wwPDB X-ray Structure Validation Summary Report (i)

Nov 19, 2024 – 03:13 pm GMT

PDB ID	:	8R7E
Title	:	MutSbeta bound to compound CHDI-00898647 in the canonical DNA-mismatch bound form
Authors	:	Thomsen, M.; Thieulin-Pardo, G.; Steinbacher, S.; Brace, G.; Tillack, K.; Johnson, P.; Ritzefeld, M.; Schaertl, S.; Frush, E.; Warfield, B.; Ballantyne, G.; Lee, J.-H.; Witte, D.; Finley, M.; Prasad, B.; Monteagudo, E.; Plotnikov, N.; Pacifici, R.; Maillard, M.; Wilkinson, H.; Iyer, R.; Dominguez, C.; Vogt, T.; Felsenfeld, D.; Haque, T.
Deposited on	:	2023-11-24
Resolution	:	2.78 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 (i) 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 (1)) were used in the production of this report:

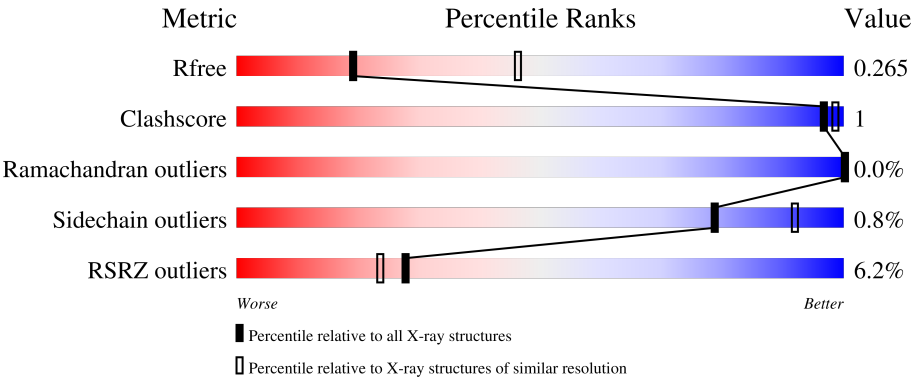
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.78 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}	164625	4924 (2.80-2.76)
Clashscore	180529	5458 (2.80-2.76)
Ramachandran outliers	177936	5386 (2.80-2.76)
Sidechain outliers	177891	5388 (2.80-2.76)
RSRZ outliers	164620	4926 (2.80-2.76)

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 <=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	930	7% 87% · 11%
1	E	930	5% 91% · 6%
2	B	918	2% 87% · 8%

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Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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Mol	Chain	Length	Quality of chain
2	F	918	9% 87% 10%
3	C	24	88% 8%
3	G	24	88% 12%
4	D	24	83% 12%
4	H	24	96%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 28977 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	825	Total	C	N	O	S	373	1	0
			6570	4183	1114	1237	36			
1	E	875	Total	C	N	O	S	339	2	0
			6956	4423	1181	1316	36			

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	840	Total	C	N	O	S	177	0	0
			6721	4289	1148	1254	30			
2	F	827	Total	C	N	O	S	347	1	0
			6618	4220	1136	1232	30			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	217	GLY	-	expression tag	UNP P20585
B	218	PRO	-	expression tag	UNP P20585
F	217	GLY	-	expression tag	UNP P20585
F	218	PRO	-	expression tag	UNP P20585

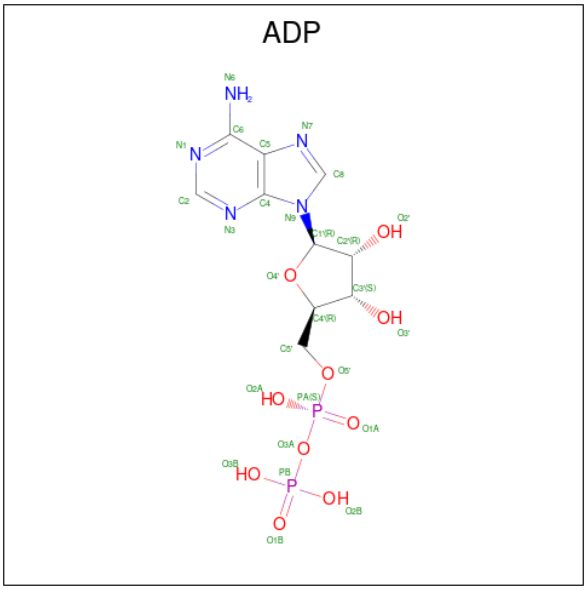
- Molecule 3 is a DNA chain called DNA (5'-D(*TP*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	22	Total	C	N	O	P	0	0	0
			449	215	82	131	21			
3	G	21	Total	C	N	O	P	0	0	0
			432	205	80	126	21			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3').

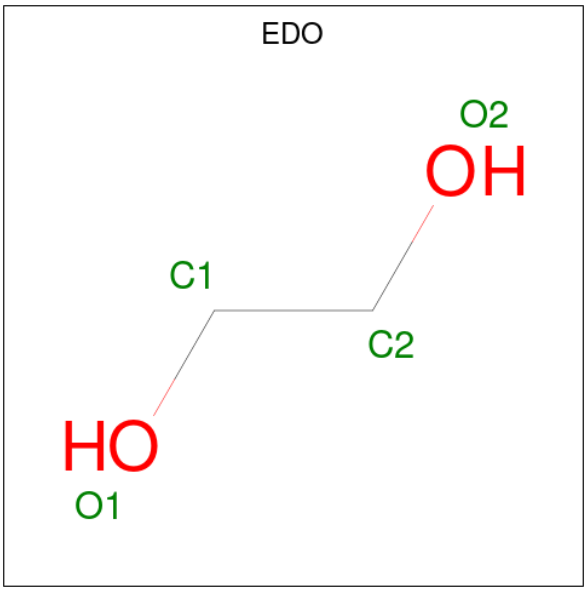
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	23	Total	C	N	O	P	0	0	0
			469	224	88	135	22			
4	H	23	Total	C	N	O	P	0	0	0
			469	224	88	135	22			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

