WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2023 – 04:31 AM EDT

PDB ID	:	1GLF
Title	:	CRYSTAL STRUCTURES OF ESCHERICHIA COLI GLYCEROL KINASE AND THE MUTANT A65T IN AN INACTIVE TETRAMER: CONFORMATIONAL CHANGES AND IMPLICATIONS FOR ALLOSTERIC REGULATION
Authors	:	Feese, M.D.; Faber, H.R.; Bystrom, C.E.; Pettigrew, D.W.; Remington, S.J.
Deposited on	:	1998-08-30
Resolution	:	2.62 Å(reported)

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

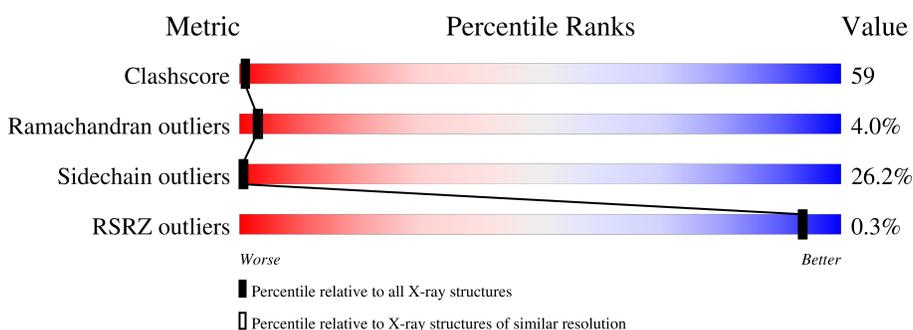|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.62 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	Percentile Ranks	Value
Clashscore		59
Ramachandran outliers		4.0%
Sidechain outliers		26.2%
RSRZ outliers		0.3%

Worse   *Better*

■ Percentile relative to all X-ray structures
⧠ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	O	501	22% 45% 24% 8% •
1	X	501	21% 49% 24% 5% •
1	Y	501	25% 47% 23% •
1	Z	501	% 23% 50% 19% 7% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

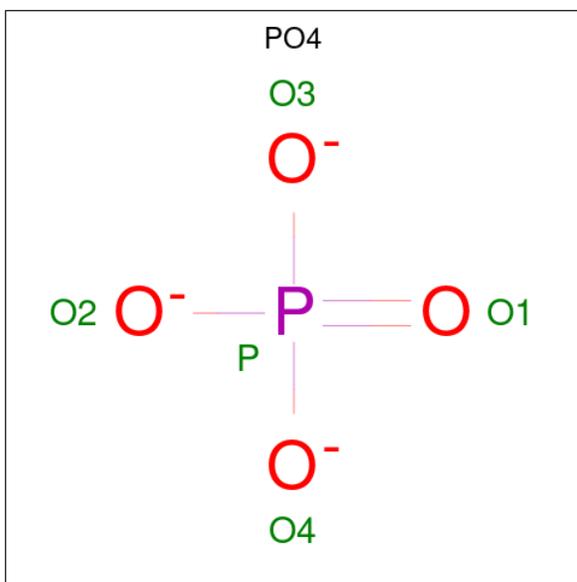| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	O	601	-	-	X	-
3	ADP	O	607	X	-	-	-
4	GOL	Z	605	-	-	X	-

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 15981 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 PROTEIN (GLYCEROL KINASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	498	Total	C	N	O	S	0	0	0
			3913	2467	684	743	19			
1	Y	499	Total	C	N	O	S	0	0	0
			3909	2465	683	742	19			
1	Z	498	Total	C	N	O	S	0	0	0
			3907	2465	682	741	19			
1	X	498	Total	C	N	O	S	0	0	0
			3910	2467	684	740	19			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	P	0	0
			5	4	1		
2	Y	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is A D E N O S I N E - 5 ' - D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
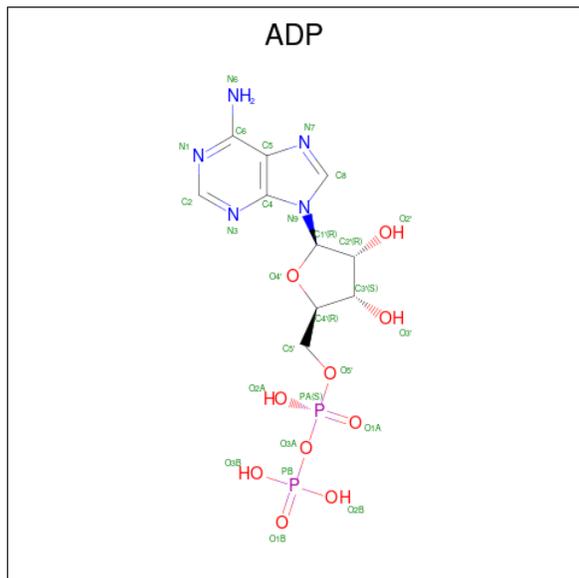
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	Y	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	Z	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	X	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

