



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:36 AM UTC

PDB ID : 4PL5 / pdb\_00004pl5  
Title : Crystal structure of murine IRE1 in complex with OICR573 inhibitor  
Authors : Sanches, M.; Duffy, N.; Talukdar, M.; Thevakumaran, N.; Chiovitti, D.; Al-  
awar, R.; Patterson, J.B.; Sicheri, F.  
Deposited on : 2014-05-16  
Resolution : 3.40 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](mailto: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>.

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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)  
Xtrriage (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

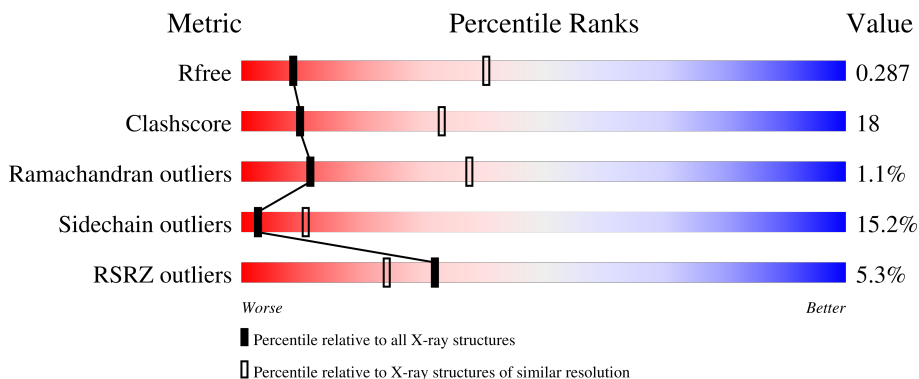
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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  $\geq 3$ , 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	435	
1	B	435	
1	C	435	
1	D	435	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12629 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	383	3117	1993	550	555	19	0	0	0
1	A	386	3124	2000	547	558	19	0	0	0
1	C	386	3133	2003	554	557	19	0	0	0
1	D	385	3090	1973	542	556	19	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

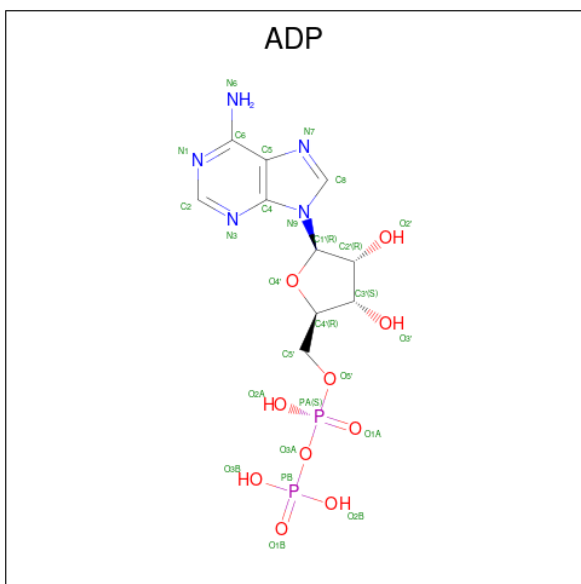
Chain	Residue	Modelled	Actual	Comment	Reference
B	543	GLY	-	expression tag	UNP Q9EQY0
B	544	ALA	-	expression tag	UNP Q9EQY0
B	545	MET	-	expression tag	UNP Q9EQY0
B	546	ASP	-	expression tag	UNP Q9EQY0
B	547	PRO	-	expression tag	UNP Q9EQY0
B	548	GLU	-	expression tag	UNP Q9EQY0
B	549	PHE	-	expression tag	UNP Q9EQY0
B	772	TYR	ASN	engineered mutation	UNP Q9EQY0
A	543	GLY	-	expression tag	UNP Q9EQY0
A	544	ALA	-	expression tag	UNP Q9EQY0
A	545	MET	-	expression tag	UNP Q9EQY0
A	546	ASP	-	expression tag	UNP Q9EQY0
A	547	PRO	-	expression tag	UNP Q9EQY0
A	548	GLU	-	expression tag	UNP Q9EQY0
A	549	PHE	-	expression tag	UNP Q9EQY0
A	772	TYR	ASN	engineered mutation	UNP Q9EQY0
C	543	GLY	-	expression tag	UNP Q9EQY0
C	544	ALA	-	expression tag	UNP Q9EQY0
C	545	MET	-	expression tag	UNP Q9EQY0
C	546	ASP	-	expression tag	UNP Q9EQY0
C	547	PRO	-	expression tag	UNP Q9EQY0

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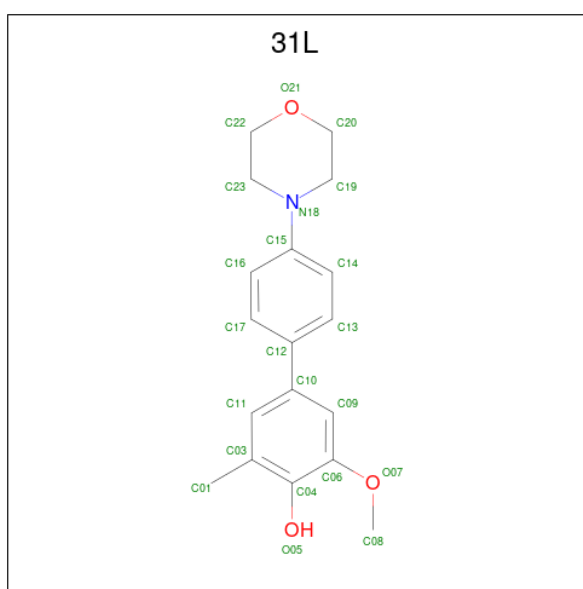
Chain	Residue	Modelled	Actual	Comment	Reference
C	548	GLU	-	expression tag	UNP Q9EQY0
C	549	PHE	-	expression tag	UNP Q9EQY0
C	772	TYR	ASN	engineered mutation	UNP Q9EQY0
D	543	GLY	-	expression tag	UNP Q9EQY0
D	544	ALA	-	expression tag	UNP Q9EQY0
D	545	MET	-	expression tag	UNP Q9EQY0
D	546	ASP	-	expression tag	UNP Q9EQY0
D	547	PRO	-	expression tag	UNP Q9EQY0
D	548	GLU	-	expression tag	UNP Q9EQY0
D	549	PHE	-	expression tag	UNP Q9EQY0
D	772	TYR	ASN	engineered mutation	UNP Q9EQY0

