



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 7, 2021 – 12:06 AM EDT

PDB ID : 3E3O
Title : Glycogen phosphorylase R state-IMP complex
Authors : Leonidas, D.D.; Zographos, S.E.; Oikonomakos, N.G.
Deposited on : 2008-08-07
Resolution : 2.60 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.23.1
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) : 2.23.1

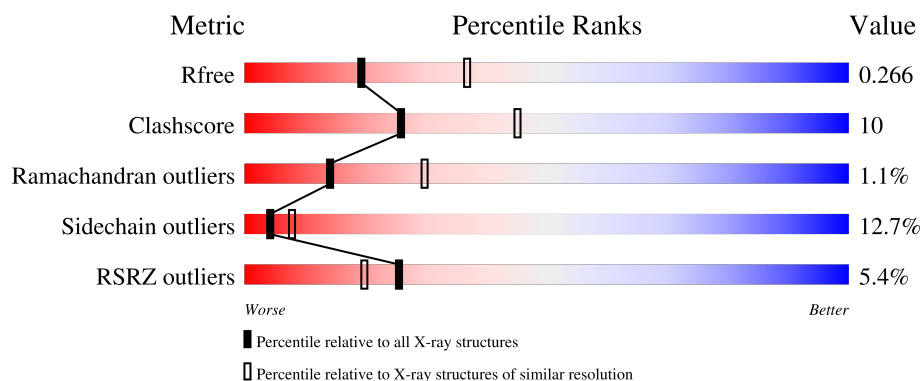
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 $\leq 5\%$. 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	842	
1	B	842	
1	C	842	
1	D	842	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26630 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 Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	P	S	0	0	0
			6601	4206	1164	1201	1	29			
1	B	812	Total	C	N	O	P	S	0	0	0
			6616	4215	1167	1204	1	29			
1	C	808	Total	C	N	O	P	S	0	0	0
			6589	4198	1165	1196	1	29			
1	D	806	Total	C	N	O	P	S	0	0	0
			6576	4190	1159	1197	1	29			

There are 4 discrepancies between the modelled and reference sequences:

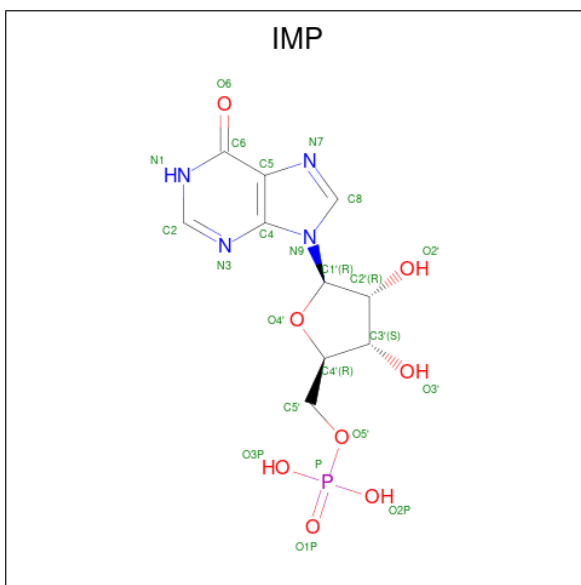
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is INOSINIC ACID (three-letter code: IMP) (formula: C₁₀H₁₃N₄O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

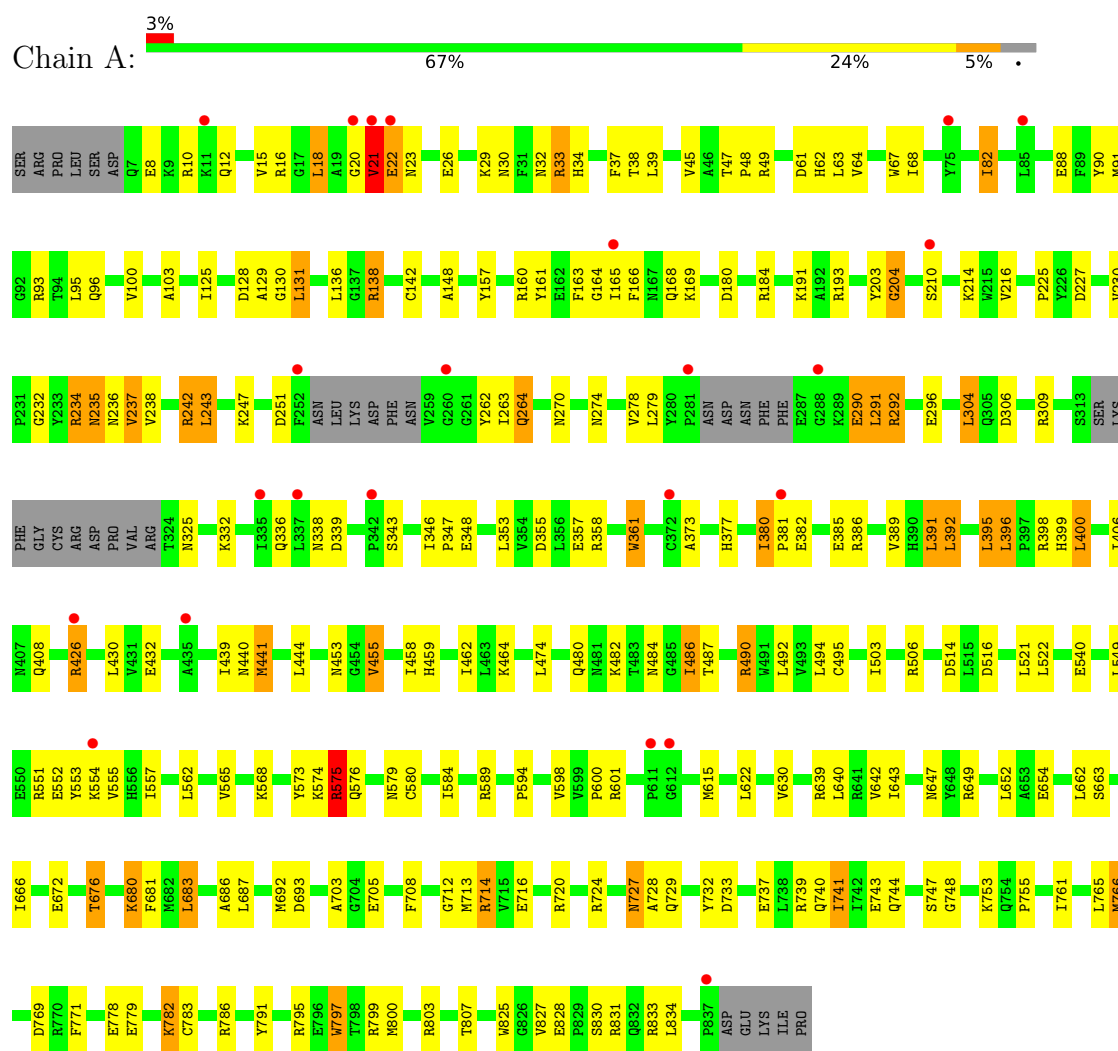
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	33	Total	O	0	0
			33	33		
4	C	33	Total	O	0	0
			33	33		
4	D	20	Total	O	0	0
			20	20		

