



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:54 AM EDT

PDB ID : 2Q83 / pdb_00002q83
Title : Crystal structure of ytaA (2635576) from Bacillus subtilis at 2.50 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2007-06-08
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

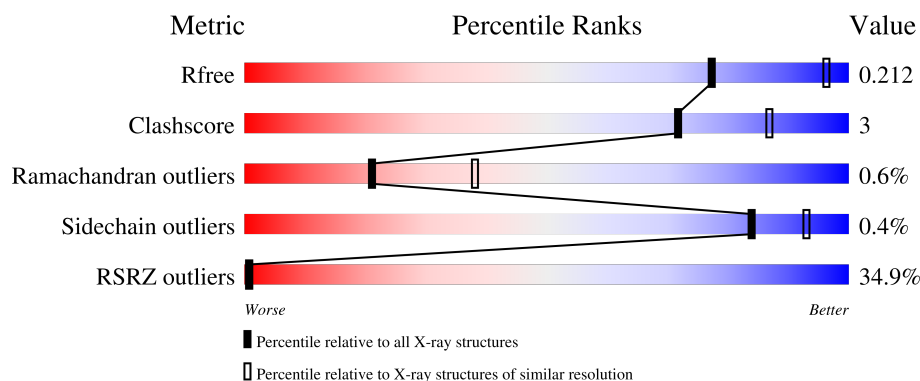
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	346	34% 87% 8% .
1	B	346	32% 88% 8% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5615 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.

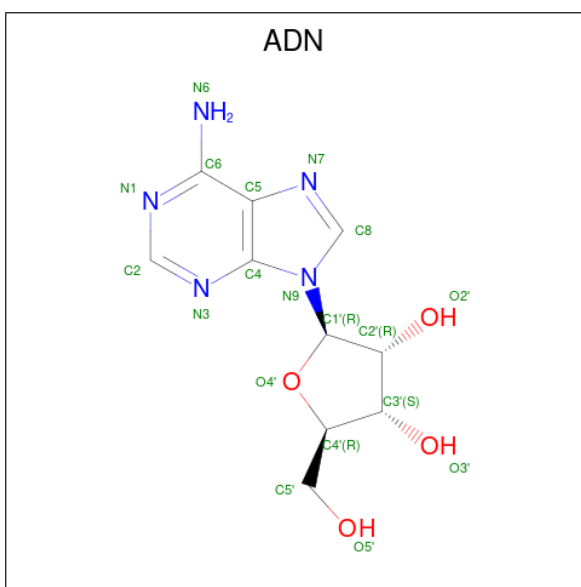
- Molecule 1 is a protein called YtaA protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	Se	0	2	0
			2657	1717	437	492	3	8			
1	B	332	Total	C	N	O	S	Se	0	2	0
			2658	1722	439	486	3	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLY	-	expression tag	UNP O34656
A	56	MSE	MET	modified residue	UNP O34656
A	96	MSE	MET	modified residue	UNP O34656
A	141	MSE	MET	modified residue	UNP O34656
A	180	MSE	MET	modified residue	UNP O34656
A	186	MSE	MET	modified residue	UNP O34656
A	273	MSE	MET	modified residue	UNP O34656
A	292	MSE	MET	modified residue	UNP O34656
A	310	MSE	MET	modified residue	UNP O34656
A	314	MSE	MET	modified residue	UNP O34656
B	12	GLY	-	expression tag	UNP O34656
B	56	MSE	MET	modified residue	UNP O34656
B	96	MSE	MET	modified residue	UNP O34656
B	141	MSE	MET	modified residue	UNP O34656
B	180	MSE	MET	modified residue	UNP O34656
B	186	MSE	MET	modified residue	UNP O34656
B	273	MSE	MET	modified residue	UNP O34656
B	292	MSE	MET	modified residue	UNP O34656
B	310	MSE	MET	modified residue	UNP O34656
B	314	MSE	MET	modified residue	UNP O34656

- Molecule 2 is ADENOSINE (CCD ID: ADN) (formula: C₁₀H₁₃N₅O₄).



