



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 2W03 / pdb_00002w03
Title : Co-complex Structure of Achromobactin Synthetase Protein D (AcsD) with adenosine, sulfate and citrate from Pectobacterium Chrysanthemi
Authors : Schmelz, S.; McMahon, S.A.; Kadi, N.; Song, L.; Oves-Costales, D.; Oke, M.; Liu, H.; Johnson, K.A.; Carter, L.; White, M.F.; Challis, G.L.; Naismith, J.H.
Deposited on : 2008-08-08
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

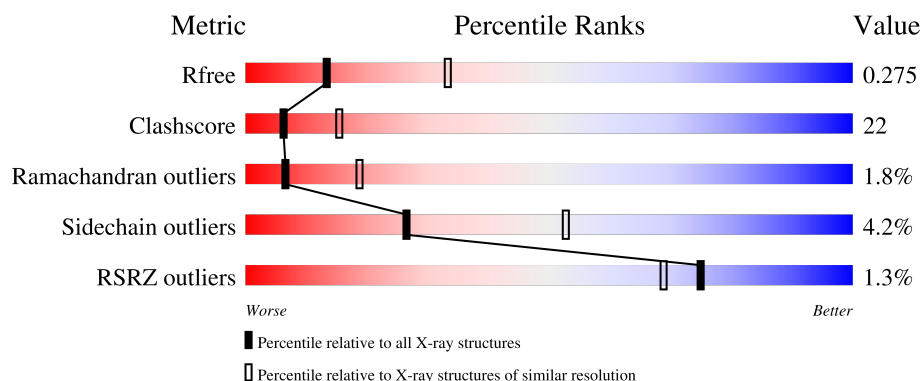
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 $\leq 5\%$. 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	620	% 52% 36% • 7%
1	B	620	% 48% 41% • 7%

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
3	SO4	B	1589	-	-	X	-

2 Entry composition [i](#)

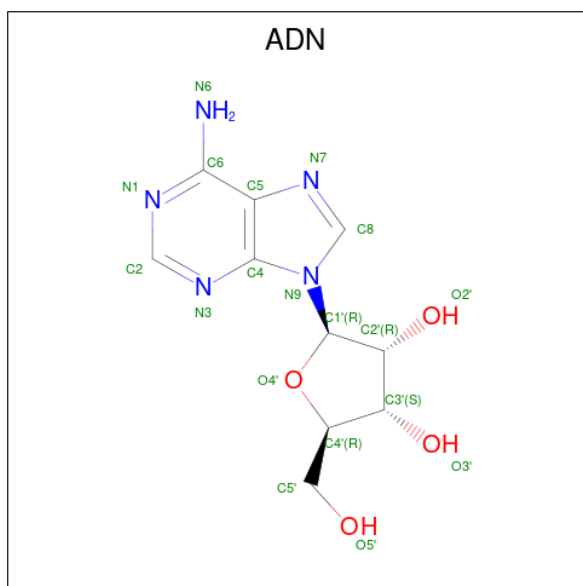
There are 5 unique types of molecules in this entry. The entry contains 9361 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACSD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	0	0
			4601	2926	834	821	20			
1	B	577	Total	C	N	O	S	0	0	0
			4626	2940	841	825	20			

- Molecule 2 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



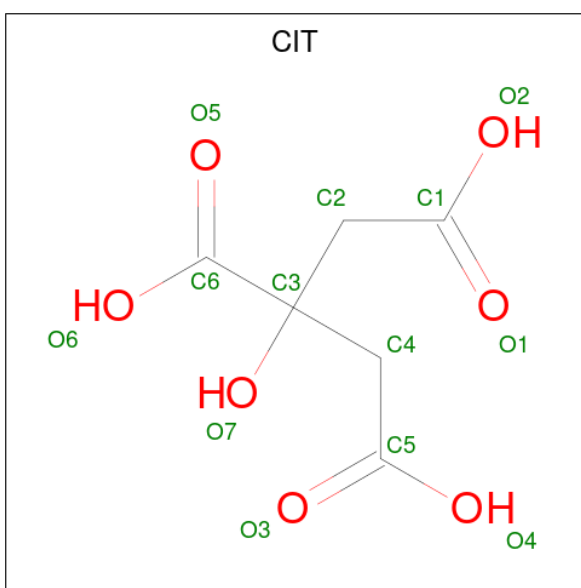
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	10	5	4		
2	B	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	33	Total 33	O 33	0	0
5	B	40	Total 40	O 40	0	0