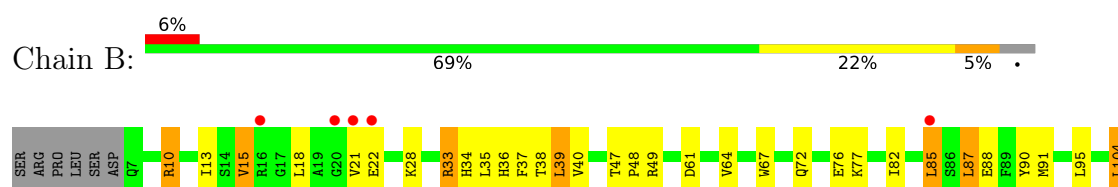
3 Residue-property plots

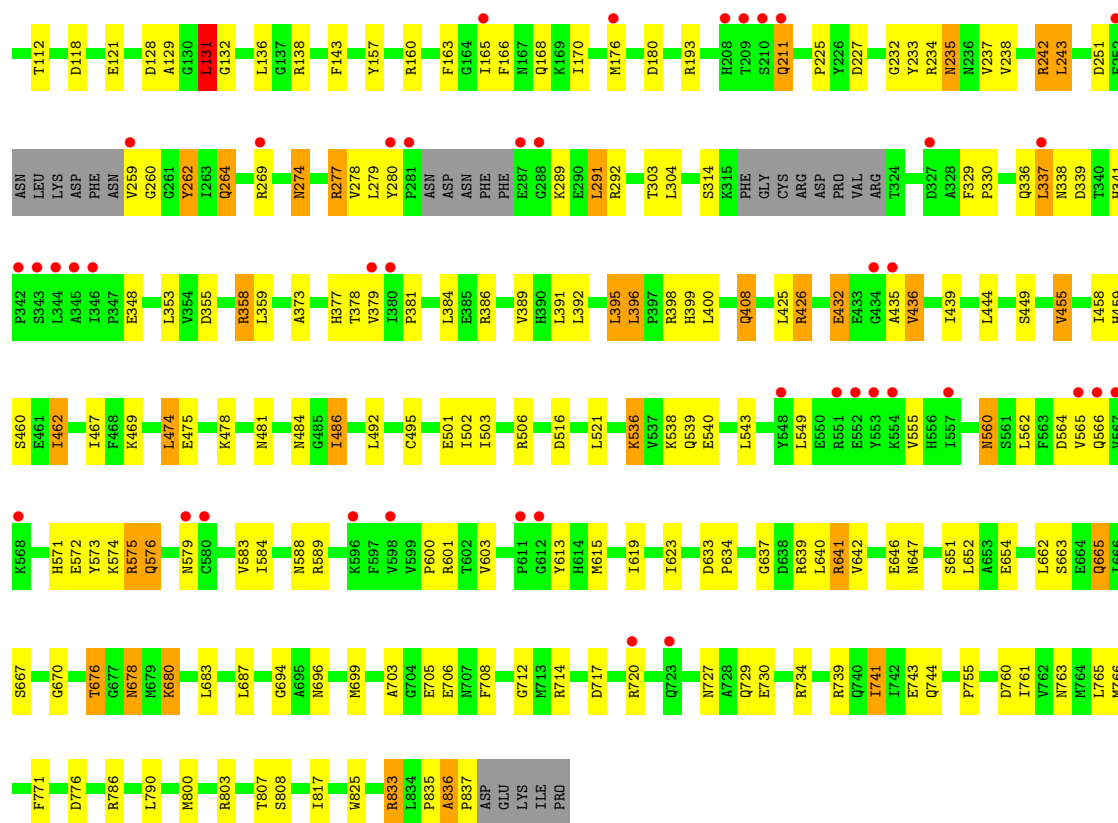
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glycogen phosphorylase, muscle form