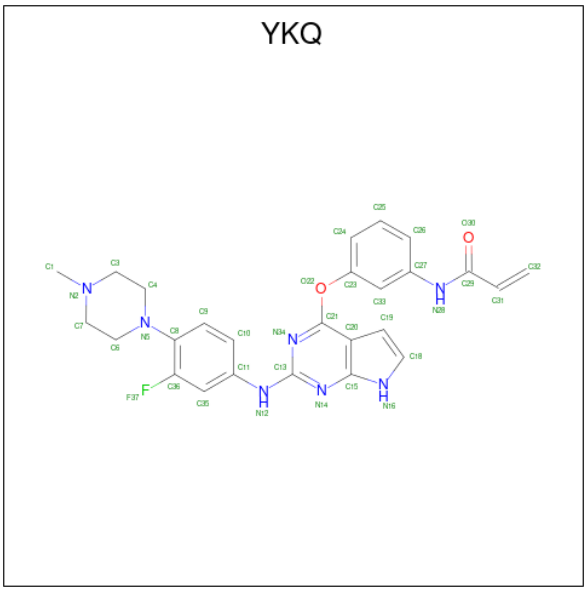


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	F	1	Total C O 4 2 2	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

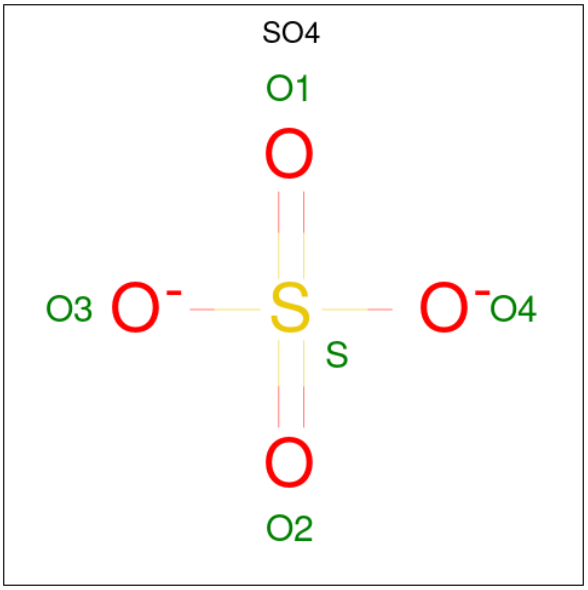
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0
7	B	1	Total Cl 1 1	0	0
7	E	3	Total Cl 3 3	0	0

- Molecule 8 is Abivertinib (three-letter code: YKQ) (formula: $C_{26}H_{26}FN_7O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	F	N	O	0	0
			36	26	1	7	2		
8	F	1	Total	C	F	N	O	5	0
			36	26	1	7	2		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 10 is water.

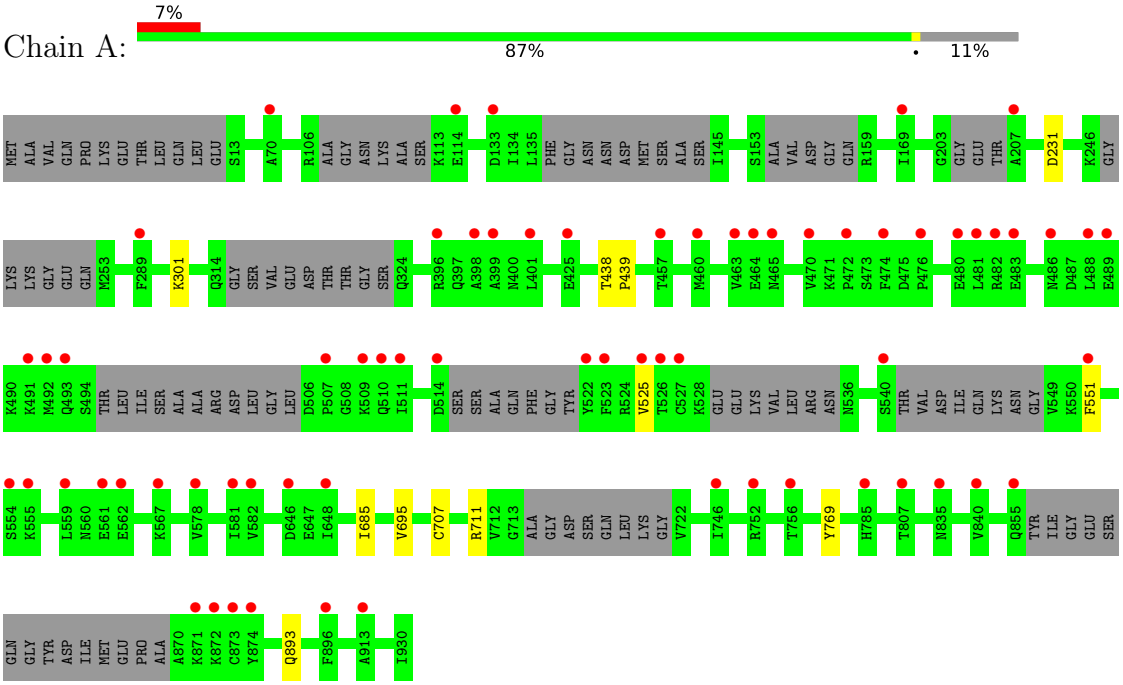
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	22	Total O 22 22	0	0
10	B	27	Total O 27 27	0	0
10	E	29	Total O 29 29	0	0
10	F	34	Total O 34 34	0	0
10	G	2	Total O 2 2	0	0
10	H	3	Total O 3 3	0	0

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.

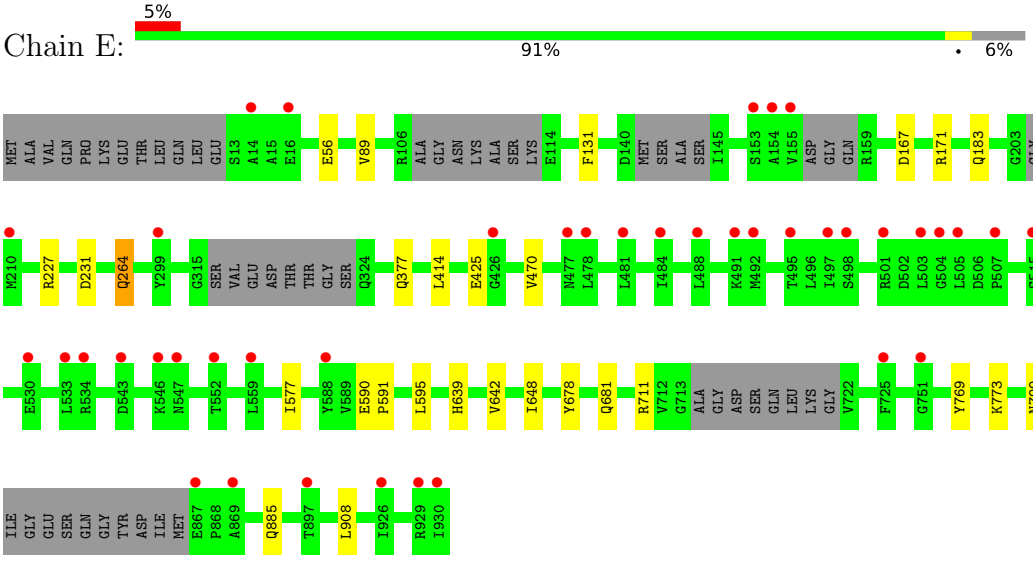
• Molecule 1: DNA mismatch repair protein Msh2