C3

OH O3

C1   C2

HO   OH

O1   O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	1	Total 6	C 3	O 3	0	0
4	Y	1	Total 6	C 3	O 3	0	0
4	Z	1	Total 6	C 3	O 3	0	0
4	X	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	46	Total 46	O 46	0	0
5	Y	51	Total 51	O 51	0	0
5	Z	53	Total 53	O 53	0	0
5	X	50	Total 50	O 50	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.
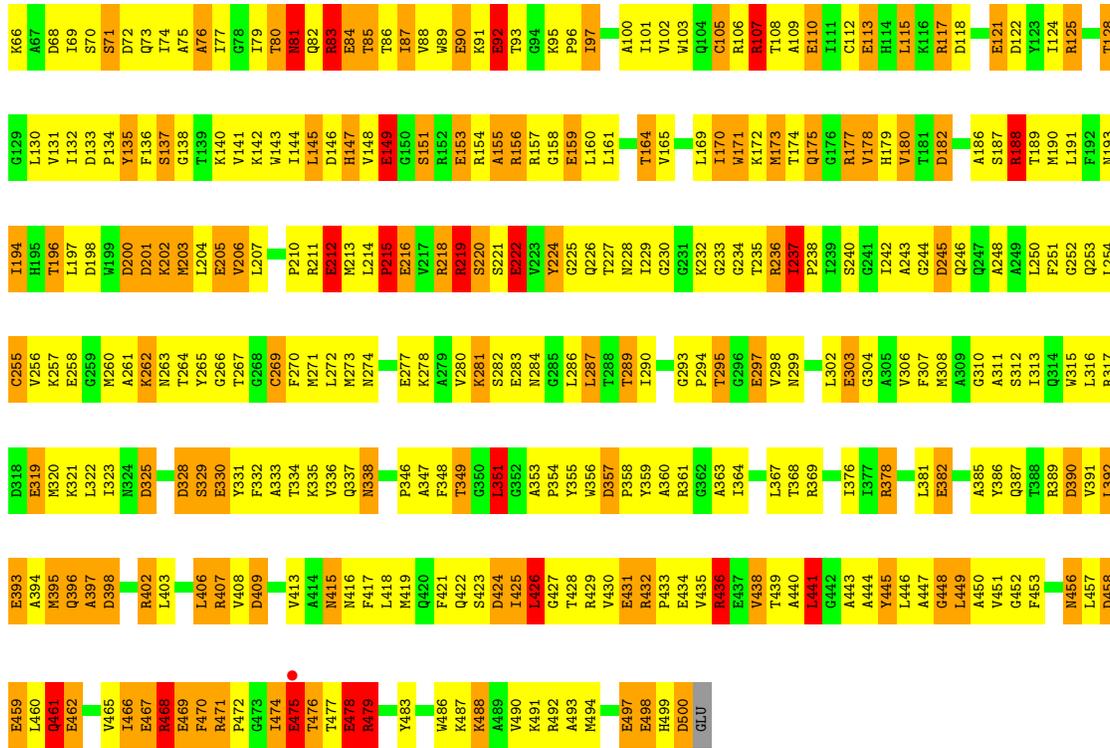
- Molecule 1: PROTEIN (GLYCEROL KINASE)
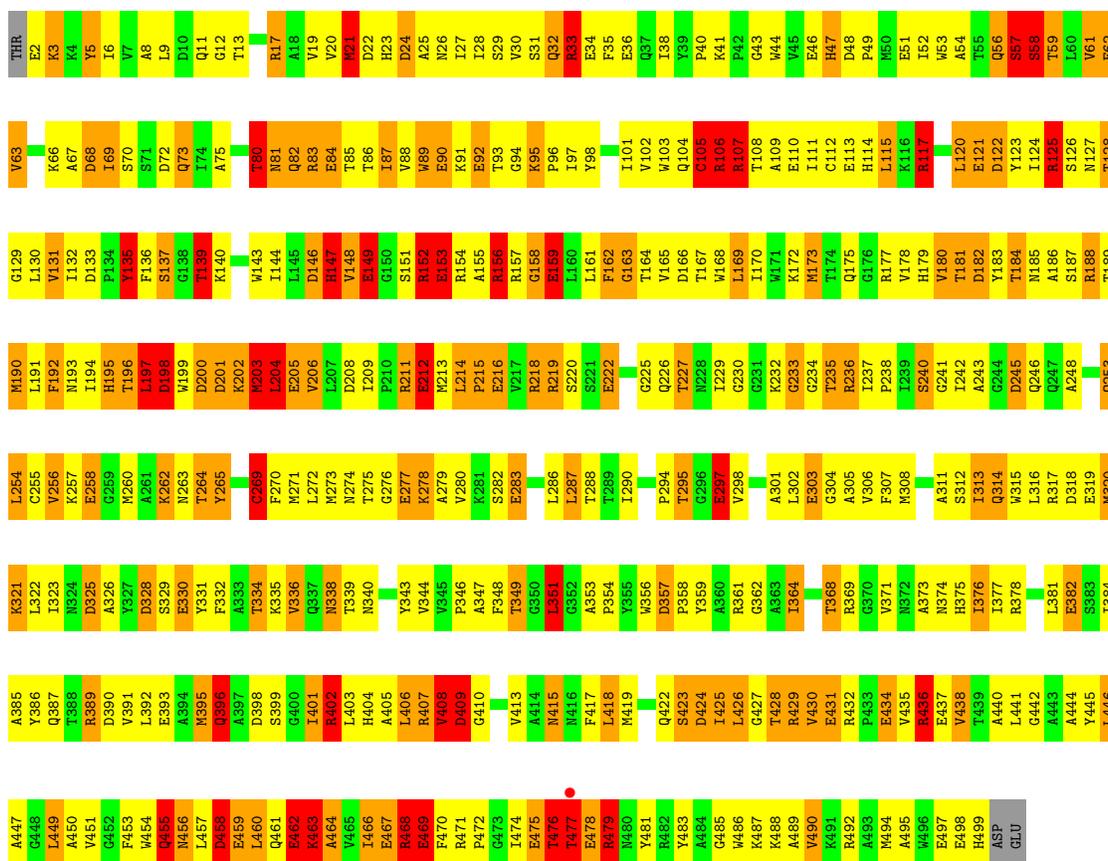
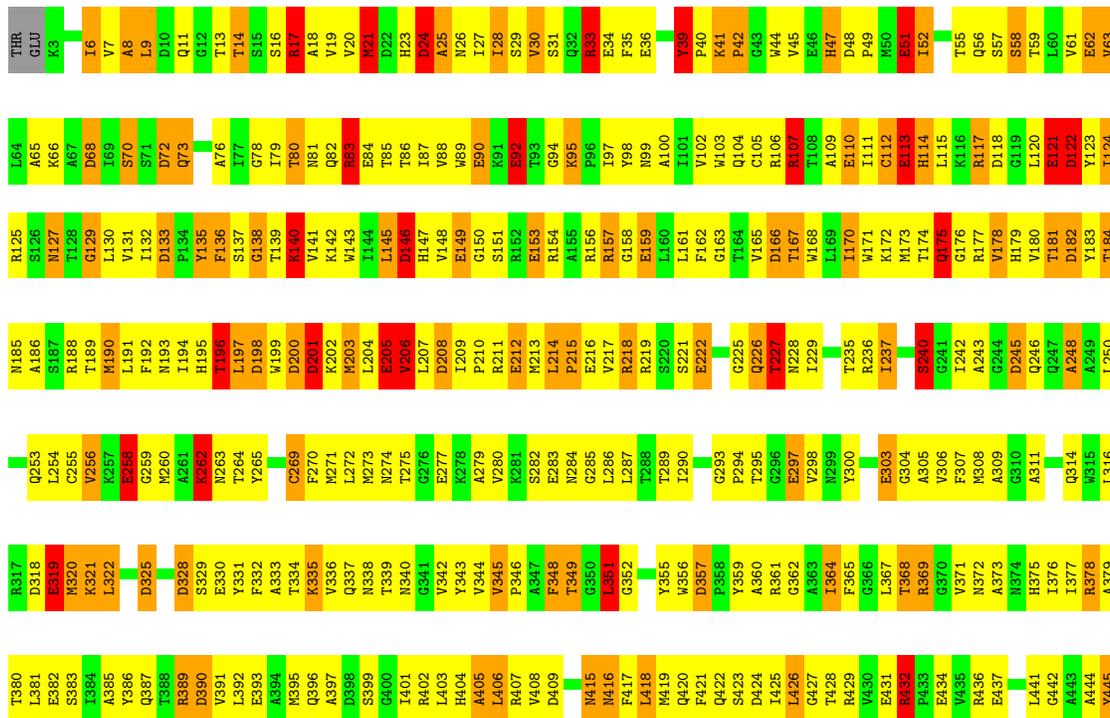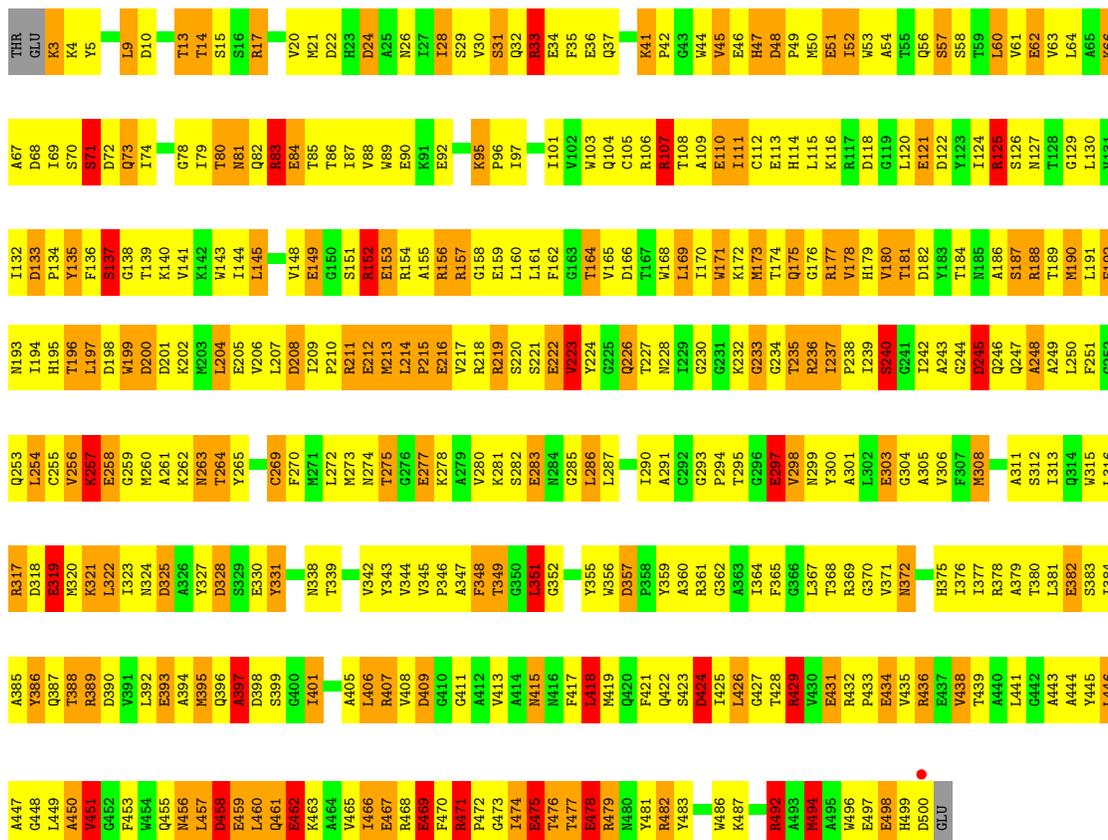- Molecule 1: PROTEIN (GLYCEROL KINASE)