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



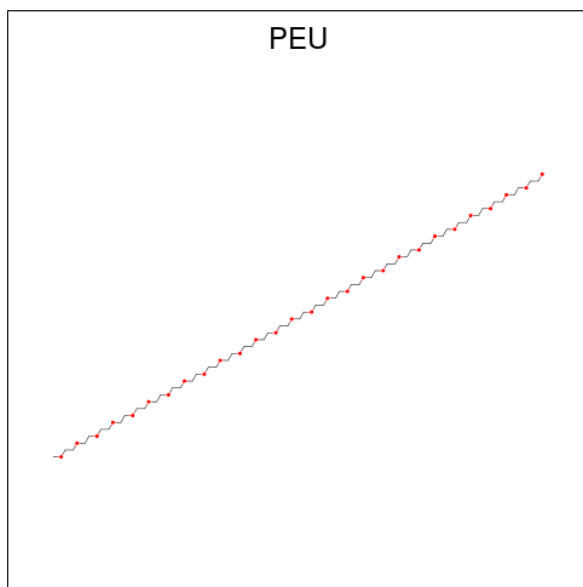
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is 3-methoxy-5-methyl-4'-(morpholin-4-yl)biphenyl-4-ol (CCD ID: 31L) (formula:  $C_{18}H_{21}NO_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 22 18 1 3	0	0

- Molecule 5 is 2,5,8,11,14,17,20,23,26,29,32,35,38,41,44,47,50,53,56,59,62,65,68,71,74,77,80-H EPTACOSAOXADOCTACONTAN-82-OL (CCD ID: PEU) (formula:  $C_{55}H_{112}O_{28}$ ).

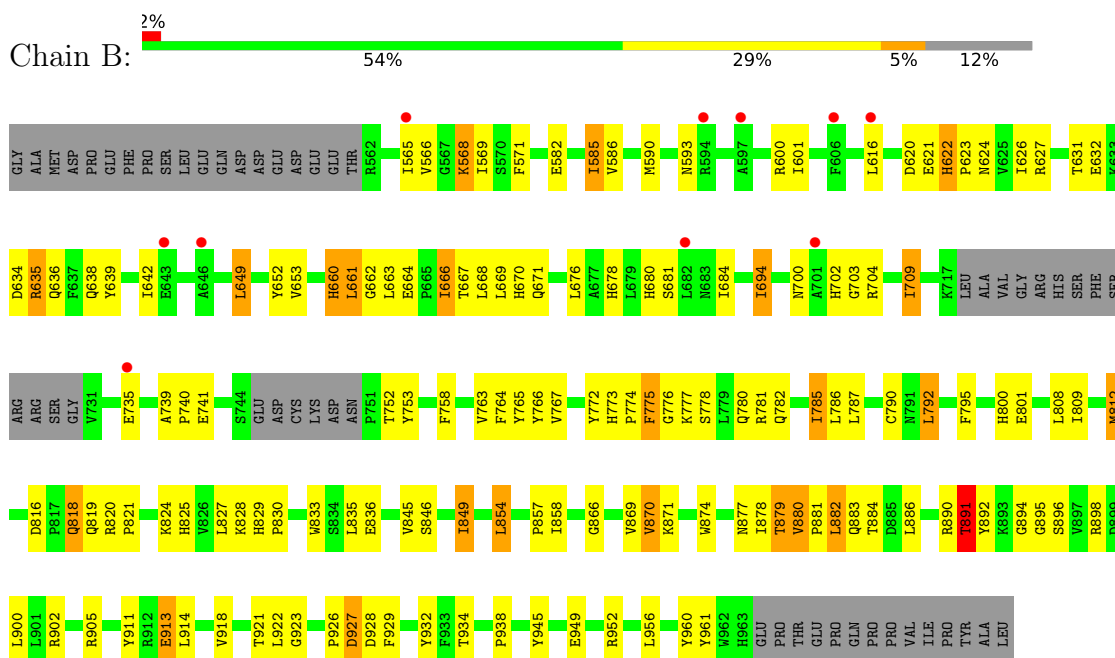


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	31	20	11	0	0

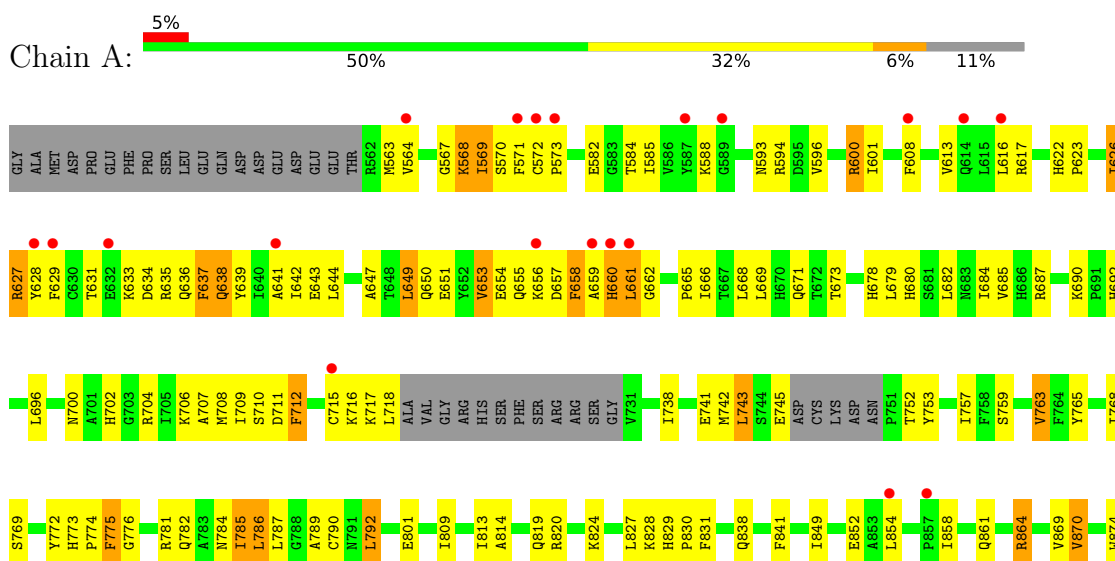
### 3 Residue-property plots

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.