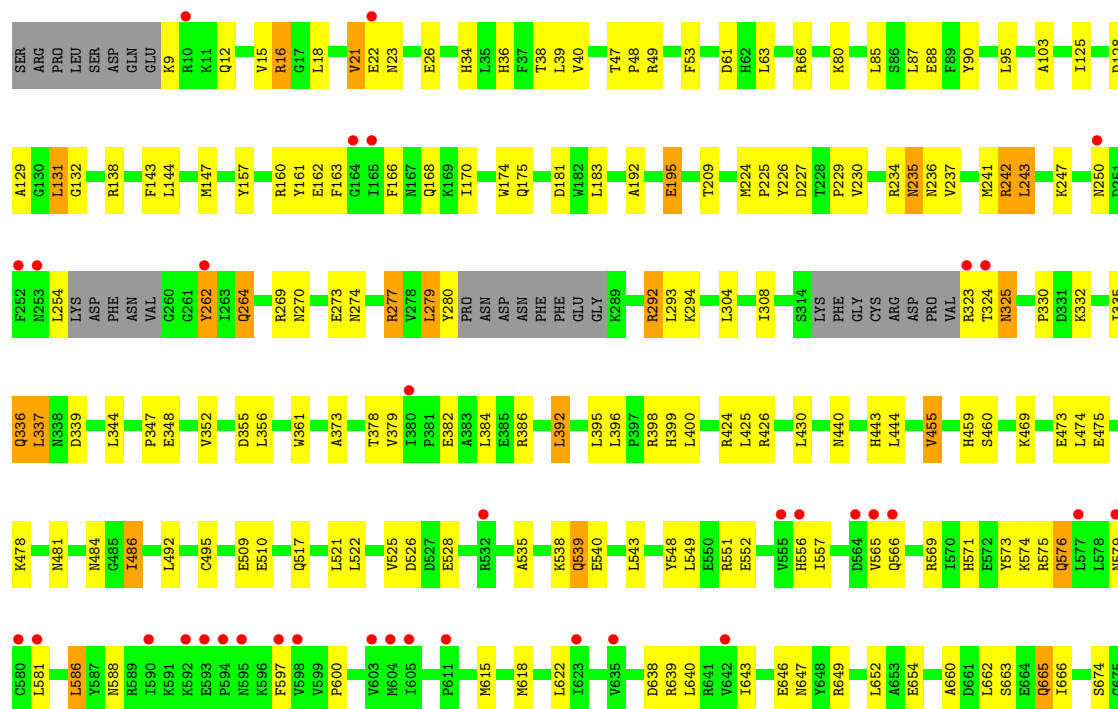


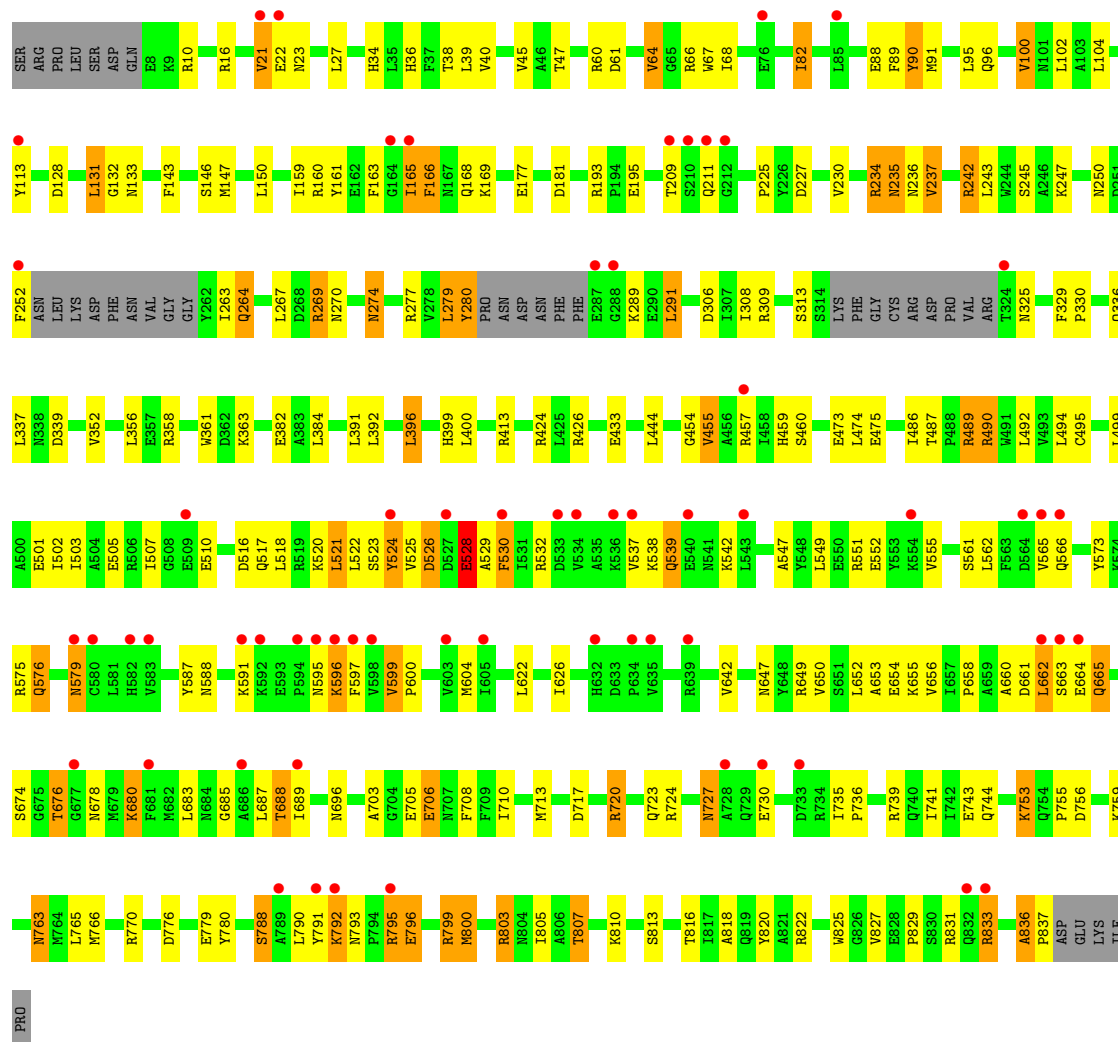
• Molecule 1: Glycogen phosphorylase, muscle form





