WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2023 – 01:33 pm GMT

PDB ID	:	2C91
Title	:	mouse succinic semialdehyde reductase, AKR7A5
Authors	:	Zhu, X.; Ellis, E.M.; Lapthorn, A.J.
Deposited on	:	2005-12-08
Resolution	:	2.30 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

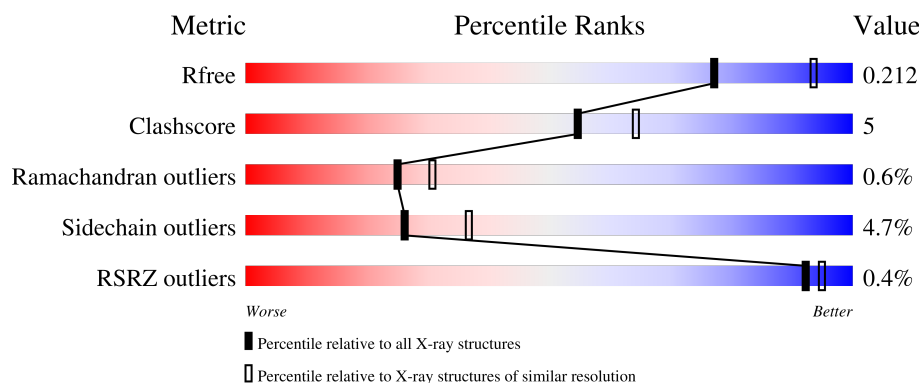|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Rfree		0.212
Clashscore		5
Ramachandran outliers		0.6%
Sidechain outliers		4.7%
RSRZ outliers		0.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	338	79% 15% · ·
1	B	338	.% 81% 12% · ·
1	C	338	81% 13% · ·
1	D	338	82% 11% · · ·
1	E	338	81% 12% · ·

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Mol	Chain	Length	Quality of chain
1	F	338	.% 81% 12% · · ·
1	G	338	77% 16% · · ·
1	H	338	.% 81% 12% · · · ·
1	I	338	.% 80% 13% · ·
1	J	338	.% 81% 13% · · ·

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	G	364	-	X	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 28440 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 AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	3	0
			2569	1617	454	480	18			
1	B	324	Total	C	N	O	S	0	0	0
			2545	1603	447	477	18			
1	C	324	Total	C	N	O	S	0	1	0
			2552	1608	447	479	18			
1	D	324	Total	C	N	O	S	0	2	0
			2564	1616	453	477	18			
1	E	324	Total	C	N	O	S	0	1	0
			2556	1611	450	477	18			
1	F	324	Total	C	N	O	S	0	0	0
			2548	1606	447	477	18			
1	G	324	Total	C	N	O	S	0	1	0
			2552	1608	447	479	18			
1	H	324	Total	C	N	O	S	0	1	0
			2538	1601	440	479	18			
1	I	324	Total	C	N	O	S	0	0	0
			2548	1606	447	477	18			
1	J	325	Total	C	N	O	S	0	1	0
			2559	1613	448	480	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ILE	VAL	conflict	UNP Q8CG76
A	122	CYS	ARG	conflict	UNP Q8CG76
B	87	ILE	VAL	conflict	UNP Q8CG76
B	122	CYS	ARG	conflict	UNP Q8CG76
C	87	ILE	VAL	conflict	UNP Q8CG76
C	122	CYS	ARG	conflict	UNP Q8CG76
D	87	ILE	VAL	conflict	UNP Q8CG76
D	122	CYS	ARG	conflict	UNP Q8CG76
E	87	ILE	VAL	conflict	UNP Q8CG76

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Chain	Residue	Modelled	Actual	Comment	Reference
E	122	CYS	ARG	conflict	UNP Q8CG76
F	87	ILE	VAL	conflict	UNP Q8CG76
F	122	CYS	ARG	conflict	UNP Q8CG76
G	87	ILE	VAL	conflict	UNP Q8CG76
G	122	CYS	ARG	conflict	UNP Q8CG76
H	87	ILE	VAL	conflict	UNP Q8CG76
H	122	CYS	ARG	conflict	UNP Q8CG76
I	87	ILE	VAL	conflict	UNP Q8CG76
I	122	CYS	ARG	conflict	UNP Q8CG76
J	87	ILE	VAL	conflict	UNP Q8CG76
J	122	CYS	ARG	conflict	UNP Q8CG76

- 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
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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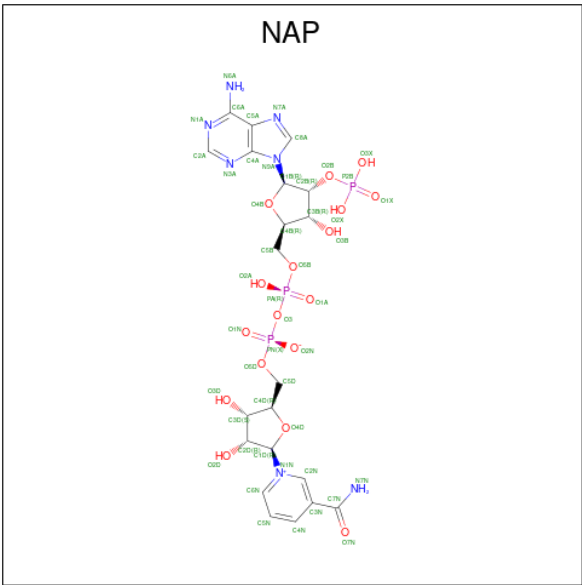
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).
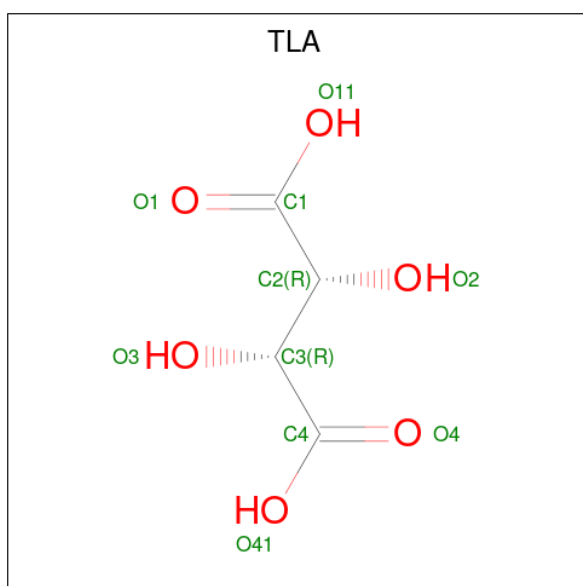
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		
3	B	1	Total	C	O	0	0
			10	4	6		
3	C	1	Total	C	O	0	0
			10	4	6		
3	D	1	Total	C	O	0	0
			10	4	6		
3	E	1	Total	C	O	0	0
			10	4	6		
3	F	1	Total	C	O	0	0
			10	4	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total 10	C 4	O 6	0	0
3	H	1	Total 10	C 4	O 6	0	0
3	I	1	Total 10	C 4	O 6	0	0
3	J	1	Total 10	C 4	O 6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
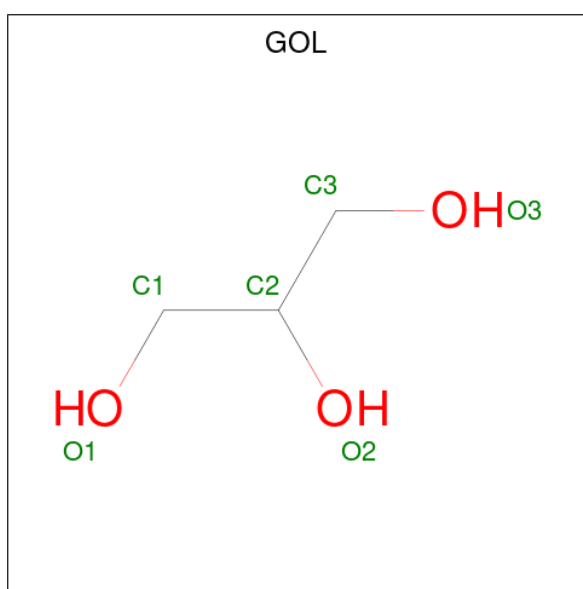
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	F	1	Total 6	C 3	O 3	0	0
4	G	1	Total 6	C 3	O 3	0	0
4	G	1	Total 6	C 3	O 3	0	0
4	G	1	Total 6	C 3	O 3	0	0
4	H	1	Total 6	C 3	O 3	0	0
4	H	1	Total 6	C 3	O 3	0	0
4	I	1	Total 6	C 3	O 3	0	0
4	I	1	Total 6	C 3	O 3	0	0
4	J	1	Total 6	C 3	O 3	0	0
4	J	1	Total 6	C 3	O 3	0	0
4	J	1	Total 6	C 3	O 3	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ —— P ══ O O1

