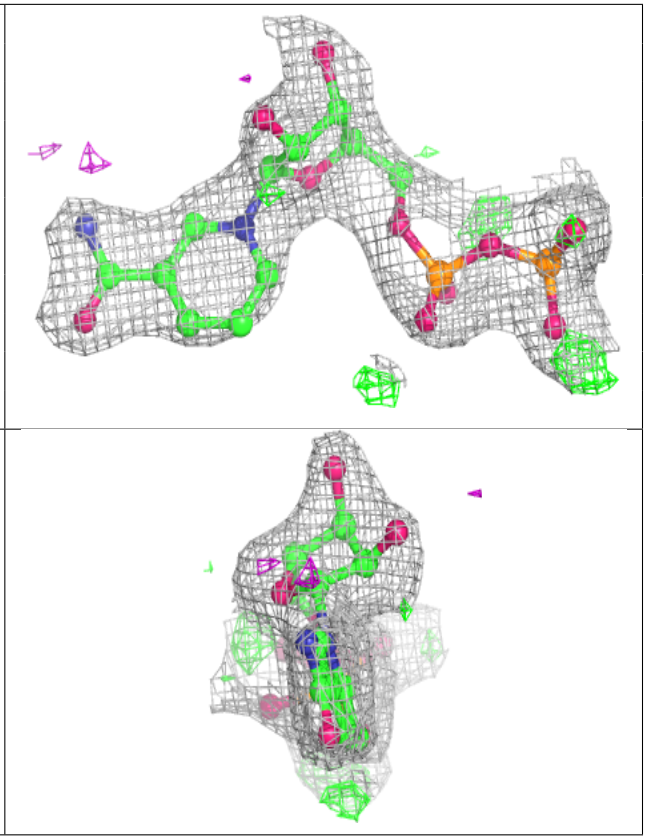
Electron density around NAP C 1001 (B):

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



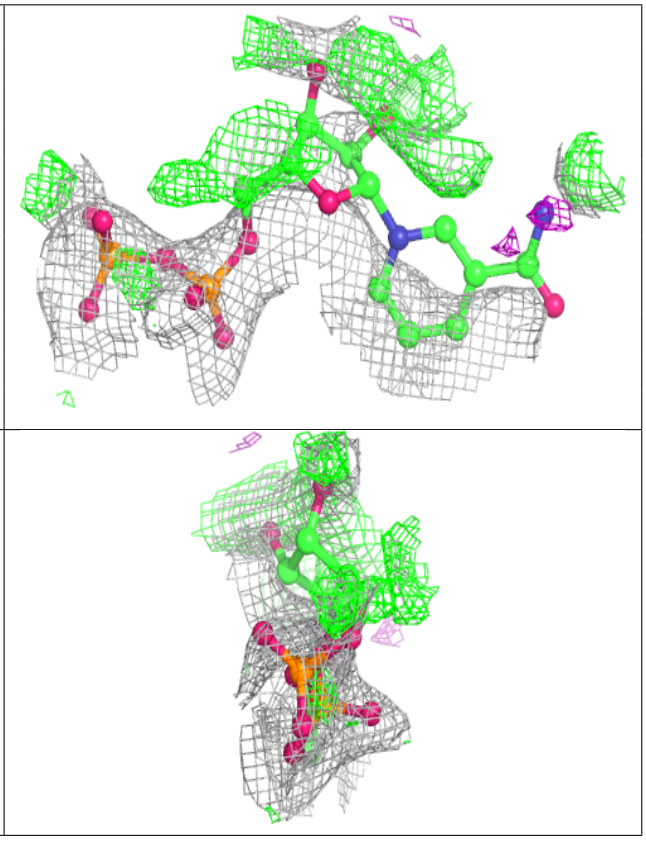
Electron density around NAP D 1001 (A):

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



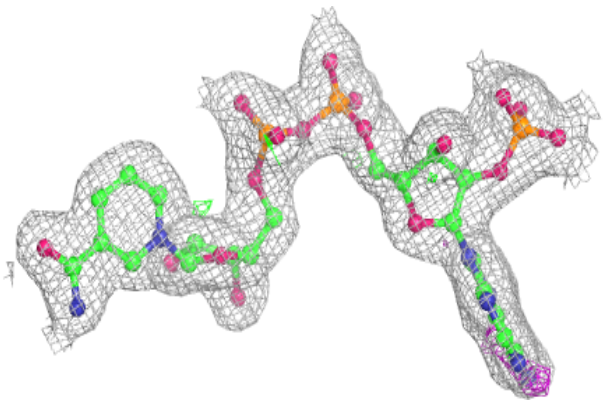
Electron density around NAP D 1001 (B):

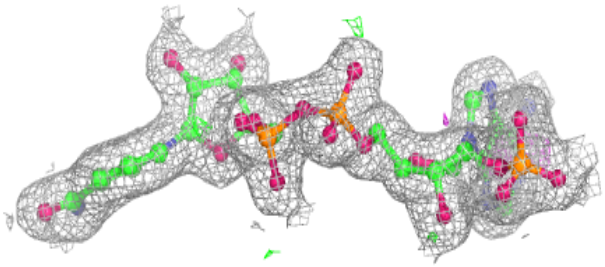
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

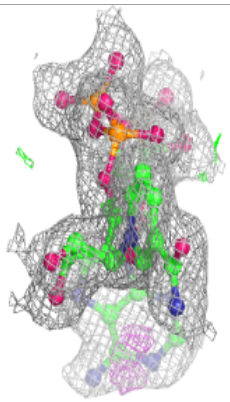


Electron density around NAP A 1001:

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

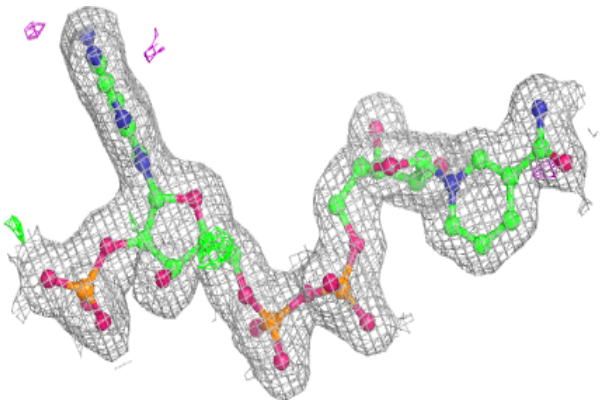


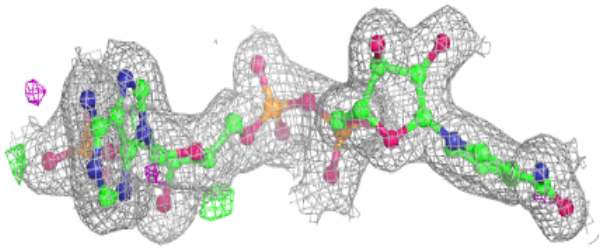


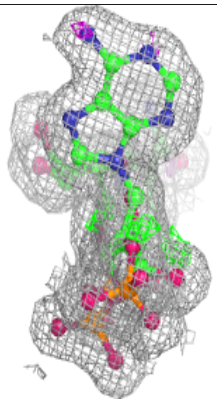


Electron density around NAP B 1001:

$2mF_o$-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.