wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 12:54 PM BST

PDB ID	:	5LW1
Title	:	Crystal structure of DARPin-DARPin rigid fusion, variant DD_232_11_D12 in complex JNK1a1 and JIP1 peptide
Authors	:	Wu, Y.; Batyuk, A.; Mittl, P.R.; Honegger, A.; Plueckthun, A.
Deposited on	:	2016-09-15
Resolution	:	3.20 Å(reported)

The following versions of software and data (see references ①) were used in the production of this report:

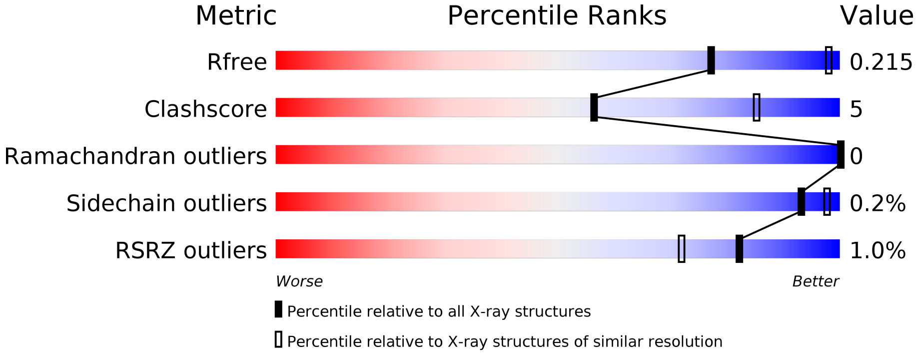
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	326	
1	D	326	
1	G	326	
2	B	373	
2	E	373	
2	H	373	

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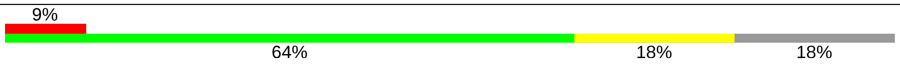
Mol	Chain	Length	Quality of chain
3	C	11	
3	F	11	
3	I	11	
4	L	6	

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
5	SO4	A	402	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16279 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 DD_232_11_D12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2441	1544	435	460	2	0	0	0
1	D	313	2381	1509	418	452	2	0	0	0
1	G	314	2386	1512	419	453	2	0	0	0

- Molecule 2 is a protein called Mitogen-activated protein kinase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	355	2873	1843	484	524	22	0	0	0
2	E	355	2873	1843	484	524	22	0	0	0
2	H	355	2873	1843	484	524	22	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP P45983
B	-8	ARG	-	expression tag	UNP P45983
B	-7	GLY	-	expression tag	UNP P45983
B	-6	SER	-	expression tag	UNP P45983
B	-5	HIS	-	expression tag	UNP P45983
B	-4	HIS	-	expression tag	UNP P45983
B	-3	HIS	-	expression tag	UNP P45983
B	-2	HIS	-	expression tag	UNP P45983
B	-1	HIS	-	expression tag	UNP P45983
B	0	HIS	-	expression tag	UNP P45983
B	1	GLY	-	expression tag	UNP P45983
E	-9	MET	-	initiating methionine	UNP P45983

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	ARG	-	expression tag	UNP P45983
E	-7	GLY	-	expression tag	UNP P45983
E	-6	SER	-	expression tag	UNP P45983
E	-5	HIS	-	expression tag	UNP P45983
E	-4	HIS	-	expression tag	UNP P45983
E	-3	HIS	-	expression tag	UNP P45983
E	-2	HIS	-	expression tag	UNP P45983
E	-1	HIS	-	expression tag	UNP P45983
E	0	HIS	-	expression tag	UNP P45983
E	1	GLY	-	expression tag	UNP P45983
H	-9	MET	-	initiating methionine	UNP P45983
H	-8	ARG	-	expression tag	UNP P45983
H	-7	GLY	-	expression tag	UNP P45983
H	-6	SER	-	expression tag	UNP P45983
H	-5	HIS	-	expression tag	UNP P45983
H	-4	HIS	-	expression tag	UNP P45983
H	-3	HIS	-	expression tag	UNP P45983
H	-2	HIS	-	expression tag	UNP P45983
H	-1	HIS	-	expression tag	UNP P45983
H	0	HIS	-	expression tag	UNP P45983
H	1	GLY	-	expression tag	UNP P45983

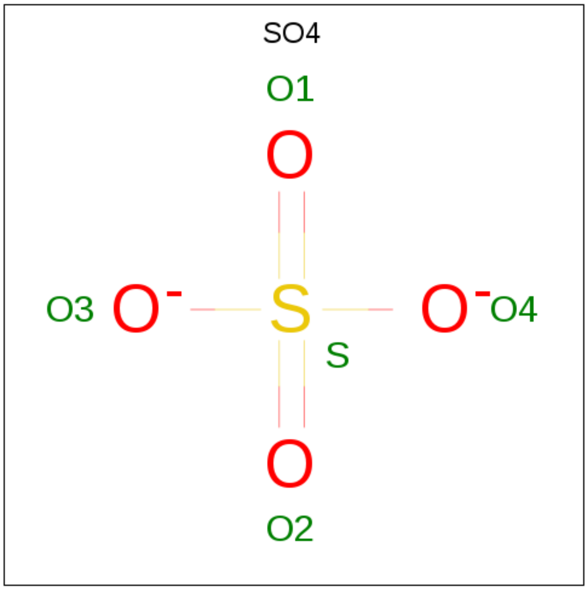
- Molecule 3 is a protein called C-Jun-amino-terminal kinase-interacting protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total 72	C 46	N 14	O 12	0	0	0
3	F	9	Total 72	C 46	N 14	O 12	0	0	0
3	I	10	Total 83	C 55	N 15	O 13	0	0	0

