W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 30, 2020 – 11:01 AM BST

PDB ID	:	3NT6
Title	:	Structure of the Shewanella loihica PV-4 NADH-dependent persulfide reductase C43S/C531S Double Mutant
Authors	:	Sazinsky, M.H.; Crane, E.J.; Warner, M.D.; Lukose, V.; Lee, K.H.; Lopez, K.
Deposited on	:	2010-07-02
Resolution	:	2.00 Å(reported)

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	:	2.13
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)	:	2.13

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.

Worse | Better

■ Percentile relative to all X-ray structures

⬚ Percentile relative to X-ray structures of similar resolution
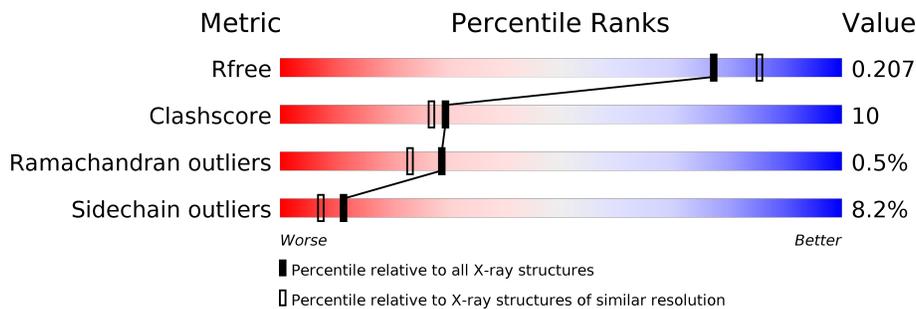
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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%

Mol	Chain	Length	Quality of chain
1	A	574	73% 21% • • •
1	B	574	74% 20% • • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9342 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 FAD-dependent pyridine nucleotide-disulphide oxidoreductase.

| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	565	Total 4295	C 2694	N 762	O 821	S 2	Se 16	0	0	0
1	B	565	Total 4294	C 2694	N 763	O 820	S 2	Se 15	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	SER	CYS	ENGINEERED MUTATION	UNP A3QAV3
A	531	SER	CYS	ENGINEERED MUTATION	UNP A3QAV3
A	567	LEU	-	EXPRESSION TAG	UNP A3QAV3
A	568	GLU	-	EXPRESSION TAG	UNP A3QAV3
A	569	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	570	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	571	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	572	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	573	HIS	-	EXPRESSION TAG	UNP A3QAV3
A	574	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	43	SER	CYS	ENGINEERED MUTATION	UNP A3QAV3
B	531	SER	CYS	ENGINEERED MUTATION	UNP A3QAV3
B	567	LEU	-	EXPRESSION TAG	UNP A3QAV3
B	568	GLU	-	EXPRESSION TAG	UNP A3QAV3
B	569	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	570	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	571	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	572	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	573	HIS	-	EXPRESSION TAG	UNP A3QAV3
B	574	HIS	-	EXPRESSION TAG	UNP A3QAV3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD
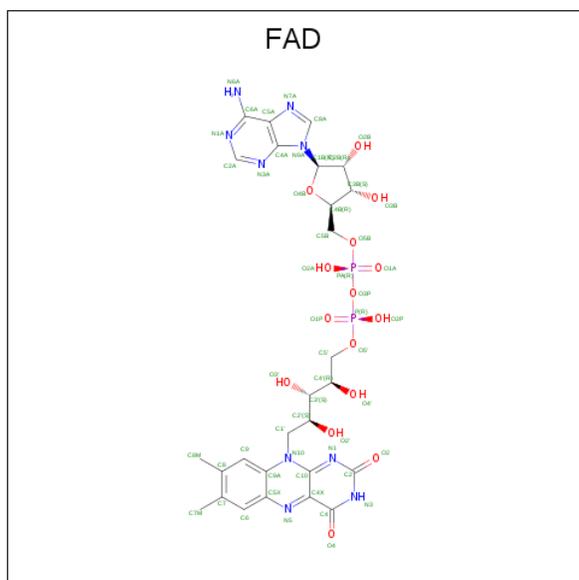
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total C N O P 53 27 9 15 2					0	0
3	B	1	Total C N O P 53 27 9 15 2					0	0