P

O⁻

O4
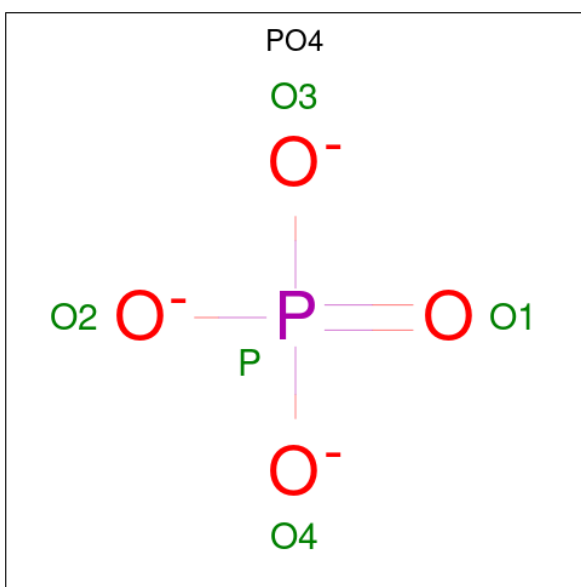
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	P 1	0	0
5	J	1	Total 5	O 4	P 1	0	0

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

MES

O1

O

C2   C6

C3   C5

H
N⁺
N4

C7

C8

S

O2S O ══ S ══ O O1S

O⁻

O3S
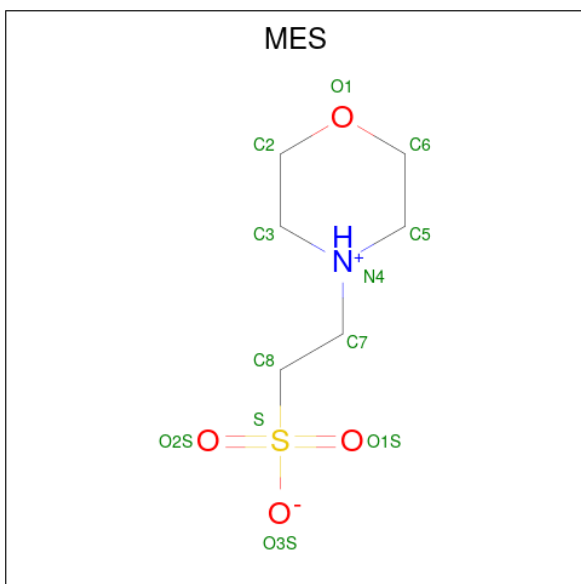
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total 12	C 6	N 1	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 12	C 6	N 1	O 4	S 1	0	0
6	D	1	Total 12	C 6	N 1	O 4	S 1	0	0
6	I	1	Total 12	C 6	N 1	O 4	S 1	0	0
6	J	1	Total 12	C 6	N 1	O 4	S 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	223	Total 223	O 223	0	0
7	B	131	Total 131	O 131	0	0
7	C	225	Total 225	O 225	0	0
7	D	272	Total 272	O 272	0	0
7	E	262	Total 262	O 262	0	0
7	F	214	Total 214	O 214	0	0
7	G	257	Total 257	O 257	0	0
7	H	159	Total 159	O 159	0	0
7	I	164	Total 164	O 164	0	0
7	J	202	Total 202	O 202	0	0

3 Residue-property plots ⓘ

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.
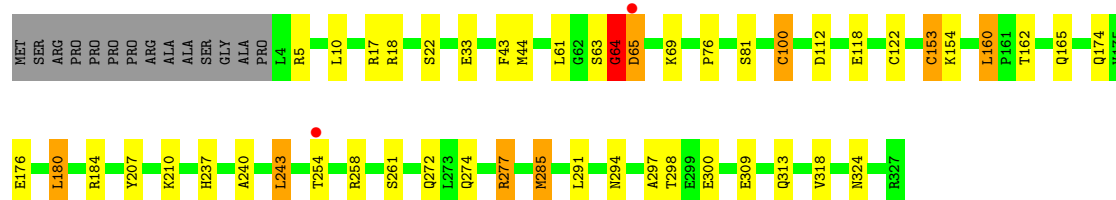
- Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2
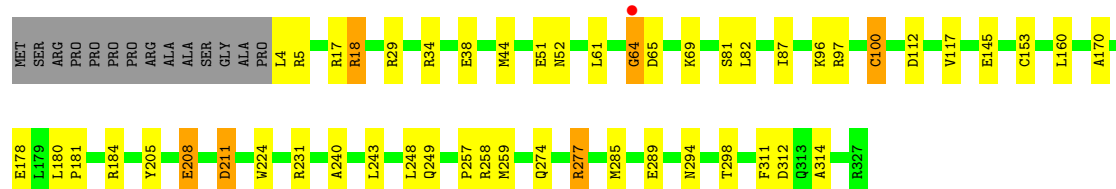
Chain A:
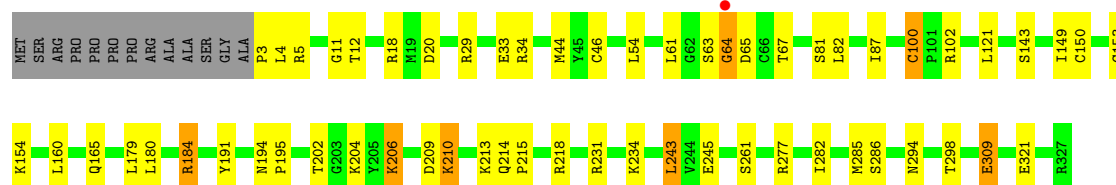
- Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain B:

- Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain C:
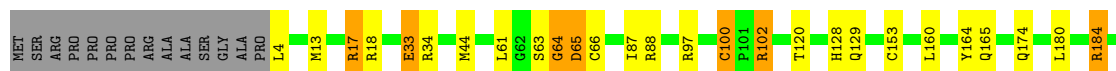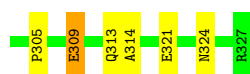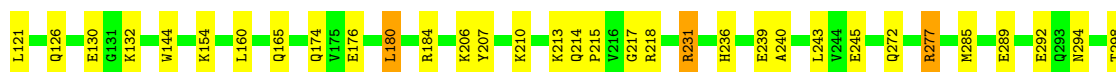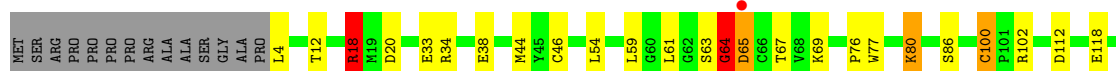

- Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain D:

Q165 L180 R184 E208 V216 A240 L243 V244 E245 L264 M267 R277 M285 S286 S287 L288 E292 Q293 N294 T298 E309 A314 R327

• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain E:

81%　　　　12%　•　•

MET SER ARG PRO PRO PRO ARG ALA ALA SER GLY ALA PRO L4 M13 R17 R18 E33 R34 M44 L61 G62 S63 G64 D65 C66 I87 R88 R97 C100 P101 R102 T120 H128 Q129 C153 L160 Y164 Q165 Q174 L180 R184

K213 V216 W224 R231 K234 E235 H236 E239 A240 L243 Q274 R277 Q278 D279 M285 L288 E292 Q293 N294 T298 E299 E309 A314 N324 R327

• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain F:

%

81%　　　　12%　•　•　•

MET SER ARG PRO PRO PRO ARG ALA ALA SER GLY ALA PRO L4 R5 M13 R17 R29 E33 M44 G62 S63 G64 D65 C66 T67 V68 K69 I87 C100 P101 R102 V117 E118 A123 Q126 E130 C153 K154 S155 N156 G157 L160 Q165

E176 L180 R184 G212 V216 N223 W224 A225 E226 R229 A240 L243 N255 R258 S261 Q274 R277 I282 M285 E289 N294 T298 A314 M317 R327

• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain G:

77%　　　　16%　•　•　•

MET SER ARG PRO PRO PRO ARG ALA ALA SER GLY ALA PRO L4 T12 R18 M19 D20 E33 R34 E38 M44 Y45 C46 L54 L59 G60 L61 G62 S63 G64 D65 C66 T67 V68 K69 P76 W77 K80 S86 C100 P101 R102 D112 E118

L121 Q126 E130 G131 K132 W144 K154 L160 Q165 Q174 V175 E176 L180 R184 K206 Y207 K210 K213 Q214 P215 V216 G217 R218 R231 H236 E239 A240 L243 V244 E245 Q272 R277 M285 E289 E292 Q293 N294 T298

P305 E309 Q313 A314 E321 N324 R327

• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain H:

%

81%　　　　12%　•　•　•

MET SER ARG PRO PRO PRO ARG ALA ALA SER GLY ALA PRO L4 E33 M44 L61 G62 S63 G64 D65 C66 K69 S81 L82 K83 I87 R88 C100 P101 R102 V117 E118 E119 T120 Q129 S143 W144 C153 L160 P161 T162 Q165 Q174 V175

E176 A177 E178 L179 L180 R184 E208 R231 E239 L243 L248 P257 S261 Q274 R277 M285 N294 A297 T298 E299 E300 P305 E309 Q313 N324 R327

• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain I:

• Molecule 1: AFLATOXIN B1 ALDEHYDE REDUCTASE MEMBER 2

Chain J:

4   Data and refinement statistics (i)
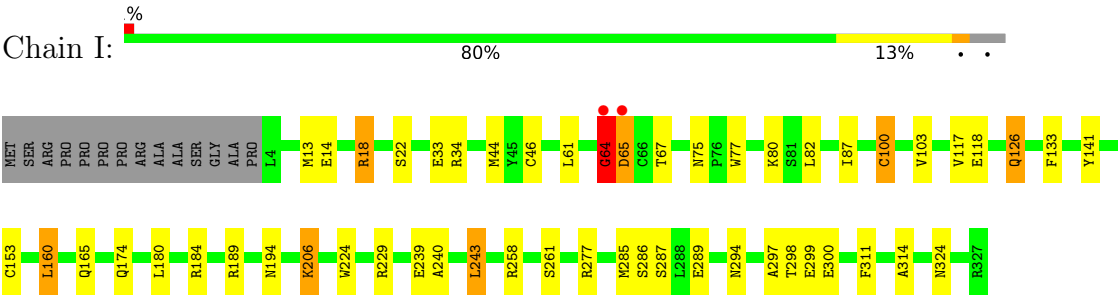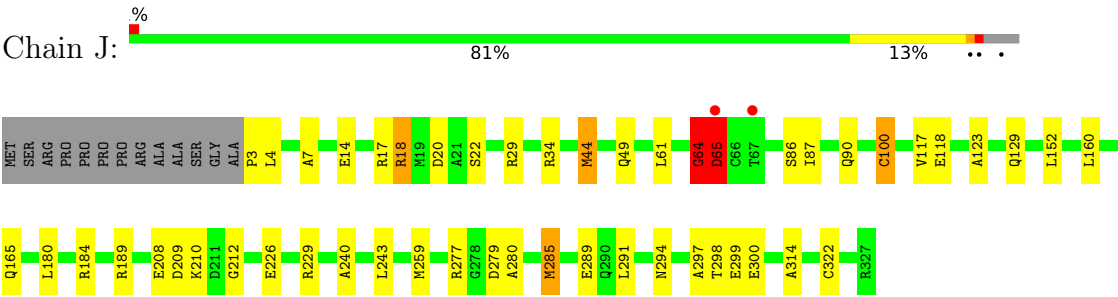
Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	98.53Å 159.24Å 96.70Å 90.02° 119.40° 78.50°	Depositor
Resolution (Å)	45.00 – 2.30 41.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.8 (45.00-2.30) 89.7 (41.88-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.160 , 0.208 0.170 , 0.212	Depositor DCC
R_{free} test set	9982 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	29.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.458 for -h-l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28440	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: TLA, PO4, MES, GOL, NAP

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	1.17	13/2647 (0.5%)	0.98	9/3584 (0.3%)
1	B	1.02	5/2608 (0.2%)	0.89	4/3533 (0.1%)
1	C	1.09	6/2620 (0.2%)	0.95	10/3549 (0.3%)
1	D	1.17	7/2633 (0.3%)	1.03	15/3565 (0.4%)
1	E	1.14	4/2622 (0.2%)	1.05	19/3552 (0.5%)
1	F	1.10	5/2611 (0.2%)	0.97	9/3537 (0.3%)
1	G	1.16	8/2620 (0.3%)	1.00	10/3549 (0.3%)
1	H	1.02	4/2604 (0.2%)	0.88	7/3531 (0.2%)
1	I	1.09	8/2611 (0.3%)	0.94	5/3537 (0.1%)
1	J	1.01	4/2625 (0.2%)	0.94	13/3556 (0.4%)
All	All	1.10	64/26201 (0.2%)	0.96	101/35493 (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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
All	All	0	10

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	118	GLU	CG-CD	9.15	1.65	1.51
1	D	309	GLU	CG-CD	8.77	1.65	1.51
1	I	100	CYS	CB-SG	-8.64	1.67	1.82
1	F	289	GLU	CG-CD	8.10	1.64	1.51
1	D	18	ARG	CG-CD	8.08	1.72	1.51