- Molecule 4 is a protein called Pepstatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	L	6	Total 48	C 34	N 5	O 9	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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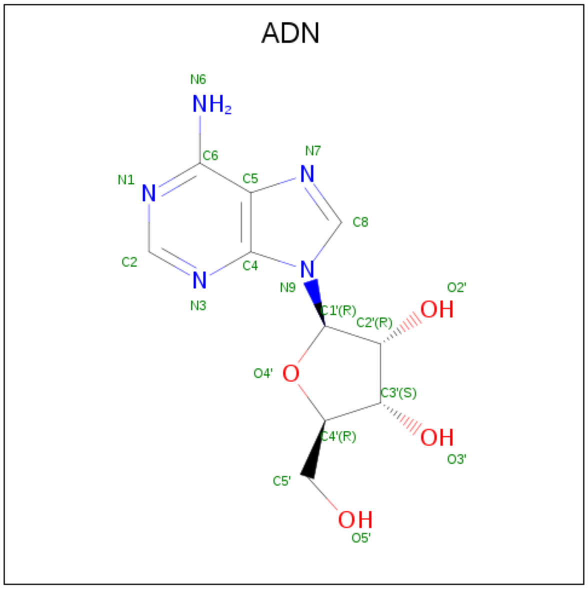
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0

- Molecule 6 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).



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

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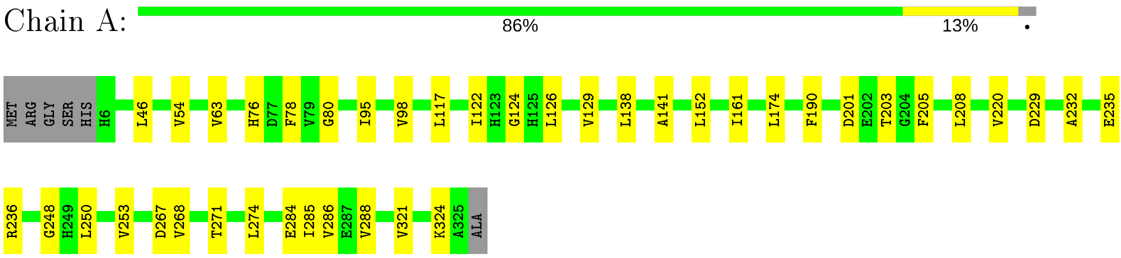
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C N O 19 10 5 4	0	0
6	H	1	Total C N O 19 10 5 4	0	0