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).
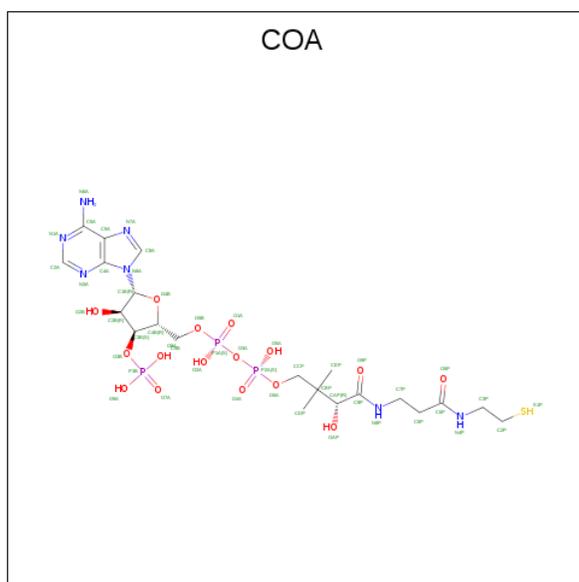
COA

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

• Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	259	Total	O	0	0
			259	259		
5	B	290	Total	O	0	0
			290	290		

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. 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. 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: FAD-dependent pyridine nucleotide-disulphide oxidoreductase
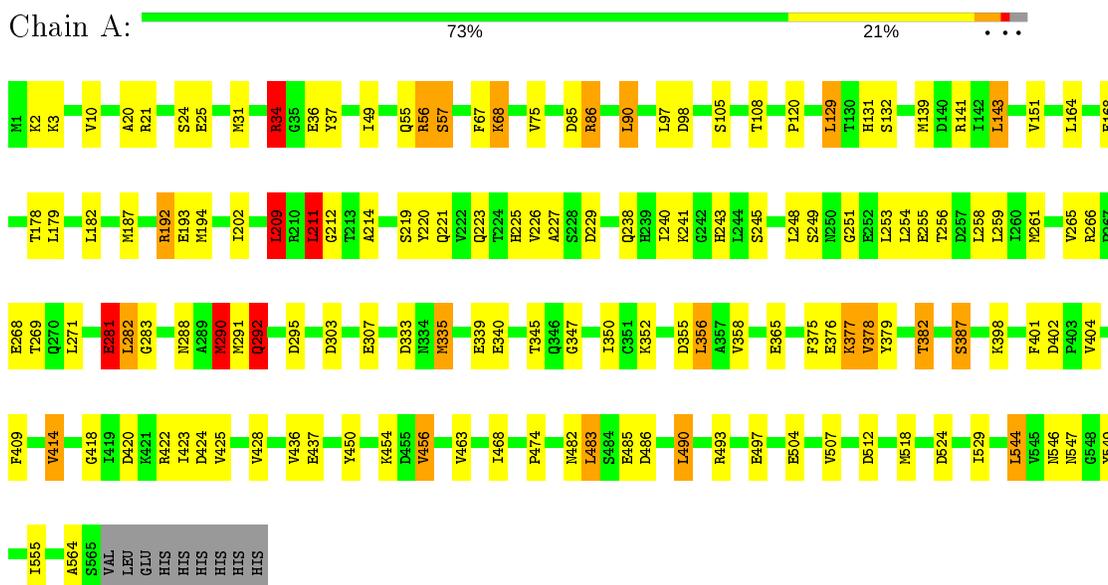
• Molecule 1: FAD-dependent pyridine nucleotide-disulphide oxidoreductase
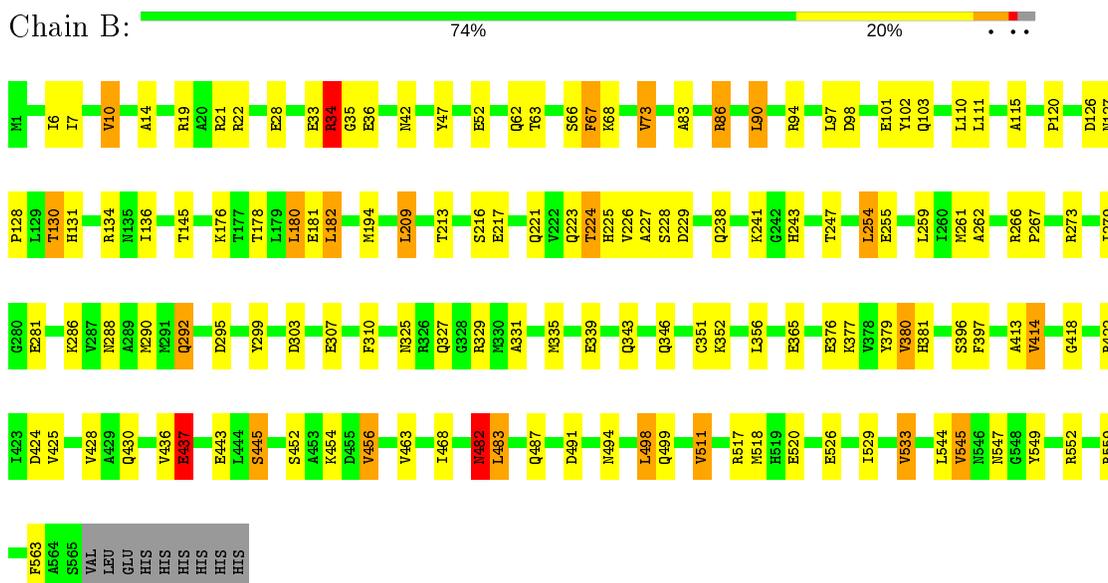
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	133.71Å 133.71Å 79.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	115.00 – 2.00 38.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (115.00-2.00) 99.9 (38.31-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.85 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.122 , 0.155 0.178 , 0.207	Depositor DCC
R_{free} test set	5160 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.0	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.34$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l 0.045 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.023 for H, K, L 0.517 for -H, H+K, -L 0.460 for -h,-k,l	Depositor
Outliers	0 of 107016 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9342	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: COA, FAD, CL

