wwPDB X-ray Structure Validation Summary Report (i)

Aug 22, 2020 – 09:39 AM BST

PDB ID	:	5J7I
Title	:	Crystal structure of a Geobacillus thermoglucosidasius Acetylating Aldehyde Dehydrogenase in complex with ADP
Authors	:	Crennell, S.J.; Extance, J.P.; Danson, M.J.
Deposited on	:	2016-04-06
Resolution	:	4.00 Å(reported)

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

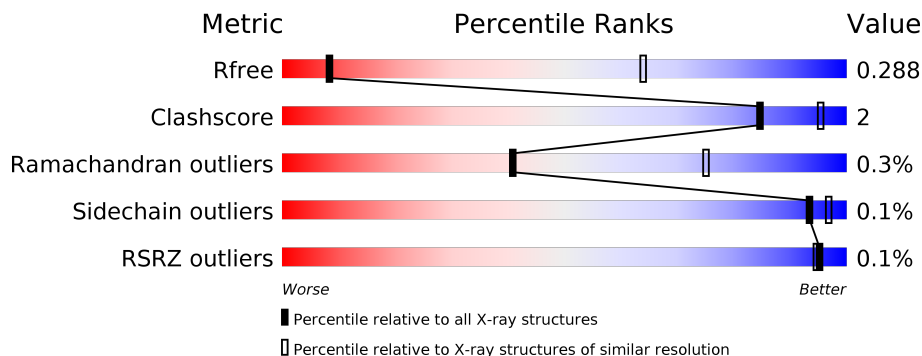|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 4.00 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	Percentile Ranks	Value
Rfree		0.288
Clashscore		2
Ramachandran outliers		0.3%
Sidechain outliers		0.1%
RSRZ outliers		0.1%

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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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% 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	488	87%　　　6%　7%
1	B	488	88%　　　5%　7%
1	C	488	89%　　　·　7%
1	D	488	88%　　　· ·　7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 27900 atoms, of which 14122 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 Acetaldehyde dehydrogenase (Acetylating).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	H	N	O	S	0	2	0
			6958	2168	3530	580	665	15			
1	B	456	Total	C	H	N	O	S	0	0	0
			6944	2164	3523	580	662	15			
1	C	455	Total	C	H	N	O	S	0	0	0
			6936	2161	3520	579	661	15			
1	D	453	Total	C	H	N	O	S	0	0	0
			6888	2147	3492	575	659	15			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A0M1QQ83
A	2	GLY	-	expression tag	UNP A0A0M1QQ83
A	3	SER	-	expression tag	UNP A0A0M1QQ83
A	4	SER	-	expression tag	UNP A0A0M1QQ83
A	5	HIS	-	expression tag	UNP A0A0M1QQ83
A	6	HIS	-	expression tag	UNP A0A0M1QQ83
A	7	HIS	-	expression tag	UNP A0A0M1QQ83
A	8	HIS	-	expression tag	UNP A0A0M1QQ83
A	9	HIS	-	expression tag	UNP A0A0M1QQ83
A	10	HIS	-	expression tag	UNP A0A0M1QQ83
A	11	SER	-	expression tag	UNP A0A0M1QQ83
A	12	SER	-	expression tag	UNP A0A0M1QQ83
A	13	GLY	-	expression tag	UNP A0A0M1QQ83
A	14	LEU	-	expression tag	UNP A0A0M1QQ83
A	15	VAL	-	expression tag	UNP A0A0M1QQ83
A	16	PRO	-	expression tag	UNP A0A0M1QQ83
A	17	ARG	-	expression tag	UNP A0A0M1QQ83
A	18	GLY	-	expression tag	UNP A0A0M1QQ83
A	19	SER	-	expression tag	UNP A0A0M1QQ83
A	20	HIS	-	expression tag	UNP A0A0M1QQ83
A	21	MET	-	expression tag	UNP A0A0M1QQ83

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ALA	-	expression tag	UNP A0A0M1QQ83
A	23	SER	-	expression tag	UNP A0A0M1QQ83
A	372	ILE	THR	conflict	UNP A0A0M1QQ83
B	1	MET	-	initiating methionine	UNP A0A0M1QQ83
B	2	GLY	-	expression tag	UNP A0A0M1QQ83
B	3	SER	-	expression tag	UNP A0A0M1QQ83
B	4	SER	-	expression tag	UNP A0A0M1QQ83
B	5	HIS	-	expression tag	UNP A0A0M1QQ83
B	6	HIS	-	expression tag	UNP A0A0M1QQ83
B	7	HIS	-	expression tag	UNP A0A0M1QQ83
B	8	HIS	-	expression tag	UNP A0A0M1QQ83
B	9	HIS	-	expression tag	UNP A0A0M1QQ83
B	10	HIS	-	expression tag	UNP A0A0M1QQ83
B	11	SER	-	expression tag	UNP A0A0M1QQ83
B	12	SER	-	expression tag	UNP A0A0M1QQ83
B	13	GLY	-	expression tag	UNP A0A0M1QQ83
B	14	LEU	-	expression tag	UNP A0A0M1QQ83
B	15	VAL	-	expression tag	UNP A0A0M1QQ83
B	16	PRO	-	expression tag	UNP A0A0M1QQ83
B	17	ARG	-	expression tag	UNP A0A0M1QQ83
B	18	GLY	-	expression tag	UNP A0A0M1QQ83
B	19	SER	-	expression tag	UNP A0A0M1QQ83
B	20	HIS	-	expression tag	UNP A0A0M1QQ83
B	21	MET	-	expression tag	UNP A0A0M1QQ83
B	22	ALA	-	expression tag	UNP A0A0M1QQ83
B	23	SER	-	expression tag	UNP A0A0M1QQ83
B	372	ILE	THR	conflict	UNP A0A0M1QQ83
C	1	MET	-	initiating methionine	UNP A0A0M1QQ83
C	2	GLY	-	expression tag	UNP A0A0M1QQ83
C	3	SER	-	expression tag	UNP A0A0M1QQ83
C	4	SER	-	expression tag	UNP A0A0M1QQ83
C	5	HIS	-	expression tag	UNP A0A0M1QQ83
C	6	HIS	-	expression tag	UNP A0A0M1QQ83
C	7	HIS	-	expression tag	UNP A0A0M1QQ83
C	8	HIS	-	expression tag	UNP A0A0M1QQ83
C	9	HIS	-	expression tag	UNP A0A0M1QQ83
C	10	HIS	-	expression tag	UNP A0A0M1QQ83
C	11	SER	-	expression tag	UNP A0A0M1QQ83
C	12	SER	-	expression tag	UNP A0A0M1QQ83
C	13	GLY	-	expression tag	UNP A0A0M1QQ83
C	14	LEU	-	expression tag	UNP A0A0M1QQ83
C	15	VAL	-	expression tag	UNP A0A0M1QQ83