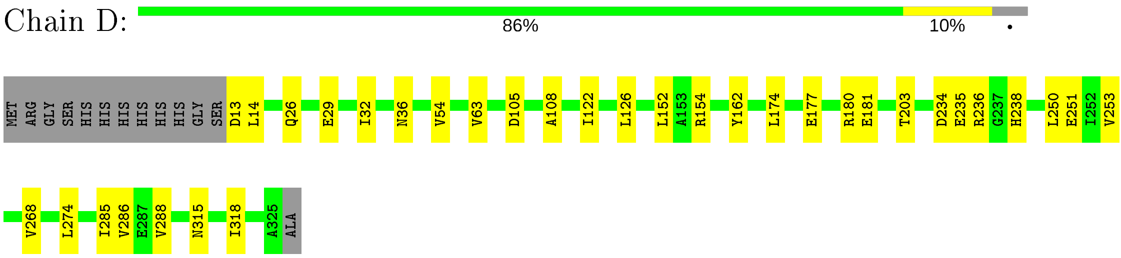
3 Residue-property plots ⓘ

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

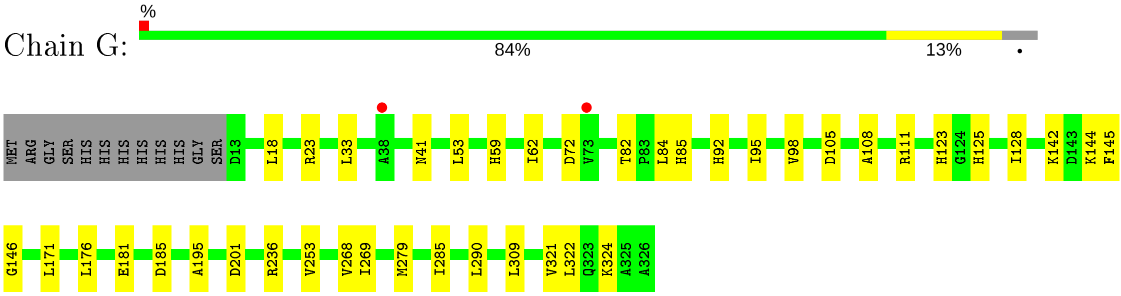
- Molecule 1: DD_232_11_D12



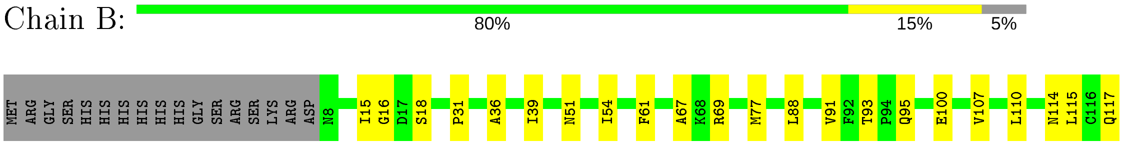
- Molecule 1: DD_232_11_D12

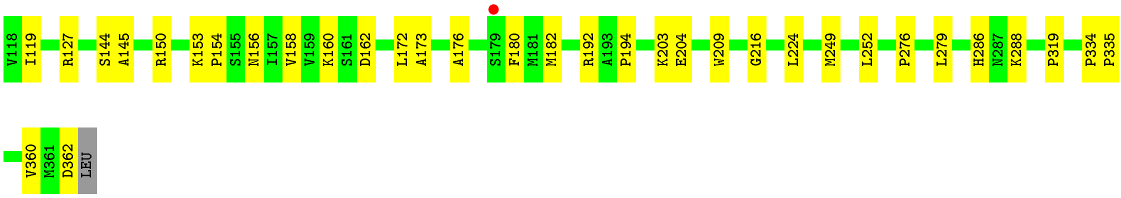


- Molecule 1: DD_232_11_D12



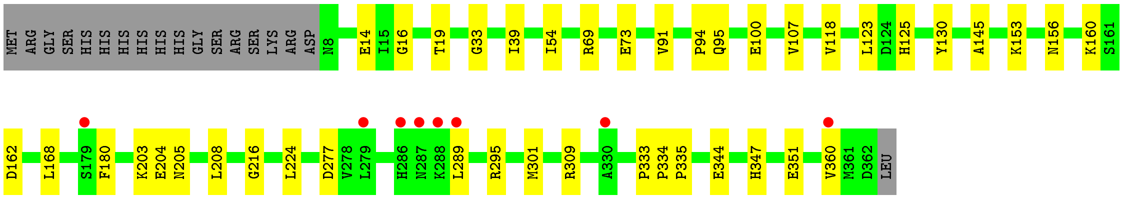
- Molecule 2: Mitogen-activated protein kinase 8





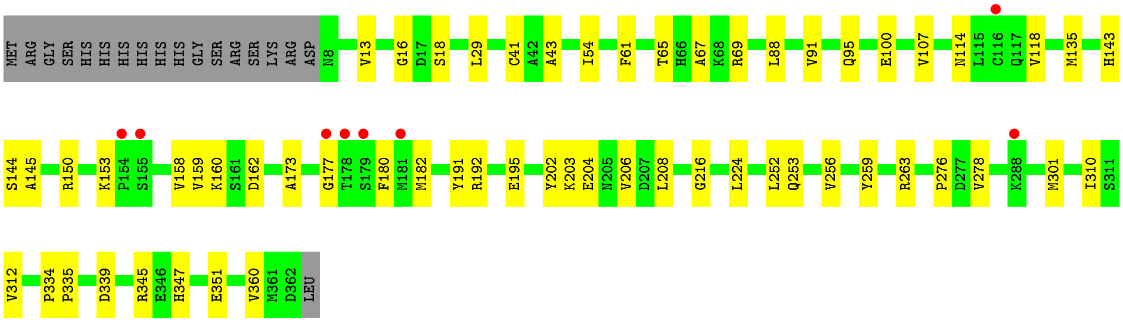
- Molecule 2: Mitogen-activated protein kinase 8

Chain E:



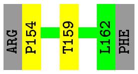
- Molecule 2: Mitogen-activated protein kinase 8

Chain H:



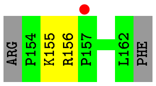
- Molecule 3: C-Jun-amino-terminal kinase-interacting protein 1

Chain C:



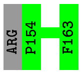
- Molecule 3: C-Jun-amino-terminal kinase-interacting protein 1

Chain F:



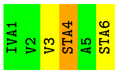
- Molecule 3: C-Jun-amino-terminal kinase-interacting protein 1

Chain I:



- Molecule 4: Pepstatin

Chain L:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	219.99Å 141.76Å 119.85Å 90.00° 97.83° 90.00°	Depositor
Resolution (Å)	49.38 – 3.20 49.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.38-3.20) 97.4 (49.38-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.175 , 0.212 0.177 , 0.215	Depositor DCC
R_{free} test set	3883 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	117.5	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 69.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16279	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.23	0/2486	0.39	0/3375
1	D	0.24	0/2421	0.40	0/3287
1	G	0.23	0/2426	0.39	0/3294
2	B	0.24	0/2939	0.41	0/3976
2	E	0.24	0/2939	0.41	0/3976
2	H	0.24	0/2939	0.42	0/3976
3	C	0.21	0/73	0.50	0/98
3	F	0.20	0/73	0.51	0/98
3	I	0.27	0/85	0.50	0/114
4	L	0.13	0/17	0.35	0/21
All	All	0.24	0/16398	0.41	0/22215