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	1.42	22/4350 (0.5%)	1.24	29/5865 (0.5%)
1	B	1.44	21/4349 (0.5%)	1.28	29/5863 (0.5%)
All	All	1.43	43/8699 (0.5%)	1.26	58/11728 (0.5%)

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

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	GLU	CB-CG	-8.84	1.35	1.52
1	B	33	GLU	CD-OE1	8.68	1.35	1.25
1	B	331	ALA	CA-CB	7.62	1.68	1.52
1	A	450	TYR	CD1-CE1	7.35	1.50	1.39
1	A	409	PHE	CE2-CZ	7.17	1.50	1.37

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	34	ARG	NE-CZ-NH1	14.21	127.40	120.30
1	A	34	ARG	NE-CZ-NH2	-11.84	114.38	120.30
1	B	22	ARG	NE-CZ-NH2	-10.86	114.87	120.30
1	B	134	ARG	NE-CZ-NH1	-10.66	114.97	120.30
1	B	511	VAL	CG1-CB-CG2	10.17	127.17	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	MSE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4295	0	4298	77	2
1	B	4294	0	4300	95	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	31	1	0
3	B	53	0	30	0	0
4	A	48	0	32	0	0
4	B	48	0	32	0	0
5	A	259	0	0	5	0
5	B	290	0	0	11	0
All	All	9342	0	8723	167	2

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 10.

The worst 5 of 167 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:B:290:MSE:CE	1:B:339:GLU:HA	1.70	1.20
1:A:192:ARG:NH2	1:A:564:ALA:O	1.74	1.19
1:A:290:MSE:HE3	1:A:339:GLU:HA	1.16	1.12
1:B:290:MSE:HE1	1:B:339:GLU:CG	1.83	1.09
1:B:290:MSE:HE1	1:B:339:GLU:HG2	1.08	1.08

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:ND1	1:A:512:ASP:OD2[2_555]	2.09	0.11
1:A:229:ASP:OD2	1:A:387:SER:OG[2_555]	2.13	0.07

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	563/574 (98%)	543 (96%)	18 (3%)	2 (0%)	34	30
1	B	563/574 (98%)	547 (97%)	12 (2%)	4 (1%)	22	16
All	All	1126/1148 (98%)	1090 (97%)	30 (3%)	6 (0%)	29	23

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	ASN
1	B	483	LEU
1	A	10	VAL
1	A	456	VAL
1	B	10	VAL

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	449/443 (101%)	416 (93%)	33 (7%)	14	9
1	B	449/443 (101%)	408 (91%)	41 (9%)	9	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	898/886 (101%)	824 (92%)	74 (8%)	11 7

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	34	ARG
1	B	103	GLN
1	B	494	ASN
1	B	42	ASN
1	B	67	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	GLN
1	B	205	GLN
1	B	482	ASN
1	B	131	HIS
1	B	221	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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	COA	B	901	-	41,50,50	1.97	3 (7%)	52,75,75	1.76	11 (21%)
3	FAD	B	900	-	51,58,58	1.72	11 (21%)	60,89,89	2.57	17 (28%)
4	COA	A	901	-	41,50,50	1.57	3 (7%)	52,75,75	2.23	14 (26%)
3	FAD	A	900	-	51,58,58	1.43	7 (13%)	60,89,89	2.12	17 (28%)