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 UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			10	10		
3	B	1	Total	O	0	0
			10	10		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



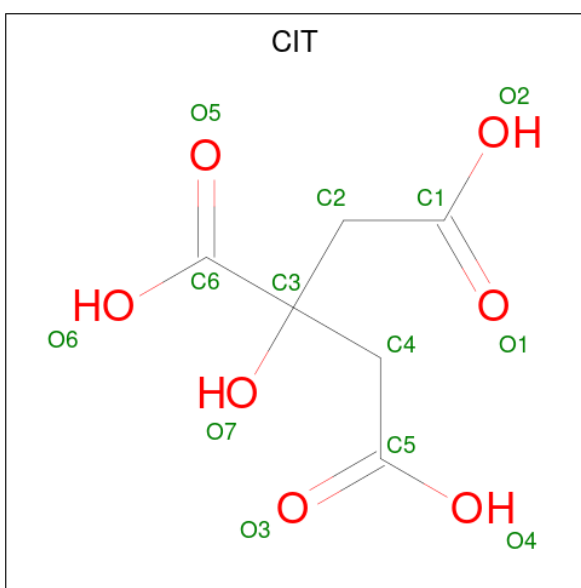
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

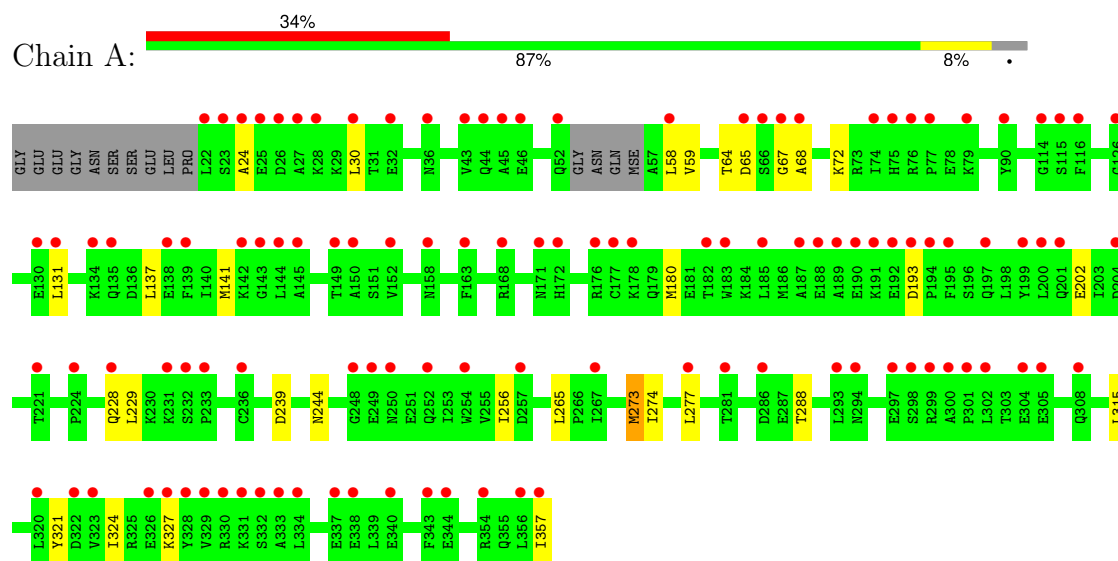
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	82	Total 82	O 82	0	0
7	B	105	Total 105	O 105	0	0

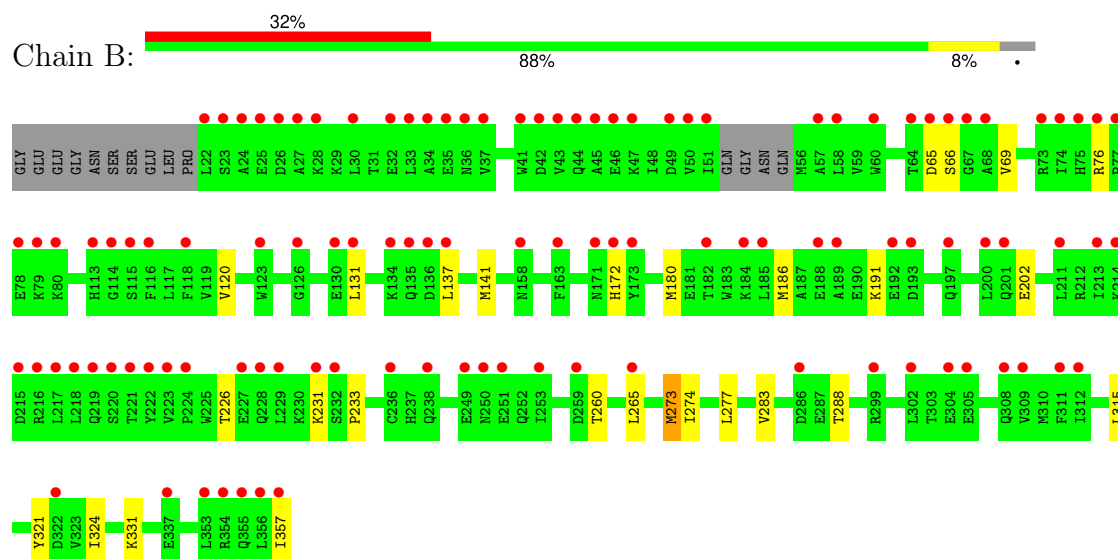
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: YtaA protein