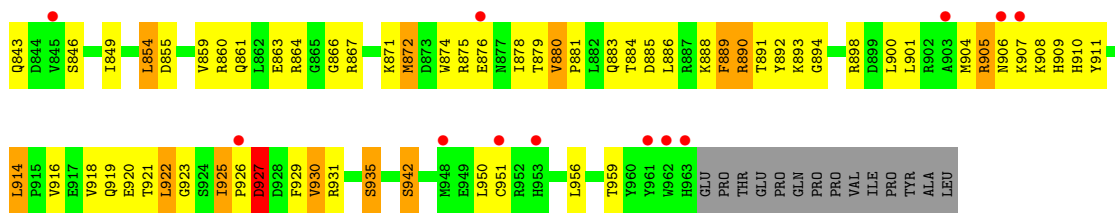
- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	319.22Å 63.03Å 140.78Å 90.00° 99.49° 90.00°	Depositor
Resolution (Å)	48.27 – 3.40 48.27 – 3.40	Depositor EDS
% Data completeness (in resolution range)	75.2 (48.27-3.40) 75.5 (48.27-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 3.40Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_1175)	Depositor
R, $R_{free}$	0.222 , 0.285 0.223 , 0.287	Depositor DCC
$R_{free}$ test set	1207 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.2	Xtrriage
Anisotropy	0.233	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 90.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ADP, PEU, MG, 31L

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	0.45	0/3202	0.89	5/4327 (0.1%)
1	B	0.43	0/3195	0.90	7/4315 (0.2%)
1	C	0.42	1/3211 (0.0%)	0.87	4/4339 (0.1%)
1	D	0.43	0/3165	0.88	4/4281 (0.1%)
All	All	0.43	1/12773 (0.0%)	0.89	20/17262 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	880	VAL	CA-CB	6.50	1.57	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	775	PHE	N-CA-C	7.83	122.59	112.26
1	A	775	PHE	N-CA-C	7.76	125.44	113.19
1	B	660	HIS	N-CA-C	6.68	118.22	111.07
1	D	888	LYS	N-CA-C	6.25	117.78	110.97
1	C	775	PHE	N-CA-C	6.22	123.72	113.89

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	3124	0	3066	112	0
1	B	3117	0	3073	95	0
1	C	3133	0	3088	111	0
1	D	3090	0	3012	127	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	1	0
2	D	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	22	0	18	3	0
5	A	31	0	40	0	0
All	All	12629	0	12345	443	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 18.

The worst 5 of 443 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:A:660:HIS:HB2	1:A:661:LEU:HA	1.53	0.90
1:B:649:LEU:HG	1:B:694:ILE:HD11	1.60	0.82
1:C:879:THR:HG21	1:C:921:THR:HG21	1.61	0.82
1:A:849:ILE:HD13	1:A:898:ARG:HG3	1.63	0.81
1:B:824:LYS:HE3	1:B:828:LYS:HD2	1.63	0.81

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	380/435 (87%)	331 (87%)	44 (12%)	5 (1%)	9	33
1	B	377/435 (87%)	348 (92%)	27 (7%)	2 (0%)	24	54
1	C	380/435 (87%)	346 (91%)	31 (8%)	3 (1%)	16	44
1	D	379/435 (87%)	345 (91%)	27 (7%)	7 (2%)	6	26
All	All	1516/1740 (87%)	1370 (90%)	129 (8%)	17 (1%)	11	38

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	659	ALA
1	C	866	GLY
1	D	661	LEU
1	B	735	GLU
1	B	927	ASP

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	337/387 (87%)	288 (86%)	49 (14%)	3	13
1	B	338/387 (87%)	289 (86%)	49 (14%)	3	13
1	C	339/387 (88%)	290 (86%)	49 (14%)	3	13
1	D	331/387 (86%)	273 (82%)	58 (18%)	2	8
All	All	1345/1548 (87%)	1140 (85%)	205 (15%)	3	10

5 of 205 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	676	LEU
1	C	925	ILE
1	D	930	VAL
1	C	750	ASN
1	C	860	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	593	ASN
1	A	680	HIS
1	D	910	HIS
1	C	877	ASN
1	D	877	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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	31L	A	1001	1	24,24,24	0.71	0	32,33,33	2.51	8 (25%)
5	PEU	A	1004	-	30,30,82	0.46	0	29,29,81	0.59	0
2	ADP	C	1001	3	28,29,29	1.48	5 (17%)	43,45,45	1.75	7 (16%)
2	ADP	B	1001	3	28,29,29	1.45	4 (14%)	43,45,45	1.78	7 (16%)
2	ADP	D	1001	3	28,29,29	1.49	4 (14%)	43,45,45	1.85	10 (23%)
2	ADP	A	1002	3	28,29,29	1.46	3 (10%)	43,45,45	1.93	9 (20%)

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	31L	A	1001	1	-	2/10/18/18	0/3/3/3
5	PEU	A	1004	-	-	12/28/28/80	-
2	ADP	C	1001	3	-	8/16/32/32	0/3/3/3
2	ADP	B	1001	3	-	7/16/32/32	0/3/3/3
2	ADP	D	1001	3	-	5/16/32/32	0/3/3/3
2	ADP	A	1002	3	-	0/16/32/32	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1002	ADP	C5-C4	5.21	1.48	1.39
2	B	1001	ADP	C5-C4	5.04	1.48	1.39
2	D	1001	ADP	C5-C4	5.03	1.48	1.39
2	C	1001	ADP	C5-C4	4.92	1.47	1.39
2	D	1001	ADP	C5-C6	2.95	1.49	1.41