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	PRO	-	expression tag	UNP A0A0M1QQ83
C	17	ARG	-	expression tag	UNP A0A0M1QQ83
C	18	GLY	-	expression tag	UNP A0A0M1QQ83
C	19	SER	-	expression tag	UNP A0A0M1QQ83
C	20	HIS	-	expression tag	UNP A0A0M1QQ83
C	21	MET	-	expression tag	UNP A0A0M1QQ83
C	22	ALA	-	expression tag	UNP A0A0M1QQ83
C	23	SER	-	expression tag	UNP A0A0M1QQ83
C	372	ILE	THR	conflict	UNP A0A0M1QQ83
D	1	MET	-	initiating methionine	UNP A0A0M1QQ83
D	2	GLY	-	expression tag	UNP A0A0M1QQ83
D	3	SER	-	expression tag	UNP A0A0M1QQ83
D	4	SER	-	expression tag	UNP A0A0M1QQ83
D	5	HIS	-	expression tag	UNP A0A0M1QQ83
D	6	HIS	-	expression tag	UNP A0A0M1QQ83
D	7	HIS	-	expression tag	UNP A0A0M1QQ83
D	8	HIS	-	expression tag	UNP A0A0M1QQ83
D	9	HIS	-	expression tag	UNP A0A0M1QQ83
D	10	HIS	-	expression tag	UNP A0A0M1QQ83
D	11	SER	-	expression tag	UNP A0A0M1QQ83
D	12	SER	-	expression tag	UNP A0A0M1QQ83
D	13	GLY	-	expression tag	UNP A0A0M1QQ83
D	14	LEU	-	expression tag	UNP A0A0M1QQ83
D	15	VAL	-	expression tag	UNP A0A0M1QQ83
D	16	PRO	-	expression tag	UNP A0A0M1QQ83
D	17	ARG	-	expression tag	UNP A0A0M1QQ83
D	18	GLY	-	expression tag	UNP A0A0M1QQ83
D	19	SER	-	expression tag	UNP A0A0M1QQ83
D	20	HIS	-	expression tag	UNP A0A0M1QQ83
D	21	MET	-	expression tag	UNP A0A0M1QQ83
D	22	ALA	-	expression tag	UNP A0A0M1QQ83
D	23	SER	-	expression tag	UNP A0A0M1QQ83
D	372	ILE	THR	conflict	UNP A0A0M1QQ83

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP
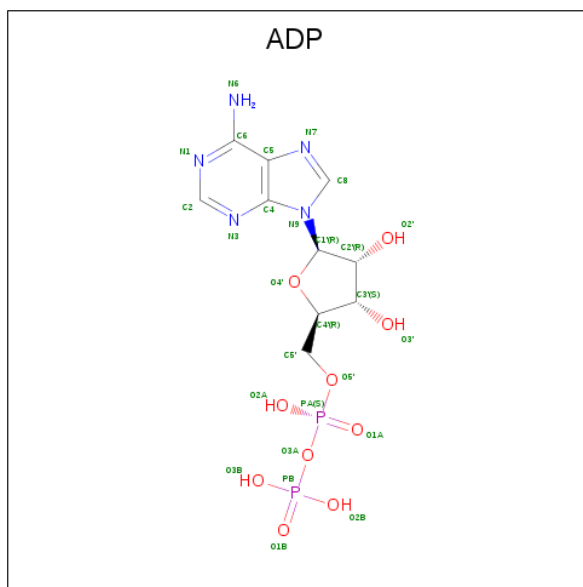
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	C	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		
2	D	1	Total	C	H	N	O	P	0	0
			39	10	12	5	10	2		

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).