• Molecule 1: YtaA protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	173.00Å 173.00Å 192.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.96 – 2.50 29.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.96-2.50) 99.9 (29.96-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.198 , 0.210 0.200 , 0.212	Depositor DCC
R_{free} test set	2988 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5615	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, UNL, EDO, 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	0.73	0/2712	1.06	4/3665 (0.1%)
1	B	0.72	0/2719	1.01	4/3671 (0.1%)
All	All	0.73	0/5431	1.03	8/7336 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	256	ILE	N-CA-C	13.87	123.73	111.81
1	B	274	ILE	N-CA-C	7.12	117.72	110.82
1	A	68	ALA	N-CA-C	6.55	120.15	110.46
1	B	202	GLU	N-CA-C	5.83	121.29	113.72
1	B	233	PRO	N-CA-C	5.47	120.90	111.77
1	B	191	LYS	N-CA-C	5.42	117.89	111.33
1	A	202	GLU	N-CA-C	5.39	120.73	113.72
1	A	274	ILE	N-CA-C	5.04	116.50	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2657	0	2570	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2658	0	2604	18	0
2	A	19	0	13	0	0
2	B	19	0	13	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	8	0	12	0	0
4	B	24	0	36	0	0
5	B	10	0	0	0	0
6	B	13	0	5	0	0
7	A	82	0	0	0	0
7	B	105	0	0	2	0
All	All	5615	0	5253	35	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 3.

All (35) 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:180:MSE:HE2	1:B:324:ILE:HD12	1.51	0.92
1:A:180:MSE:HE2	1:A:324:ILE:HD12	1.64	0.79
1:A:30:LEU:HD22	1:A:58:LEU:HD21	1.66	0.76
1:A:315:LEU:HD11	1:A:357:ILE:HD13	1.71	0.73
1:A:229:LEU:HD12	1:A:265:LEU:HD23	1.71	0.72
1:B:180:MSE:HE2	1:B:324:ILE:CD1	2.20	0.71
1:B:76:ARG:NH2	1:B:260:THR:HG22	2.06	0.69
1:B:315:LEU:HD11	1:B:357:ILE:HD13	1.78	0.65
1:B:172:HIS:ND1	7:B:461:HOH:O	2.30	0.65
1:B:137:LEU:HD21	1:B:288:THR:HG23	1.81	0.63
1:A:64:THR:OG1	1:A:67:GLY:O	2.16	0.62
1:B:180:MSE:HE3	1:B:321:TYR:HA	1.87	0.56
1:A:193:ASP:OD2	1:A:327:LYS:NZ	2.41	0.54
1:A:137:LEU:HD21	1:A:288:THR:HG23	1.89	0.54
1:A:141:MSE:HE1	1:A:273:MSE:HG2	1.91	0.52
1:B:131:LEU:HD13	1:B:277:LEU:HD13	1.93	0.50
1:B:69:VAL:CG1	1:B:120:VAL:HG13	2.43	0.49
1:B:226:THR:HG22	1:B:265:LEU:CD1	2.42	0.49
1:A:141:MSE:HA	1:A:141:MSE:HE2	1.95	0.48
1:B:226:THR:HG22	1:B:265:LEU:HD11	1.94	0.48
1:A:59:VAL:HG22	1:A:72:LYS:HG3	1.96	0.48
1:A:315:LEU:HD11	1:A:357:ILE:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:MSE:HE2	1:B:141:MSE:HA	1.97	0.46
1:A:228[A]:GLN:NE2	1:B:231:LYS:O	2.49	0.46
1:A:180:MSE:HE3	1:A:321:TYR:HB2	2.00	0.44
1:B:186:MSE:HE1	1:B:331:LYS:HE3	1.99	0.44
1:B:76:ARG:HH22	1:B:260:THR:HG22	1.81	0.44
1:A:239:ASP:O	1:A:244:ASN:ND2	2.51	0.43
1:B:141:MSE:HE1	1:B:273:MSE:HG2	2.01	0.43
1:A:315:LEU:CD1	1:A:357:ILE:HG21	2.48	0.42
1:A:131:LEU:HD13	1:A:277:LEU:HD13	2.02	0.42
1:A:229:LEU:HD12	1:A:265:LEU:CD2	2.47	0.41
1:B:283:VAL:HG22	7:B:442:HOH:O	2.20	0.41
1:B:315:LEU:CD1	1:B:357:ILE:HG21	2.50	0.41
1:A:273:MSE:HE3	1:A:273:MSE:HA	2.03	0.41