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	31L	O07-C06-C04	8.38	123.30	114.53
2	C	1001	ADP	C5-C4-N3	-5.93	118.55	126.72
2	B	1001	ADP	C5-C4-N3	-5.92	118.56	126.72
2	A	1002	ADP	C5-C4-N3	-5.74	118.82	126.72
2	D	1001	ADP	C5-C4-N3	-5.40	119.28	126.72

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

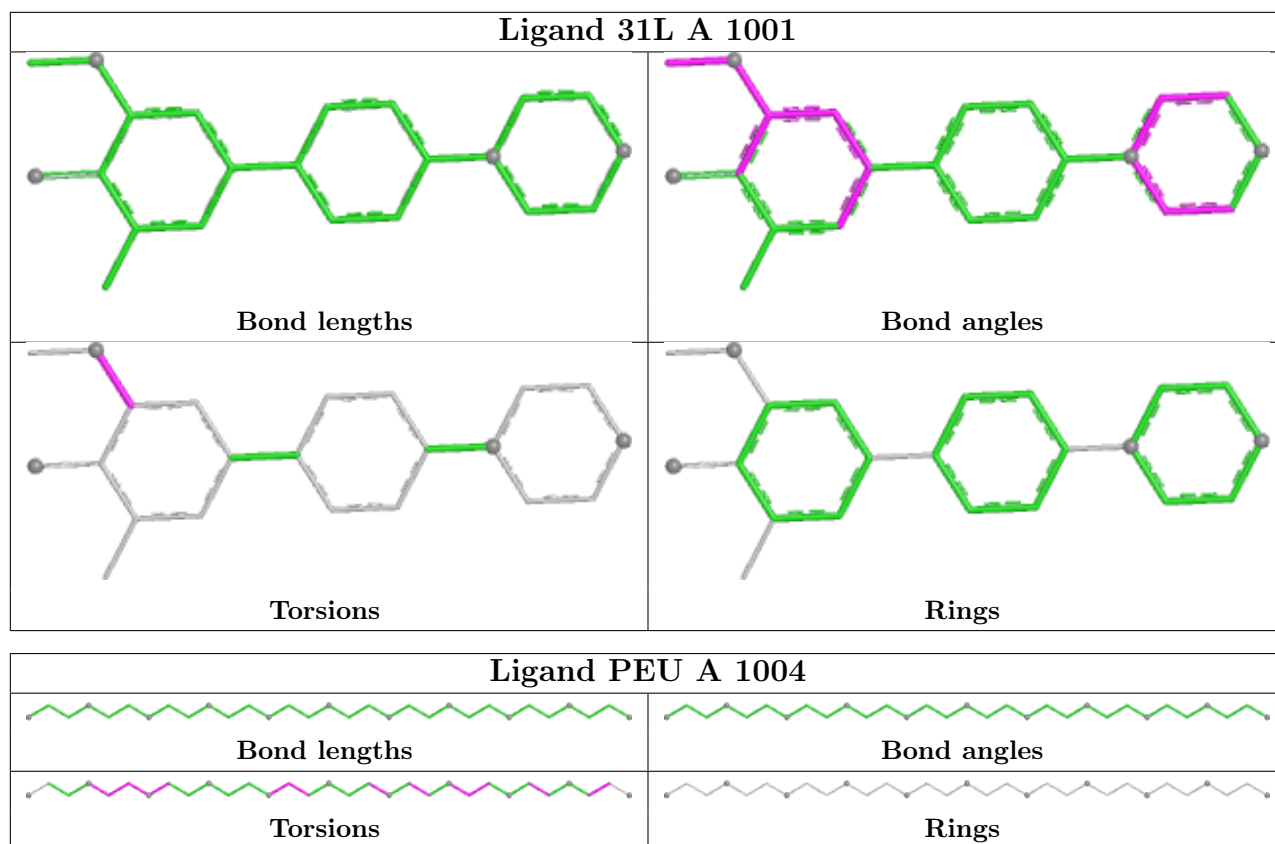
Mol	Chain	Res	Type	Atoms
2	B	1001	ADP	O4'-C4'-C5'-O5'
2	C	1001	ADP	C5'-O5'-PA-O1A
2	C	1001	ADP	C5'-O5'-PA-O3A
2	C	1001	ADP	O4'-C4'-C5'-O5'
2	C	1001	ADP	C3'-C4'-C5'-O5'