MET
ASN
ASN
ARG
ASN
ASN
HIS
D7
V8
L9
S10
I13
S14
E15
K16
L19
H20
L23
I27
K28
E29
F30
A31
I32
P33
Y36
E40
M45
K46
P49
P50
D55
G56
A57
D58
W59
K60
G61
I62
M65
I66
G67
P68
D70
L74
F75
V78



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.65Å 69.14Å 94.19Å 95.43° 101.45° 95.06°	Depositor
Resolution (Å)	91.67 – 2.95 91.67 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.2 (91.67-2.95) 98.2 (91.67-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.267 0.212 , 0.275	Depositor DCC
R_{free} test set	1474 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9361	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, SO4, CIT

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	0.89	1/4721 (0.0%)	1.17	16/6415 (0.2%)
1	B	0.91	0/4746	1.15	16/6448 (0.2%)
All	All	0.90	1/9467 (0.0%)	1.16	32/12863 (0.2%)

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	2	3
1	B	0	3
All	All	2	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	THR	CA-CB	6.48	1.64	1.53

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ALA	N-CA-C	14.32	130.92	113.16
1	B	481	ASP	CB-CA-C	-9.90	105.15	116.54
1	A	302	ASN	N-CA-C	9.77	121.62	110.97
1	A	481	ASP	N-CA-C	8.71	122.90	111.75
1	A	477	ARG	N-CA-C	8.38	123.06	113.01

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	351	ALA	CA
1	A	482	ASP	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	GLY	Peptide
1	A	300	ILE	Peptide
1	A	480	ASP	Peptide
1	B	268	GLY	Peptide
1	B	97	GLN	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	4601	0	4519	183	0
1	B	4626	0	4545	227	0
2	A	19	0	13	0	0
2	B	19	0	13	4	0
3	A	5	0	0	0	0
3	B	5	0	0	2	0
4	B	13	0	5	1	0
5	A	33	0	0	0	0
5	B	40	0	0	5	0
All	All	9361	0	9095	410	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 22.

The worst 5 of 410 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:124:ARG:CD	1:B:571:ALA:HA	1.67	1.23
1:B:124:ARG:HD3	1:B:571:ALA:CA	1.68	1.23
1:B:563:LYS:NZ	1:B:576:ARG:HH22	1.41	1.15
1:A:303:CYS:SG	1:A:305:ARG:NH2	2.29	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ILE:HD13	1:B:492:LEU:HD13	1.32	1.04

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	568/620 (92%)	501 (88%)	59 (10%)	8 (1%)	9	24
1	B	571/620 (92%)	494 (86%)	65 (11%)	12 (2%)	5	16
All	All	1139/1240 (92%)	995 (87%)	124 (11%)	20 (2%)	6	19

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	ASP
1	B	351	ALA
1	B	482	ASP
1	A	464	ASP
1	A	515	ILE

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	485/522 (93%)	467 (96%)	18 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	487/522 (93%)	464 (95%)	23 (5%)	23	49
All	All	972/1044 (93%)	931 (96%)	41 (4%)	26	53

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	300	ILE
1	B	541	GLN
1	B	362	GLU
1	B	474	LEU
1	B	569	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	288	HIS
1	B	329	HIS
1	B	577	GLN
1	B	405	HIS
1	B	307	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	1589	-	4,4,4	0.33	0	6,6,6	0.56	0
2	ADN	B	1588	-	21,21,21	1.25	3 (14%)	31,31,31	2.00	7 (22%)
4	CIT	B	1590	-	12,12,12	1.32	1 (8%)	17,17,17	1.73	4 (23%)
3	SO4	B	1589	-	4,4,4	0.43	0	6,6,6	0.54	0
2	ADN	A	1588	-	21,21,21	1.30	3 (14%)	31,31,31	2.02	7 (22%)

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	ADN	B	1588	-	-	2/6/22/22	0/3/3/3
4	CIT	B	1590	-	-	8/16/16/16	-
2	ADN	A	1588	-	-	3/6/22/22	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1588	ADN	C5-N7	-3.60	1.32	1.39
2	A	1588	ADN	C5-N7	-3.21	1.33	1.39
2	B	1588	ADN	C8-N9	-2.53	1.33	1.37
2	A	1588	ADN	C1'-N9	2.23	1.52	1.46
2	A	1588	ADN	C8-N9	-2.15	1.33	1.37

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1588	ADN	C5-C4-N3	-5.87	118.63	126.72
2	B	1588	ADN	C5-C4-N3	-5.51	119.12	126.72
2	A	1588	ADN	N3-C2-N1	-4.35	122.00	128.58
2	B	1588	ADN	N3-C4-N9	4.29	134.46	127.17
2	A	1588	ADN	N3-C4-N9	4.11	134.16	127.17