APR
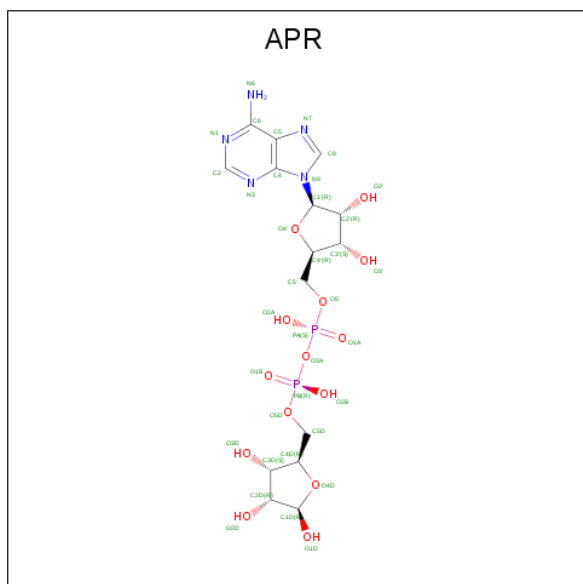
| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	P	0	0
			57	15	21	5	14	2		

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.
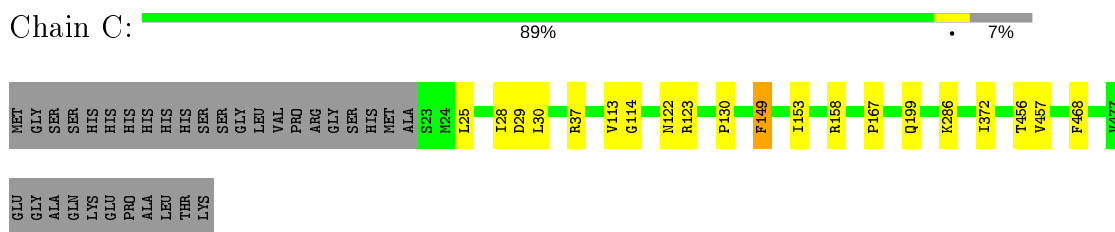
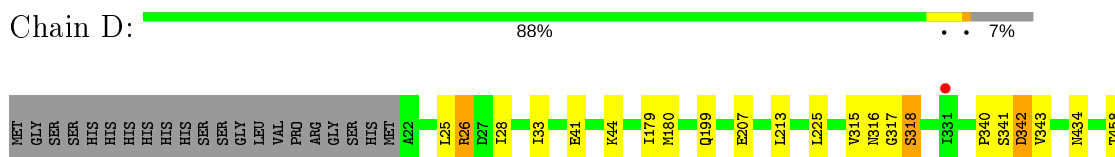- Molecule 1: Acetaldehyde dehydrogenase (Acetylating)
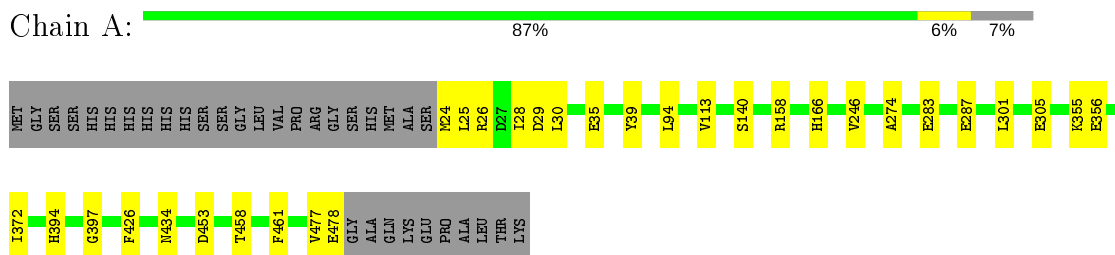
Chain A:

- Molecule 1: Acetaldehyde dehydrogenase (Acetylating)

Chain B:

- Molecule 1: Acetaldehyde dehydrogenase (Acetylating)

Chain C:

- Molecule 1: Acetaldehyde dehydrogenase (Acetylating)

Chain D:
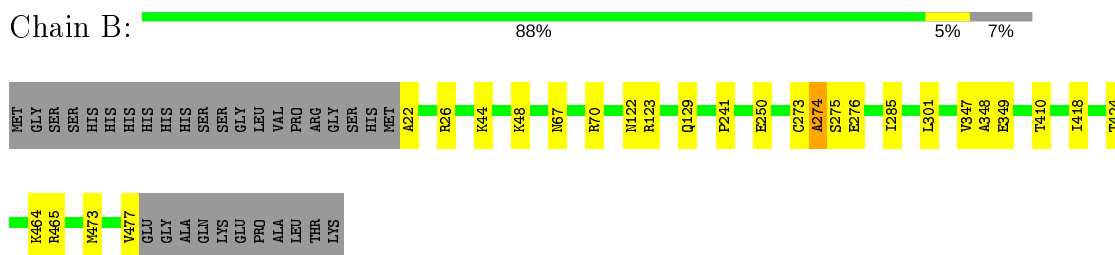
F461 P474 LYS LYS VAL GLU GLY ALA GLN LYS GLU PRO ALA LEU THR LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.05Å 109.54Å 204.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.67 – 4.00 49.10 – 4.00	Depositor EDS
% Data completeness (in resolution range)	78.4 (42.67-4.00) 78.0 (49.10-4.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.63 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.230 , 0.282 0.235 , 0.288	Depositor DCC
R_{free} test set	718 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.9	EDS
L-test for twinning [2]	$<|L|> = 0.45$, $<L^2> = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	27900	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: APR, SCY, ADP

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	0.34	0/3473	0.62	0/4696
1	B	0.32	0/3457	0.60	0/4676
1	C	0.32	0/3452	0.60	2/4669 (0.0%)
1	D	0.32	0/3432	0.59	0/4644
All	All	0.32	0/13814	0.60	2/18685 (0.0%)

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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	149	PHE	CB-CG-CD1	-7.12	115.82	120.80
1	C	149	PHE	CB-CG-CD2	6.83	125.58	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	342	ASP	Mainchain

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	3428	3530	3516	23	1
1	B	3421	3523	3527	18	2
1	C	3416	3520	3521	18	0
1	D	3396	3492	3492	15	0
2	A	27	12	12	0	0
2	C	27	12	12	2	0
2	D	27	12	12	1	0
3	B	36	21	20	1	0
All	All	13778	14122	14112	65	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 2.