• Molecule 1: Glycogen phosphorylase, muscle form





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.68Å 188.45Å 87.85Å 90.00° 109.10° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.60) 99.3 (29.67-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.201 , 0.267 0.201 , 0.266	Depositor DCC
R_{free} test set	5573 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26630	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, LLP, IMP

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	0.55	3/6721 (0.0%)	0.71	8/9091 (0.1%)
1	B	0.48	0/6736	0.65	2/9110 (0.0%)
1	C	0.49	0/6708	0.65	1/9072 (0.0%)
1	D	0.66	16/6695 (0.2%)	0.67	5/9055 (0.1%)
All	All	0.55	19/26860 (0.1%)	0.67	16/36328 (0.0%)

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	C	0	1

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	528	GLU	CG-CD	11.22	1.68	1.51
1	D	524	TYR	CG-CD2	10.60	1.52	1.39
1	D	524	TYR	CE1-CZ	10.11	1.51	1.38
1	D	796	GLU	CD-OE2	9.90	1.36	1.25
1	D	661	ASP	CG-OD2	7.83	1.43	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	GLY	N-CA-C	-9.41	89.57	113.10
1	D	799	ARG	NE-CZ-NH2	-8.73	115.93	120.30
1	D	524	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	D	803	ARG	NE-CZ-NH2	-7.76	116.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	NE-CZ-NH2	-7.76	116.42	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	324	THR	Peptide

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	6601	0	6554	147	0
1	B	6616	0	6572	139	0
1	C	6589	0	6550	134	0
1	D	6576	0	6528	151	0
2	A	5	0	0	0	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	23	0	11	1	0
3	B	23	0	11	0	0
3	C	23	0	11	0	0
3	D	23	0	11	1	0
4	A	30	0	0	0	0
4	B	33	0	0	2	0
4	C	33	0	0	2	0
4	D	20	0	0	1	0
All	All	26630	0	26248	552	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 10.

The worst 5 of 552 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:D:836:ALA:HB1	1:D:837:PRO:HA	1.30	1.06
1:A:395:LEU:HD12	1:A:396:LEU:HD22	1.38	1.02
1:A:455:VAL:H	1:A:459:HIS:HD2	1.15	0.94
1:B:85:LEU:HD21	1:B:303:THR:HG21	1.49	0.94
1:A:783:CYS:SG	1:A:786:ARG:NH2	2.42	0.93

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	801/842 (95%)	744 (93%)	46 (6%)	11 (1%)	11	22
1	B	803/842 (95%)	758 (94%)	36 (4%)	9 (1%)	14	30
1	C	799/842 (95%)	751 (94%)	40 (5%)	8 (1%)	15	32
1	D	797/842 (95%)	724 (91%)	65 (8%)	8 (1%)	15	32
All	All	3200/3368 (95%)	2977 (93%)	187 (6%)	36 (1%)	14	30

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	166	PHE
1	C	21	VAL
1	C	22	GLU
1	C	166	PHE
1	A	166	PHE

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	699/730 (96%)	604 (86%)	95 (14%)	3	6
1	B	701/730 (96%)	615 (88%)	86 (12%)	4	9
1	C	698/730 (96%)	617 (88%)	81 (12%)	5	10
1	D	697/730 (96%)	604 (87%)	93 (13%)	4	7
All	All	2795/2920 (96%)	2440 (87%)	355 (13%)	4	8

5 of 355 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	517	GLN
1	D	269	ARG
1	C	576	GLN
1	C	783	CYS
1	D	392	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	576	GLN
1	D	274	ASN
1	C	665	GLN
1	D	34	HIS
1	D	453	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
1	LLP	A	680	1	23,24,25	1.76	4 (17%)	25,32,34	1.32	4 (16%)
1	LLP	B	680	1	23,24,25	1.80	4 (17%)	25,32,34	1.65	5 (20%)
1	LLP	C	680	1	23,24,25	1.69	5 (21%)	25,32,34	1.44	5 (20%)
1	LLP	D	680	1	23,24,25	1.66	4 (17%)	25,32,34	1.35	6 (24%)

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
1	LLP	A	680	1	-	0/16/17/19	0/1/1/1
1	LLP	B	680	1	-	0/16/17/19	0/1/1/1
1	LLP	C	680	1	-	3/16/17/19	0/1/1/1
1	LLP	D	680	1	-	5/16/17/19	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	680	LLP	O3-C3	-6.12	1.22	1.37
1	A	680	LLP	O3-C3	-5.90	1.23	1.37
1	D	680	LLP	O3-C3	-5.76	1.23	1.37
1	C	680	LLP	O3-C3	-5.56	1.24	1.37
1	A	680	LLP	C4-C4'	2.91	1.52	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	680	LLP	OP4-C5'-C5	4.25	117.44	109.35
1	A	680	LLP	OP4-C5'-C5	3.42	115.87	109.35
1	B	680	LLP	CE-NZ-C4'	-3.10	109.37	118.90
1	B	680	LLP	OP2-P-OP4	-3.03	98.68	106.73
1	C	680	LLP	C5-C6-N1	-2.90	118.99	123.82

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	680	LLP	C5'-OP4-P-OP3
1	D	680	LLP	C5'-OP4-P-OP1
1	D	680	LLP	C5'-OP4-P-OP2
1	D	680	LLP	C5'-OP4-P-OP3
1	C	680	LLP	C5'-OP4-P-OP2