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

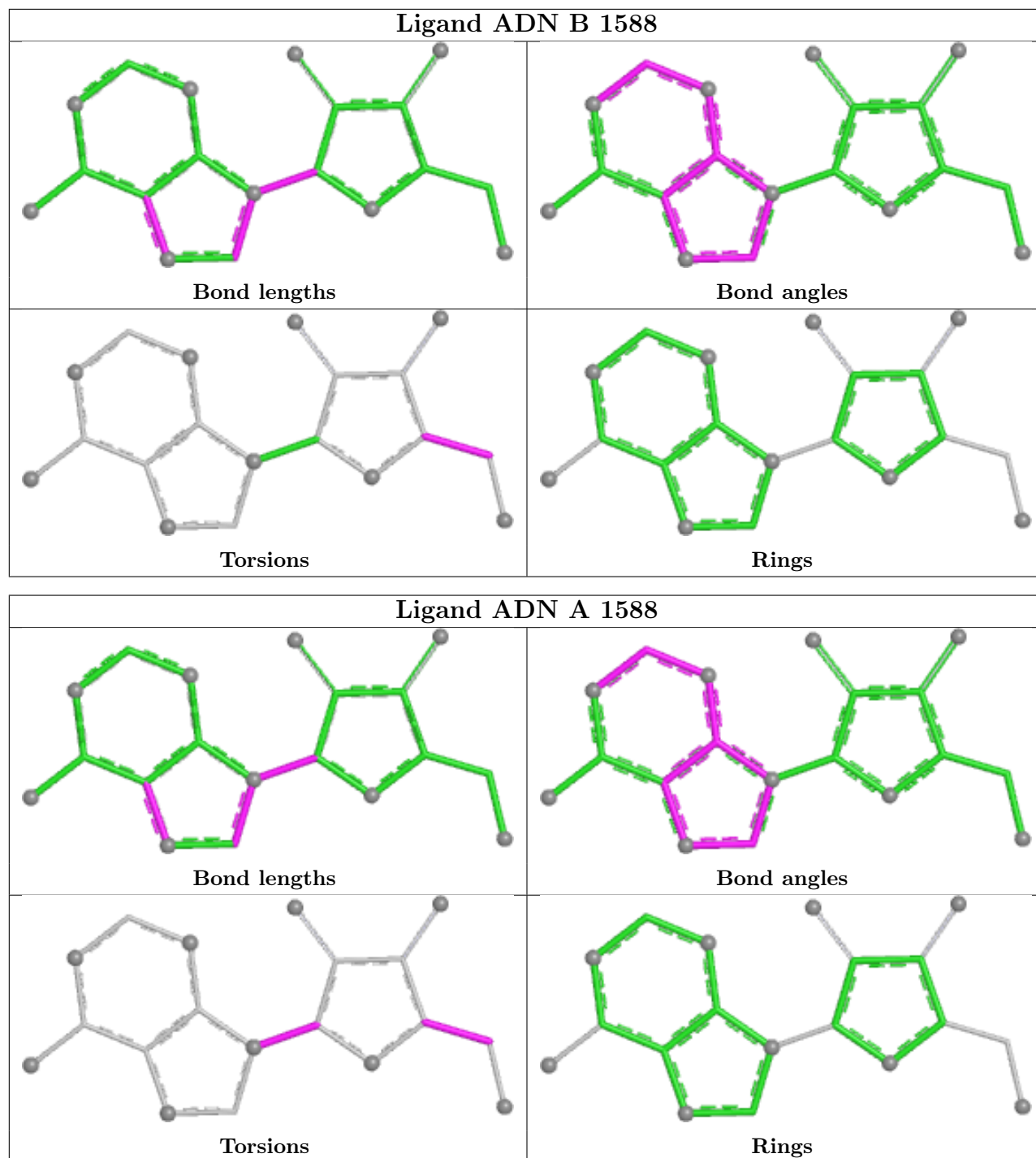
Mol	Chain	Res	Type	Atoms
4	B	1590	CIT	C2-C3-C4-C5
4	B	1590	CIT	O7-C3-C4-C5
4	B	1590	CIT	C6-C3-C4-C5
4	B	1590	CIT	C2-C3-C6-O5
4	B	1590	CIT	C2-C3-C6-O6