• Molecule 1: PROTEIN (GLYCEROL KINASE)

• Molecule 1: PROTEIN (GLYCEROL KINASE)

Chain X:

21%   49%   24%   5% •
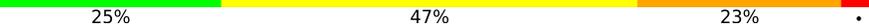
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.10Å 117.40Å 108.40Å 90.00° 93.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.62 20.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	84.0 (20.00-2.62) 84.4 (20.00-2.62)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.63Å)	Xtriage
Refinement program	TNT 5F-6	Depositor
R, R_{free}	0.146 , (Not available) 0.138 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	24.5	Xtriage
Anisotropy	1.015	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 117.9	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	0.97	EDS
Total number of atoms	15981	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4046e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

[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: PO4, GOL, ADP

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	O	1.34	41/3993 (1.0%)	1.82	99/5416 (1.8%)
1	X	1.34	36/3990 (0.9%)	1.75	79/5411 (1.5%)
1	Y	1.32	38/3989 (1.0%)	1.77	84/5412 (1.6%)
1	Z	1.32	32/3987 (0.8%)	1.79	88/5408 (1.6%)
All	All	1.33	147/15959 (0.9%)	1.78	350/21647 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	1	1
1	Y	1	0
All	All	2	1

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	121	GLU	CD-OE1	10.08	1.36	1.25
1	O	475	GLU	CD-OE1	9.83	1.36	1.25
1	Y	277	GLU	CD-OE1	9.55	1.36	1.25
1	X	478	GLU	CD-OE1	9.33	1.35	1.25
1	Z	149	GLU	CD-OE1	9.21	1.35	1.25

The worst 5 of 350 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	479	ARG	NE-CZ-NH2	-21.02	109.79	120.30
1	O	479	ARG	NE-CZ-NH1	15.27	127.93	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	200	ASP	CB-CG-OD1	-14.20	105.52	118.30
1	O	245	ASP	CB-CG-OD2	-13.98	105.72	118.30
1	Y	177	ARG	NE-CZ-NH1	12.26	126.43	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	Y	155	ALA	CA
1	X	31	SER	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	478	GLU	Sidechain

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	O	3913	0	3830	495	0
1	X	3910	0	3833	478	0
1	Y	3909	0	3822	435	0
1	Z	3907	0	3826	459	0
2	O	5	0	0	2	0
2	Y	5	0	0	1	0
3	O	27	0	11	1	0
3	X	27	0	11	1	0
3	Y	27	0	12	0	0
3	Z	27	0	12	0	0
4	O	6	0	8	2	0
4	X	6	0	8	2	0
4	Y	6	0	8	3	0
4	Z	6	0	8	9	0
5	O	46	0	0	9	0
5	X	50	0	0	6	0
5	Y	51	0	0	11	0
5	Z	53	0	0	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15981	0	15389	1827	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 59.

The worst 5 of 1827 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:Y:200:ASP:HB3	1:Y:203:MET:HB2	1.14	1.13
1:Y:155:ALA:HB2	1:Y:160:LEU:HB2	1.10	1.08
1:Z:468:ARG:HH11	1:Z:468:ARG:HG3	1.17	1.07
1:O:84:GLU:HB2	1:O:103:TRP:HB3	1.31	1.06
1:X:422:GLN:HE21	1:X:426:LEU:HD22	1.18	1.06

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	O	496/501 (99%)	409 (82%)	65 (13%)	22 (4%)	2	3
1	X	496/501 (99%)	411 (83%)	69 (14%)	16 (3%)	4	5
1	Y	497/501 (99%)	414 (83%)	60 (12%)	23 (5%)	2	2
1	Z	496/501 (99%)	425 (86%)	52 (10%)	19 (4%)	3	4
All	All	1985/2004 (99%)	1659 (84%)	246 (12%)	80 (4%)	3	3

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	149	GLU
1	O	159	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	203	MET
1	O	204	LEU
1	O	233	GLY

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	O	406/412 (98%)	294 (72%)	112 (28%)	0	1
1	X	405/412 (98%)	295 (73%)	110 (27%)	0	1
1	Y	405/412 (98%)	305 (75%)	100 (25%)	0	1
1	Z	405/412 (98%)	303 (75%)	102 (25%)	0	1
All	All	1621/1648 (98%)	1197 (74%)	424 (26%)	0	1

5 of 424 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	73	GLN
1	Z	364	ILE
1	X	401	ILE
1	Z	112	CYS
1	Z	205	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	415	ASN
1	X	415	ASN
1	Z	226	GLN
1	X	337	GLN
1	X	499	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	$\#|Z| > 2$
2	PO4	Y	602	-	4,4,4	2.76	3 (75%)	6,6,6	0.86	0
3	ADP	Y	608	-	24,29,29	1.17	2 (8%)	29,45,45	2.58	9 (31%)
2	PO4	O	601	-	4,4,4	2.07	1 (25%)	6,6,6	1.07	0
4	GOL	Y	604	-	5,5,5	0.69	0	5,5,5	0.49	0
3	ADP	X	610	-	24,29,29	1.35	3 (12%)	29,45,45	2.82	6 (20%)
4	GOL	X	606	-	5,5,5	0.62	0	5,5,5	0.74	0
4	GOL	O	603	-	5,5,5	0.61	0	5,5,5	0.25	0
3	ADP	Z	609	-	24,29,29	0.86	0	29,45,45	2.27	7 (24%)
3	ADP	O	607	-	24,29,29	1.43	2 (8%)	29,45,45	3.20	8 (27%)
4	GOL	Z	605	-	5,5,5	0.52	0	5,5,5	0.70	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
3	ADP	Y	608	-	-	8/12/32/32	0/3/3/3
4	GOL	Y	604	-	-	0/4/4/4	-
3	ADP	X	610	-	-	8/12/32/32	0/3/3/3
4	GOL	X	606	-	-	2/4/4/4	-
4	GOL	O	603	-	-	2/4/4/4	-
3	ADP	Z	609	-	-	2/12/32/32	0/3/3/3
3	ADP	O	607	-	1/1/6/6	0/12/32/32	0/3/3/3
4	GOL	Z	605	-	-	3/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	607	ADP	O2'-C2'	4.17	1.52	1.43
3	O	607	ADP	C2'-C1'	-4.02	1.47	1.53
3	X	610	ADP	C2-N3	3.65	1.38	1.32
2	O	601	PO4	P-O4	-3.48	1.44	1.54
2	Y	602	PO4	P-O2	3.34	1.64	1.54

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	607	ADP	C1'-N9-C4	-12.88	104.00	126.64
3	X	610	ADP	C1'-N9-C4	-9.87	109.31	126.64
3	Y	608	ADP	C1'-N9-C4	-9.79	109.44	126.64
3	X	610	ADP	O2'-C2'-C3'	8.09	138.00	111.82
3	Z	609	ADP	C1'-N9-C4	7.85	140.43	126.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	O	607	ADP	C2'

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Y	608	ADP	PA-O3A-PB-O2B
3	Y	608	ADP	C5'-O5'-PA-O1A
3	Y	608	ADP	C5'-O5'-PA-O2A
3	Y	608	ADP	C3'-C4'-C5'-O5'
3	X	610	ADP	PA-O3A-PB-O2B