The worst 5 of 101 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	97	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	E	184	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	G	80	LYS	CD-CE-NZ	-9.83	89.09	111.70
1	D	97	ARG	NE-CZ-NH1	9.57	125.09	120.30
1	D	18	ARG	NE-CZ-NH1	9.55	125.07	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	GLY	Peptide
1	B	64	GLY	Peptide
1	C	64	GLY	Peptide
1	D	64	GLY	Peptide
1	E	64	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2569	0	2484	35	0
1	B	2545	0	2453	24	0
1	C	2552	0	2464	21	0
1	D	2564	0	2488	21	0
1	E	2556	0	2475	26	0
1	F	2548	0	2462	29	0
1	G	2552	0	2464	37	0
1	H	2538	0	2435	22	0
1	I	2548	0	2462	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2559	0	2470	20	0
2	A	48	0	25	2	0
2	B	48	0	25	3	0
2	C	48	0	25	0	0
2	D	48	0	25	1	0
2	E	48	0	25	1	0
2	F	48	0	25	3	0
2	G	48	0	24	1	0
2	H	48	0	25	4	0
2	I	48	0	25	3	0
2	J	48	0	25	2	0
3	A	10	0	4	0	0
3	B	10	0	4	2	0
3	C	10	0	4	3	0
3	D	10	0	4	0	0
3	E	10	0	4	1	0
3	F	10	0	4	1	0
3	G	10	0	4	0	0
3	H	10	0	4	2	0
3	I	10	0	4	1	0
3	J	10	0	4	1	0
4	A	12	0	16	2	0
4	B	18	0	24	0	0
4	C	18	0	24	0	0
4	D	18	0	24	0	0
4	E	18	0	24	0	0
4	F	6	0	8	0	0
4	G	18	0	24	5	0
4	H	12	0	16	2	0
4	I	12	0	16	1	0
4	J	18	0	24	0	0
5	A	5	0	0	0	0
5	J	5	0	0	0	0
6	B	12	0	12	0	0
6	C	12	0	12	0	0
6	D	12	0	12	0	0
6	I	12	0	12	0	0
6	J	12	0	12	0	0
7	A	223	0	0	9	0
7	B	131	0	0	3	0
7	C	225	0	0	7	0
7	D	272	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	262	0	0	7	0
7	F	214	0	0	9	0
7	G	257	0	0	8	0
7	H	159	0	0	2	0
7	I	164	0	0	9	0
7	J	202	0	0	8	0
All	All	28440	0	25206	267	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 267 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:E:100:CYS:SG	7:E:2088:HOH:O	1.95	1.23
1:C:100:CYS:SG	7:C:2071:HOH:O	2.05	1.10
1:F:44:MET:SD	7:F:2025:HOH:O	2.10	1.08
1:A:100:CYS:SG	7:A:2061:HOH:O	2.10	1.06
1:I:13:MET:HG2	7:I:2008:HOH:O	1.61	0.99

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	326/338 (96%)	320 (98%)	4 (1%)	2 (1%)	25	31
1	B	322/338 (95%)	314 (98%)	6 (2%)	2 (1%)	25	31
1	C	323/338 (96%)	314 (97%)	7 (2%)	2 (1%)	25	31
1	D	324/338 (96%)	317 (98%)	5 (2%)	2 (1%)	25	31
1	E	323/338 (96%)	316 (98%)	6 (2%)	1 (0%)	41	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	322/338 (95%)	312 (97%)	8 (2%)	2 (1%)	25	31
1	G	323/338 (96%)	316 (98%)	5 (2%)	2 (1%)	25	31
1	H	323/338 (96%)	316 (98%)	5 (2%)	2 (1%)	25	31
1	I	322/338 (95%)	314 (98%)	6 (2%)	2 (1%)	25	31
1	J	324/338 (96%)	313 (97%)	8 (2%)	3 (1%)	17	20
All	All	3232/3380 (96%)	3152 (98%)	60 (2%)	20 (1%)	25	31

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	ASP
1	B	65	ASP
1	C	65	ASP
1	D	65	ASP
1	E	65	ASP

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	269/276 (98%)	260 (97%)	9 (3%)	38	53
1	B	265/276 (96%)	250 (94%)	15 (6%)	20	28
1	C	267/276 (97%)	253 (95%)	14 (5%)	23	32
1	D	268/276 (97%)	257 (96%)	11 (4%)	30	43
1	E	267/276 (97%)	258 (97%)	9 (3%)	37	51
1	F	266/276 (96%)	251 (94%)	15 (6%)	21	29
1	G	267/276 (97%)	254 (95%)	13 (5%)	25	35
1	H	264/276 (96%)	249 (94%)	15 (6%)	20	28
1	I	266/276 (96%)	251 (94%)	15 (6%)	21	29
1	J	267/276 (97%)	255 (96%)	12 (4%)	27	39
All	All	2666/2760 (97%)	2538 (95%)	128 (5%)	26	36

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	299	GLU
1	J	44	MET
1	D	285	MET
1	D	243	LEU
1	J	117	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	52	ASN
1	G	126	GLN
1	J	272	GLN
1	F	128	HIS
1	F	274	GLN

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 ⓘ

52 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
4	GOL	B	362	-	5,5,5	0.77	0	5,5,5	1.29	1 (20%)
6	MES	D	364	-	12,12,12	1.82	1 (8%)	14,16,16	2.98	8 (57%)
2	NAP	J	350	-	45,52,52	1.59	4 (8%)	56,80,80	1.69	13 (23%)
4	GOL	E	363	-	5,5,5	0.78	0	5,5,5	0.96	0
2	NAP	F	350	-	45,52,52	1.85	4 (8%)	56,80,80	1.49	9 (16%)
3	TLA	F	360	-	9,9,9	0.99	1 (11%)	12,12,12	1.97	4 (33%)
4	GOL	D	363	-	5,5,5	1.45	0	5,5,5	1.73	1 (20%)
2	NAP	D	350	-	45,52,52	1.72	7 (15%)	56,80,80	1.31	4 (7%)
4	GOL	H	362	-	5,5,5	0.72	0	5,5,5	1.08	0
4	GOL	B	361	-	5,5,5	0.55	0	5,5,5	0.53	0
4	GOL	J	364	-	5,5,5	0.56	0	5,5,5	0.73	0
6	MES	B	364	-	12,12,12	2.05	1 (8%)	14,16,16	3.45	11 (78%)
4	GOL	C	362	-	5,5,5	0.56	0	5,5,5	1.17	1 (20%)
4	GOL	H	361	-	5,5,5	0.43	0	5,5,5	0.60	0
2	NAP	A	350	-	45,52,52	1.91	9 (20%)	56,80,80	1.27	4 (7%)
3	TLA	A	360	-	9,9,9	1.16	1 (11%)	12,12,12	1.71	4 (33%)
4	GOL	D	362	-	5,5,5	0.53	0	5,5,5	0.77	0
2	NAP	B	350	-	45,52,52	1.75	8 (17%)	56,80,80	1.74	10 (17%)
4	GOL	C	361	-	5,5,5	0.69	0	5,5,5	1.36	0
4	GOL	E	361	-	5,5,5	0.57	0	5,5,5	0.93	0
6	MES	J	368	-	12,12,12	1.74	3 (25%)	14,16,16	2.46	5 (35%)
4	GOL	C	363	-	5,5,5	0.82	0	5,5,5	1.38	0
4	GOL	I	362	-	5,5,5	0.70	0	5,5,5	1.38	1 (20%)
2	NAP	E	350	-	45,52,52	1.72	5 (11%)	56,80,80	1.64	8 (14%)
3	TLA	C	360	-	9,9,9	1.65	2 (22%)	12,12,12	1.75	4 (33%)
4	GOL	A	361	-	5,5,5	0.53	0	5,5,5	0.71	0
3	TLA	B	360	-	9,9,9	2.12	3 (33%)	12,12,12	1.25	2 (16%)
5	PO4	J	367	-	4,4,4	0.96	0	6,6,6	0.61	0
2	NAP	G	350	-	45,52,52	1.93	8 (17%)	56,80,80	1.53	12 (21%)
3	TLA	G	360	-	9,9,9	1.78	4 (44%)	12,12,12	1.19	1 (8%)
4	GOL	I	361	-	5,5,5	0.53	0	5,5,5	0.87	0
4	GOL	J	366	-	5,5,5	0.88	0	5,5,5	0.93	0
3	TLA	H	360	-	9,9,9	1.66	2 (22%)	12,12,12	0.81	0
4	GOL	A	363	-	5,5,5	0.83	0	5,5,5	0.92	0
6	MES	I	363	-	12,12,12	2.08	3 (25%)	14,16,16	2.67	5 (35%)
4	GOL	J	363	-	5,5,5	0.44	0	5,5,5	1.05	0
4	GOL	G	364	-	5,5,5	0.97	0	5,5,5	1.58	2 (40%)
3	TLA	J	360	-	9,9,9	1.65	1 (11%)	12,12,12	0.92	1 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	GOL	G	362	-	5,5,5	0.63	0	5,5,5	1.26	1 (20%)
5	PO4	A	364	-	4,4,4	0.79	0	6,6,6	2.39	3 (50%)
3	TLA	E	360	-	9,9,9	1.70	2 (22%)	12,12,12	1.33	2 (16%)
4	GOL	B	363	-	5,5,5	0.71	0	5,5,5	0.93	0
4	GOL	E	362	-	5,5,5	0.65	0	5,5,5	0.67	0
3	TLA	D	360	-	9,9,9	1.88	3 (33%)	12,12,12	2.00	4 (33%)
6	MES	C	364	-	12,12,12	2.06	1 (8%)	14,16,16	2.64	6 (42%)
2	NAP	I	350	-	45,52,52	1.73	3 (6%)	56,80,80	1.51	8 (14%)
2	NAP	H	350	-	45,52,52	1.91	5 (11%)	56,80,80	1.68	12 (21%)
4	GOL	F	361	-	5,5,5	0.73	0	5,5,5	1.52	2 (40%)
4	GOL	D	361	-	5,5,5	0.63	0	5,5,5	0.36	0
2	NAP	C	350	-	45,52,52	1.55	5 (11%)	56,80,80	1.47	8 (14%)
3	TLA	I	360	-	9,9,9	1.81	2 (22%)	12,12,12	1.53	3 (25%)
4	GOL	G	363	-	5,5,5	0.62	0	5,5,5	1.19	1 (20%)