Chain A:



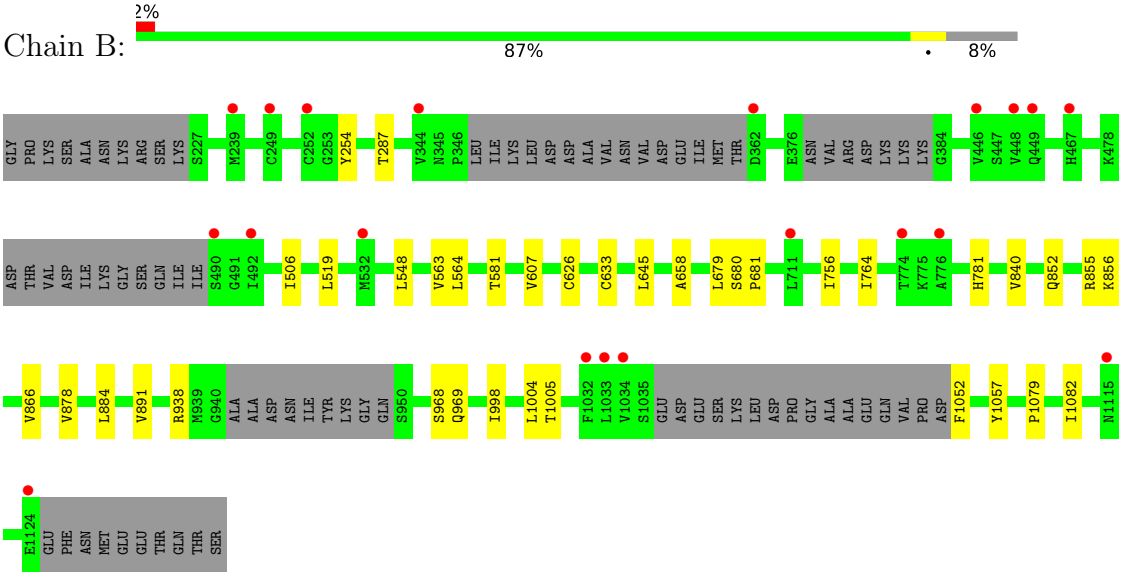
• Molecule 1: DNA mismatch repair protein Msh2

Chain E:



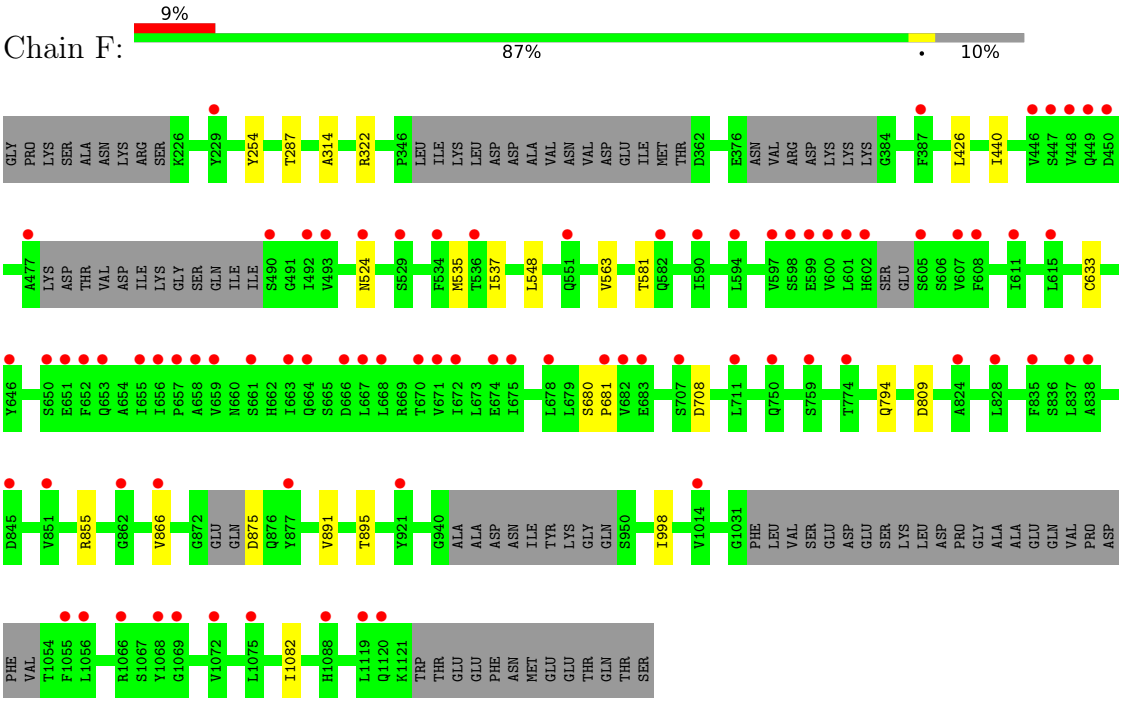
• Molecule 2: DNA mismatch repair protein Msh3

Chain B:



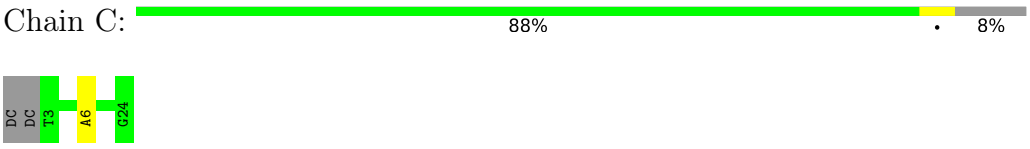
• Molecule 2: DNA mismatch repair protein Msh3

Chain F:



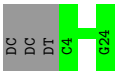
• Molecule 3: DNA (5'-D(*TP*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3')

Chain C:



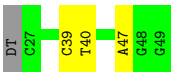
• Molecule 3: DNA (5'-D(*TP*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3')