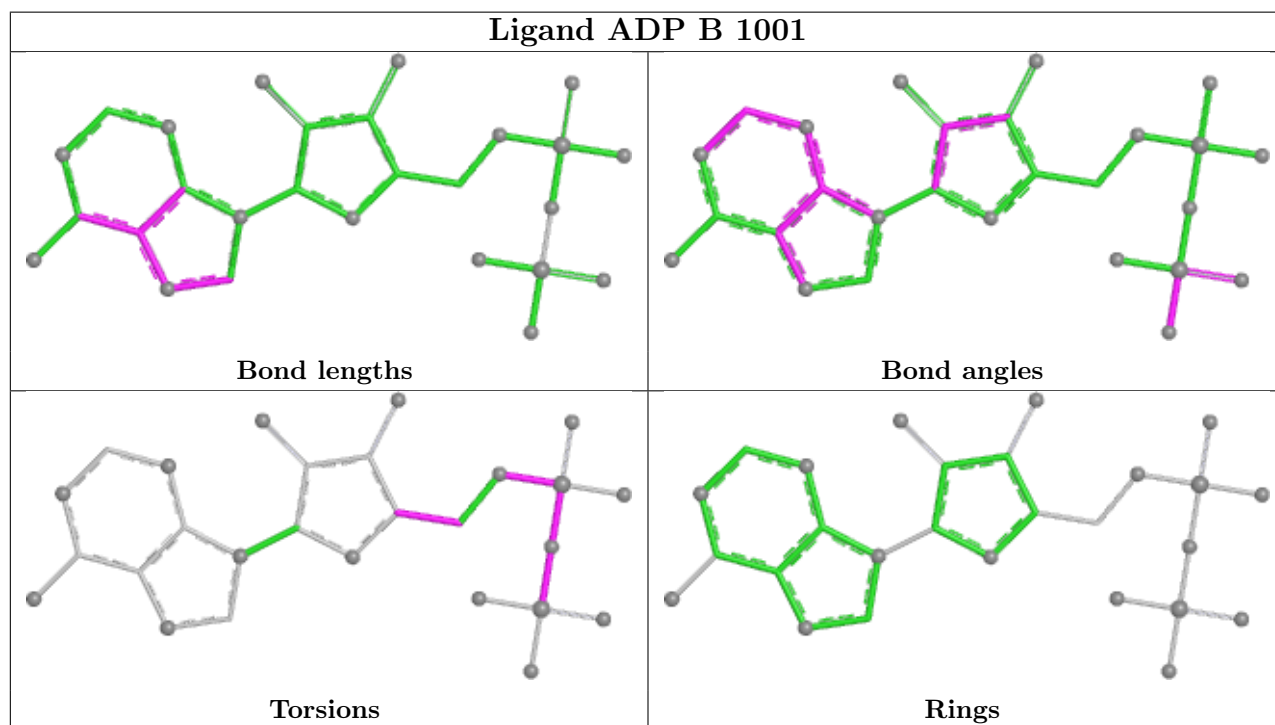
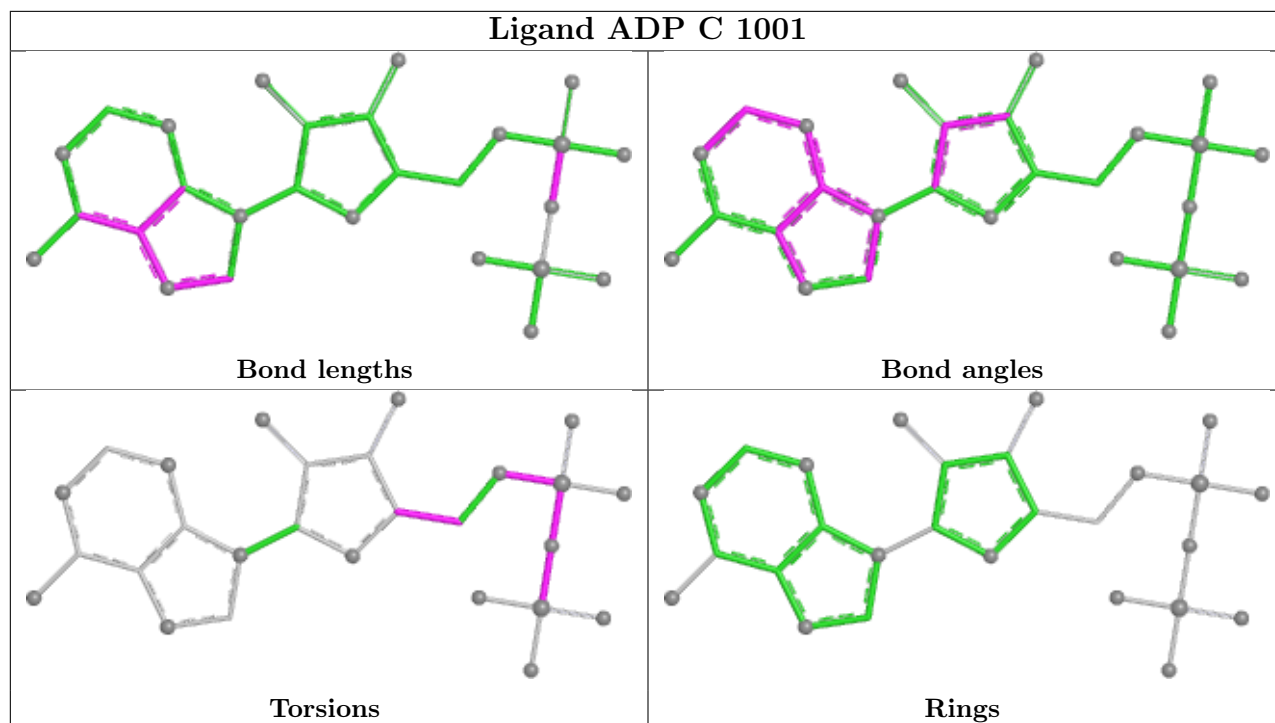
There are no ring outliers.