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	680	LLP	2	0
1	B	680	LLP	2	0
1	C	680	LLP	2	0
1	D	680	LLP	6	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	SO4	D	901	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	B	902	-	4,4,4	0.14	0	6,6,6	0.49	0
2	SO4	A	901	-	4,4,4	0.15	0	6,6,6	0.26	0
2	SO4	B	901	-	4,4,4	0.17	0	6,6,6	0.10	0
2	SO4	D	900	-	4,4,4	0.17	0	6,6,6	0.33	0
3	IMP	B	920	-	21,25,25	1.48	3 (14%)	23,38,38	1.77	4 (17%)
2	SO4	C	901	-	4,4,4	0.13	0	6,6,6	0.30	0
3	IMP	D	920	-	21,25,25	1.46	3 (14%)	23,38,38	1.54	3 (13%)
3	IMP	C	920	-	21,25,25	1.59	3 (14%)	23,38,38	1.66	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	900	-	4,4,4	0.15	0	6,6,6	0.43	0
3	IMP	A	920	-	21,25,25	1.50	3 (14%)	23,38,38	1.60	4 (17%)
2	SO4	C	900	-	4,4,4	0.15	0	6,6,6	0.15	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	IMP	C	920	-	-	0/6/26/26	0/3/3/3
3	IMP	A	920	-	-	0/6/26/26	0/3/3/3
3	IMP	B	920	-	-	2/6/26/26	0/3/3/3
3	IMP	D	920	-	-	3/6/26/26	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	920	IMP	C2-N3	4.46	1.39	1.32
3	A	920	IMP	C2-N3	4.44	1.39	1.32
3	C	920	IMP	C2-N3	4.12	1.38	1.32
3	B	920	IMP	C2-N3	3.91	1.38	1.32
3	B	920	IMP	C6-N1	3.66	1.39	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	920	IMP	N3-C2-N1	-6.19	119.01	128.68
3	C	920	IMP	N3-C2-N1	-5.95	119.37	128.68
3	D	920	IMP	N3-C2-N1	-5.57	119.97	128.68
3	A	920	IMP	N3-C2-N1	-5.17	120.59	128.68
3	A	920	IMP	C3'-C2'-C1'	3.12	105.67	100.98

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	920	IMP	C5'-O5'-P-O1P
3	B	920	IMP	C3'-C4'-C5'-O5'
3	B	920	IMP	O4'-C4'-C5'-O5'
3	D	920	IMP	C5'-O5'-P-O2P

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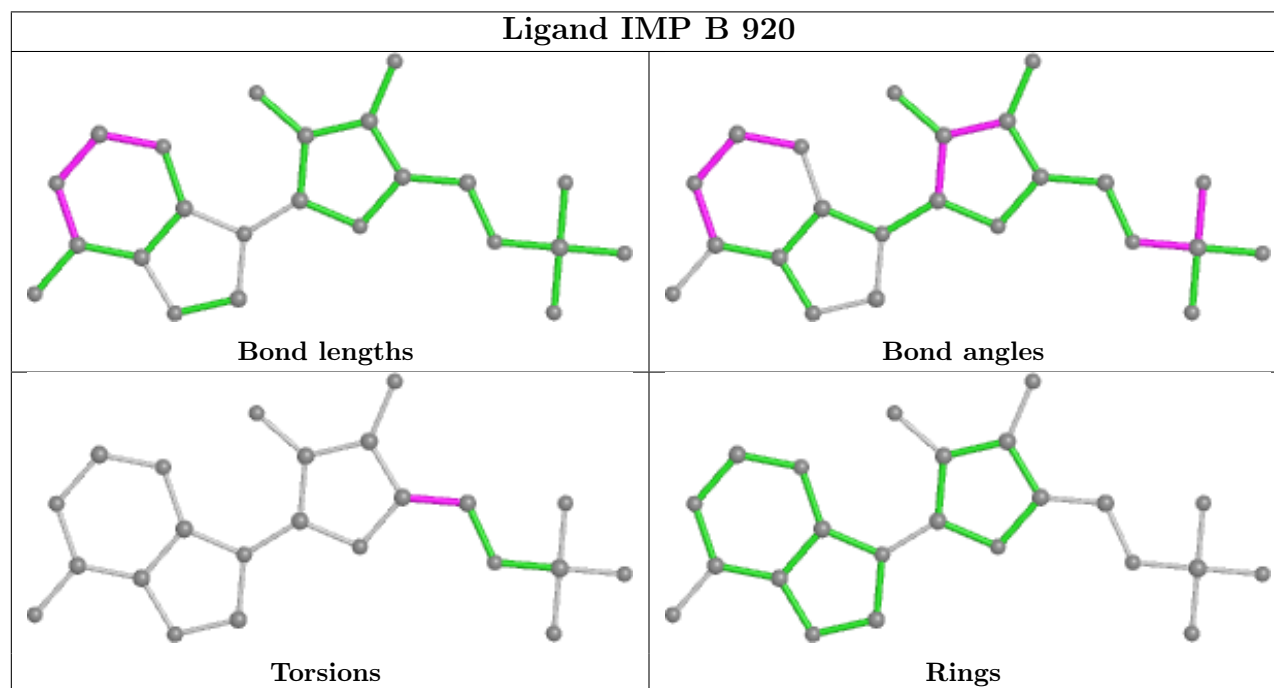
Mol	Chain	Res	Type	Atoms
3	D	920	IMP	C5'-O5'-P-O3P

There are no ring outliers.