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	602	PO4	1	0
2	O	601	PO4	2	0
4	Y	604	GOL	3	0
3	X	610	ADP	1	0
4	X	606	GOL	2	0
4	O	603	GOL	2	0
3	O	607	ADP	1	0
4	Z	605	GOL	9	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 ADP Y 608

Bond lengths   Bond angles

Torsions   Rings

Ligand ADP X 610

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP Z 609

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP O 607

Bond lengths

Bond angles

Torsions

Rings
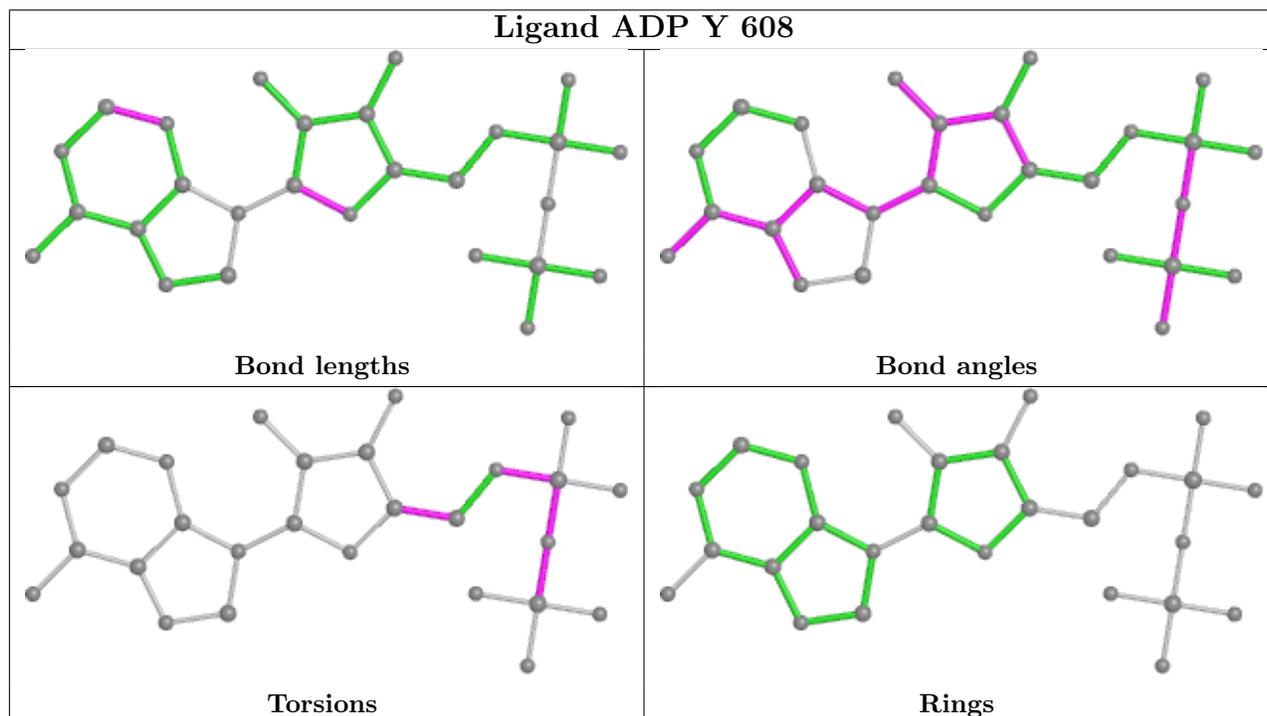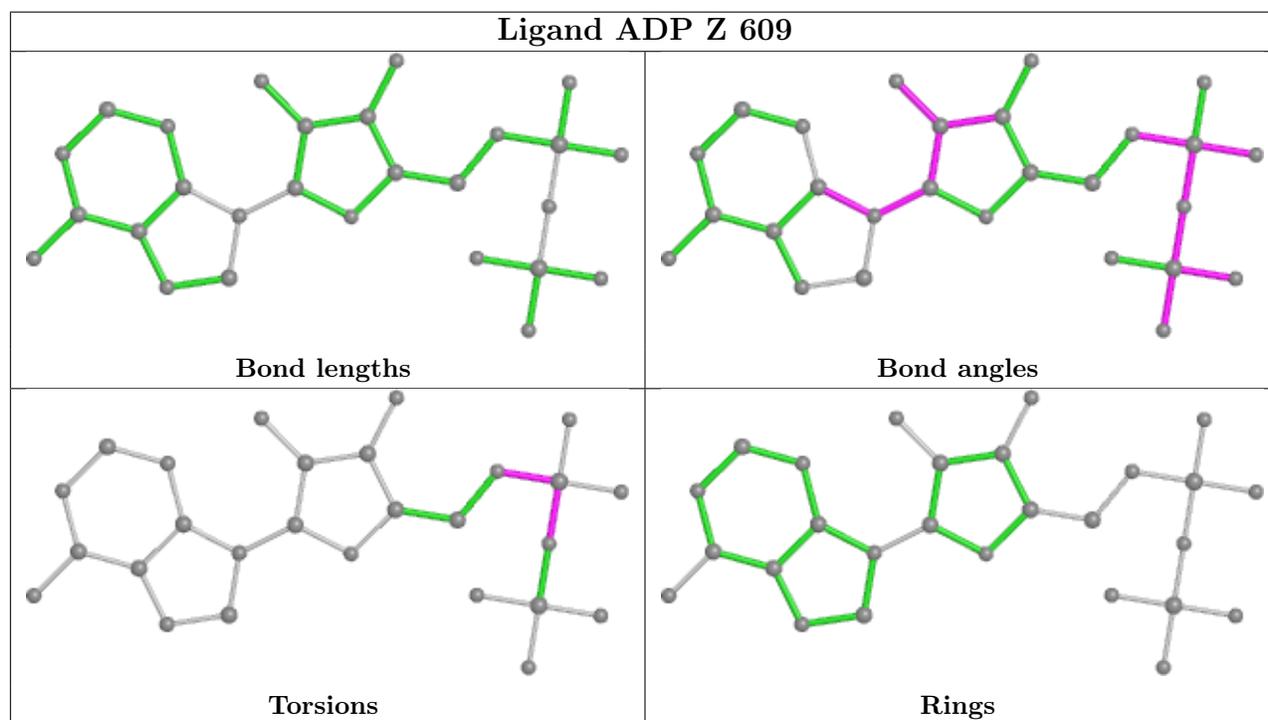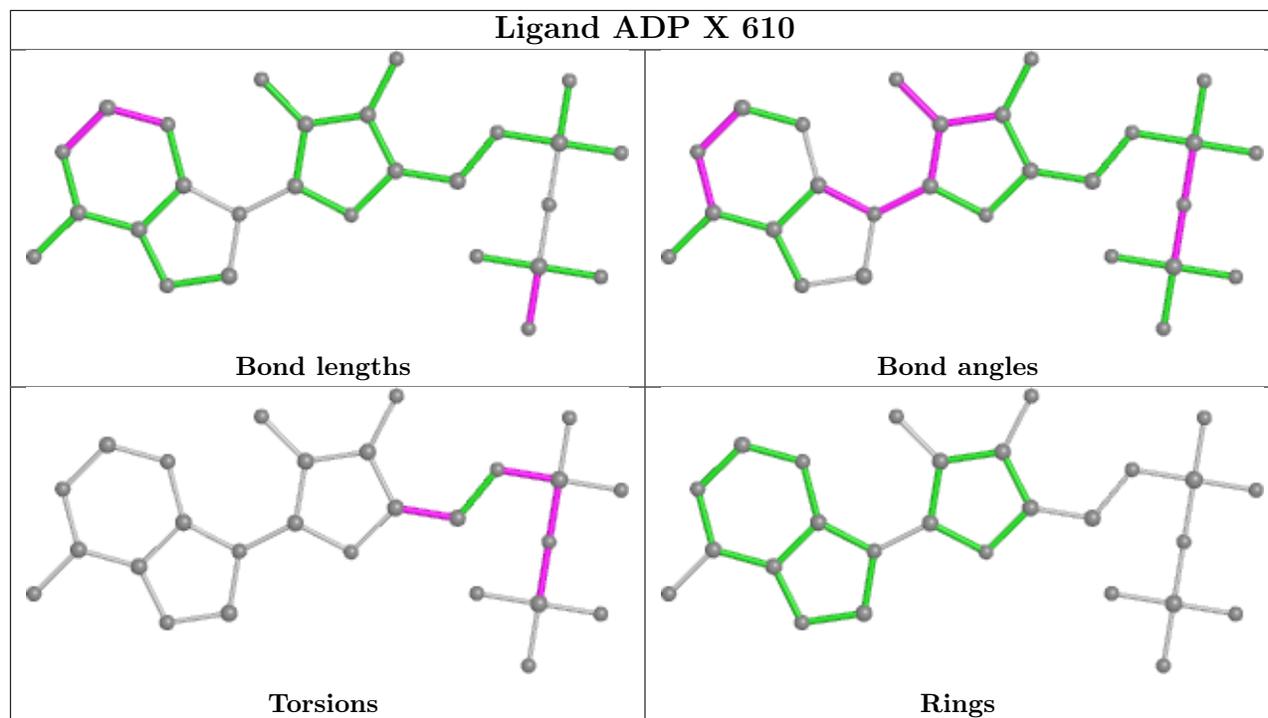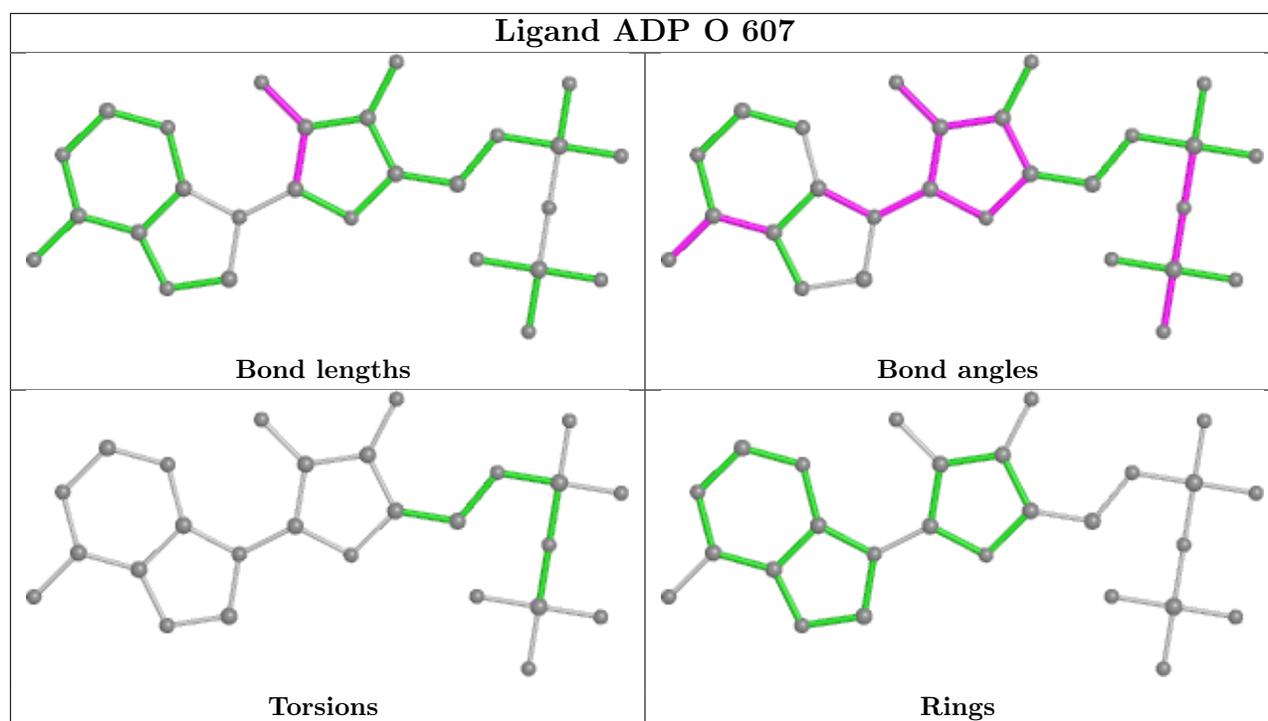
5.7 Other polymers ⓘ