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	330/346 (95%)	321 (97%)	7 (2%)	2 (1%)	21	38
1	B	330/346 (95%)	318 (96%)	10 (3%)	2 (1%)	21	38
All	All	660/692 (95%)	639 (97%)	17 (3%)	4 (1%)	21	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	ALA
1	A	65	ASP
1	B	66	SER
1	B	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	273/298 (92%)	272 (100%)	1 (0%)	84	93
1	B	276/298 (93%)	275 (100%)	1 (0%)	84	93
All	All	549/596 (92%)	547 (100%)	2 (0%)	84	93

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

Mol	Chain	Res	Type
1	A	273	MSE
1	B	273	MSE

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

Mol	Chain	Res	Type
1	A	97	ASN
1	A	179	GLN
1	A	252	GLN
1	B	158	ASN
1	B	171	ASN
1	B	197	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 2 are unknown - leaving 13 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	EDO	B	358	-	3,3,3	0.49	0	2,2,2	0.28	0
4	EDO	A	358	-	3,3,3	0.52	0	2,2,2	0.13	0
4	EDO	B	9	-	3,3,3	0.47	0	2,2,2	0.19	0
5	SO4	B	6	-	4,4,4	0.19	0	6,6,6	0.20	0
4	EDO	A	8	-	3,3,3	0.43	0	2,2,2	0.33	0
4	EDO	B	11	-	3,3,3	0.40	0	2,2,2	0.48	0
5	SO4	B	7	-	4,4,4	0.25	0	6,6,6	0.12	0
6	CIT	B	3	-	12,12,12	1.09	0	17,17,17	1.99	7 (41%)
2	ADN	B	2	-	21,21,21	1.63	3 (14%)	31,31,31	2.14	9 (29%)
4	EDO	B	359	-	3,3,3	0.51	0	2,2,2	0.26	0
4	EDO	B	360	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	B	10	-	3,3,3	0.48	0	2,2,2	0.27	0
2	ADN	A	1	-	21,21,21	1.72	4 (19%)	31,31,31	2.26	14 (45%)

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	EDO	B	358	-	-	1/1/1/1	-
4	EDO	A	358	-	-	0/1/1/1	-
4	EDO	B	9	-	-	1/1/1/1	-
4	EDO	A	8	-	-	1/1/1/1	-
4	EDO	B	11	-	-	1/1/1/1	-
6	CIT	B	3	-	-	5/16/16/16	-
2	ADN	B	2	-	-	2/6/22/22	0/3/3/3
4	EDO	B	359	-	-	0/1/1/1	-
4	EDO	B	360	-	-	0/1/1/1	-
4	EDO	B	10	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADN	A	1	-	-	2/6/22/22	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	ADN	C5-C4	5.06	1.48	1.39
2	B	2	ADN	C5-C4	4.82	1.47	1.39
2	B	2	ADN	C5-C6	3.47	1.50	1.41
2	A	1	ADN	C5-C6	3.45	1.50	1.41
2	A	1	ADN	C8-N7	3.25	1.37	1.31
2	B	2	ADN	C8-N7	2.83	1.37	1.31
2	A	1	ADN	C4-N9	-2.13	1.33	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	ADN	C5-C4-N3	-5.87	118.64	126.72
2	A	1	ADN	C4-C5-N7	-5.02	104.84	110.58
2	A	1	ADN	C5-C4-N3	-4.75	120.18	126.72
2	B	2	ADN	C4-C5-N7	-4.53	105.40	110.58
2	A	1	ADN	O4'-C1'-N9	4.19	116.14	108.09
2	B	2	ADN	N3-C4-N9	3.96	133.90	127.17
2	B	2	ADN	C2-N3-C4	3.89	121.32	111.83
2	A	1	ADN	C6-C5-N7	3.70	139.22	132.09
2	A	1	ADN	C2-N3-C4	3.43	120.20	111.83
6	B	3	CIT	O6-C6-C3	3.38	119.63	113.14
6	B	3	CIT	O7-C3-C4	-3.33	101.78	109.38
2	A	1	ADN	C5-N7-C8	3.13	108.38	103.45
2	B	2	ADN	C5-N7-C8	3.12	108.36	103.45
2	B	2	ADN	C6-C5-N7	2.96	137.80	132.09
2	A	1	ADN	C4-N9-C1'	-2.84	119.99	126.63
2	B	2	ADN	N3-C2-N1	-2.81	124.33	128.58
6	B	3	CIT	O4-C5-C4	2.78	123.15	114.35
2	A	1	ADN	N3-C2-N1	-2.63	124.60	128.58
2	B	2	ADN	C4-N9-C8	2.57	108.43	105.74
2	B	2	ADN	N9-C8-N7	-2.53	110.35	113.94
2	A	1	ADN	N9-C8-N7	-2.51	110.38	113.94
2	A	1	ADN	N3-C4-N9	2.48	131.38	127.17
2	A	1	ADN	C5-C4-N9	2.41	108.44	105.81
6	B	3	CIT	O2-C1-C2	2.40	121.95	114.35
6	B	3	CIT	O4-C5-O3	-2.25	117.53	123.33
6	B	3	CIT	O6-C6-O5	-2.23	116.73	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ADN	C1'-N9-C8	2.23	132.03	127.09
6	B	3	CIT	O7-C3-C6	-2.15	105.91	108.96
2	A	1	ADN	C4-N9-C8	2.13	107.97	105.74
2	A	1	ADN	C4'-O4'-C1'	-2.11	104.81	109.47