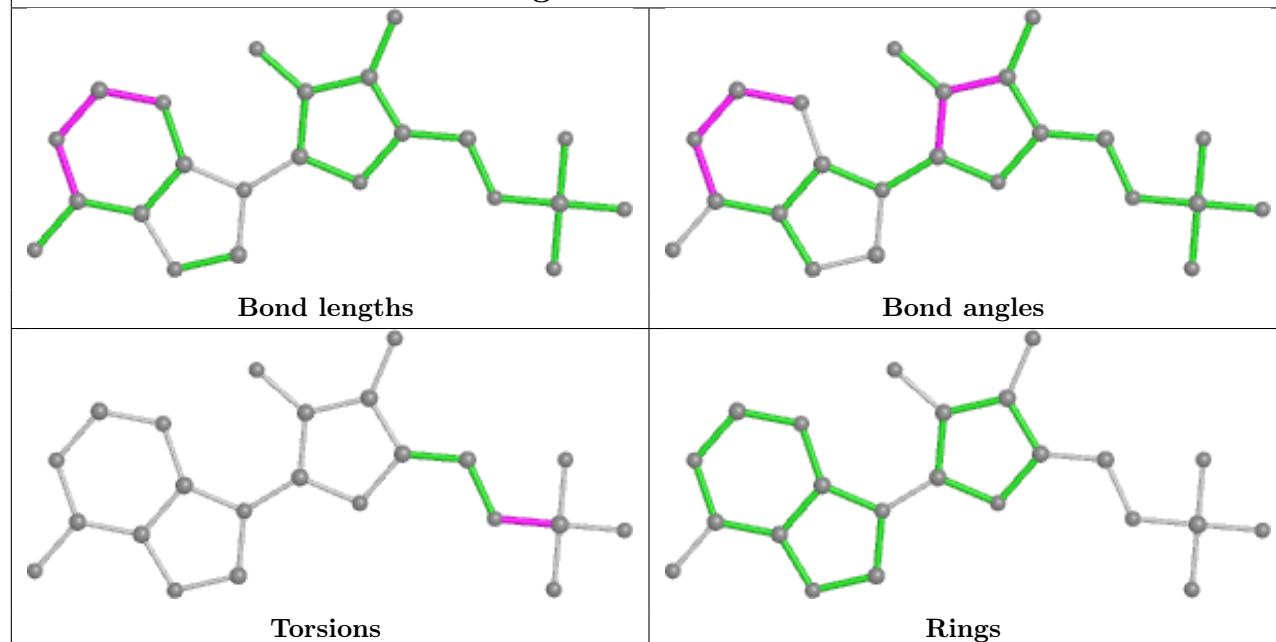
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	920	IMP	1	0
3	A	920	IMP	1	0

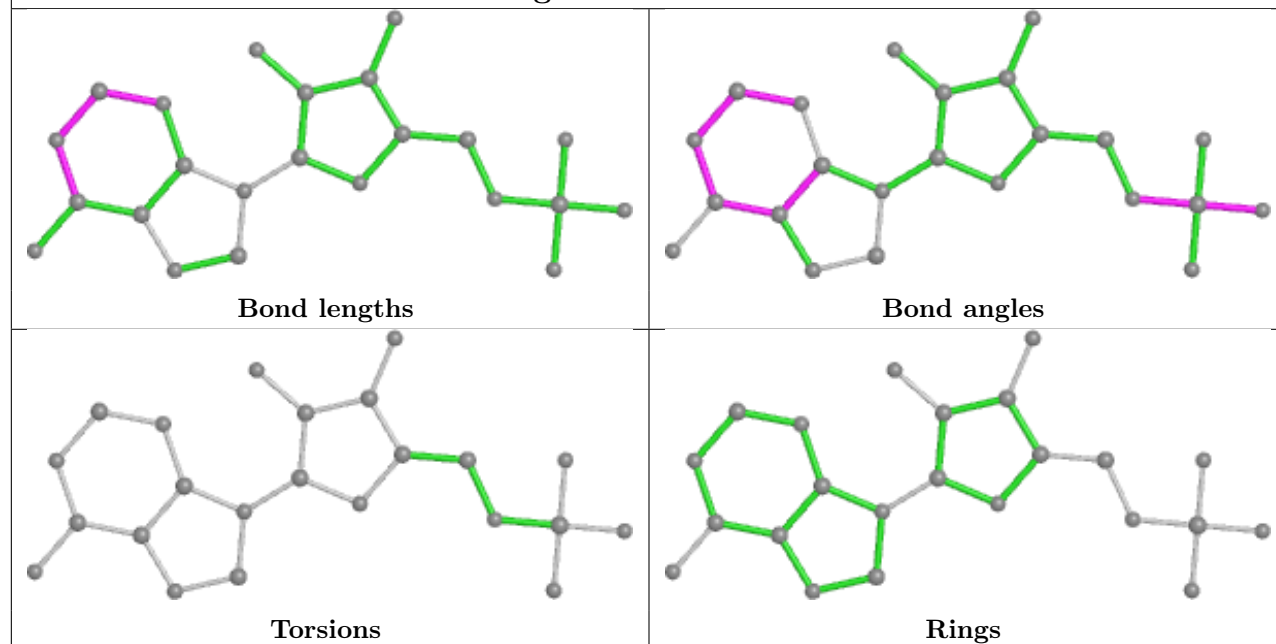
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