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
4	GOL	B	362	-	-	2/4/4/4	-
6	MES	D	364	-	-	5/6/14/14	0/1/1/1
2	NAP	J	350	-	-	3/31/67/67	0/5/5/5
4	GOL	E	363	-	-	0/4/4/4	-
2	NAP	F	350	-	-	2/31/67/67	0/5/5/5
3	TLA	F	360	-	-	6/12/12/12	-
4	GOL	D	363	-	-	4/4/4/4	-
2	NAP	D	350	-	-	2/31/67/67	0/5/5/5
4	GOL	H	362	-	-	3/4/4/4	-
4	GOL	B	361	-	-	0/4/4/4	-
4	GOL	J	364	-	-	2/4/4/4	-
6	MES	B	364	-	-	4/6/14/14	0/1/1/1
4	GOL	C	362	-	-	0/4/4/4	-
4	GOL	H	361	-	-	2/4/4/4	-
2	NAP	A	350	-	-	1/31/67/67	0/5/5/5
3	TLA	A	360	-	-	6/12/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	362	-	-	0/4/4/4	-
2	NAP	B	350	-	-	3/31/67/67	0/5/5/5
4	GOL	C	361	-	-	1/4/4/4	-
4	GOL	E	361	-	-	3/4/4/4	-
6	MES	J	368	-	-	4/6/14/14	0/1/1/1
4	GOL	C	363	-	-	4/4/4/4	-
4	GOL	I	362	-	-	2/4/4/4	-
2	NAP	E	350	-	-	4/31/67/67	0/5/5/5
3	TLA	C	360	-	-	6/12/12/12	-
4	GOL	A	361	-	-	2/4/4/4	-
3	TLA	B	360	-	-	4/12/12/12	-
2	NAP	G	350	-	-	4/31/67/67	0/5/5/5
3	TLA	G	360	-	-	6/12/12/12	-
4	GOL	I	361	-	-	2/4/4/4	-
4	GOL	J	366	-	-	3/4/4/4	-
3	TLA	H	360	-	-	4/12/12/12	-
4	GOL	A	363	-	-	0/4/4/4	-
6	MES	I	363	-	-	4/6/14/14	0/1/1/1
4	GOL	J	363	-	-	0/4/4/4	-
4	GOL	G	364	-	-	4/4/4/4	-
3	TLA	J	360	-	-	4/12/12/12	-
4	GOL	G	362	-	-	4/4/4/4	-
3	TLA	E	360	-	-	6/12/12/12	-
4	GOL	B	363	-	-	0/4/4/4	-
4	GOL	E	362	-	-	2/4/4/4	-
3	TLA	D	360	-	-	6/12/12/12	-
6	MES	C	364	-	-	4/6/14/14	0/1/1/1
2	NAP	I	350	-	-	2/31/67/67	0/5/5/5
2	NAP	H	350	-	-	3/31/67/67	0/5/5/5
4	GOL	F	361	-	-	2/4/4/4	-
4	GOL	D	361	-	-	0/4/4/4	-
2	NAP	C	350	-	-	2/31/67/67	0/5/5/5
3	TLA	I	360	-	-	6/12/12/12	-
4	GOL	G	363	-	-	2/4/4/4	-

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	350	NAP	O7N-C7N	8.97	1.41	1.24
2	A	350	NAP	O7N-C7N	8.69	1.40	1.24
2	H	350	NAP	O7N-C7N	8.65	1.40	1.24
2	D	350	NAP	O7N-C7N	8.27	1.40	1.24
2	E	350	NAP	O7N-C7N	7.68	1.38	1.24

The worst 5 of 161 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	350	NAP	N3A-C2A-N1A	-7.03	117.69	128.68
6	J	368	MES	C5-N4-C3	7.00	124.58	108.83
2	E	350	NAP	N3A-C2A-N1A	-6.98	117.76	128.68
6	D	364	MES	C5-N4-C3	6.97	124.52	108.83
6	B	364	MES	O1S-S-C8	6.53	114.78	106.92

There are no chirality outliers.

5 of 145 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	350	NAP	O4D-C1D-N1N-C2N
2	B	350	NAP	O4D-C1D-N1N-C6N
2	C	350	NAP	C2B-O2B-P2B-O1X
2	E	350	NAP	C2B-O2B-P2B-O1X
2	E	350	NAP	O4D-C1D-N1N-C6N

There are no ring outliers.

20 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	350	NAP	2	0
2	F	350	NAP	3	0
3	F	360	TLA	1	0
2	D	350	NAP	1	0
4	H	361	GOL	2	0
2	A	350	NAP	2	0
2	B	350	NAP	3	0
4	I	362	GOL	1	0
2	E	350	NAP	1	0
3	C	360	TLA	3	0
4	A	361	GOL	2	0
3	B	360	TLA	2	0
2	G	350	NAP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	360	TLA	2	0
4	G	364	GOL	5	0
3	J	360	TLA	1	0
3	E	360	TLA	1	0
2	I	350	NAP	3	0
2	H	350	NAP	4	0
3	I	360	TLA	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 J 350

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP F 350

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 350

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 350

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 350

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP E 350

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP G 350

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP I 350

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP H 350

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 350

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	325/338 (96%)	-0.43	1 (0%)	94	96	30, 36, 47, 72	0
1	B	324/338 (95%)	-0.31	2 (0%)	89	92	29, 36, 47, 71	0
1	C	324/338 (95%)	-0.46	1 (0%)	94	96	30, 36, 47, 72	0
1	D	324/338 (95%)	-0.38	0	100	100	30, 36, 47, 73	0
1	E	324/338 (95%)	-0.43	0	100	100	30, 36, 47, 72	0
1	F	324/338 (95%)	-0.42	3 (0%)	84	88	30, 36, 47, 72	0
1	G	324/338 (95%)	-0.38	1 (0%)	94	96	30, 36, 47, 72	0
1	H	324/338 (95%)	-0.30	2 (0%)	89	92	30, 36, 46, 71	0
1	I	324/338 (95%)	-0.40	2 (0%)	89	92	29, 36, 47, 72	0
1	J	325/338 (96%)	-0.39	2 (0%)	89	92	30, 36, 47, 72	0
All	All	3242/3380 (95%)	-0.39	14 (0%)	92	95	29, 36, 47, 73	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	GLY	4.5
1	H	64	GLY	3.8
1	F	65	ASP	3.6
1	A	64	GLY	3.5
1	I	65	ASP	3.0