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
4	L	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L	3	VAL	Mainchain
4	L	4	STA	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2441	0	2434	24	0
1	D	2381	0	2391	22	0
1	G	2386	0	2396	26	0
2	B	2873	0	2889	34	0
2	E	2873	0	2889	26	0
2	H	2873	0	2889	37	0
3	C	72	0	82	2	0
3	F	72	0	82	2	0
3	I	83	0	91	0	0
4	L	48	0	60	2	0
5	A	10	0	0	0	0
5	B	25	0	0	1	0
5	D	20	0	0	0	0
5	E	20	0	0	0	0
5	G	20	0	0	0	0
5	H	20	0	0	2	0
5	I	5	0	0	0	0
6	B	19	0	13	1	0
6	E	19	0	13	1	0
6	H	19	0	13	0	0
All	All	16279	0	16242	161	0

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

The worst 5 of 161 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)
2:H:202:TYR:HB2	2:H:206:VAL:HG21	1.54	0.89
2:B:77:MET:HG3	2:B:88:LEU:HB2	1.66	0.78
1:G:82:THR:HG22	1:G:84:LEU:H	1.52	0.73
2:E:277:ASP:OD1	2:E:295:ARG:NH2	2.26	0.69
2:H:150:ARG:NH1	2:H:177:GLY:O	2.26	0.69

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/326 (98%)	311 (98%)	7 (2%)	0	100	100
1	D	311/326 (95%)	304 (98%)	7 (2%)	0	100	100
1	G	312/326 (96%)	305 (98%)	7 (2%)	0	100	100
2	B	353/373 (95%)	342 (97%)	11 (3%)	0	100	100
2	E	353/373 (95%)	342 (97%)	11 (3%)	0	100	100
2	H	353/373 (95%)	344 (98%)	9 (2%)	0	100	100
3	C	7/11 (64%)	7 (100%)	0	0	100	100
3	F	7/11 (64%)	7 (100%)	0	0	100	100
3	I	8/11 (73%)	8 (100%)	0	0	100	100
4	L	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
All	All	2025/2136 (95%)	1972 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	251/255 (98%)	251 (100%)	0	100	100
1	D	245/255 (96%)	245 (100%)	0	100	100
1	G	245/255 (96%)	244 (100%)	1 (0%)	91	95
2	B	319/335 (95%)	318 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	319/335 (95%)	319 (100%)	0	100	100
2	H	319/335 (95%)	317 (99%)	2 (1%)	86	94
3	C	9/11 (82%)	9 (100%)	0	100	100
3	F	9/11 (82%)	9 (100%)	0	100	100
3	I	10/11 (91%)	10 (100%)	0	100	100
4	L	2/2 (100%)	2 (100%)	0	100	100
All	All	1728/1805 (96%)	1724 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	ASP
1	G	185	ASP
2	H	65	THR
2	H	253	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	69	ASN
1	G	238	HIS
2	E	134	GLN
2	B	293	GLN
1	G	41	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\#\|Z\| > 2$
4	STA	L	6	4	8,11,11	0.64	0	7,14,14	0.85	0
4	STA	L	4	4	10,10,11	0.74	0	9,12,14	1.38	1 (11%)

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	STA	L	6	4	-	4/10/12/12	-
4	STA	L	4	4	-	2/11/11/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	4	STA	CG-CB-CA	-2.79	109.81	115.82

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	6	STA	N-CA-CB-CG
4	L	6	STA	N-CA-CH-OH
4	L	6	STA	N-CA-CH-CM
4	L	4	STA	CA-CB-CG-CD1
4	L	4	STA	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	6	STA	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

27 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	$\#\|Z\| > 2$
5	SO4	A	402	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	B	405	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	B	402	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	I	201	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	D	403	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	E	403	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	D	404	-	4,4,4	0.14	0	6,6,6	0.05	0
6	ADN	E	401	-	18,21,21	1.66	3 (16%)	18,31,31	3.31	5 (27%)
5	SO4	B	406	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	D	402	-	4,4,4	0.14	0	6,6,6	0.05	0
6	ADN	B	401	-	18,21,21	1.68	3 (16%)	18,31,31	3.20	3 (16%)
5	SO4	H	402	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	E	405	-	4,4,4	0.14	0	6,6,6	0.05	0
6	ADN	H	401	-	18,21,21	1.67	3 (16%)	18,31,31	3.25	3 (16%)
5	SO4	G	403	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	G	404	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	404	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	G	402	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	401	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	H	404	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	H	403	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	G	401	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	D	401	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	E	404	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	H	405	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	E	402	-	4,4,4	0.15	0	6,6,6	0.04	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
6	ADN	H	401	-	-	0/2/22/22	0/3/3/3
6	ADN	B	401	-	-	2/2/22/22	0/3/3/3
6	ADN	E	401	-	-	2/2/22/22	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	401	ADN	C6-N6	4.70	1.51	1.34
6	H	401	ADN	C6-N6	4.69	1.51	1.34
6	E	401	ADN	C6-N6	4.66	1.51	1.34
6	B	401	ADN	C4-N3	-3.25	1.31	1.35
6	H	401	ADN	C4-N3	-3.23	1.31	1.35