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1588	ADN	4	0
4	B	1590	CIT	1	0
3	B	1589	SO4	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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	574/620 (92%)	-0.14	6 (1%) 79 74	8, 20, 31, 38	0
1	B	577/620 (93%)	-0.03	9 (1%) 70 63	6, 20, 31, 46	2 (0%)
All	All	1151/1240 (92%)	-0.08	15 (1%) 75 69	6, 20, 31, 46	2 (0%)

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	571	ALA	6.3
1	B	304	VAL	5.9
1	B	144	VAL	5.4
1	A	571	ALA	4.5
1	A	482	ASP	4.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

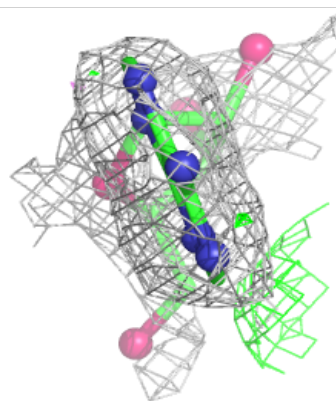
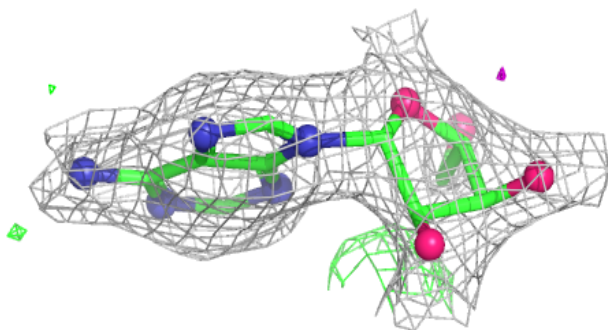
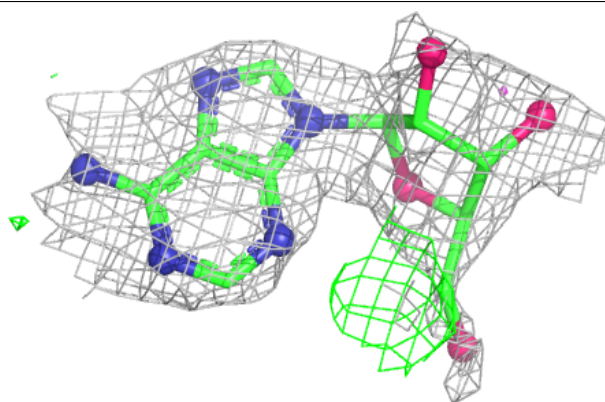
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADN	A	1588	19/19	0.86	0.12	42,43,45,46	0
2	ADN	B	1588	19/19	0.93	0.09	30,31,36,38	0
4	CIT	B	1590	13/13	0.93	0.08	16,29,32,33	0
3	SO4	A	1589	5/5	0.97	0.07	19,24,25,25	0
3	SO4	B	1589	5/5	0.98	0.06	18,21,22,22	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.

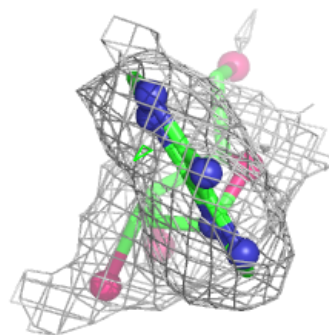
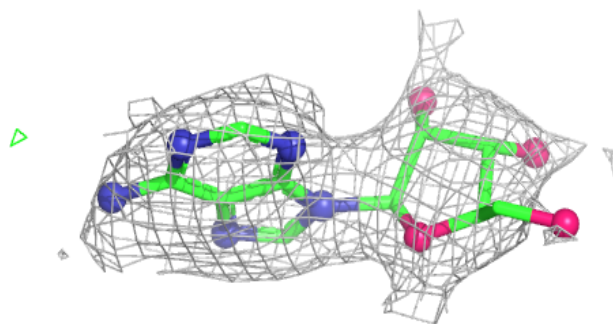
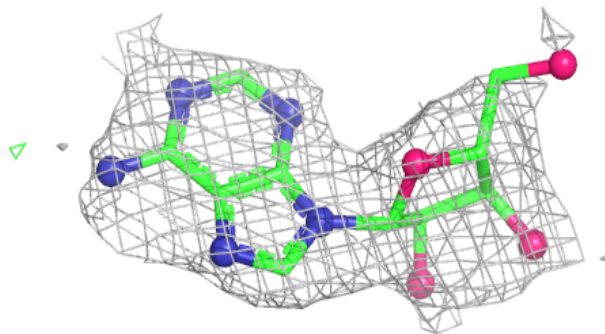
Electron density around ADN A 1588:

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 ADN B 1588:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.