The worst 5 of 65 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:26:ARG:NH1	1:D:41:GLU:OE2	2.15	0.80
1:B:129:GLN:OE1	1:B:464:LYS:NZ	2.20	0.74
1:A:434:ASN:ND2	1:B:122:ASN:O	2.27	0.67
1:D:341:SER:O	1:D:343:VAL:N	2.34	0.60
1:B:301:LEU:HD12	1:B:347:VAL:O	2.02	0.59

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:B:22:ALA:N	1:B:349:GLU:OE2[4_545]	2.16	0.04
1:A:24:MET:O	1:B:123:ARG:NH2[3_554]	2.19	0.01

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	454/488 (93%)	441 (97%)	13 (3%)	0	100	100
1	B	453/488 (93%)	442 (98%)	10 (2%)	1 (0%)	47	79
1	C	452/488 (93%)	444 (98%)	8 (2%)	0	100	100
1	D	450/488 (92%)	435 (97%)	11 (2%)	4 (1%)	17	55
All	All	1809/1952 (93%)	1762 (97%)	42 (2%)	5 (0%)	41	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	26	ARG
1	D	316	ASN
1	D	318	SER
1	B	274	ALA
1	D	342	ASP

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	365/389 (94%)	365 (100%)	0	100	100
1	B	363/389 (93%)	363 (100%)	0	100	100
1	C	363/389 (93%)	363 (100%)	0	100	100
1	D	360/389 (92%)	358 (99%)	2 (1%)	86	92
All	All	1451/1556 (93%)	1449 (100%)	2 (0%)	93	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	25	LEU
1	D	26	ARG

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

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	SCY	D	273	1	7,8,9	0.93	0	3,9,11	0.71	0
1	SCY	B	273	1	7,8,9	1.15	0	3,9,11	0.63	0
1	SCY	C	273	1	7,8,9	1.00	0	3,9,11	0.69	0
1	SCY	A	273	1	7,8,9	1.01	0	3,9,11	0.84	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
1	SCY	D	273	1	-	2/5/7/9	-
1	SCY	B	273	1	-	2/5/7/9	-
1	SCY	C	273	1	-	3/5/7/9	-
1	SCY	A	273	1	-	5/5/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	273	SCY	N-CA-CB-SG
1	D	273	SCY	C-CA-CB-SG
1	B	273	SCY	N-CA-CB-SG
1	B	273	SCY	C-CA-CB-SG
1	C	273	SCY	CA-CB-SG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	273	SCY	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	ADP	D	501	-	24,29,29	0.99	2 (8%)	29,45,45	1.33	4 (13%)
2	ADP	A	501	-	24,29,29	0.94	1 (4%)	29,45,45	1.37	3 (10%)
3	APR	B	501	-	34,39,39	3.69	14 (41%)	40,60,60	1.92	6 (15%)
2	ADP	C	501	-	24,29,29	1.02	3 (12%)	29,45,45	1.13	1 (3%)

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
2	ADP	D	501	-	-	8/12/32/32	0/3/3/3
2	ADP	A	501	-	-	0/12/32/32	0/3/3/3
3	APR	B	501	-	-	8/18/54/54	0/4/4/4
2	ADP	C	501	-	-	2/12/32/32	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	APR	O4D-C1D	-9.94	1.31	1.43
3	B	501	APR	O4'-C1'	-8.38	1.29	1.41
3	B	501	APR	C3'-C4'	-7.97	1.32	1.53
3	B	501	APR	O4'-C4'	7.46	1.61	1.45
3	B	501	APR	C3D-C4D	-6.86	1.35	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	APR	C5-C6-N6	6.72	130.57	120.35
3	B	501	APR	N3-C2-N1	-5.36	120.29	128.68
3	B	501	APR	N6-C6-N1	-4.23	109.79	118.57
3	B	501	APR	C3'-C2'-C1'	4.11	107.17	100.98
2	A	501	ADP	N3-C2-N1	-3.76	122.80	128.68