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	401	ADN	C5-C6-N6	10.27	135.96	120.35
6	B	401	ADN	C5-C6-N6	10.16	135.79	120.35
6	E	401	ADN	C5-C6-N6	10.11	135.72	120.35
6	H	401	ADN	N6-C6-N1	-6.93	104.19	118.57
6	E	401	ADN	N6-C6-N1	-6.90	104.24	118.57

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	401	ADN	O4'-C4'-C5'-O5'
6	B	401	ADN	C3'-C4'-C5'-O5'
6	E	401	ADN	O4'-C4'-C5'-O5'
6	E	401	ADN	C3'-C4'-C5'-O5'

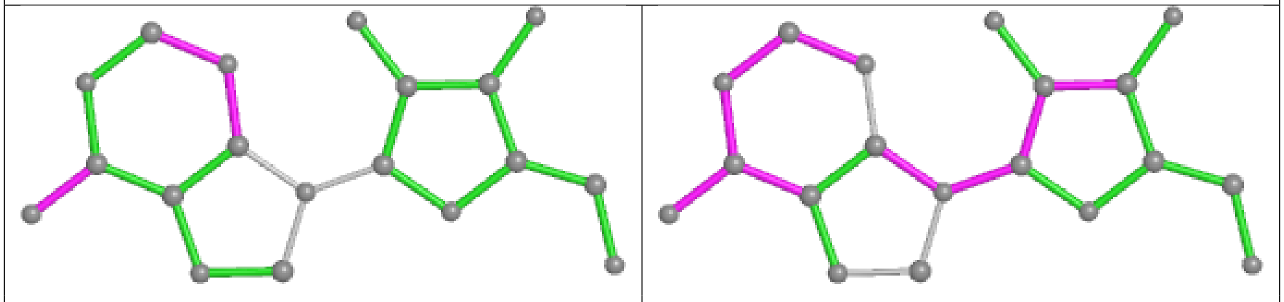
There are no ring outliers.

5 monomers are involved in 5 short contacts:

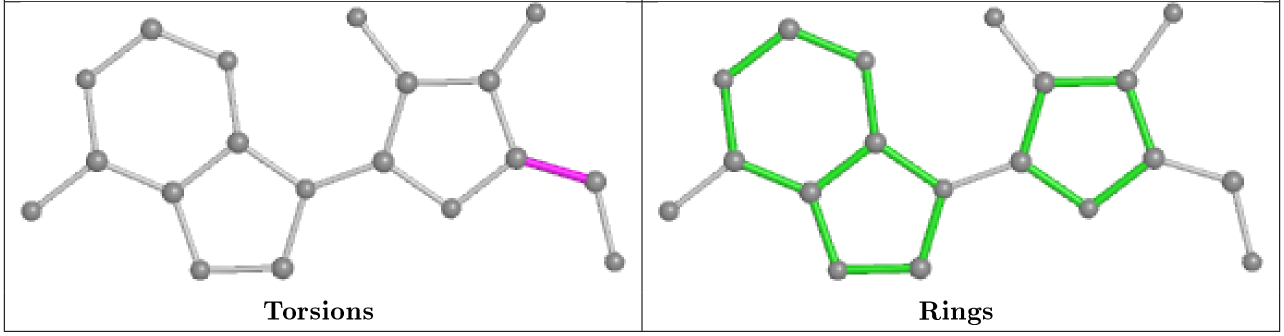
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	401	ADN	1	0
6	B	401	ADN	1	0
5	H	402	SO4	1	0
5	B	404	SO4	1	0
5	H	403	SO4	1	0