There are no chirality outliers.

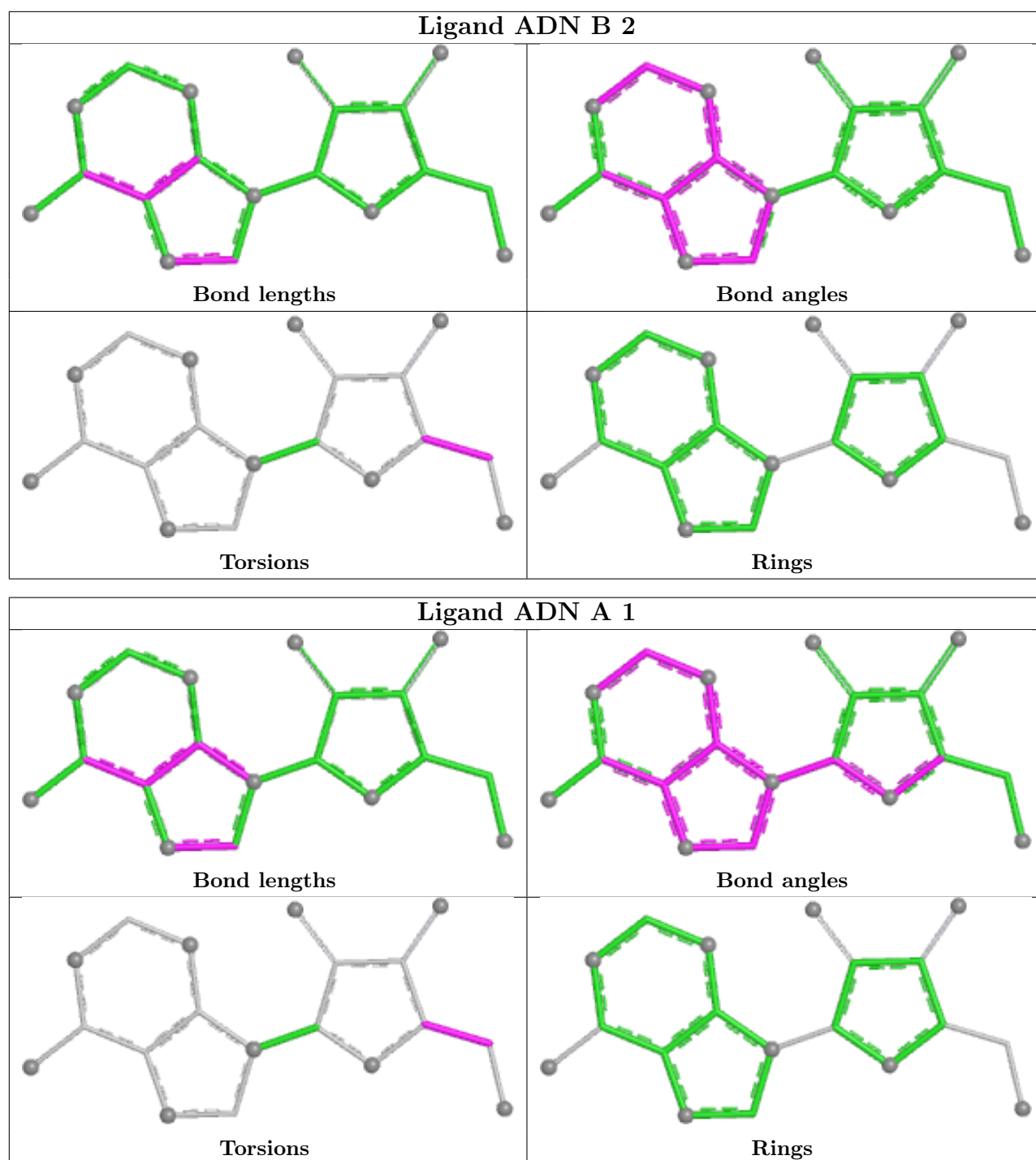
All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	ADN	O4'-C4'-C5'-O5'
6	B	3	CIT	C2-C3-C6-O5
6	B	3	CIT	C2-C3-C6-O6
6	B	3	CIT	O7-C3-C6-O5
6	B	3	CIT	O7-C3-C6-O6
2	A	1	ADN	C3'-C4'-C5'-O5'
2	B	2	ADN	O4'-C4'-C5'-O5'
2	B	2	ADN	C3'-C4'-C5'-O5'
4	B	9	EDO	O1-C1-C2-O2
4	B	11	EDO	O1-C1-C2-O2
6	B	3	CIT	O7-C3-C4-C5
4	B	358	EDO	O1-C1-C2-O2
4	A	8	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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