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

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

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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, 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
4	GOL	D	363	6/6	0.77	0.22	48,53,55,55	0
4	GOL	G	364	6/6	0.88	0.29	58,62,62,64	0
4	GOL	C	363	6/6	0.89	0.14	49,60,61,62	0
4	GOL	J	366	6/6	0.90	0.12	51,53,53,54	0
4	GOL	B	362	6/6	0.92	0.26	57,61,62,63	0
4	GOL	J	363	6/6	0.95	0.15	39,42,42,46	0
4	GOL	A	361	6/6	0.95	0.10	37,40,45,46	0
5	PO4	A	364	5/5	0.95	0.10	59,59,63,65	0
4	GOL	H	361	6/6	0.96	0.12	37,44,45,46	0
4	GOL	D	361	6/6	0.96	0.09	29,29,33,33	0
3	TLA	B	360	10/10	0.96	0.09	34,37,41,42	0
4	GOL	A	363	6/6	0.96	0.12	39,42,42,43	0
6	MES	I	363	12/12	0.96	0.21	55,60,61,61	0
3	TLA	A	360	10/10	0.97	0.09	28,33,35,35	0
4	GOL	F	361	6/6	0.97	0.15	36,39,41,42	0
4	GOL	G	362	6/6	0.97	0.08	31,36,37,39	0
3	TLA	C	360	10/10	0.97	0.11	29,33,38,41	0
4	GOL	B	361	6/6	0.97	0.14	33,40,42,42	0
3	TLA	F	360	10/10	0.97	0.10	31,36,39,39	0
4	GOL	C	361	6/6	0.97	0.10	38,45,47,50	0
3	TLA	G	360	10/10	0.97	0.09	31,33,35,35	0
6	MES	D	364	12/12	0.97	0.09	48,62,66,67	0
3	TLA	I	360	10/10	0.97	0.09	27,35,37,40	0
6	MES	J	368	12/12	0.97	0.16	53,57,59,60	0
4	GOL	B	363	6/6	0.98	0.09	30,33,34,35	0
2	NAP	H	350	48/48	0.98	0.08	24,33,37,43	0
4	GOL	G	363	6/6	0.98	0.14	34,36,36,38	0
4	GOL	C	362	6/6	0.98	0.10	33,36,39,39	0
2	NAP	B	350	48/48	0.98	0.09	27,32,38,43	0
4	GOL	H	362	6/6	0.98	0.17	30,34,36,36	0
4	GOL	I	361	6/6	0.98	0.18	44,47,48,48	0
4	GOL	I	362	6/6	0.98	0.12	33,34,36,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
3	TLA	D	360	10/10	0.98	0.10	25,31,34,36	0
4	GOL	J	364	6/6	0.98	0.14	45,48,49,50	0
4	GOL	D	362	6/6	0.98	0.08	33,34,35,36	0
3	TLA	J	360	10/10	0.98	0.08	29,33,34,37	0
5	PO4	J	367	5/5	0.98	0.14	60,60,65,67	0
6	MES	B	364	12/12	0.98	0.16	50,61,65,65	0
6	MES	C	364	12/12	0.98	0.14	57,62,64,64	0
4	GOL	E	361	6/6	0.98	0.12	33,36,36,37	0
4	GOL	E	362	6/6	0.98	0.12	31,33,36,36	0
4	GOL	E	363	6/6	0.98	0.14	28,31,31,32	0
2	NAP	E	350	48/48	0.99	0.08	20,27,31,36	0
2	NAP	F	350	48/48	0.99	0.08	23,29,34,36	0
3	TLA	E	360	10/10	0.99	0.09	26,31,35,35	0
2	NAP	G	350	48/48	0.99	0.08	19,27,31,35	0
2	NAP	A	350	48/48	0.99	0.08	21,26,31,35	0
3	TLA	H	360	10/10	0.99	0.13	30,36,41,43	0
2	NAP	I	350	48/48	0.99	0.07	22,31,35,36	0
2	NAP	J	350	48/48	0.99	0.07	23,30,35,40	0
2	NAP	C	350	48/48	0.99	0.07	23,29,35,37	0
2	NAP	D	350	48/48	0.99	0.09	20,25,32,37	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.
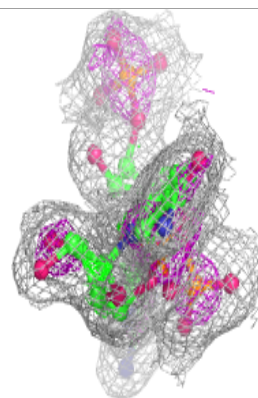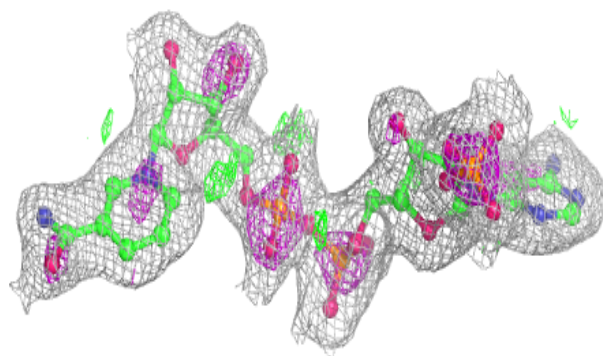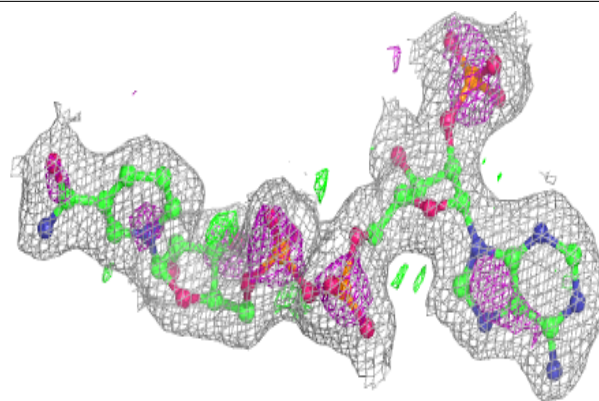
Electron density around NAP H 350:

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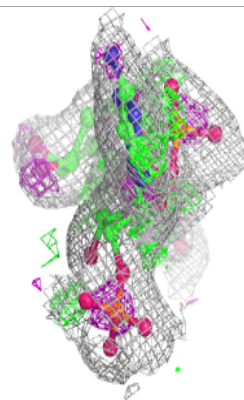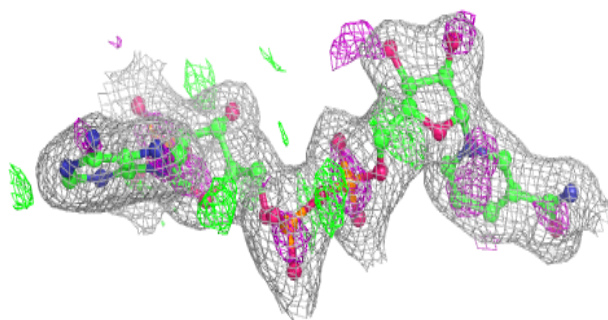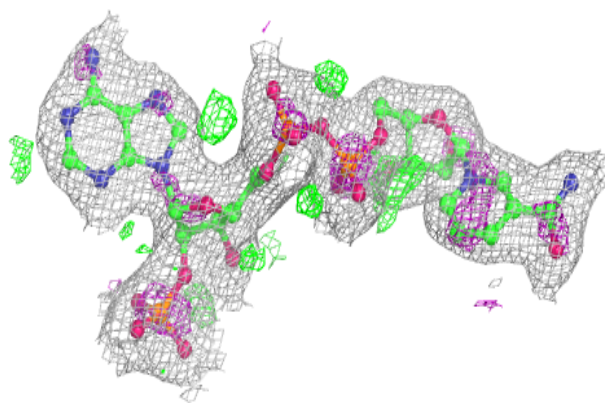
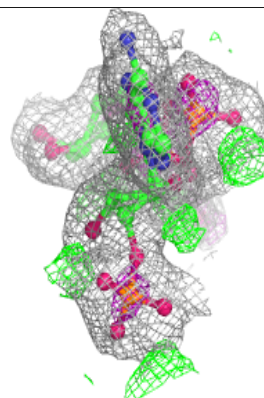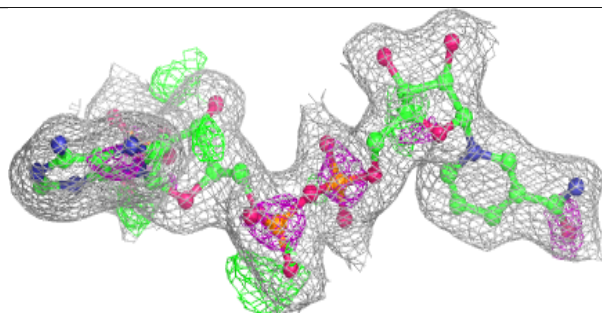

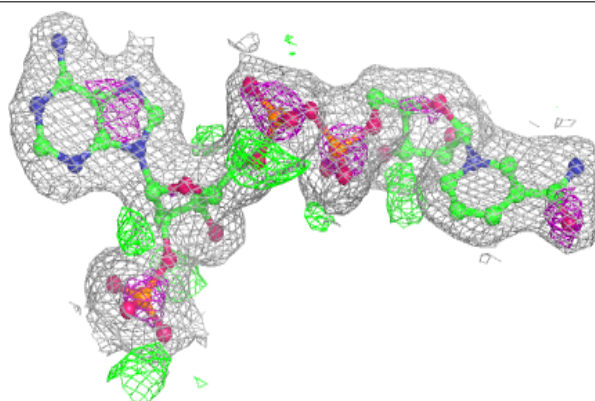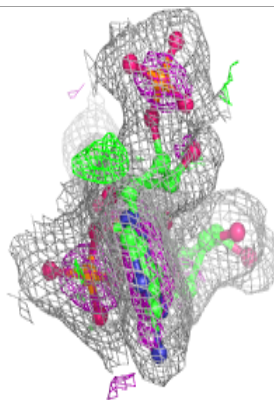**Electron density around NAP B 350:**

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
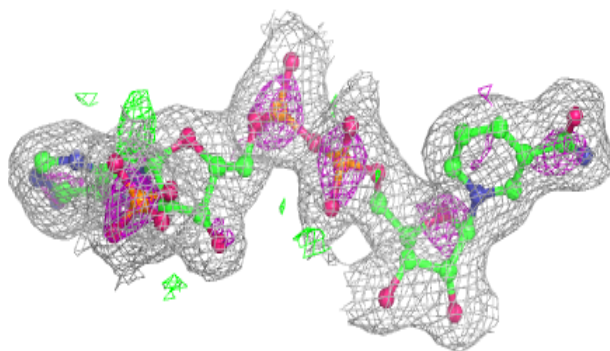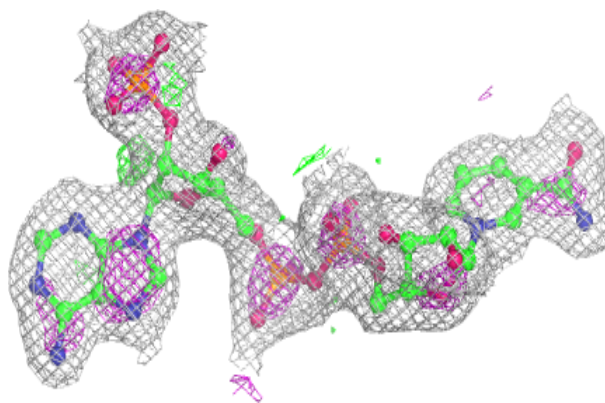and green (positive)
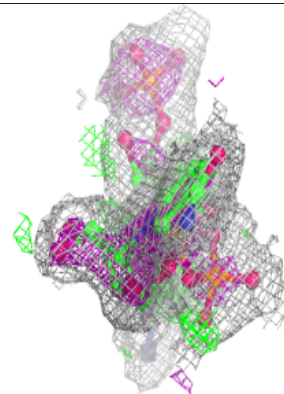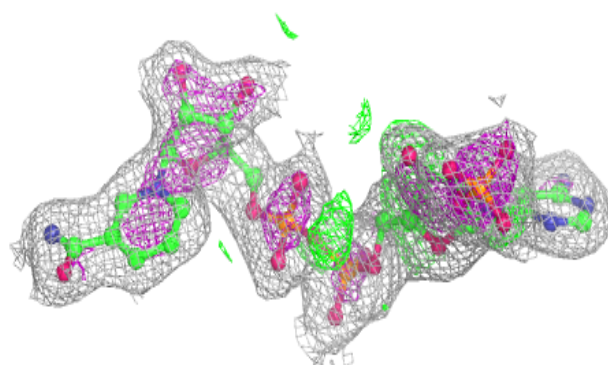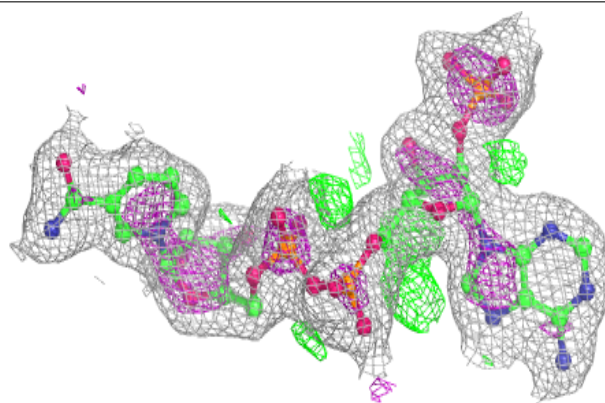
Electron density around NAP E 350:

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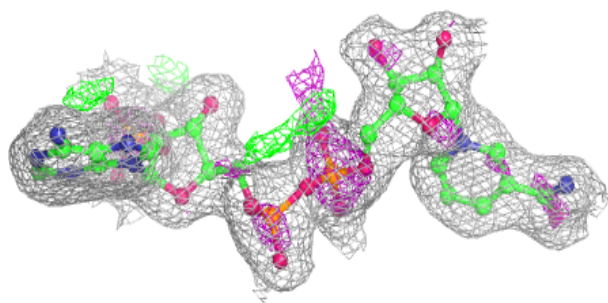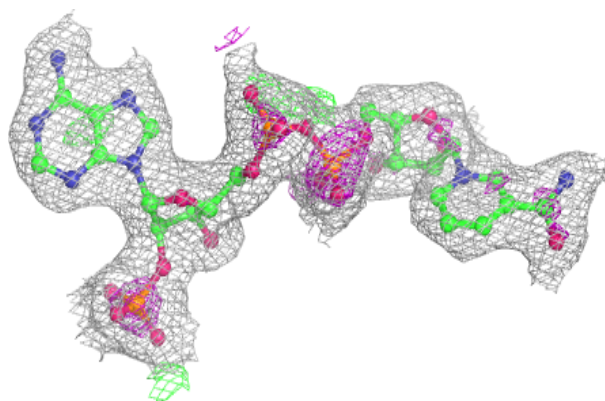