There are no chirality outliers.
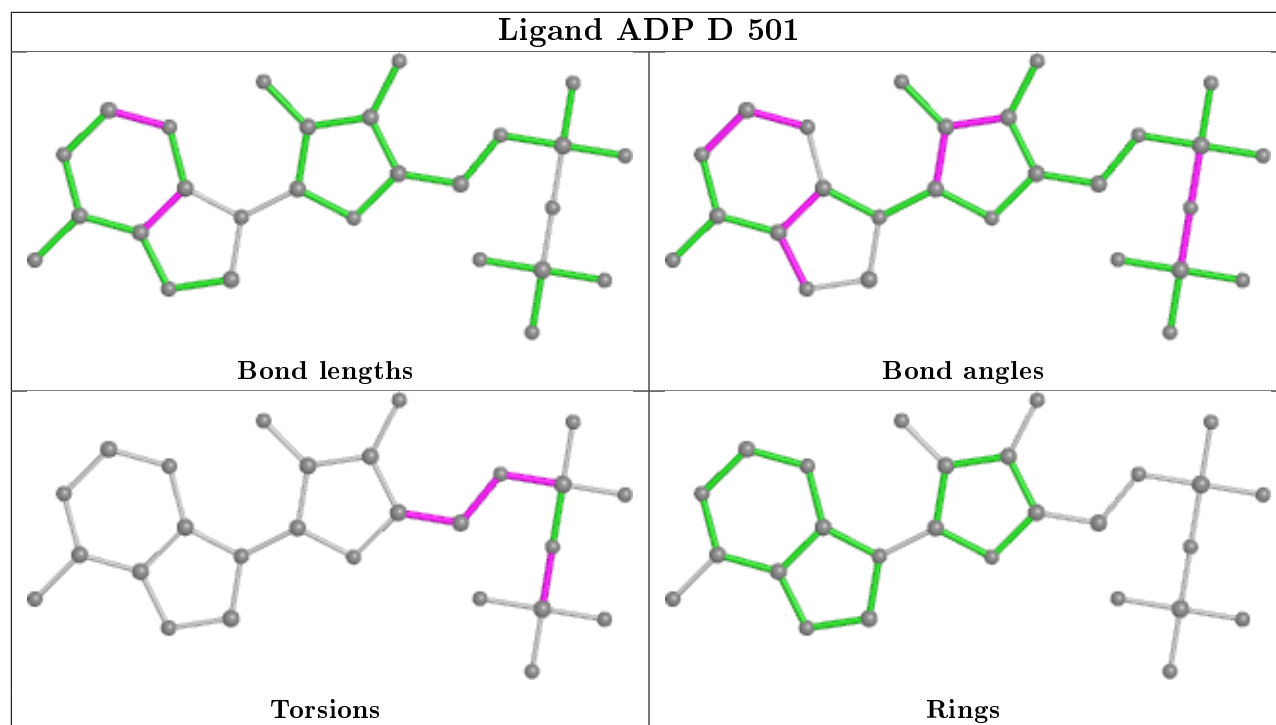
5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	ADP	PA-O3A-PB-O3B
2	D	501	ADP	O4'-C4'-C5'-O5'
2	D	501	ADP	C3'-C4'-C5'-O5'
3	B	501	APR	C5'-O5'-PA-O1A
3	B	501	APR	C5'-O5'-PA-O2A

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	ADP	1	0
3	B	501	APR	1	0
2	C	501	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ADP D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand APR B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 501