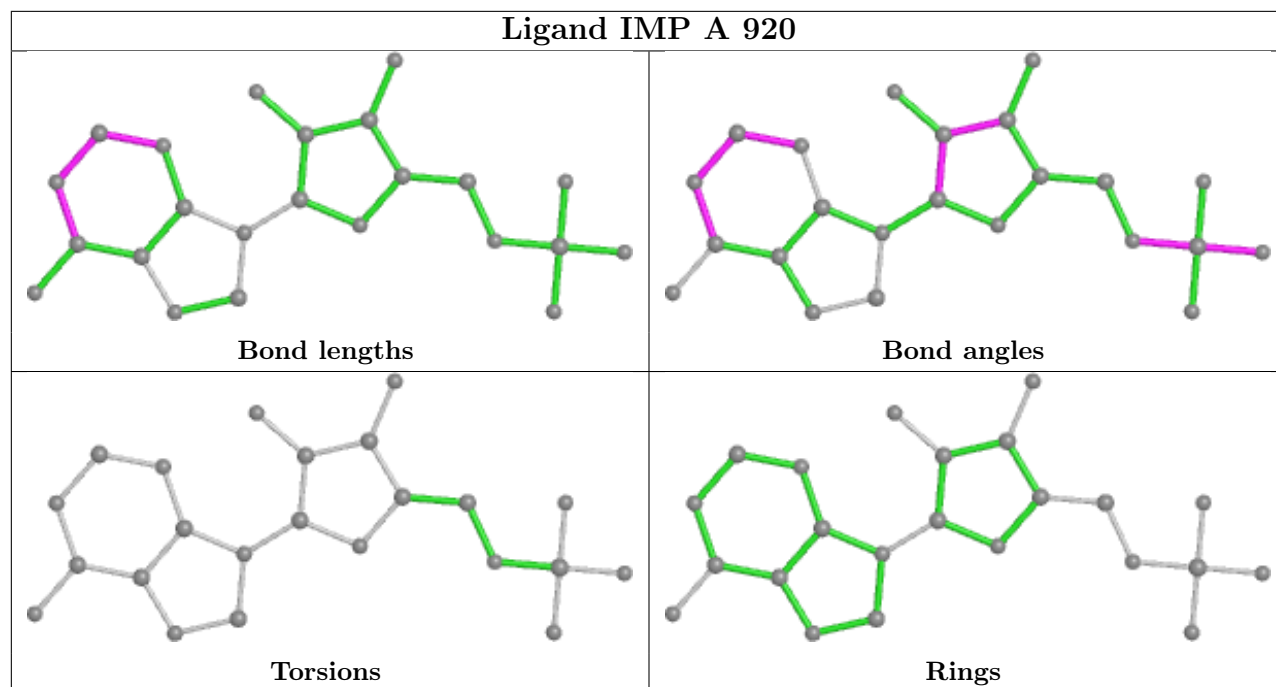


Ligand IMP D 920



Ligand IMP C 920





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 [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, 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	809/842 (96%)	-0.01	23 (2%)	53	46	23, 38, 53, 73	0
1	B	811/842 (96%)	0.11	47 (5%)	23	17	18, 43, 64, 70	0
1	C	807/842 (95%)	0.11	41 (5%)	28	22	21, 44, 66, 72	0
1	D	805/842 (95%)	0.29	63 (7%)	13	9	27, 47, 70, 75	0
All	All	3232/3368 (95%)	0.13	174 (5%)	25	20	18, 43, 66, 75	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	324	THR	7.7
1	B	259	VAL	6.8
1	D	22	GLU	6.6
1	A	281	PRO	6.6
1	D	288	GLY	5.7

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	LLP	B	680	24/25	0.93	0.21	37,39,42,43	0
1	LLP	A	680	24/25	0.96	0.19	22,24,34,36	0
1	LLP	C	680	24/25	0.96	0.16	38,41,45,45	0
1	LLP	D	680	24/25	0.98	0.25	42,44,46,47	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

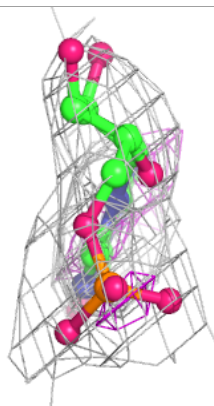
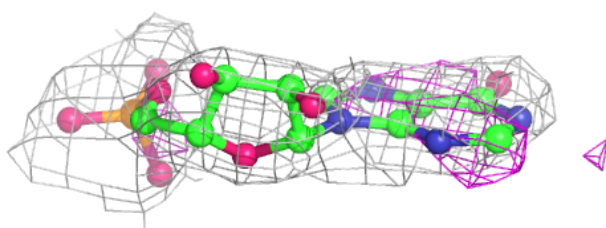
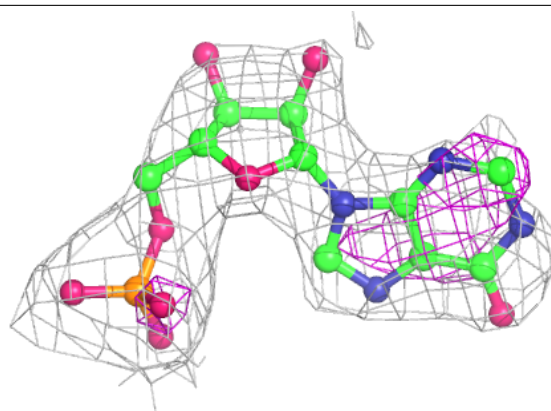
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	C	901	5/5	0.86	0.22	100,101,101,101	0
2	SO4	D	900	5/5	0.88	0.18	94,94,95,96	0
2	SO4	A	901	5/5	0.89	0.19	98,99,99,100	0
3	IMP	A	920	23/23	0.92	0.32	73,80,82,82	0
2	SO4	B	902	5/5	0.93	0.20	83,84,85,85	0
2	SO4	B	900	5/5	0.93	0.12	83,84,84,85	0
2	SO4	D	901	5/5	0.94	0.11	104,104,104,104	0
3	IMP	D	920	23/23	0.94	0.26	51,70,72,73	0
2	SO4	C	900	5/5	0.95	0.15	97,98,98,98	0
2	SO4	B	901	5/5	0.95	0.14	81,81,82,82	0
3	IMP	C	920	23/23	0.97	0.15	44,54,56,56	0
3	IMP	B	920	23/23	0.97	0.23	44,58,58,59	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.