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	COA	B	901	-	-	6/44/64/64	0/3/3/3
3	FAD	B	900	-	-	1/30/50/50	0/6/6/6
4	COA	A	901	-	-	8/44/64/64	0/3/3/3
3	FAD	A	900	-	-	2/30/50/50	0/6/6/6

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	COA	O9P-C9P	9.80	1.42	1.23
4	A	901	COA	O9P-C9P	7.50	1.38	1.23
3	B	900	FAD	C10-N1	5.61	1.40	1.33
4	B	901	COA	C2A-N3A	5.24	1.40	1.32
3	A	900	FAD	C2A-N3A	3.86	1.38	1.32

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	900	FAD	N3A-C2A-N1A	-8.59	115.25	128.68
4	A	901	COA	N3A-C2A-N1A	-7.92	116.30	128.68
3	B	900	FAD	C1'-N10-C9A	7.74	124.39	118.29
3	B	900	FAD	C4-N3-C2	7.05	121.09	115.14
3	A	900	FAD	N3A-C2A-N1A	-6.60	118.37	128.68

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	901	COA	S1P-C2P-C3P-N4P
4	A	901	COA	OAP-CAP-CBP-CEP
4	A	901	COA	CAP-C9P-N8P-C7P
4	B	901	COA	O5P-C5P-N4P-C3P
4	B	901	COA	C6P-C5P-N4P-C3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	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 COA B 901