Chain G:



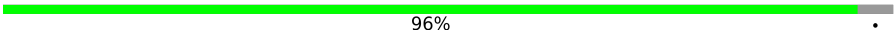
• Molecule 4: DNA (5'-D(*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP *AP*GP*AP*TP*AP*GP*G)-3')

Chain D:



• Molecule 4: DNA (5'-D(*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP *AP*GP*AP*TP*AP*GP*G)-3')

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	100.47Å 104.10Å 122.02Å 109.33° 91.81° 109.50°	Depositor
Resolution (Å)	113.66 – 2.78 113.66 – 2.78	Depositor EDS
% Data completeness (in resolution range)	72.8 (113.66-2.78) 72.8 (113.66-2.78)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.223 , 0.266 0.224 , 0.265	Depositor DCC
R_{free} test set	5400 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	62.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	28977	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: SO4, CL, ADP, EDO, YKQ

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	0.69	0/6669	0.76	0/8975
1	E	0.69	0/7066	0.77	0/9518
2	B	0.68	0/6845	0.77	0/9240
2	F	0.68	0/6737	0.77	0/9089
3	C	0.30	0/503	0.75	0/775
3	G	0.32	0/484	0.73	0/745
4	D	0.33	0/526	0.79	0/810
4	H	0.31	0/526	0.76	0/810
All	All	0.66	0/29356	0.77	0/39962

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6570	0	6637	5	0
1	E	6956	0	7010	12	0
2	B	6721	0	6816	22	0
2	F	6618	0	6720	9	0
3	C	449	0	250	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	432	0	237	0	0
4	D	469	0	260	2	0
4	H	469	0	260	0	0
5	A	27	0	12	0	0
5	E	27	0	12	0	0
6	A	4	0	6	0	0
6	B	8	0	12	0	0
6	E	4	0	6	0	0
6	F	4	0	6	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	E	3	0	0	0	0
8	B	36	0	0	0	0
8	F	36	0	0	0	0
9	B	15	0	0	0	0
9	F	10	0	0	0	0
10	A	22	0	0	0	0
10	B	27	0	0	0	0
10	E	29	0	0	2	0
10	F	34	0	0	0	0
10	G	2	0	0	0	0
10	H	3	0	0	0	0
All	All	28977	0	28244	48	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 1.

The worst 5 of 48 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:E:183:GLN:HG3	10:E:1111:HOH:O	1.97	0.63
1:E:470:VAL:HG21	1:E:577:ILE:HD11	1.82	0.61
2:B:1079:PRO:HG2	2:B:1082:ILE:HD13	1.89	0.54
2:F:891:VAL:HG21	2:F:998:ILE:HG12	1.91	0.52
2:B:884:LEU:HB3	2:B:1004:LEU:HD22	1.92	0.51

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	800/930 (86%)	772 (96%)	28 (4%)	0	100 100
1	E	861/930 (93%)	833 (97%)	28 (3%)	0	100 100
2	B	828/918 (90%)	798 (96%)	30 (4%)	0	100 100
2	F	812/918 (88%)	783 (96%)	28 (3%)	1 (0%)	48 76
All	All	3301/3696 (89%)	3186 (96%)	114 (4%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	322	ARG

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	725/804 (90%)	722 (100%)	3 (0%)	89 96
1	E	764/804 (95%)	754 (99%)	10 (1%)	65 86
2	B	750/818 (92%)	745 (99%)	5 (1%)	81 93
2	F	738/818 (90%)	731 (99%)	7 (1%)	75 91
All	All	2977/3244 (92%)	2952 (99%)	25 (1%)	79 92

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	711	ARG
1	E	908	LEU
2	F	895	THR
1	E	885	GLN
2	F	524	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	462	GLN
1	E	645	GLN
2	F	524	ASN
1	E	885	GLN
2	B	852	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 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	$\#\|Z\|>2$
6	EDO	B	1207	-	3,3,3	0.09	0	2,2,2	0.21	0
9	SO4	F	1202	-	4,4,4	0.43	0	6,6,6	0.12	0
9	SO4	B	1205	-	4,4,4	0.37	0	6,6,6	0.04	0
5	ADP	E	1001	-	24,29,29	0.64	0	29,45,45	0.82	1 (3%)
6	EDO	B	1204	-	3,3,3	0.11	0	2,2,2	0.39	0
9	SO4	B	1202	-	4,4,4	0.38	0	6,6,6	0.07	0
6	EDO	F	1204	-	3,3,3	0.05	0	2,2,2	0.25	0
9	SO4	B	1203	-	4,4,4	0.38	0	6,6,6	0.06	0
9	SO4	F	1203	-	4,4,4	0.39	0	6,6,6	0.04	0
8	YKQ	B	1201	-	38,40,40	0.70	0	48,56,56	2.63	13 (27%)
5	ADP	A	1001	-	24,29,29	0.68	0	29,45,45	0.72	1 (3%)
6	EDO	E	1004	-	3,3,3	0.11	0	2,2,2	0.38	0
6	EDO	A	1002	-	3,3,3	0.11	0	2,2,2	0.33	0
8	YKQ	F	1201	-	38,40,40	0.89	2 (5%)	48,56,56	2.61	14 (29%)

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	EDO	B	1207	-	-	0/1/1/1	-
5	ADP	E	1001	-	-	1/12/32/32	0/3/3/3
6	EDO	B	1204	-	-	1/1/1/1	-
6	EDO	F	1204	-	-	1/1/1/1	-
8	YKQ	B	1201	-	-	6/18/34/34	0/5/5/5
5	ADP	A	1001	-	-	3/12/32/32	0/3/3/3
6	EDO	E	1004	-	-	1/1/1/1	-
6	EDO	A	1002	-	-	1/1/1/1	-
8	YKQ	F	1201	-	-	4/18/34/34	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	1201	YKQ	C21-C20	-2.89	1.39	1.43
8	F	1201	YKQ	C13-N12	2.20	1.41	1.36

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1201	YKQ	C20-C21-N34	-10.35	117.18	124.40
8	F	1201	YKQ	C20-C21-N34	-10.14	117.33	124.40
8	F	1201	YKQ	C31-C29-N28	9.42	120.04	113.84
8	B	1201	YKQ	C31-C29-N28	5.63	117.55	113.84
8	B	1201	YKQ	C13-N14-C15	5.23	121.22	115.28