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 ADN E 401

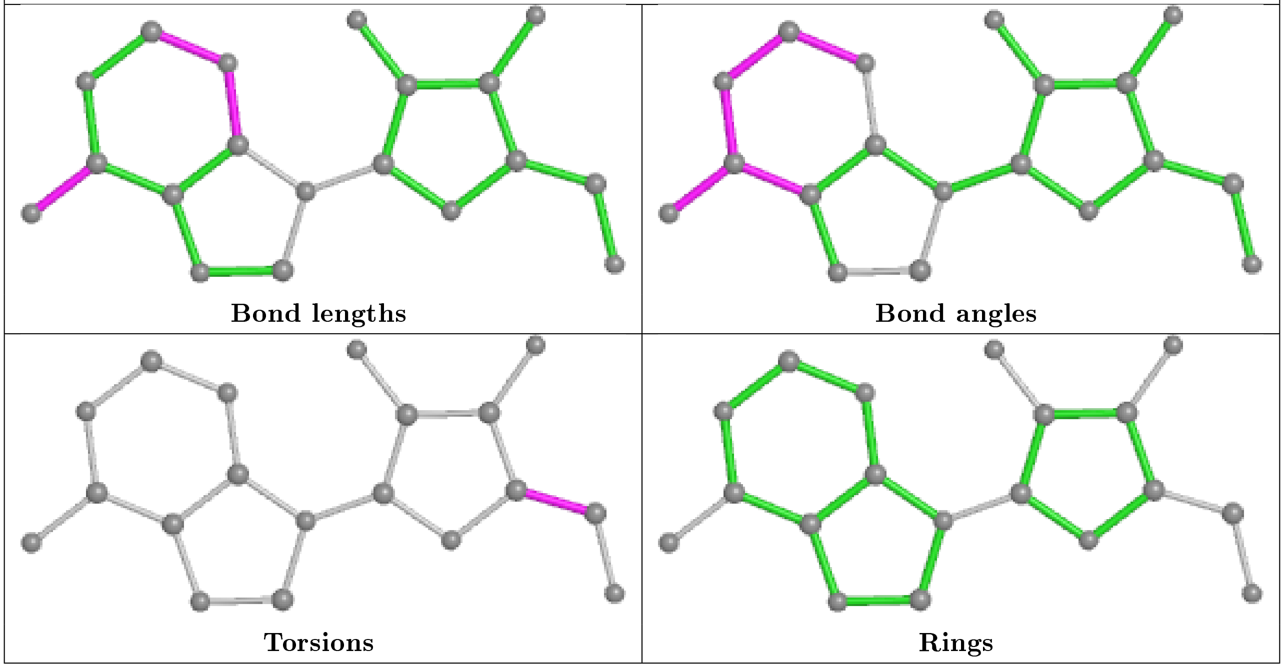


Bond lengths **Bond angles**

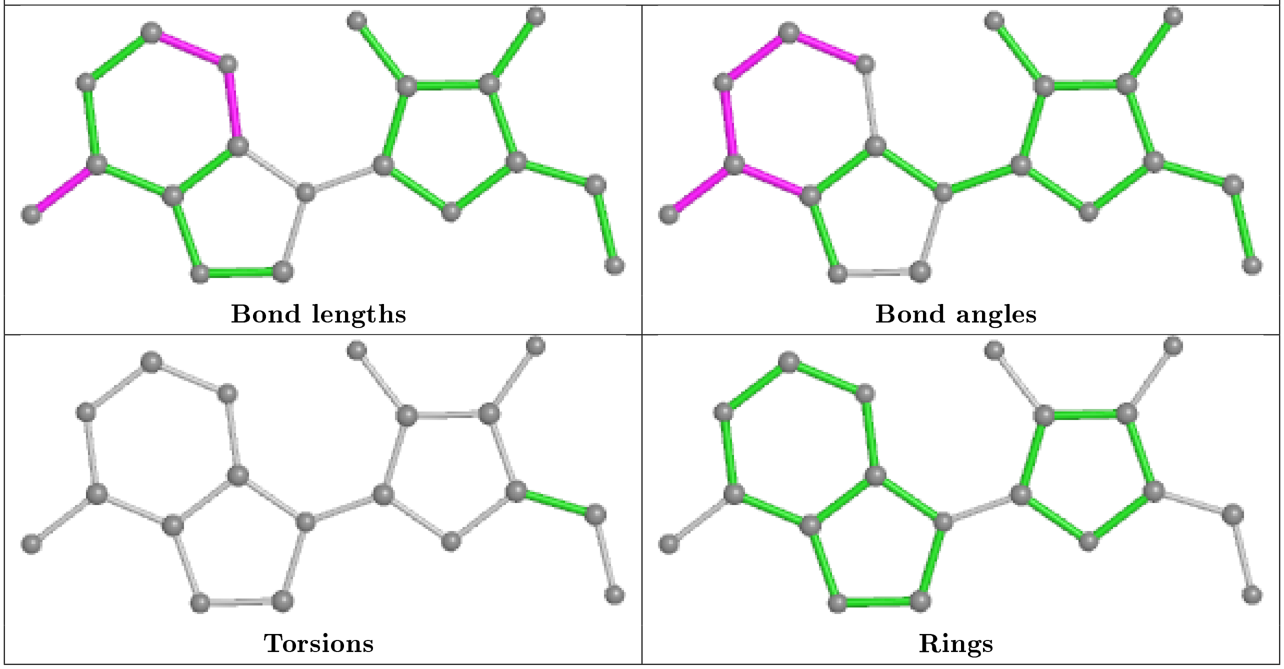


Torsions **Rings**

Ligand ADN B 401



Ligand ADN H 401



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^{2})	Q<0.9
1	A	320/326 (98%)	-0.42	0	100	100	62, 87, 131, 199	0
1	D	313/326 (96%)	-0.30	0	100	100	65, 102, 133, 166	0
1	G	314/326 (96%)	-0.24	2 (0%)	89	83	67, 105, 153, 183	0
2	B	355/373 (95%)	-0.25	1 (0%)	94	92	62, 92, 137, 177	0
2	E	355/373 (95%)	0.00	8 (2%)	60	47	78, 126, 172, 204	0
2	H	355/373 (95%)	-0.10	8 (2%)	60	47	68, 98, 139, 202	0
3	C	9/11 (81%)	-0.35	0	100	100	102, 124, 140, 142	0
3	F	9/11 (81%)	0.79	1 (11%)	5	3	135, 160, 175, 191	0
3	I	10/11 (90%)	-0.29	0	100	100	95, 119, 146, 170	0
4	L	3/6 (50%)	0.34	0	100	100	174, 174, 182, 194	0
All	All	2043/2136 (95%)	-0.21	20 (0%)	82	72	62, 102, 152, 204	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	287	ASN	5.1
2	H	116	CYS	3.8
2	H	155	SER	2.9
2	E	330	ALA	2.9
2	E	289	LEU	2.7