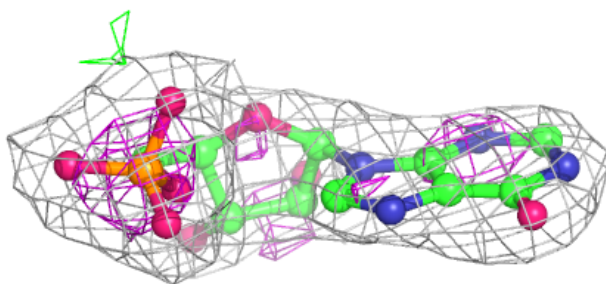
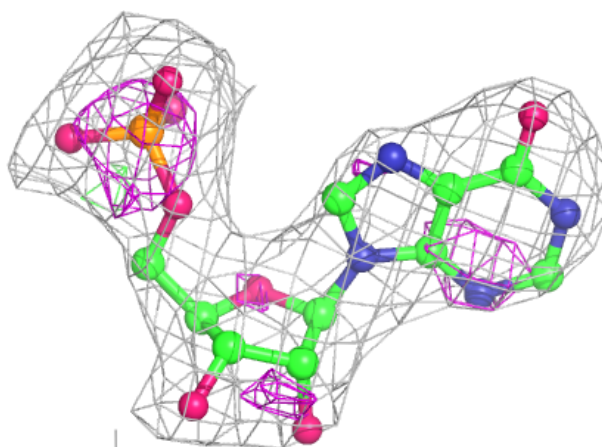
Electron density around IMP A 920:

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



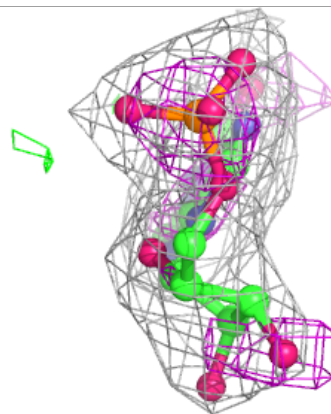
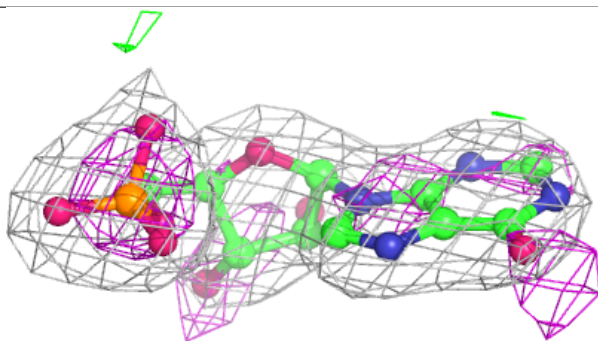
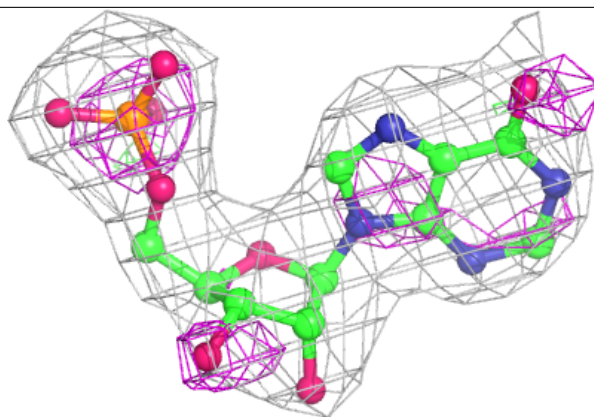
Electron density around IMP D 920:

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

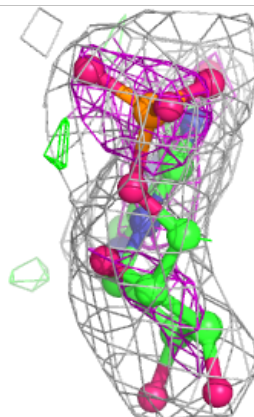
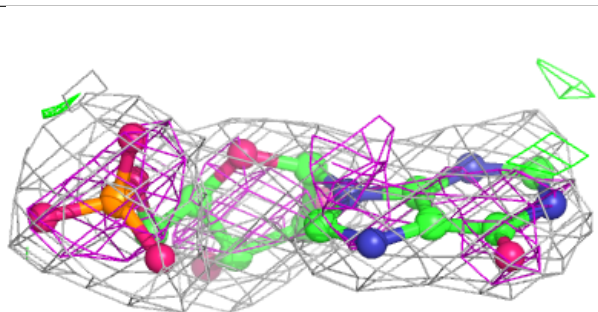
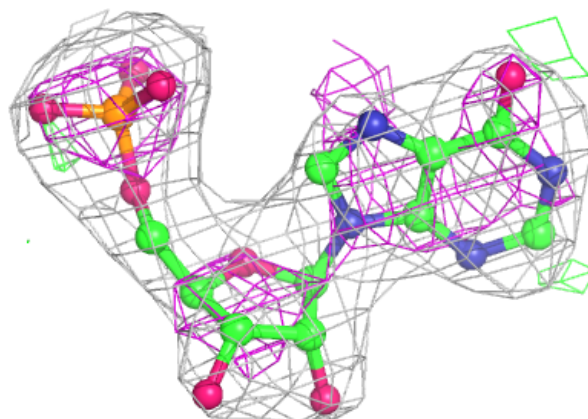


Electron density around IMP C 920:

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

**Electron density around IMP B 920:**

$2mF_o-DF_c$ (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.