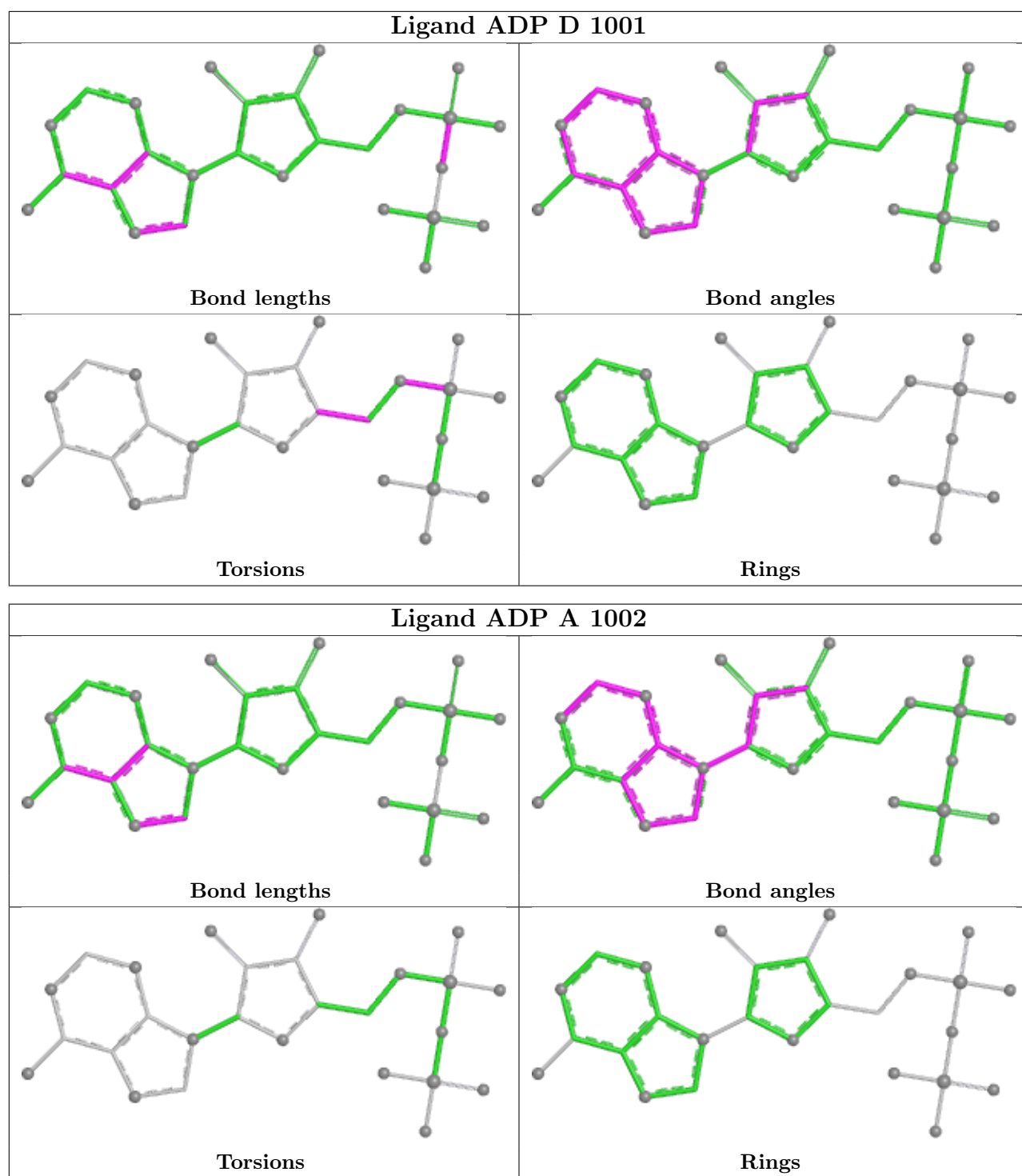
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	31L	3	0
2	C	1001	ADP	1	0
2	D	1001	ADP	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 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	386/435 (88%)	0.24	22 (5%) 29 22	13, 62, 119, 153	0
1	B	383/435 (88%)	0.23	10 (2%) 57 42	20, 68, 114, 134	0
1	C	386/435 (88%)	0.24	8 (2%) 63 48	29, 74, 122, 164	0
1	D	385/435 (88%)	0.85	41 (10%) 11 11	55, 105, 155, 183	0
All	All	1540/1740 (88%)	0.39	81 (5%) 32 24	13, 78, 135, 183	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	660	HIS	4.7
1	A	659	ALA	4.1
1	C	596	VAL	4.1
1	D	962	TRP	4.1
1	A	661	LEU	4.0

### 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](#)

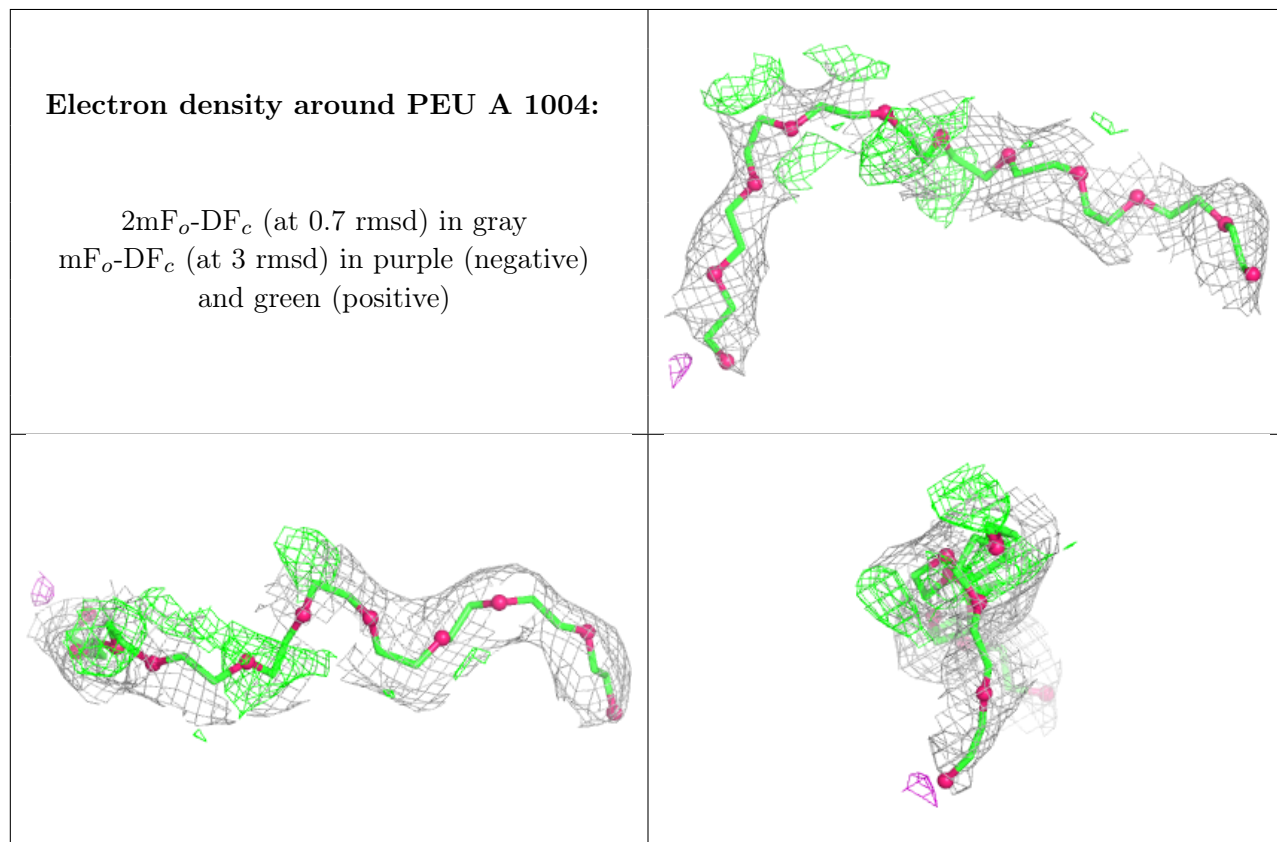
There are no oligosaccharides in this entry.