Bond lengths

Bond angles

Torsions

Rings
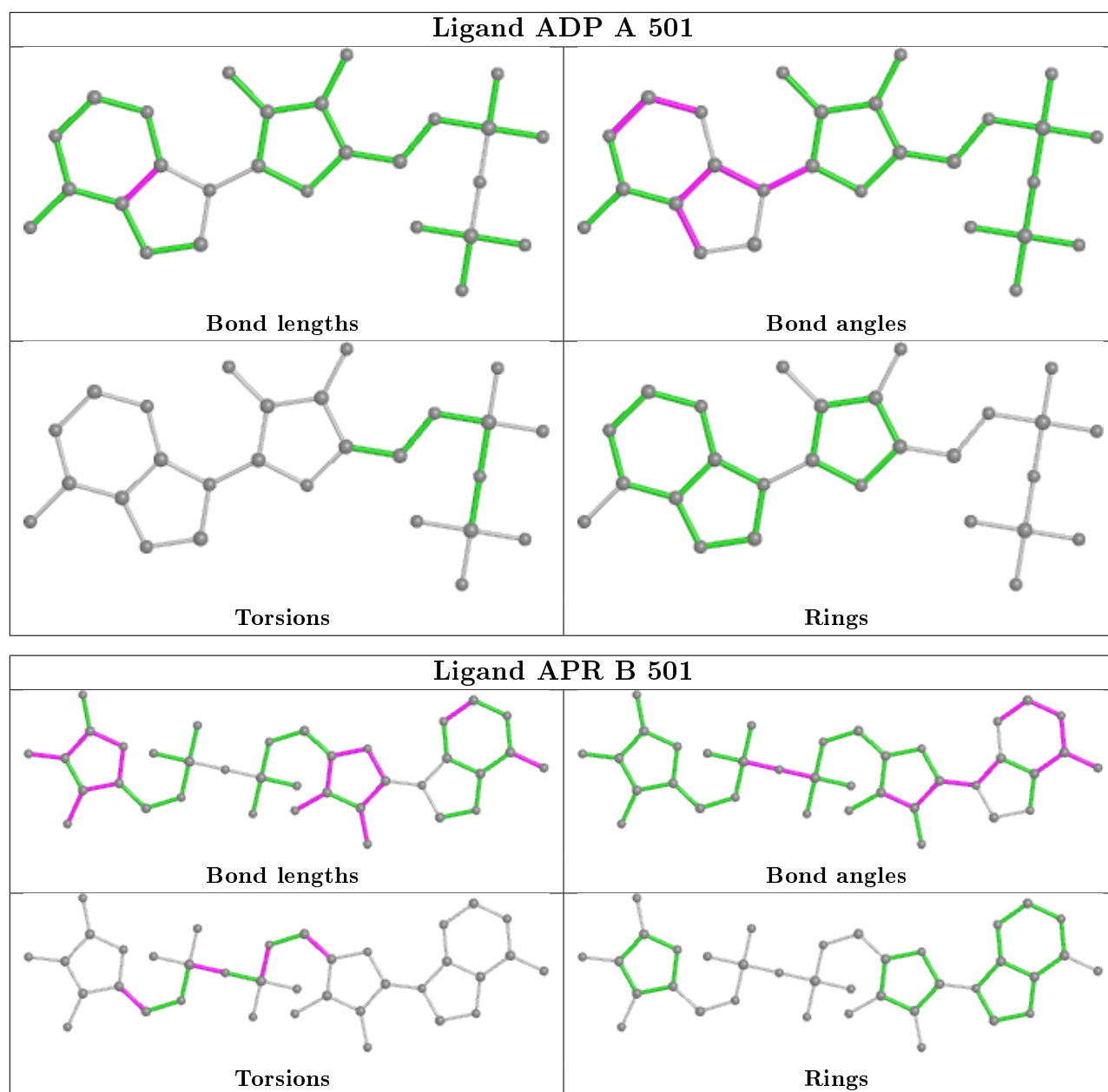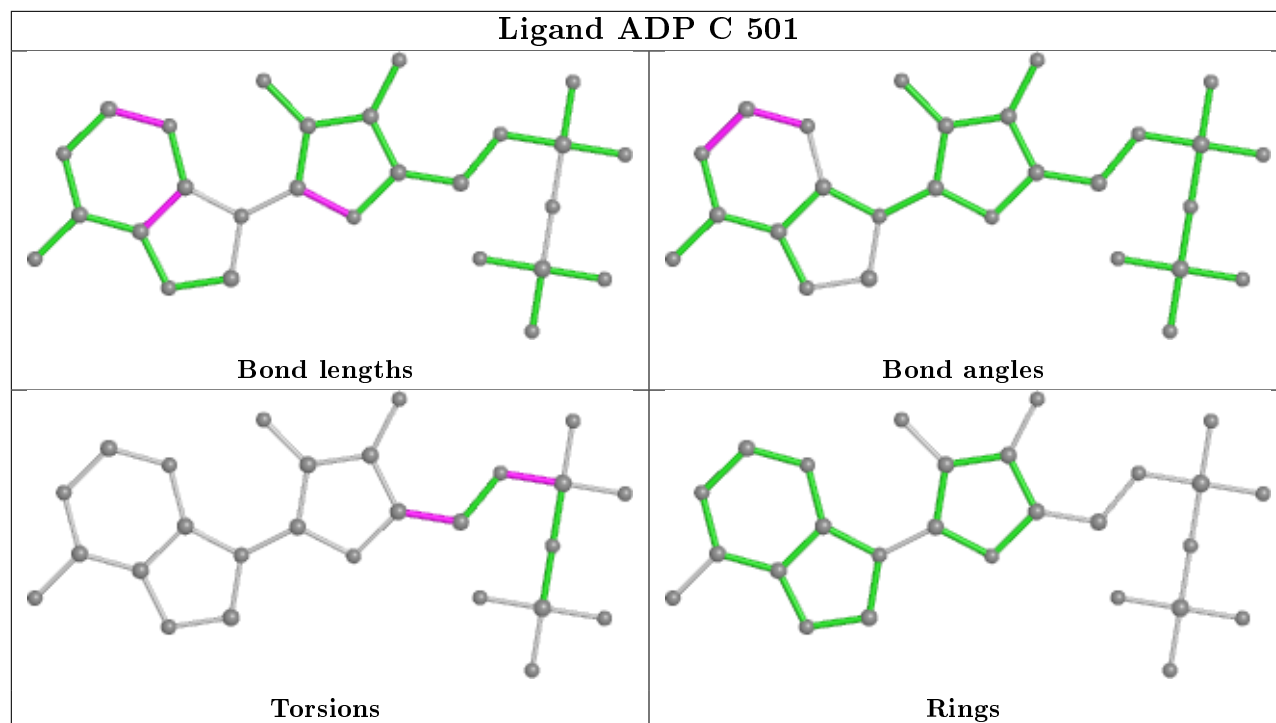
5.7 Other polymers (i)

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)

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	454/488 (93%)	-0.21	0	100	100	36, 46, 59, 85	0
1	B	455/488 (93%)	-0.38	0	100	100	37, 48, 62, 76	0
1	C	454/488 (93%)	-0.26	0	100	100	40, 59, 72, 95	0
1	D	452/488 (92%)	-0.08	1 (0%)	95	93	43, 65, 87, 98	0
All	All	1815/1952 (92%)	-0.23	1 (0%)	95	94	36, 53, 78, 98	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	331	ILE	2.0