Bond lengths   Bond angles

Torsions   Rings

Ligand FAD B 900

Bond lengths

Bond angles

Torsions

Rings

Ligand COA A 901

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD A 900

Bond lengths

Bond angles

Torsions

Rings
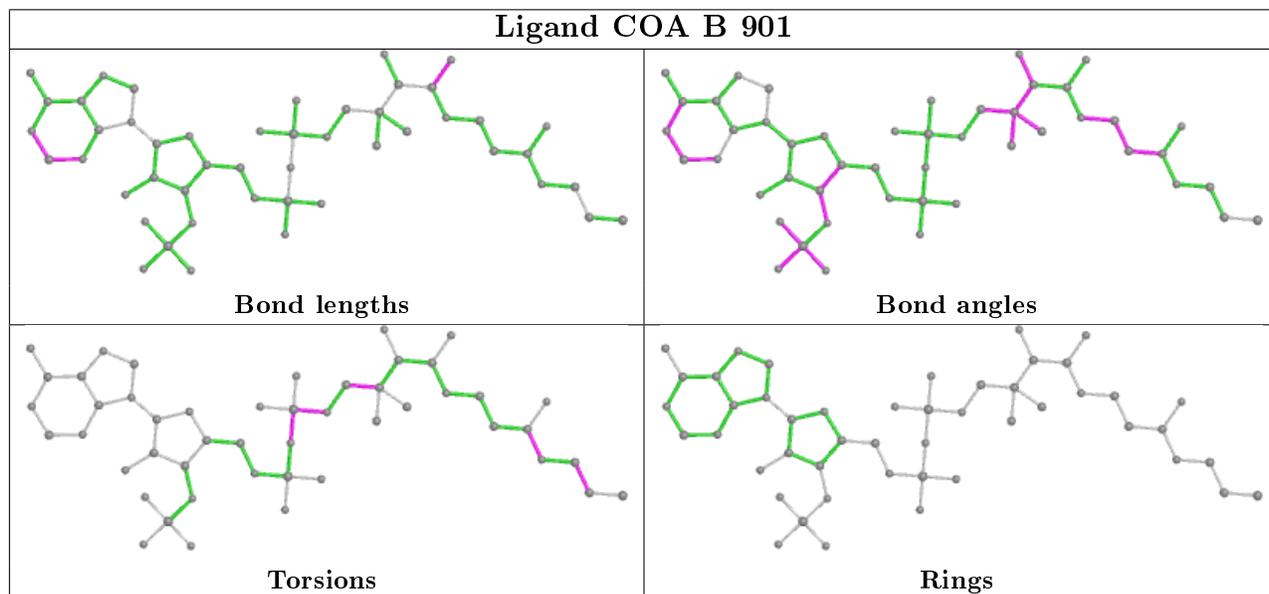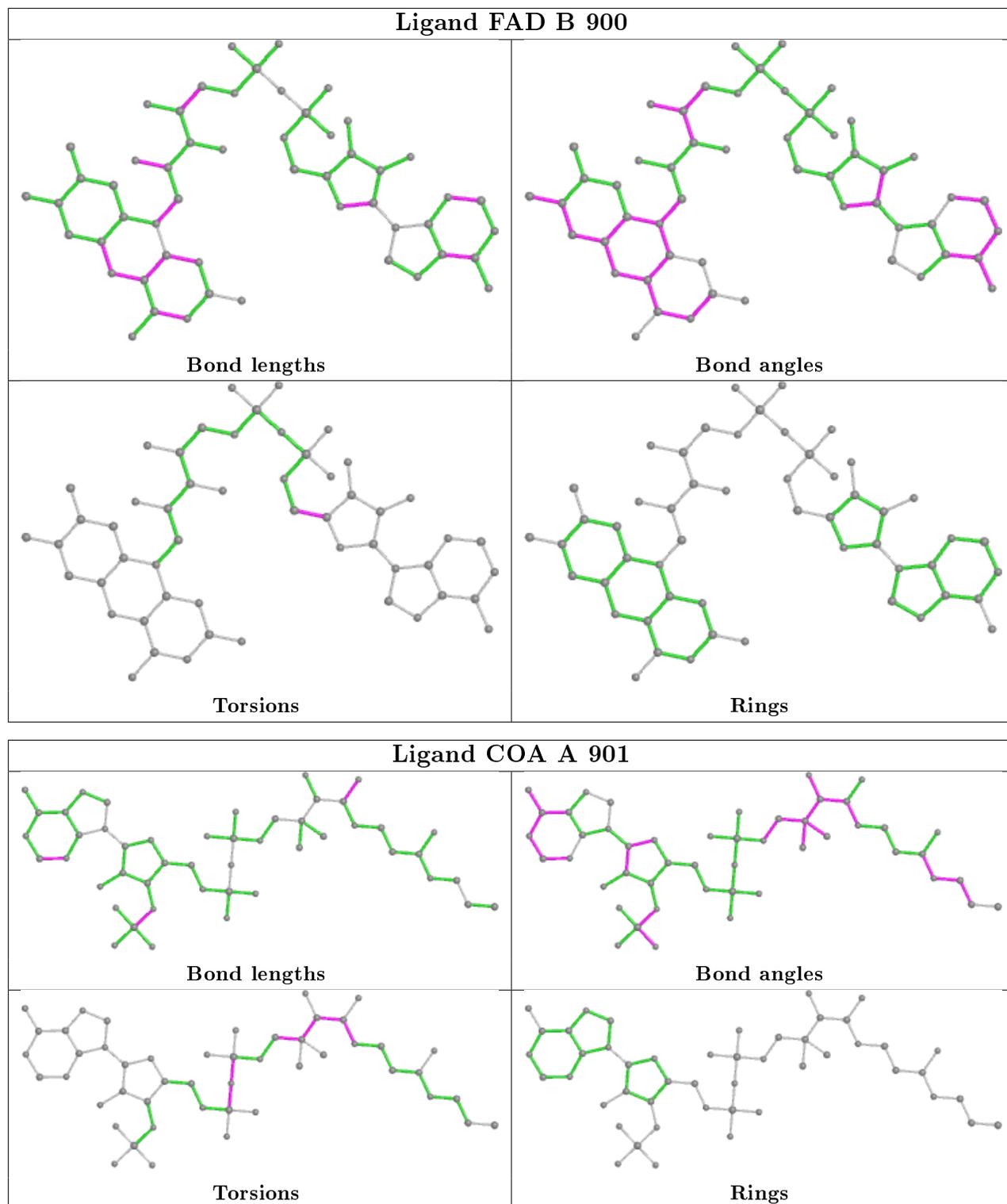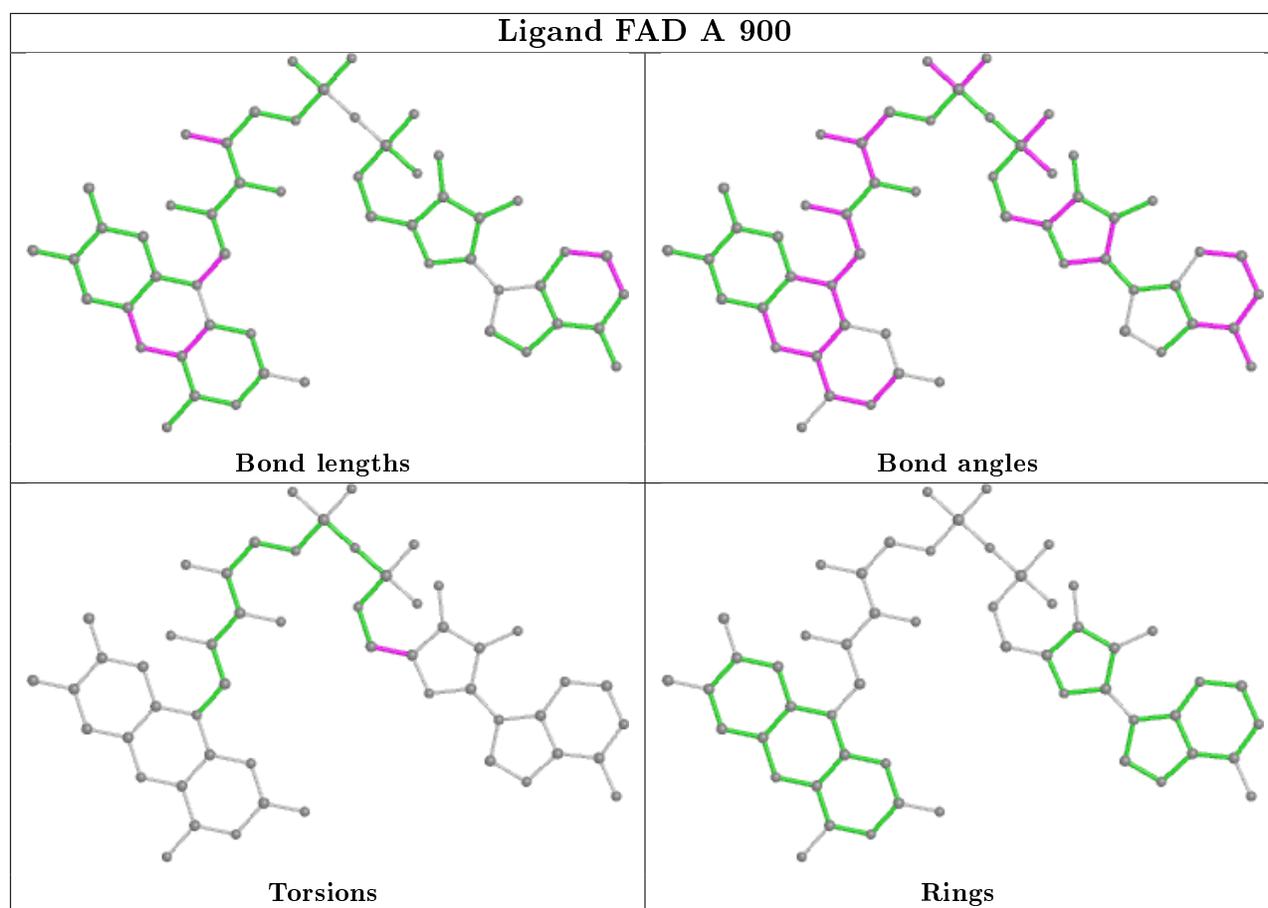
5.7 Other polymers (i)