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

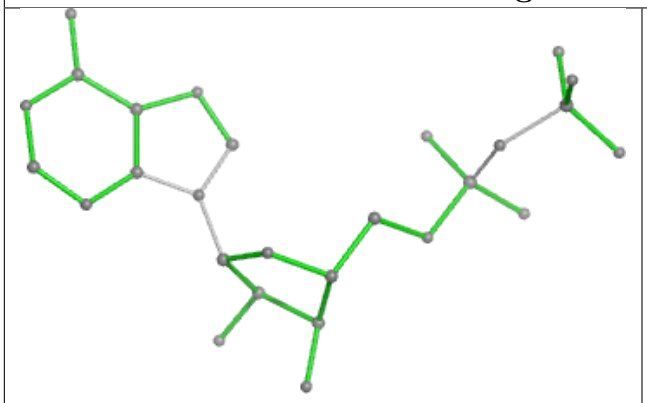
Mol	Chain	Res	Type	Atoms
8	B	1201	YKQ	C36-C8-N5-C6
5	E	1001	ADP	O4'-C4'-C5'-O5'
8	B	1201	YKQ	C26-C27-N28-C29
8	B	1201	YKQ	C33-C27-N28-C29
8	F	1201	YKQ	C33-C27-N28-C29

There are no ring outliers.

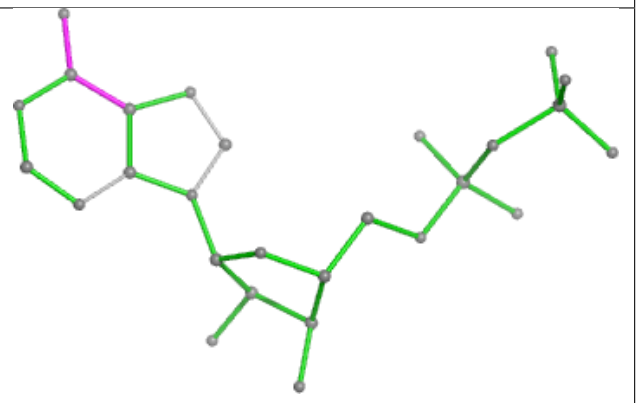
No monomer is involved in short contacts.

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 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.