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(Å ²)	Q<0.9
1	A	324/346 (93%)	1.78	116 (35%)  	26, 48, 65, 78	2 (0%)
1	B	323/346 (93%)	1.72	110 (34%)  	26, 48, 65, 83	2 (0%)
All	All	647/692 (93%)	1.75	226 (34%)  	26, 48, 65, 83	4 (0%)

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	ASP	8.1
1	A	52	GLN	6.5
1	A	75	HIS	6.4
1	B	22	LEU	6.3
1	B	24	ALA	6.3
1	B	26	ASP	6.2
1	B	75	HIS	6.2
1	A	22	LEU	5.6
1	B	57	ALA	5.6
1	A	26	ASP	5.6
1	B	66	SER	5.4
1	A	189	ALA	5.2
1	B	67	GLY	5.1
1	A	329	VAL	5.1
1	A	231	LYS	4.9
1	A	66	SER	4.9
1	A	194	PRO	4.8
1	B	228[A]	GLN	4.8
1	A	65	ASP	4.8
1	A	331	LYS	4.8
1	B	44	GLN	4.7
1	B	43	VAL	4.4
1	A	77	PRO	4.4
1	A	228[A]	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	300	ALA	4.4
1	B	115	SER	4.4
1	A	46	GLU	4.4
1	A	25	GLU	4.3
1	B	25	GLU	4.3
1	A	328	TYR	4.1
1	A	301	PRO	4.0
1	B	163	PHE	4.0
1	A	116	PHE	3.8
1	A	185	LEU	3.8
1	B	305	GLU	3.8
1	B	23	SER	3.8
1	A	183	TRP	3.8
1	B	113	HIS	3.8
1	A	299	ARG	3.8
1	A	182	THR	3.7
1	A	67	GLY	3.7
1	A	36	ASN	3.7
1	B	77	PRO	3.7
1	B	116	PHE	3.7
1	B	64	THR	3.6
1	A	44	GLN	3.6
1	A	172	HIS	3.5
1	B	27	ALA	3.5
1	A	23	SER	3.5
1	A	24	ALA	3.5
1	A	332	SER	3.5
1	A	188	GLU	3.4
1	A	297	GLU	3.4
1	B	35	GLU	3.4
1	A	192	GLU	3.3
1	A	115	SER	3.3
1	A	130	GLU	3.3
1	B	304	GLU	3.3
1	B	76	ARG	3.3
1	B	216	ARG	3.3
1	B	36	ASN	3.2
1	B	217	LEU	3.2
1	A	142	LYS	3.2
1	B	28	LYS	3.2
1	A	58	LEU	3.2
1	B	309	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	193	ASP	3.1
1	A	201	GLN	3.1
1	B	45	ALA	3.1
1	B	42	ASP	3.1
1	A	327	LYS	3.0
1	B	355	GLN	3.0
1	B	222	TYR	3.0
1	A	294	ASN	3.0
1	A	135	GLN	3.0
1	B	197	GLN	3.0
1	A	191	LYS	2.9
1	B	47	LYS	2.9
1	B	37	VAL	2.9
1	B	229	LEU	2.9
1	A	250	ASN	2.9
1	B	33	LEU	2.9
1	B	32	GLU	2.9
1	B	357	ILE	2.9
1	A	76	ARG	2.9
1	B	221	THR	2.9
1	B	220	SER	2.8
1	A	149	THR	2.8
1	B	188	GLU	2.8
1	B	30	LEU	2.8
1	B	302	LEU	2.8
1	B	312	ILE	2.8
1	B	265	LEU	2.8
1	A	252	GLN	2.8
1	B	201	GLN	2.8
1	A	176	ARG	2.8
1	B	259	ASP	2.8
1	B	172	HIS	2.8
1	B	123	TRP	2.8
1	A	68	ALA	2.8
1	B	231	LYS	2.8
1	A	200	LEU	2.7
1	A	305	GLU	2.7
1	B	219	GLN	2.7
1	A	286	ASP	2.7
1	B	46	GLU	2.7
1	A	293	LEU	2.7