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

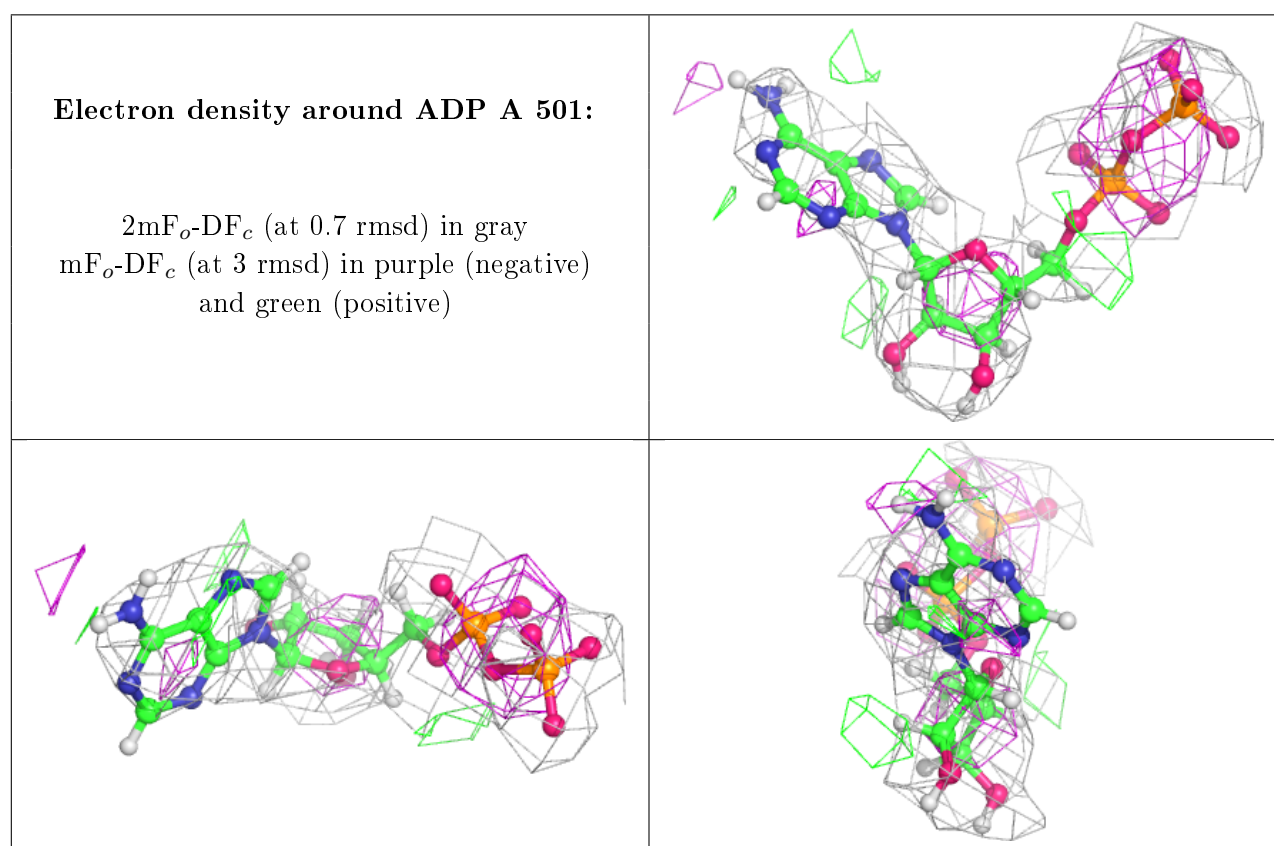| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	SCY	D	273	9/10	0.89	0.30	19,45,45,45	0
1	SCY	C	273	9/10	0.91	0.19	19,45,45,45	0
1	SCY	B	273	9/10	0.93	0.18	19,41,41,41	0
1	SCY	A	273	9/10	0.95	0.25	19,38,38,38	0