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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 FAD B 900:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
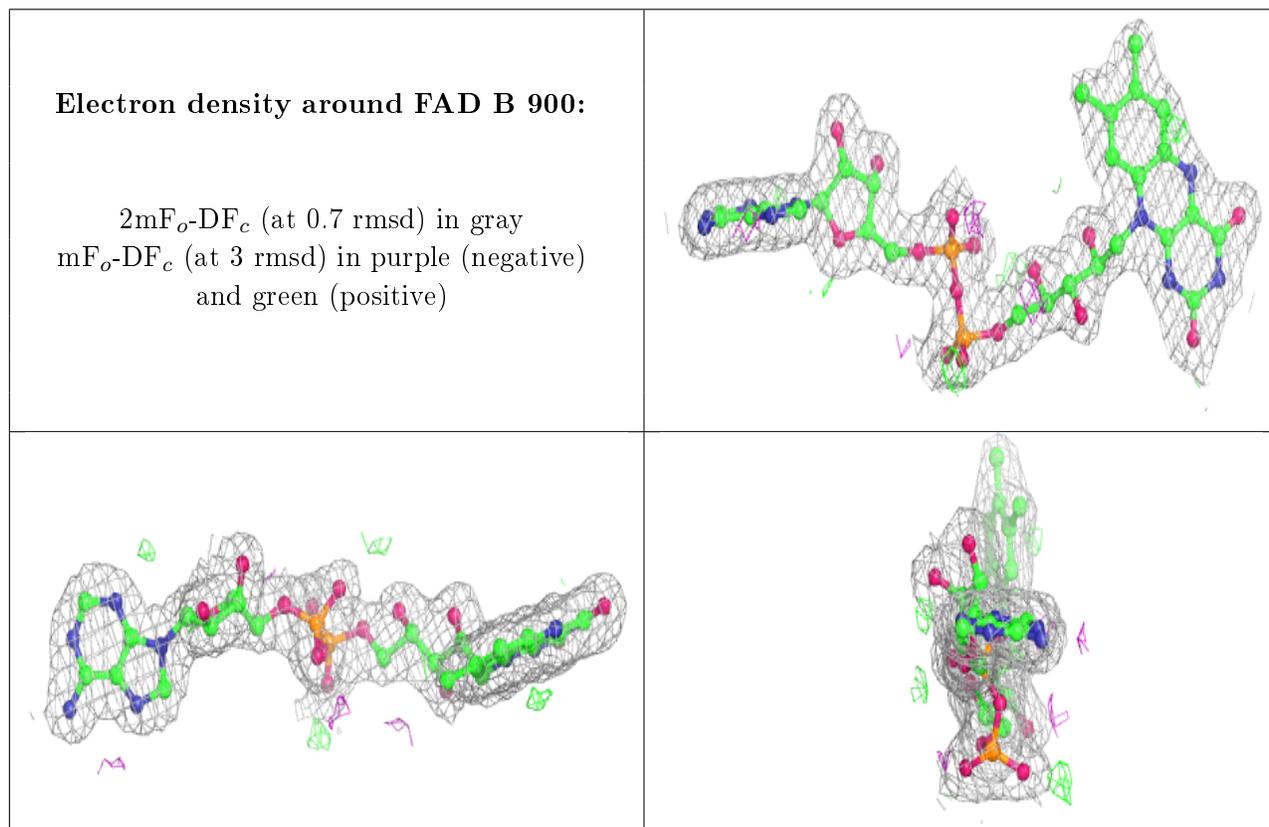
Electron density around FAD A 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
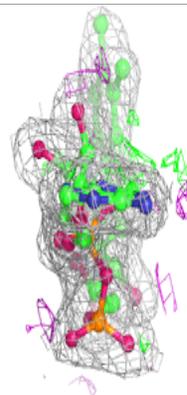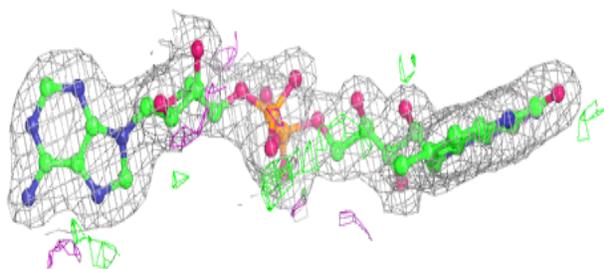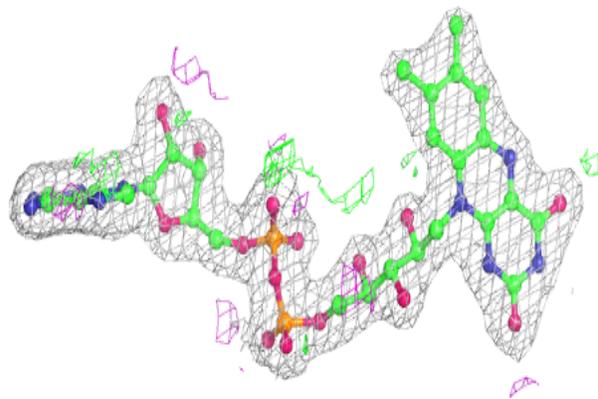
Electron density around COA B 901:

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

Electron density around COA A 901:

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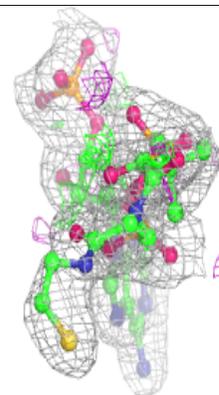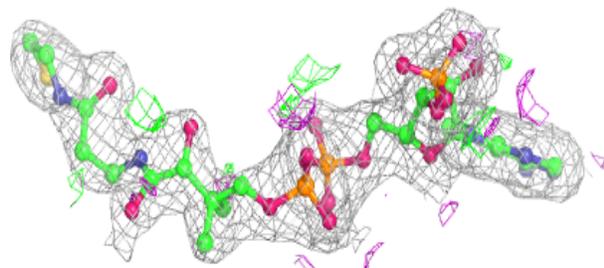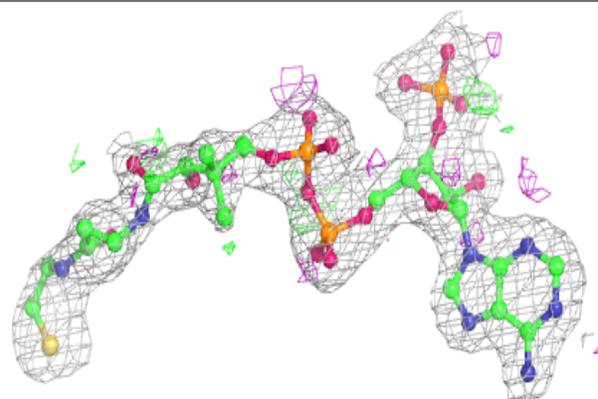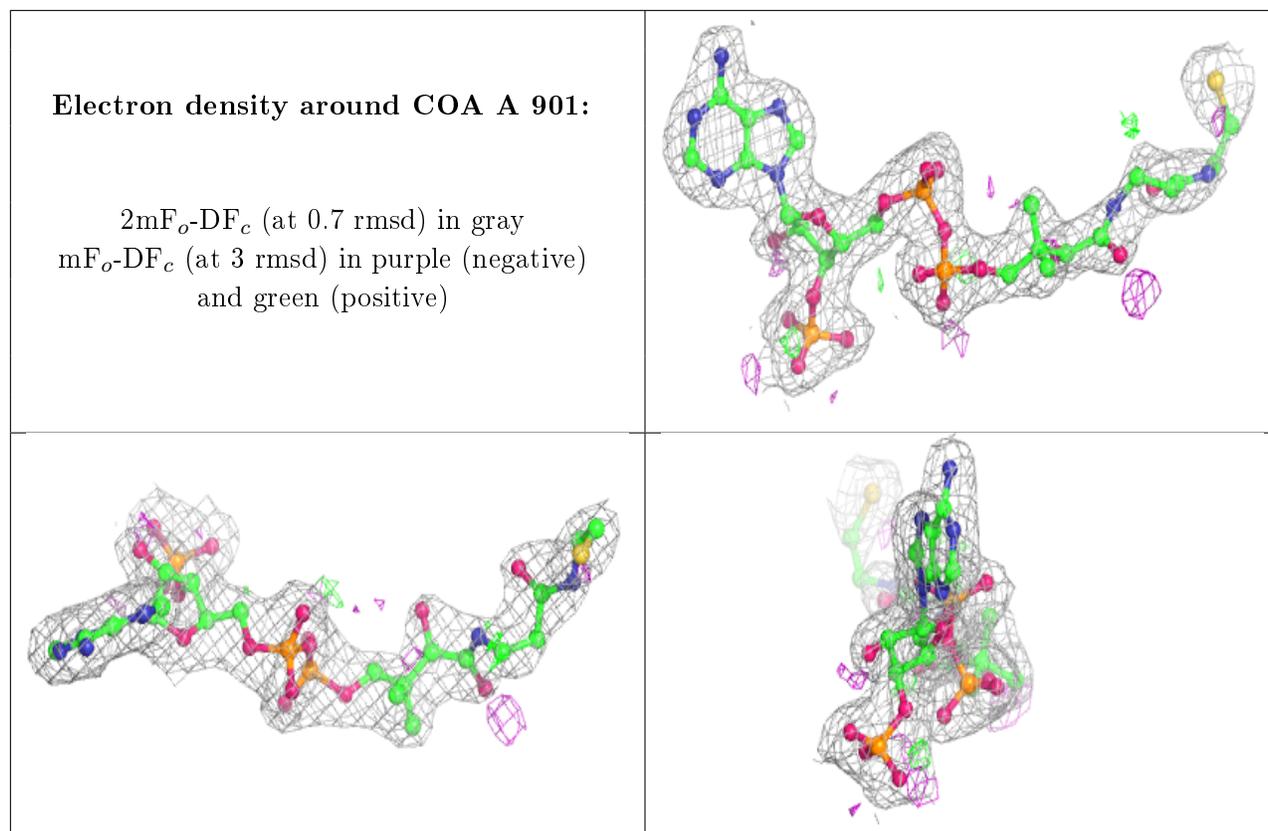
6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.