### 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, 95<sup>th</sup> 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.

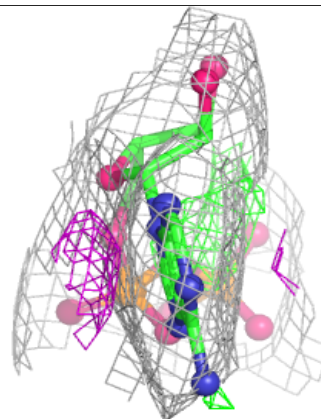
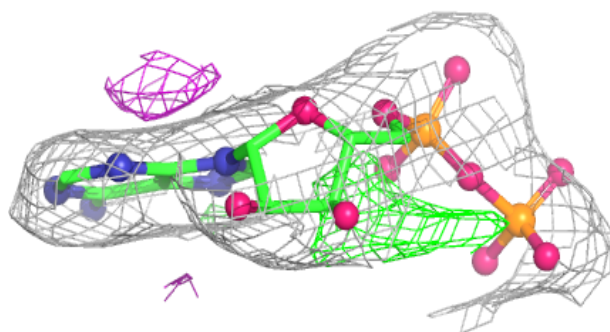
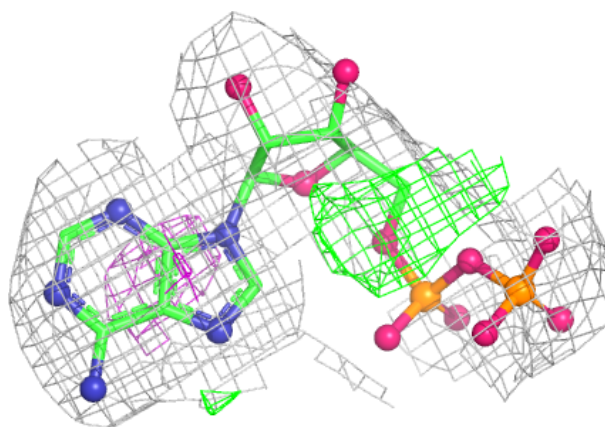
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEU	A	1004	31/83	0.72	0.20	36,76,91,98	0
3	MG	D	1002	1/1	0.83	0.14	109,109,109,109	0
2	ADP	D	1001	27/27	0.85	0.14	64,85,125,184	0
4	31L	A	1001	22/22	0.87	0.20	71,96,107,115	0
2	ADP	B	1001	27/27	0.92	0.09	25,54,79,132	0
2	ADP	C	1001	27/27	0.93	0.11	56,66,81,91	0
3	MG	A	1003	1/1	0.94	0.11	46,46,46,46	0
2	ADP	A	1002	27/27	0.94	0.10	21,46,74,154	0
3	MG	B	1002	1/1	0.97	0.08	35,35,35,35	0
3	MG	C	1002	1/1	0.98	0.10	34,34,34,34	0

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

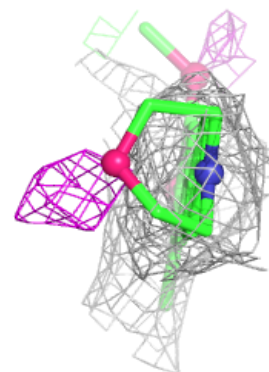
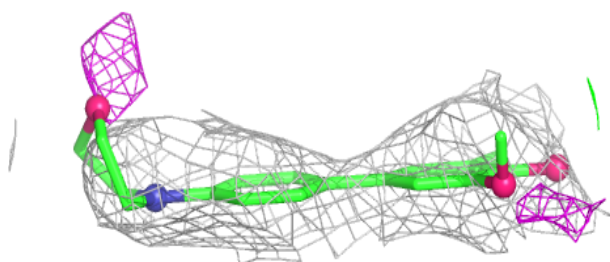
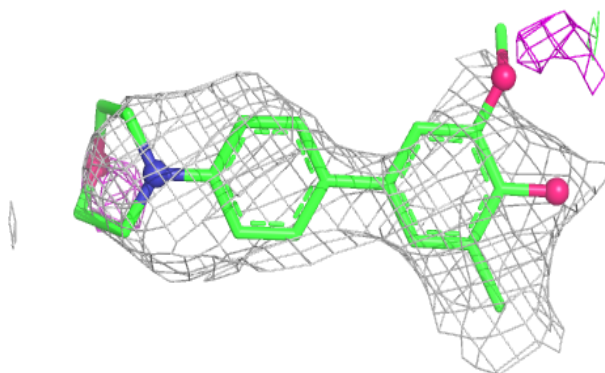


**Electron density around ADP D 1001:**

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

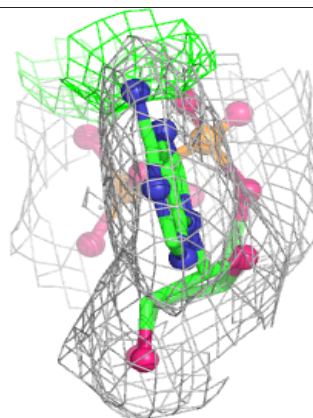
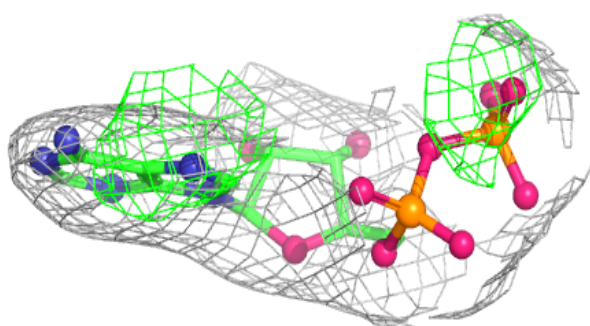
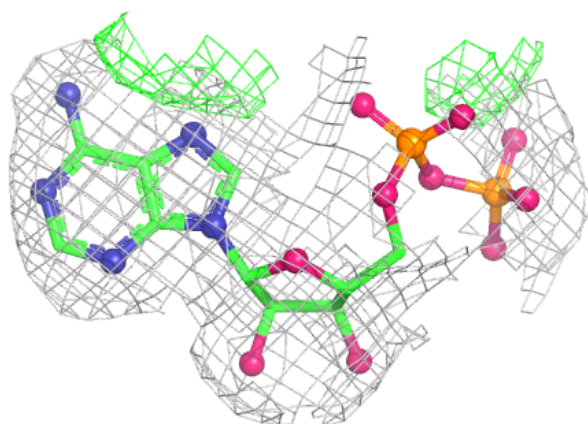
**Electron density around 31L A 1001:**