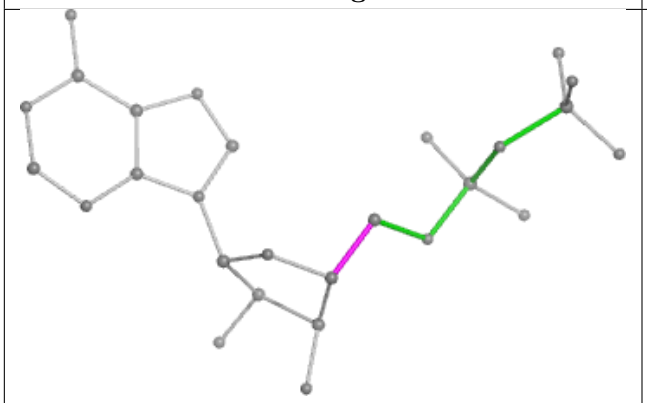
Ligand ADP E 1001



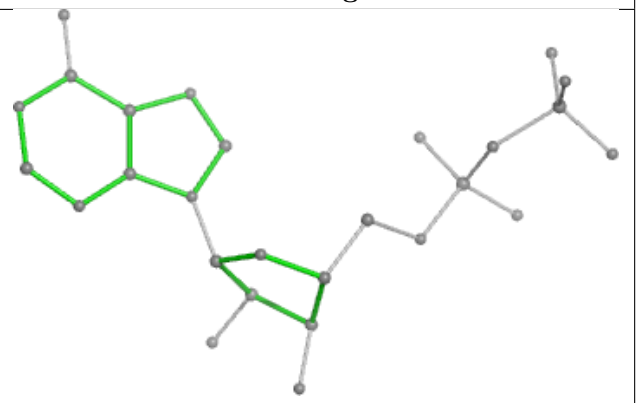
Bond lengths



Bond angles

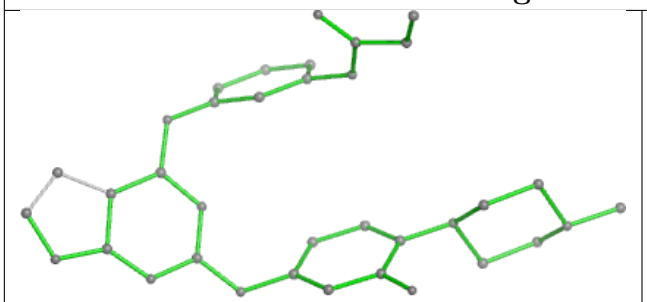


Torsions

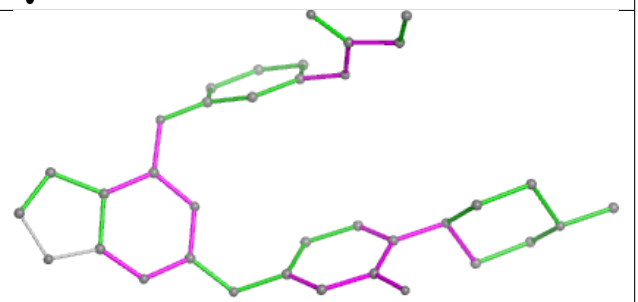


Rings

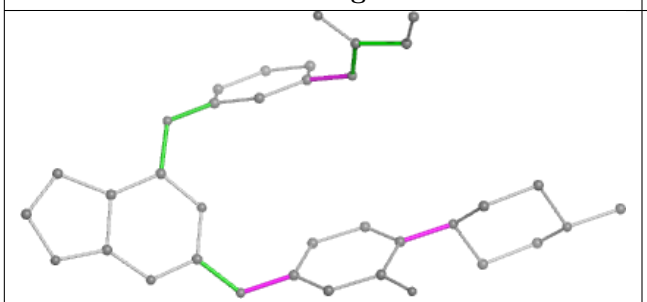
Ligand YKQ B 1201



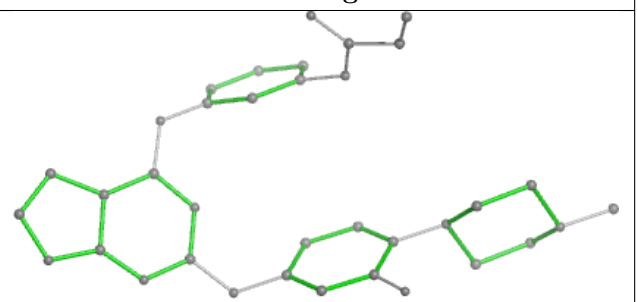
Bond lengths



Bond angles

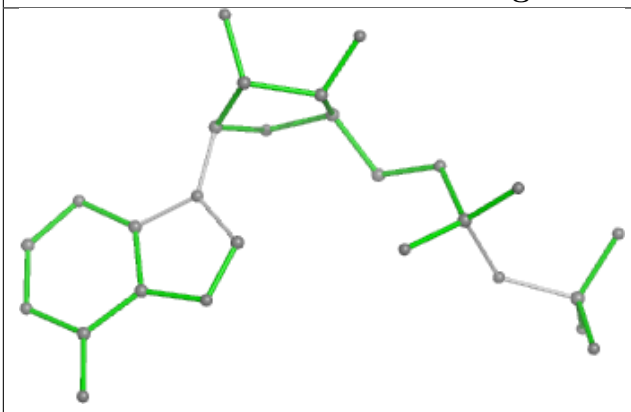


Torsions

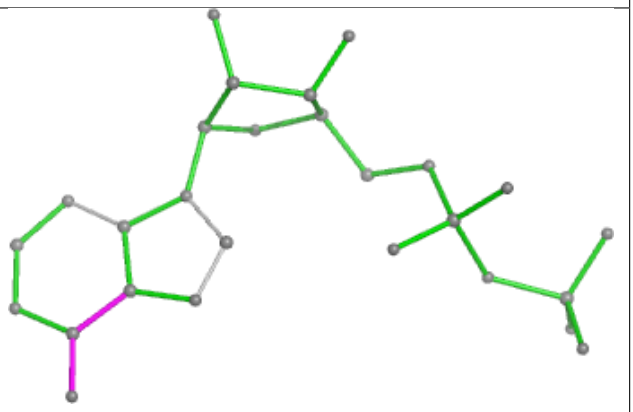


Rings

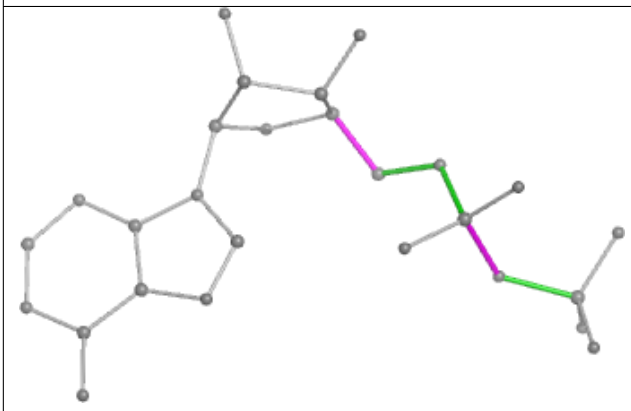
Ligand ADP A 1001



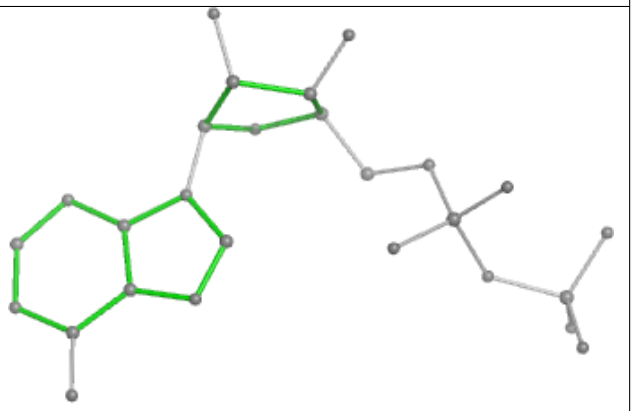
Bond lengths



Bond angles

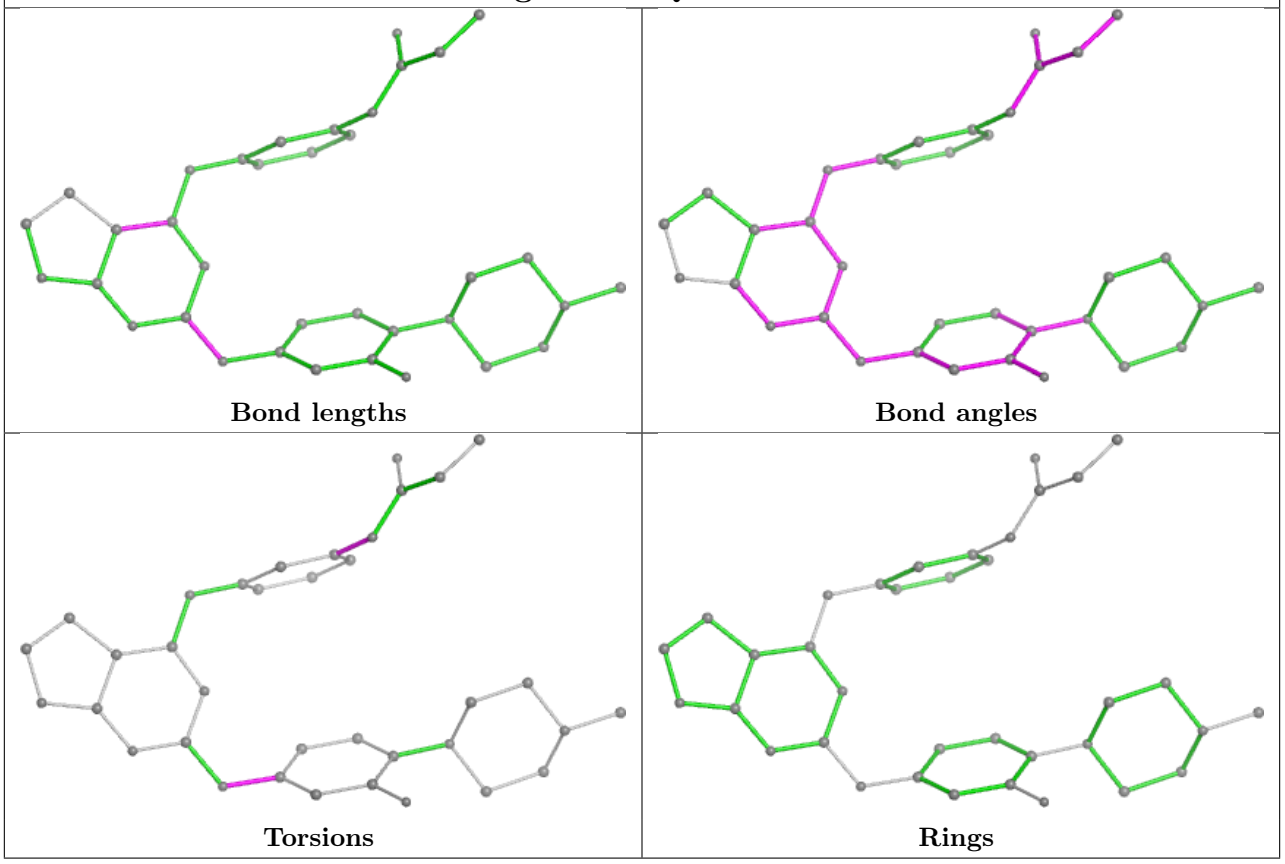


Torsions



Rings

Ligand YKQ F 1201



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, 95^{th} 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	825/930 (88%)	0.52	67 (8%) 19 17	25, 64, 118, 168	124 (15%)
1	E	875/930 (94%)	0.37	46 (5%) 33 28	24, 59, 108, 138	123 (14%)
2	B	840/918 (91%)	0.12	20 (2%) 59 53	25, 54, 87, 139	67 (7%)
2	F	827/918 (90%)	0.63	82 (9%) 14 12	31, 64, 113, 159	132 (15%)
3	C	22/24 (91%)	0.13	0 100 100	53, 97, 141, 145	0
3	G	21/24 (87%)	-0.27	0 100 100	41, 81, 130, 145	0
4	D	23/24 (95%)	-0.09	0 100 100	47, 93, 136, 146	0
4	H	23/24 (95%)	-0.14	0 100 100	43, 70, 140, 161	0
All	All	3456/3792 (91%)	0.40	215 (6%) 28 24	24, 60, 111, 168	446 (12%)

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	490	SER	4.7
2	F	774	THR	4.7
2	F	1069	GLY	4.3
1	E	503	LEU	4.2