Electron density around NAP F 350:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
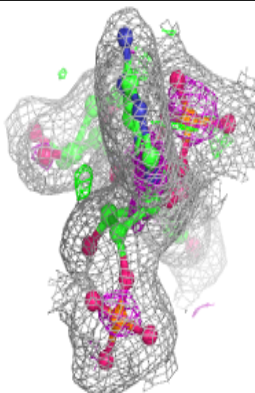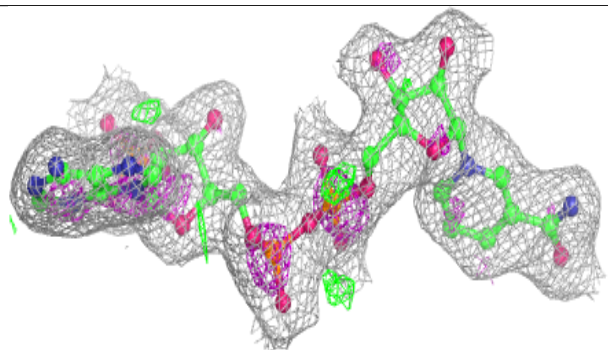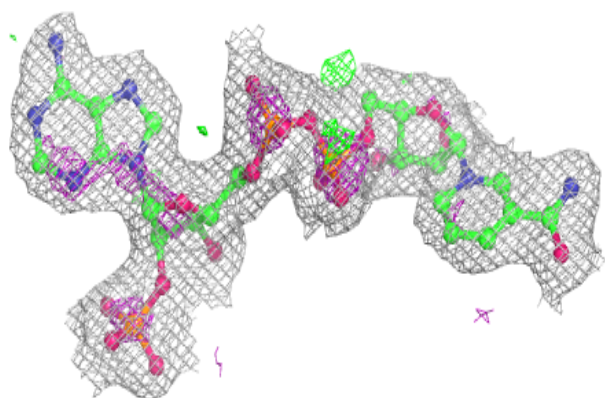
Electron density around NAP G 350:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
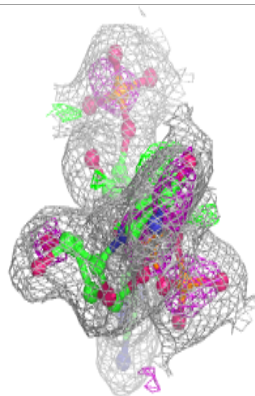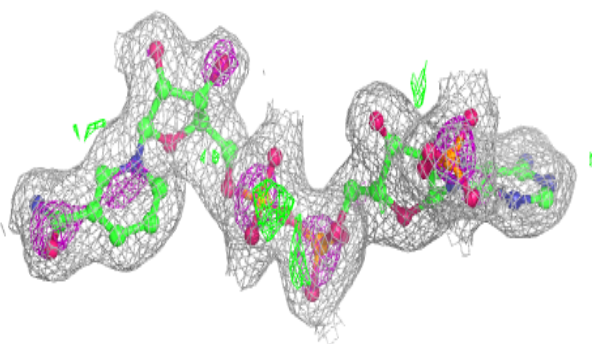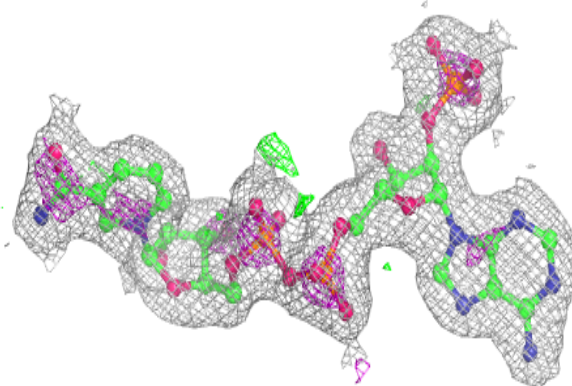
Electron density around NAP A 350:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
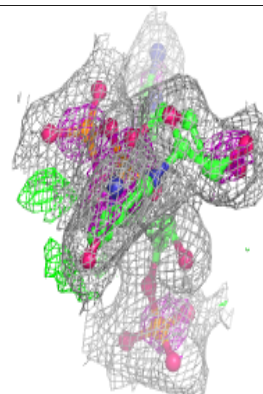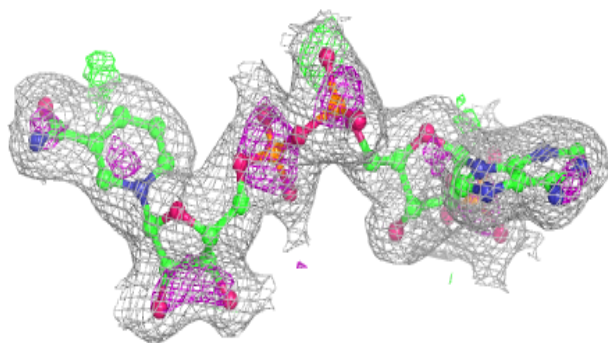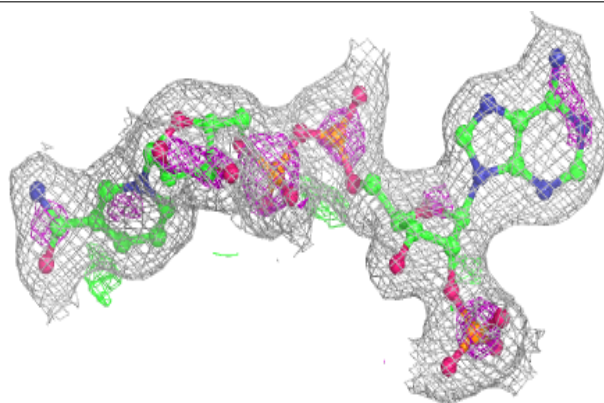
Electron density around NAP I 350:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
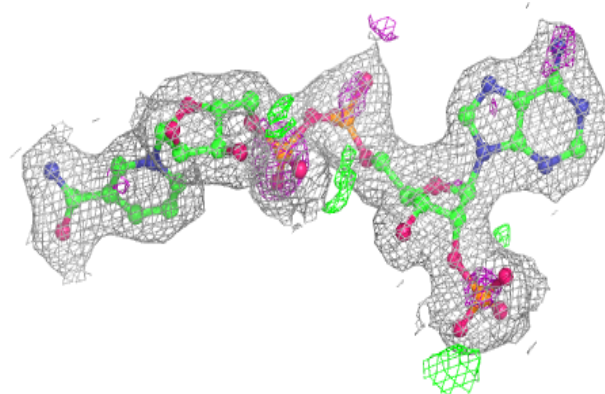

Electron density around NAP J 350:

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 350:

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

Electron density around NAP D 350:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
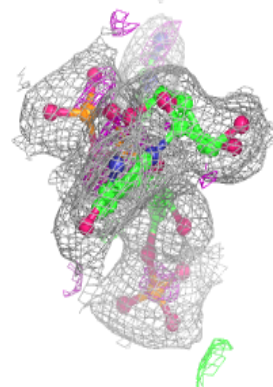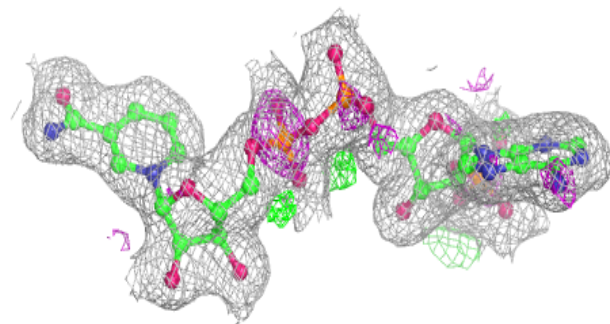
6.5 Other polymers (i)

There are no such residues in this entry.