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

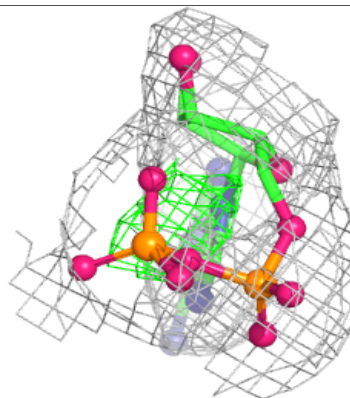
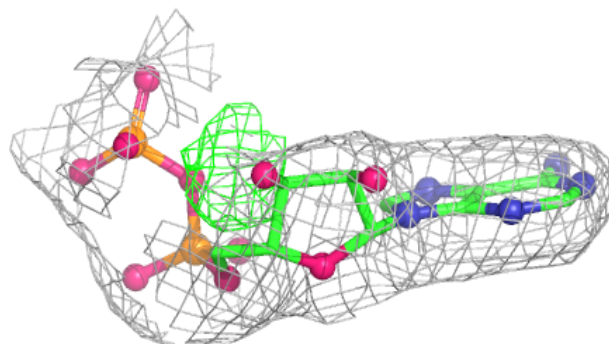
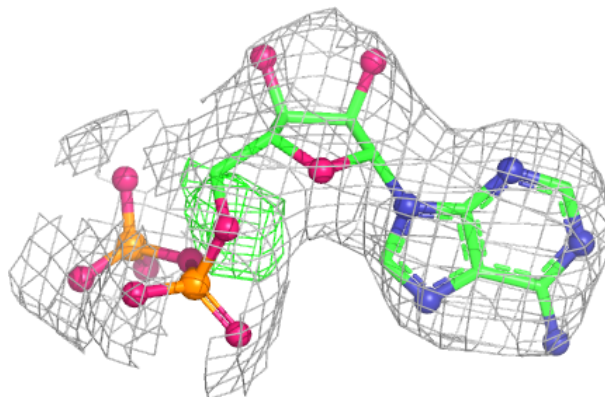


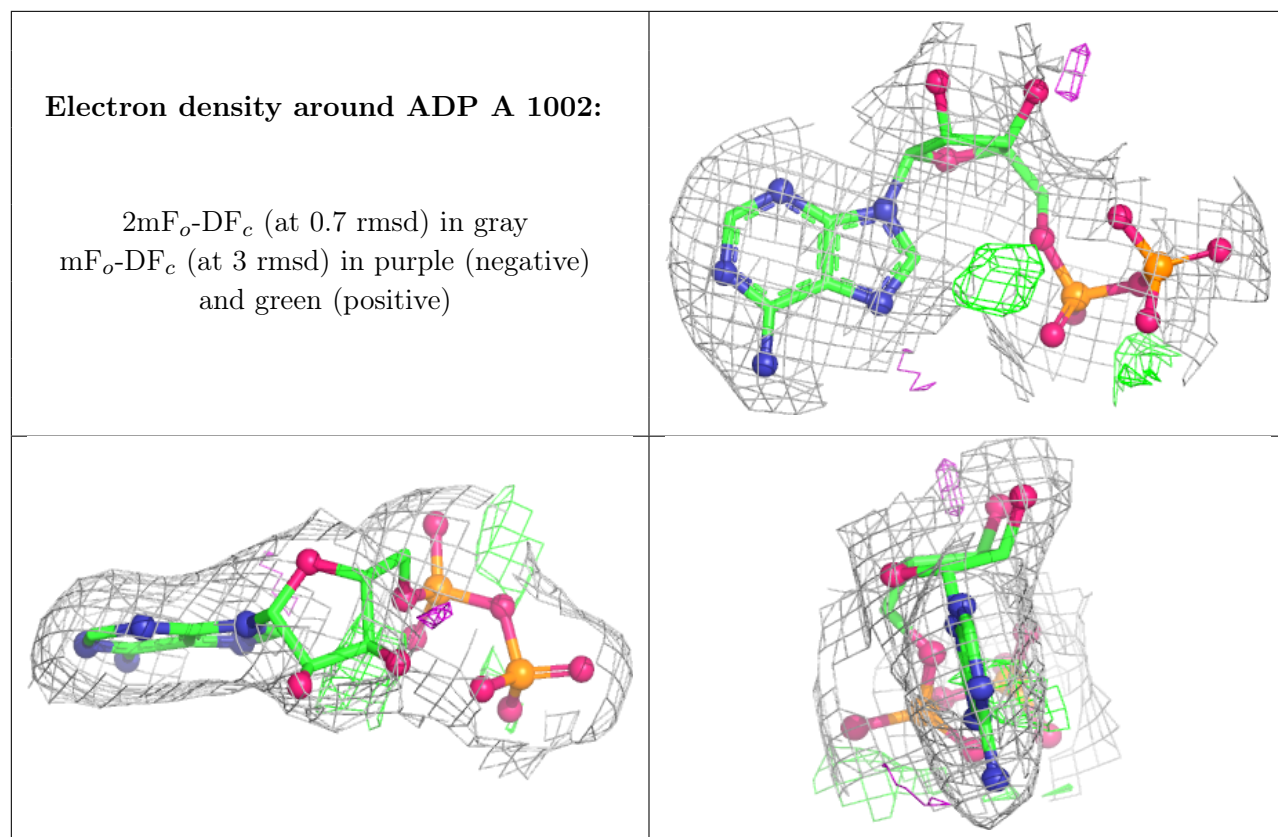
**Electron density around ADP B 1001:**

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

**Electron density around ADP C 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 [i](#)

There are no such residues in this entry.