6.3 Carbohydrates (i)
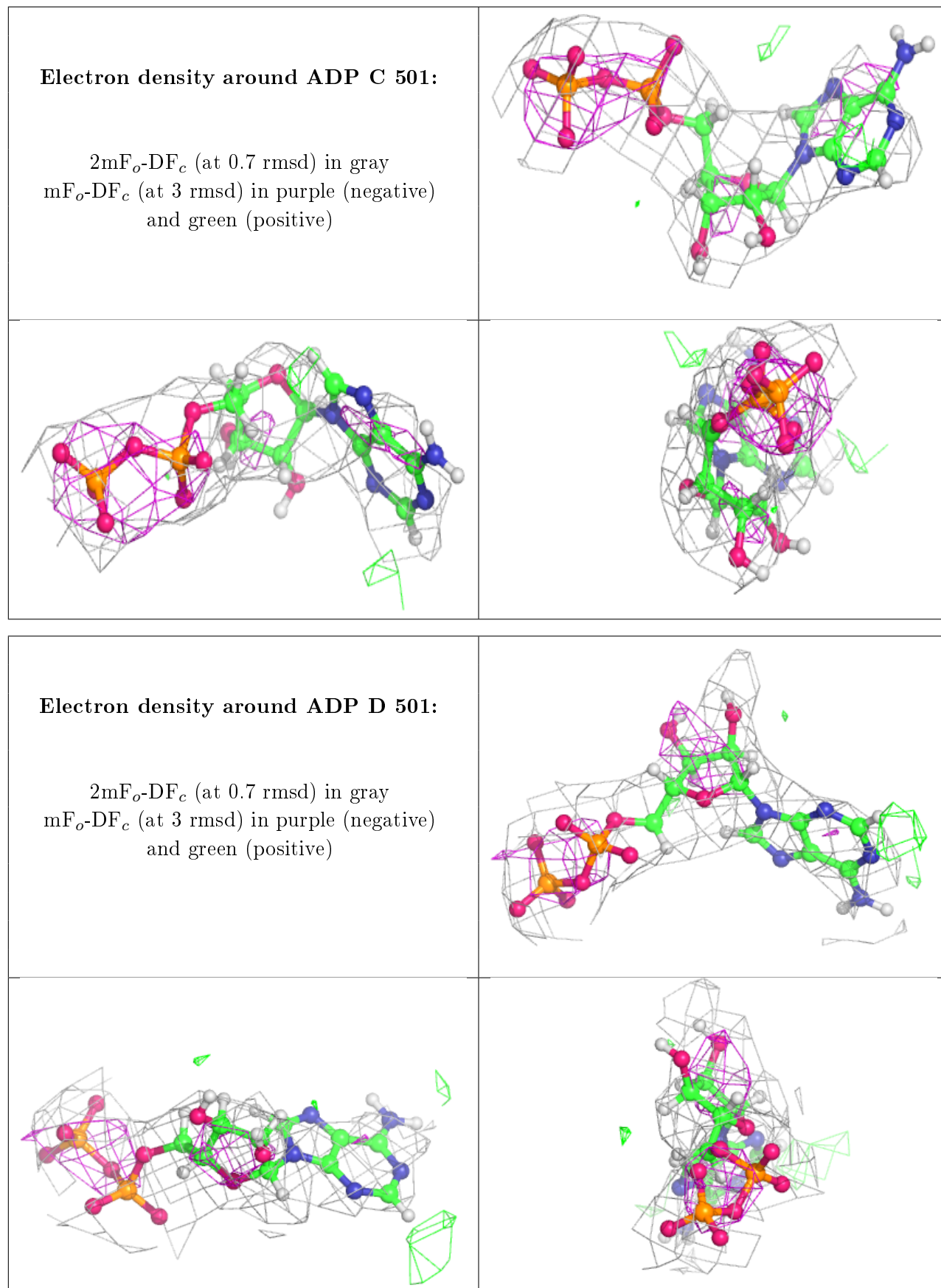
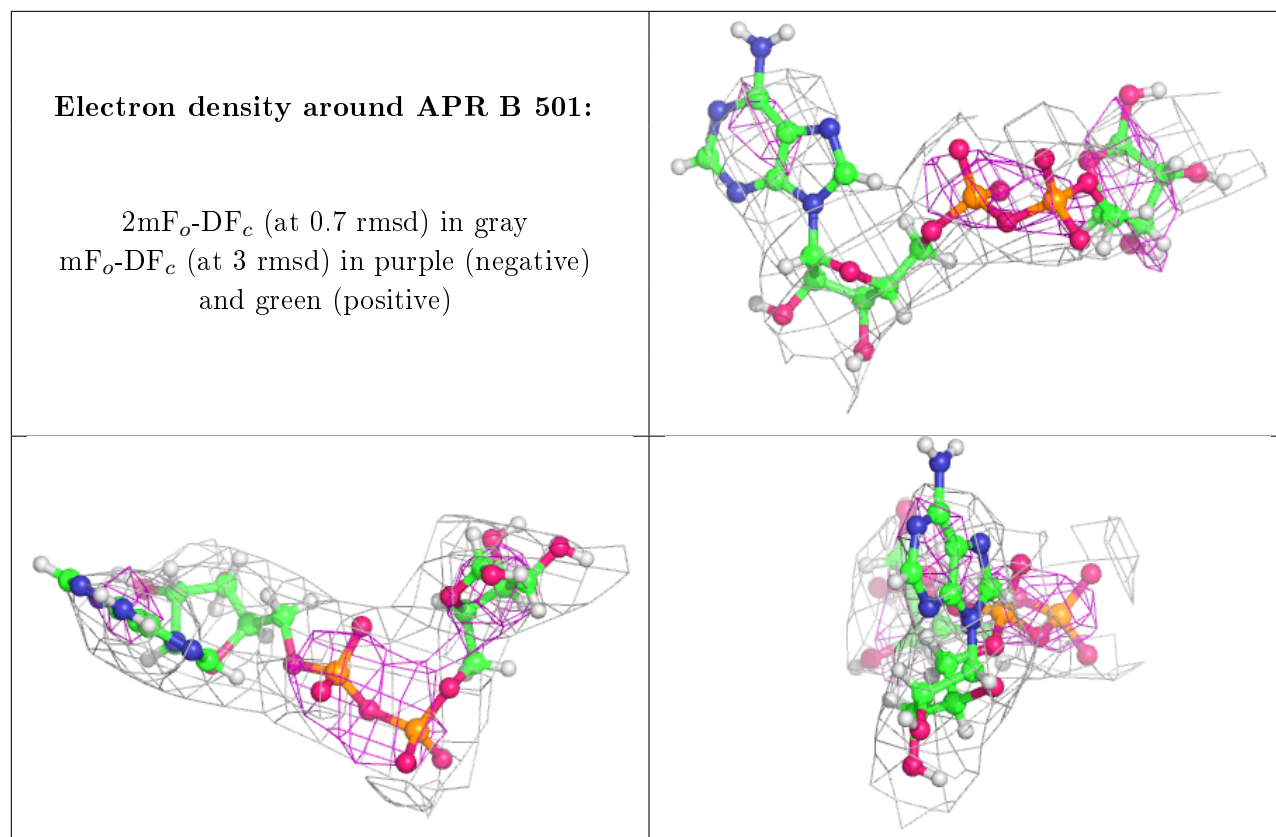There are no monosaccharides in this entry.

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
2	ADP	A	501	27/27	0.81	0.40	19,44,44,44	0
2	ADP	C	501	27/27	0.84	0.36	19,50,50,50	0
2	ADP	D	501	27/27	0.85	0.36	19,55,55,55	0
3	APR	B	501	36/36	0.87	0.29	19,47,47,47	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 ADP A 501:

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

Electron density around ADP C 501:

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

Electron density around ADP D 501:

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

Electron density around APR B 501:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.