1	B	218	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	333	ALA	2.7
1	B	73	ARG	2.7
1	B	308	GLN	2.7
1	A	171	ASN	2.7
1	A	320	LEU	2.7
1	A	114	GLY	2.6
1	B	126	GLY	2.6
1	B	158	ASN	2.6
1	B	356	LEU	2.6
1	A	74	ILE	2.6
1	A	330[A]	ARG	2.6
1	A	178	LYS	2.6
1	B	171	ASN	2.6
1	A	199	TYR	2.6
1	B	60	TRP	2.6
1	B	50	VAL	2.6
1	A	298	SER	2.6
1	B	232	SER	2.6
1	A	354	ARG	2.5
1	A	138	GLU	2.5
1	B	182	THR	2.5
1	B	354	ARG	2.5
1	A	248	GLY	2.5
1	B	213	ILE	2.5
1	B	185	LEU	2.5
1	B	214	LYS	2.5
1	B	223	VAL	2.5
1	A	322	ASP	2.5
1	A	152	VAL	2.5
1	B	34	ALA	2.4
1	B	224	PRO	2.4
1	A	249	GLU	2.4
1	A	334	LEU	2.4
1	A	131	LEU	2.4
1	A	43	VAL	2.4
1	A	45	ALA	2.4
1	A	326	GLU	2.4
1	B	227	GLU	2.4
1	B	251	GLU	2.4
1	A	168	ARG	2.4
1	B	135	GLN	2.4
1	B	80	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	74	ILE	2.3
1	B	236	CYS	2.3
1	B	173	TYR	2.3
1	A	28	LYS	2.3
1	A	126	GLY	2.3
1	A	302	LEU	2.3
1	B	200	LEU	2.3
1	A	195	PHE	2.3
1	A	236	CYS	2.3
1	B	189	ALA	2.3
1	B	238	GLN	2.3
1	A	257	ASP	2.3
1	A	79	LYS	2.3
1	B	78	GLU	2.3
1	A	150	ALA	2.3
1	A	254	TRP	2.3
1	A	267	ILE	2.3
1	A	357	ILE	2.3
1	A	27	ALA	2.2
1	B	250	ASN	2.2
1	A	197	GLN	2.2
1	A	134	LYS	2.2
1	B	353	LEU	2.2
1	A	187	ALA	2.2
1	B	58	LEU	2.2
1	B	211	LEU	2.2
1	B	337	GLU	2.2
1	B	118	PHE	2.2
1	B	79	LYS	2.2
1	A	277	LEU	2.2
1	A	356	LEU	2.2
1	A	337	GLU	2.2
1	A	338	GLU	2.2
1	A	340	GLU	2.2
1	B	192	GLU	2.2
1	A	163	PHE	2.2
1	A	343	PHE	2.2
1	B	68	ALA	2.2
1	A	90	TYR	2.2
1	B	114	GLY	2.2
1	B	131	LEU	2.2
1	A	232	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	32	GLU	2.2
1	A	344	GLU	2.2
1	B	49	ASP	2.2
1	B	249	GLU	2.2
1	A	224	PRO	2.2
1	B	311	PHE	2.2
1	A	323	VAL	2.1
1	A	143	GLY	2.1
1	A	177	CYS	2.1
1	B	136	ASP	2.1
1	A	139	PHE	2.1
1	B	41	TRP	2.1
1	A	158	ASN	2.1
1	A	144	LEU	2.1
1	A	281	THR	2.1
1	B	299	ARG	2.1
1	B	184	LYS	2.1
1	A	145	ALA	2.1
1	A	30	LEU	2.1
1	A	221	THR	2.1
1	A	190	GLU	2.1
1	B	130	GLU	2.1
1	A	204	ASP	2.1
1	B	322	ASP	2.1
1	A	308	GLN	2.1
1	B	51	ILE	2.1
1	B	134	LYS	2.1
1	B	193	ASP	2.1
1	B	286	ASP	2.1
1	B	137	LEU	2.0
1	A	304	GLU	2.0
1	B	253	ILE	2.0
1	B	215	ASP	2.0
1	A	233	PRO	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