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	O	498/501 (99%)	-0.90	1 (0%)	95	95	7, 28, 61, 75	0
1	X	498/501 (99%)	-0.92	1 (0%)	95	95	7, 27, 60, 75	0
1	Y	499/501 (99%)	-0.91	1 (0%)	95	95	6, 27, 59, 73	0
1	Z	498/501 (99%)	-1.01	3 (0%)	89	88	6, 24, 58, 75	0
All	All	1993/2004 (99%)	-0.94	6 (0%)	94	93	6, 26, 60, 75	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	500	ASP	3.1
1	O	477	THR	2.9
1	Y	475	GLU	2.7
1	Z	473	GLY	2.6
1	X	500	ASP	2.2

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

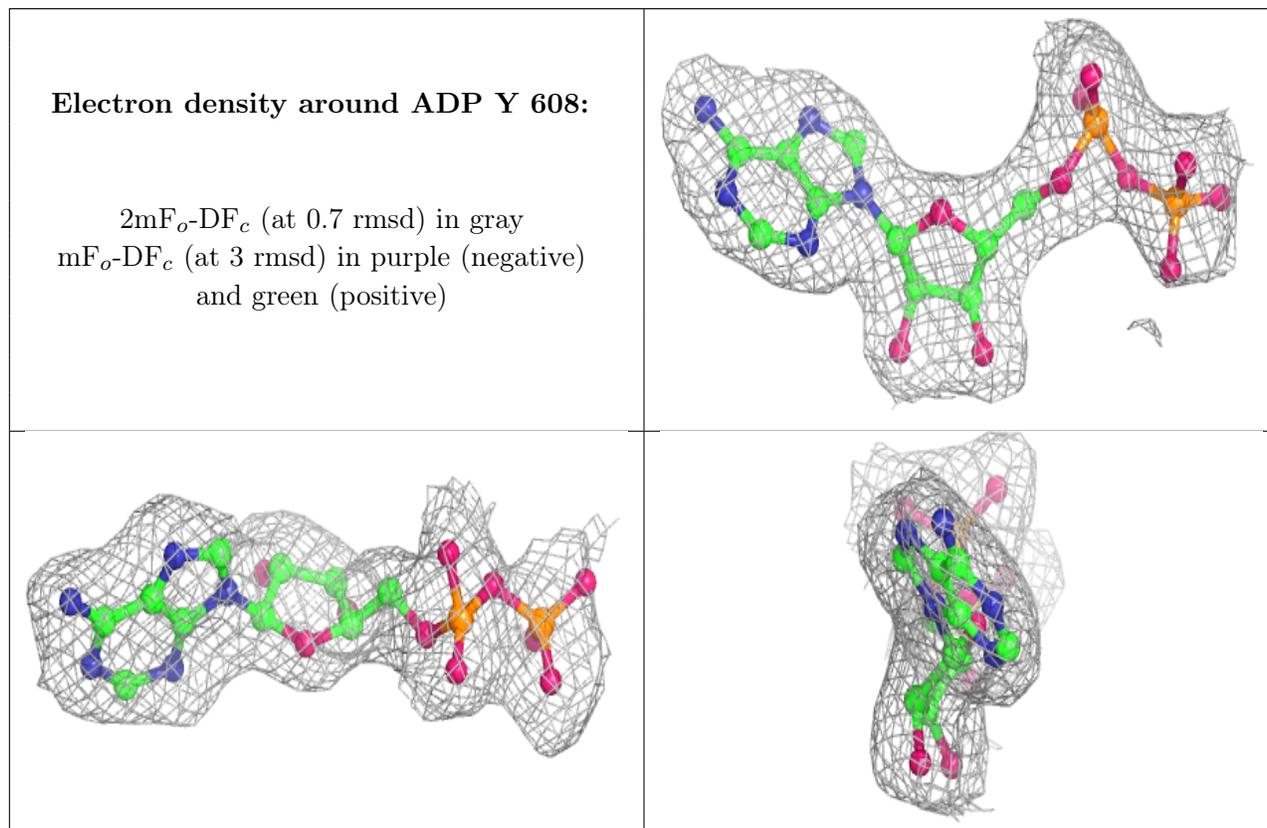There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	PO4	Y	602	5/5	0.97	0.12	29,31,53,75	0
4	GOL	O	603	6/6	0.97	0.12	5,7,49,55	0
3	ADP	Y	608	27/27	0.98	0.08	5,27,75,75	0
3	ADP	Z	609	27/27	0.98	0.09	5,26,57,75	0
3	ADP	X	610	27/27	0.98	0.10	5,49,75,75	0
3	ADP	O	607	27/27	0.98	0.09	5,39,75,75	0
4	GOL	X	606	6/6	0.98	0.10	5,18,38,43	0
4	GOL	Y	604	6/6	0.99	0.13	5,19,42,48	0
4	GOL	Z	605	6/6	0.99	0.08	5,10,25,51	0
2	PO4	O	601	5/5	0.99	0.09	5,31,56,59	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 Y 608:

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

Electron density around ADP Z 609:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
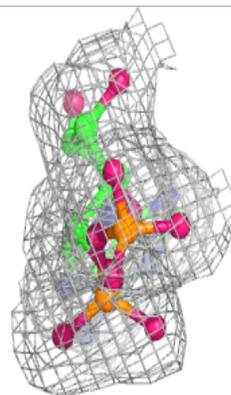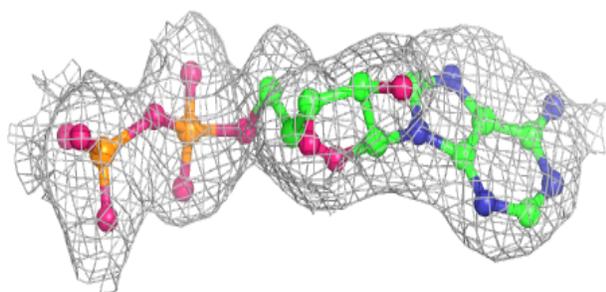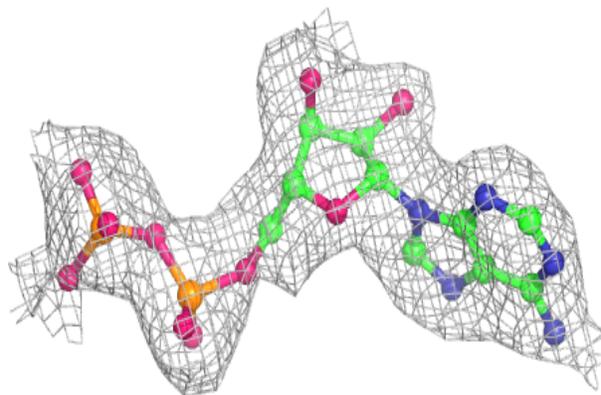
Electron density around ADP X 610:

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

Electron density around ADP O 607:

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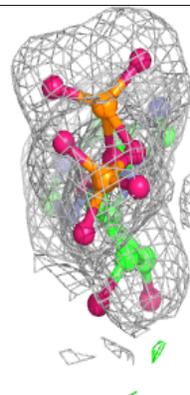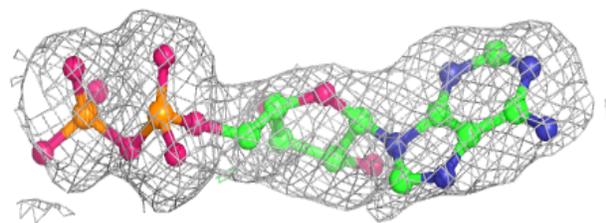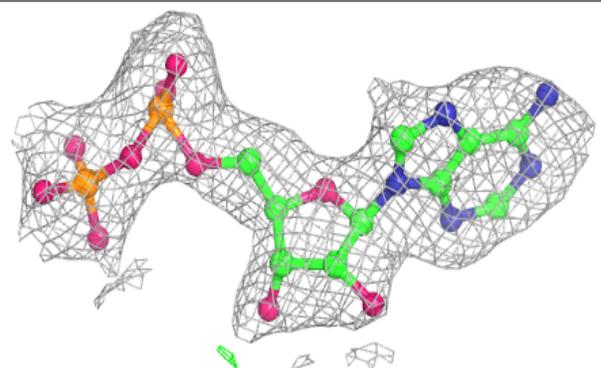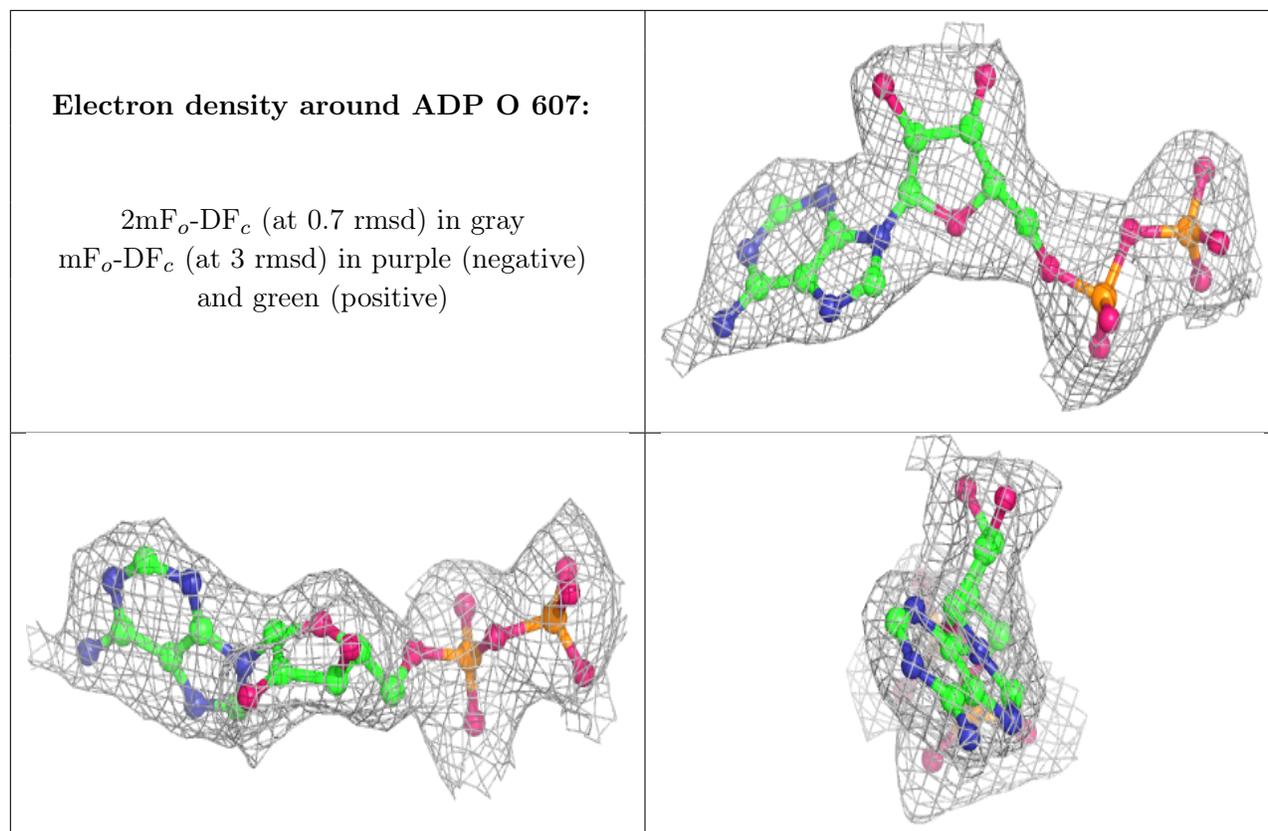
6.5 Other polymers (i)

There are no such residues in this entry.