1	E	504	GLY	4.1

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 monosaccharides in this entry.

6.4 Ligands (i)

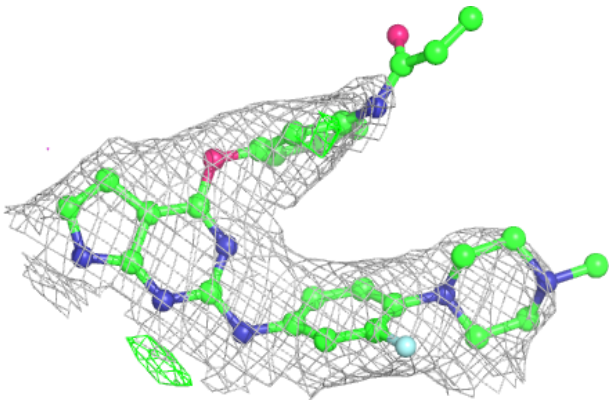
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

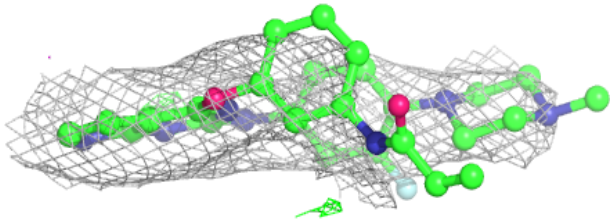
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SO4	F	1203	5/5	0.77	0.09	127,128,130,132	0
9	SO4	B	1203	5/5	0.81	0.09	110,111,112,112	0
9	SO4	F	1202	5/5	0.84	0.14	91,92,94,100	0
8	YKQ	F	1201	36/36	0.85	0.14	70,90,105,108	5
6	EDO	A	1002	4/4	0.87	0.21	66,69,70,70	0
7	CL	E	1002	1/1	0.90	0.09	74,74,74,74	0
9	SO4	B	1205	5/5	0.90	0.12	102,104,106,106	0
6	EDO	B	1204	4/4	0.91	0.10	46,47,47,47	0
6	EDO	E	1004	4/4	0.91	0.14	63,63,63,64	0
6	EDO	B	1207	4/4	0.93	0.14	56,57,57,59	0
7	CL	E	1005	1/1	0.93	0.06	78,78,78,78	0
8	YKQ	B	1201	36/36	0.93	0.10	45,57,75,77	0
5	ADP	E	1001	27/27	0.93	0.07	52,57,61,62	0
6	EDO	F	1204	4/4	0.94	0.12	44,45,46,48	0
9	SO4	B	1202	5/5	0.94	0.11	70,72,74,74	0
5	ADP	A	1001	27/27	0.94	0.07	43,48,56,59	0
7	CL	A	1003	1/1	0.96	0.05	57,57,57,57	0
7	CL	B	1206	1/1	0.97	0.05	63,63,63,63	0
7	CL	E	1003	1/1	0.97	0.05	76,76,76,76	0

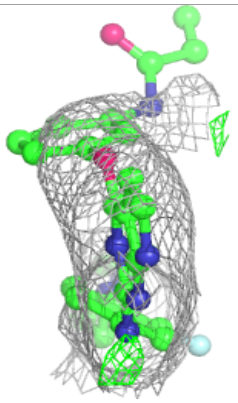
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YKQ F 1201:

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

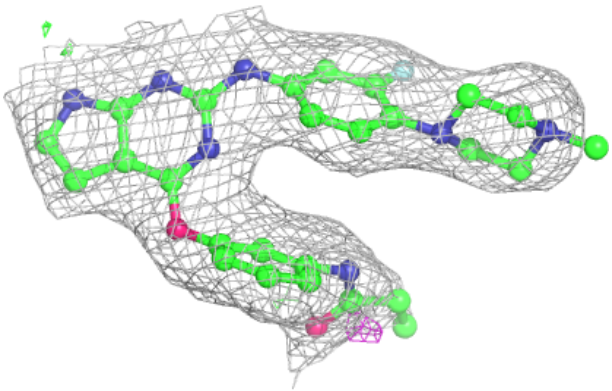


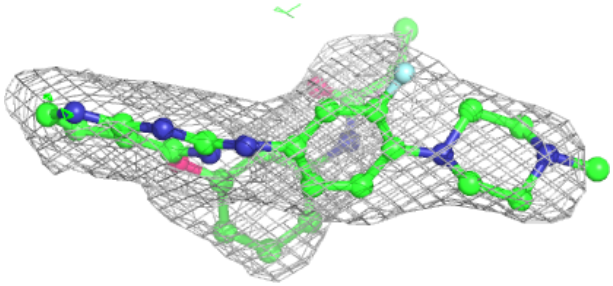


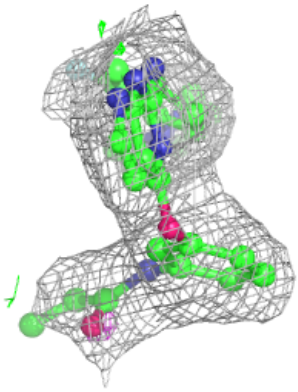


Electron density around YKQ B 1201:

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

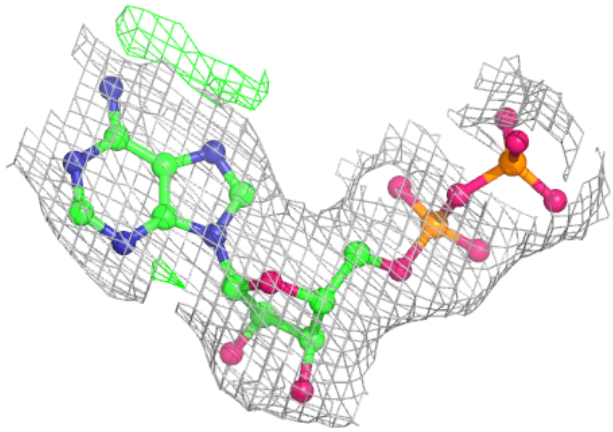


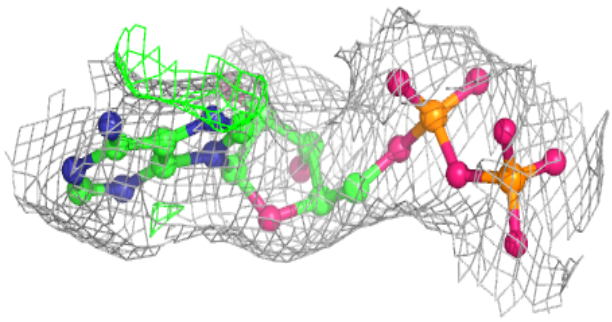


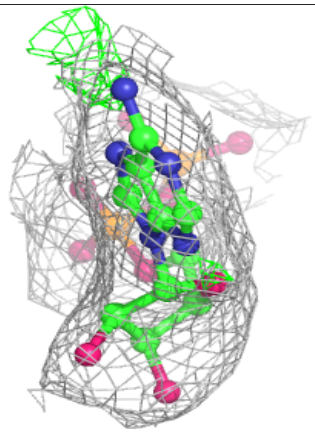


Electron density around ADP E 1001:

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

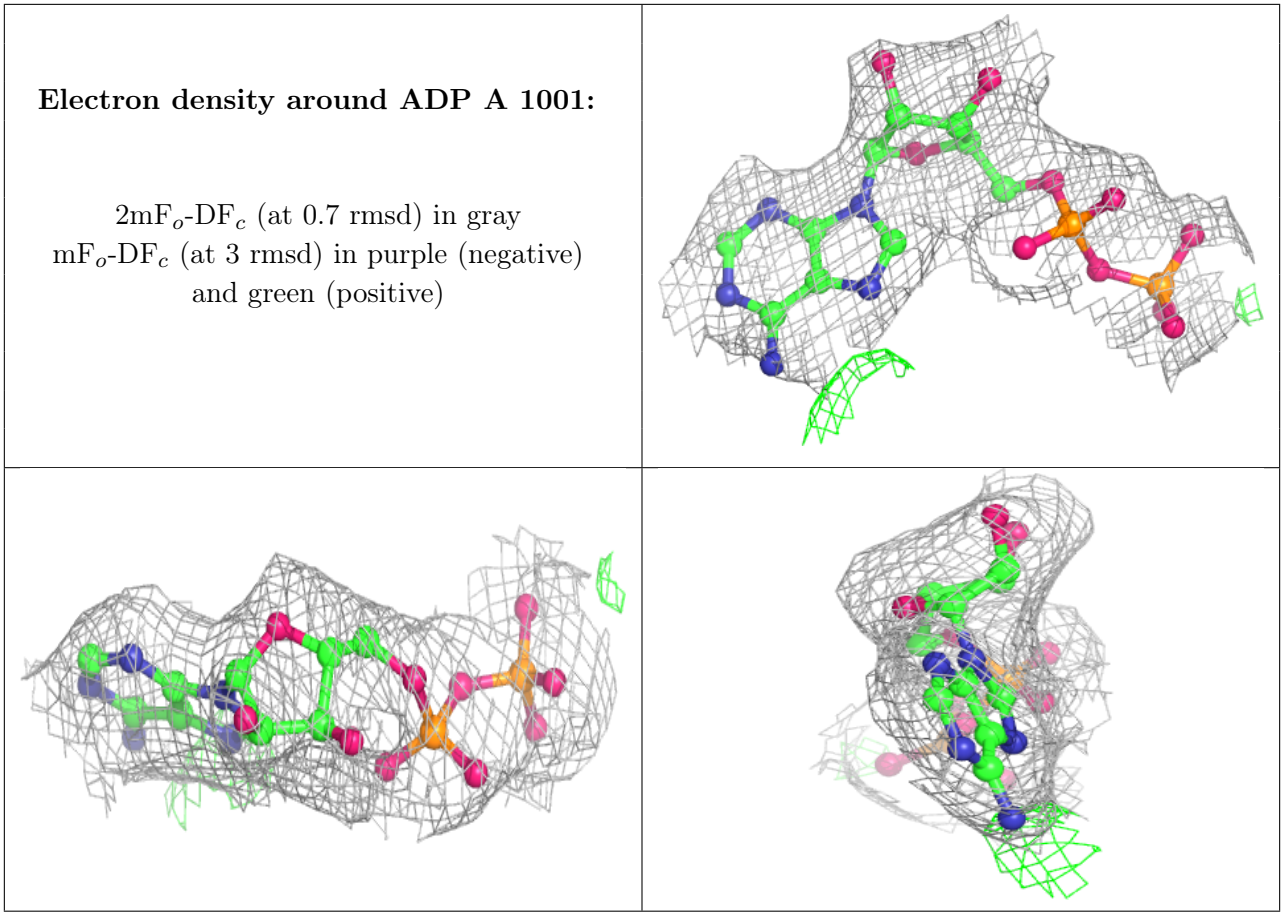






Electron density around ADP A 1001:

$2mF_o$-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.