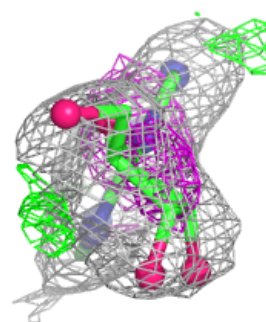
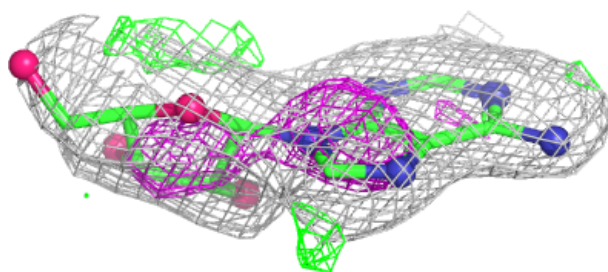
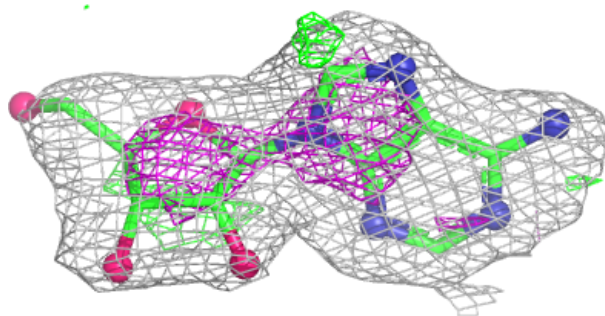
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UNL	A	5	10/-	0.51	0.24	75,104,112,113	0
4	EDO	B	360	4/4	0.53	0.38	91,92,94,94	0
5	SO4	B	6	5/5	0.57	0.27	65,66,68,70	5
6	CIT	B	3	13/13	0.58	0.26	90,101,105,105	0
4	EDO	B	10	4/4	0.61	0.36	80,86,86,87	0
3	UNL	B	4	10/-	0.72	0.19	79,82,92,94	0
2	ADN	A	1	19/19	0.74	0.23	60,67,88,91	0
2	ADN	B	2	19/19	0.74	0.23	76,80,96,97	0
4	EDO	B	358	4/4	0.76	0.35	63,74,76,76	0
5	SO4	B	7	5/5	0.79	0.24	55,55,58,59	5
4	EDO	B	9	4/4	0.79	0.25	72,77,79,82	0
4	EDO	A	358	4/4	0.80	0.34	74,79,80,83	0
4	EDO	B	359	4/4	0.80	0.28	73,78,79,79	0
4	EDO	A	8	4/4	0.81	0.21	74,77,78,79	0
4	EDO	B	11	4/4	0.81	0.32	61,63,67,70	0

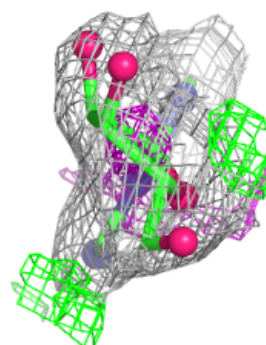
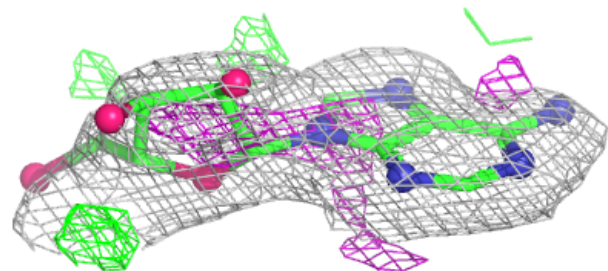
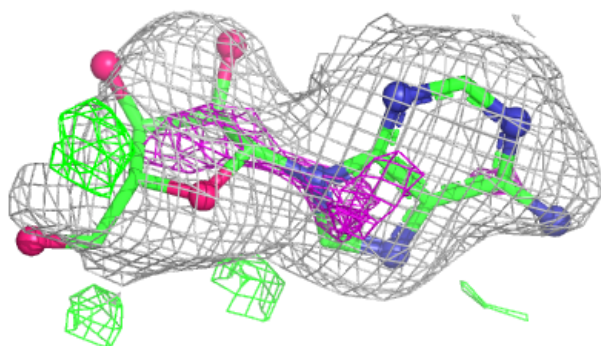
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADN A 1:

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

**Electron density around ADN B 2:**

$2mF_o-DF_c$ (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.