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	STA	L	6	12/12	0.83	0.41	90,124,145,154	0
4	STA	L	4	11/12	0.84	0.23	134,136,169,179	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

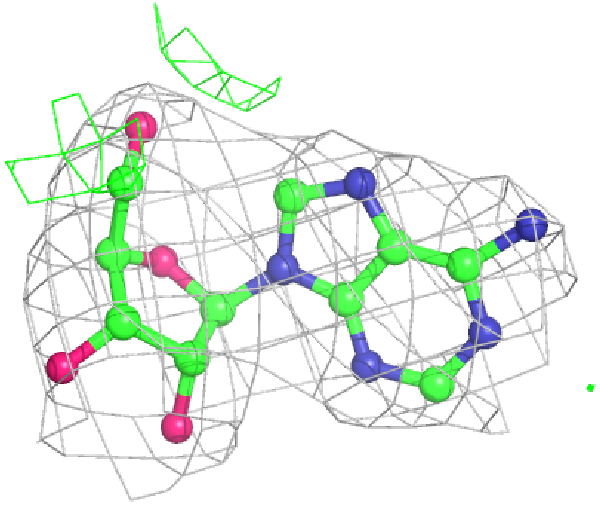
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

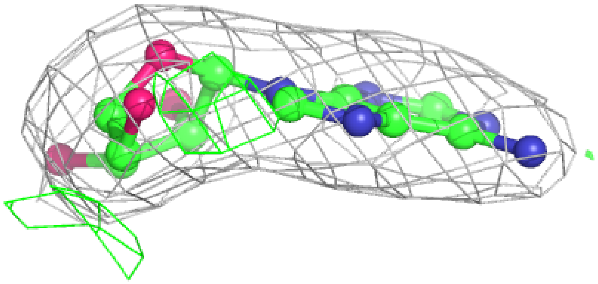
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	SO4	G	402	5/5	0.63	0.27	210,210,213,215	0
5	SO4	A	402	5/5	0.64	0.46	144,148,155,166	0
5	SO4	D	404	5/5	0.71	0.31	199,200,201,202	0
5	SO4	E	405	5/5	0.77	0.26	191,194,197,201	0
5	SO4	D	403	5/5	0.77	0.29	205,207,208,210	0
5	SO4	H	403	5/5	0.79	0.12	164,172,173,175	0
5	SO4	H	405	5/5	0.79	0.33	181,182,183,188	0
5	SO4	G	404	5/5	0.80	0.16	174,177,178,178	0
5	SO4	B	403	5/5	0.84	0.19	188,192,192,195	0
5	SO4	A	401	5/5	0.85	0.18	135,141,147,156	0
5	SO4	B	406	5/5	0.86	0.15	176,177,180,184	0
5	SO4	I	201	5/5	0.87	0.36	139,140,147,155	0
5	SO4	D	402	5/5	0.89	0.12	164,168,168,169	0
5	SO4	B	402	5/5	0.90	0.21	119,138,138,146	0
5	SO4	H	404	5/5	0.90	0.21	174,177,179,184	0
6	ADN	E	401	19/19	0.92	0.20	74,84,88,89	0
5	SO4	B	405	5/5	0.92	0.46	148,150,153,155	0
5	SO4	D	401	5/5	0.92	0.13	156,159,163,163	0
5	SO4	E	403	5/5	0.92	0.11	140,141,145,151	0
6	ADN	B	401	19/19	0.93	0.22	75,80,82,87	0
5	SO4	G	403	5/5	0.93	0.13	188,189,192,193	0
5	SO4	E	404	5/5	0.94	0.49	156,159,160,162	0
5	SO4	G	401	5/5	0.94	0.12	153,153,160,164	0
6	ADN	H	401	19/19	0.95	0.36	61,69,77,78	0
5	SO4	E	402	5/5	0.96	0.39	94,98,102,106	0
5	SO4	H	402	5/5	0.97	0.38	77,84,86,97	0
5	SO4	B	404	5/5	0.98	0.36	63,69,82,85	0

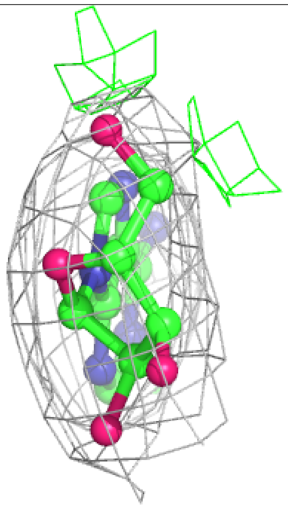
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADN E 401:

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

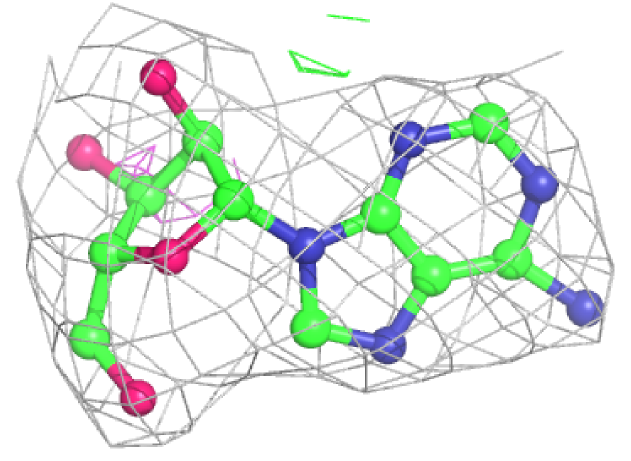


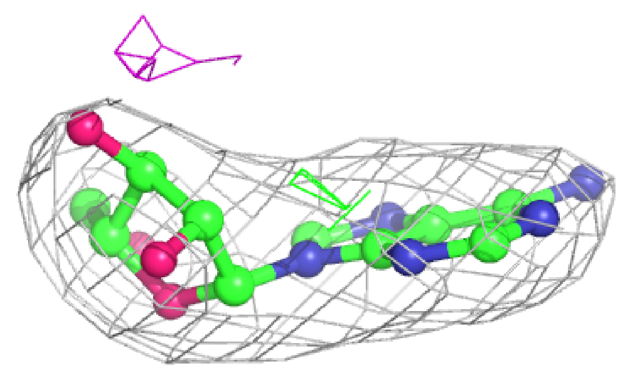


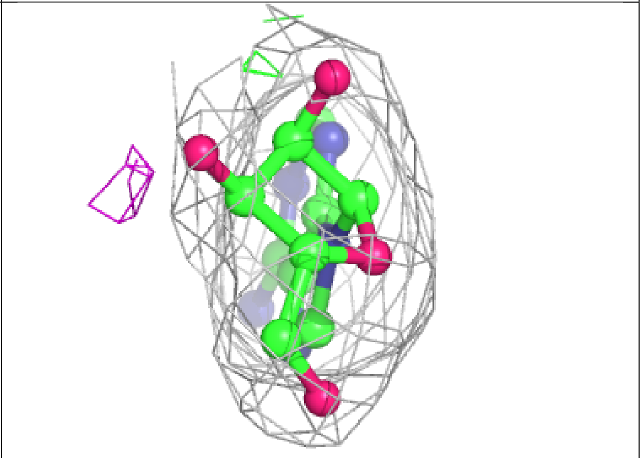


Electron density around ADN B 401:

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

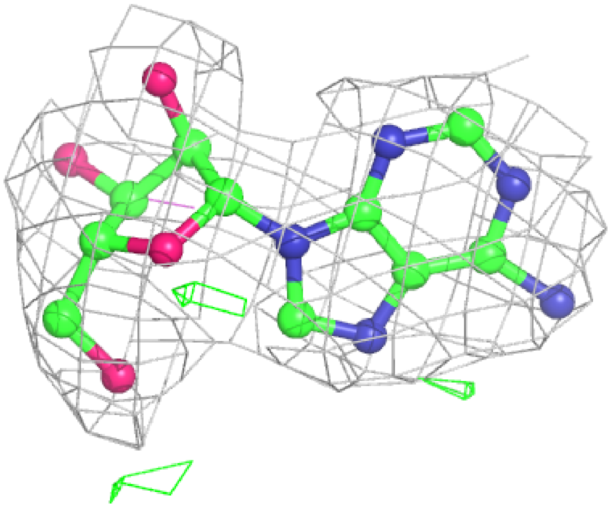


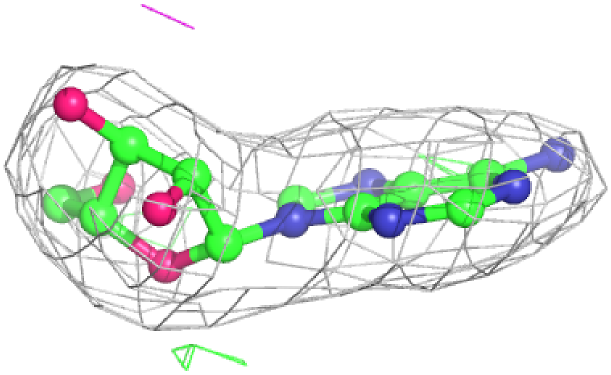


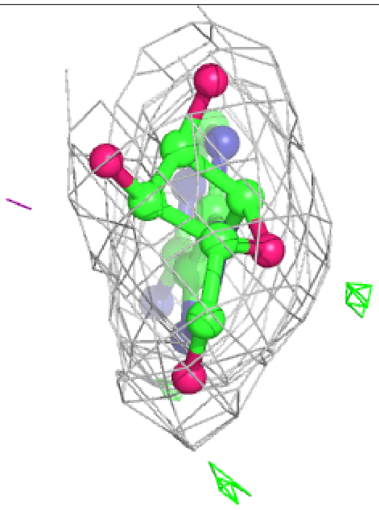


Electron density around ADN H 401:

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 ⓘ

There are no such residues in this entry.