Full wwPDB X-ray Structure Validation Report (i)

Feb 25, 2024 – 04:12 AM EST

PDB ID	:	5C03
Title	:	Crystal Structure of kinase
Authors	:	Min, X.; Wang, Z.; Walker, N.
Deposited on	:	2015-06-12
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i)) were used in the production of this report:

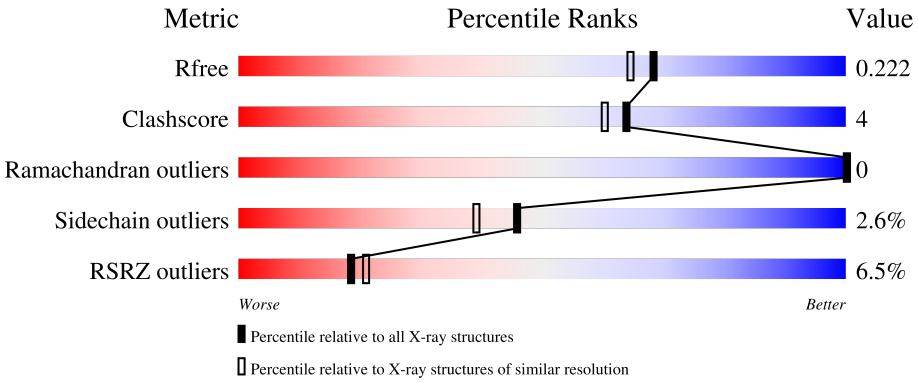
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	342	4% 71% 5% 24%
1	B	342	6% 68% 7% 24%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4568 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 Non-receptor tyrosine-protein kinase TYK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	1	0
			2067	1306	376	374	11			
1	B	260	Total	C	N	O	S	0	3	0
			2085	1317	379	377	12			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	530	MET	-	expression tag	UNP P29597
A	531	SER	-	expression tag	UNP P29597
A	532	TYR	-	expression tag	UNP P29597
A	533	TYR	-	expression tag	UNP P29597
A	534	HIS	-	expression tag	UNP P29597
A	535	HIS	-	expression tag	UNP P29597
A	536	HIS	-	expression tag	UNP P29597
A	537	HIS	-	expression tag	UNP P29597
A	538	HIS	-	expression tag	UNP P29597
A	539	HIS	-	expression tag	UNP P29597
A	540	ASP	-	expression tag	UNP P29597
A	541	TYR	-	expression tag	UNP P29597
A	542	ASP	-	expression tag	UNP P29597
A	543	ILE	-	expression tag	UNP P29597
A	544	PRO	-	expression tag	UNP P29597
A	545	THR	-	expression tag	UNP P29597
A	546	THR	-	expression tag	UNP P29597
A	547	GLU	-	expression tag	UNP P29597
A	548	ASN	-	expression tag	UNP P29597
A	549	LEU	-	expression tag	UNP P29597
A	550	TYR	-	expression tag	UNP P29597
A	551	PHE	-	expression tag	UNP P29597
A	552	GLN	-	expression tag	UNP P29597
A	553	GLY	-	expression tag	UNP P29597
A	554	ALA	-	expression tag	UNP P29597

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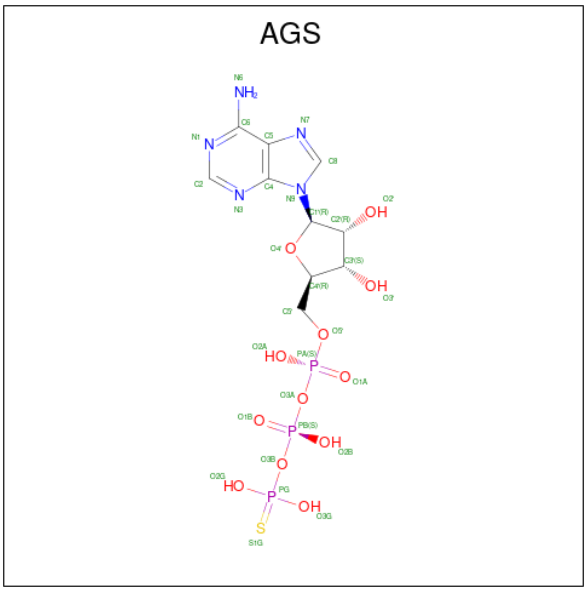
Chain	Residue	Modelled	Actual	Comment	Reference
A	555	MET	-	expression tag	UNP P29597
B	530	MET	-	expression tag	UNP P29597
B	531	SER	-	expression tag	UNP P29597
B	532	TYR	-	expression tag	UNP P29597
B	533	TYR	-	expression tag	UNP P29597
B	534	HIS	-	expression tag	UNP P29597
B	535	HIS	-	expression tag	UNP P29597
B	536	HIS	-	expression tag	UNP P29597
B	537	HIS	-	expression tag	UNP P29597
B	538	HIS	-	expression tag	UNP P29597
B	539	HIS	-	expression tag	UNP P29597
B	540	ASP	-	expression tag	UNP P29597
B	541	TYR	-	expression tag	UNP P29597
B	542	ASP	-	expression tag	UNP P29597
B	543	ILE	-	expression tag	UNP P29597
B	544	PRO	-	expression tag	UNP P29597
B	545	THR	-	expression tag	UNP P29597
B	546	THR	-	expression tag	UNP P29597
B	547	GLU	-	expression tag	UNP P29597
B	548	ASN	-	expression tag	UNP P29597
B	549	LEU	-	expression tag	UNP P29597
B	550	TYR	-	expression tag	UNP P29597
B	551	PHE	-	expression tag	UNP P29597
B	552	GLN	-	expression tag	UNP P29597
B	553	GLY	-	expression tag	UNP P29597
B	554	ALA	-	expression tag	UNP P29597
B	555	MET	-	expression tag	UNP P29597

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).

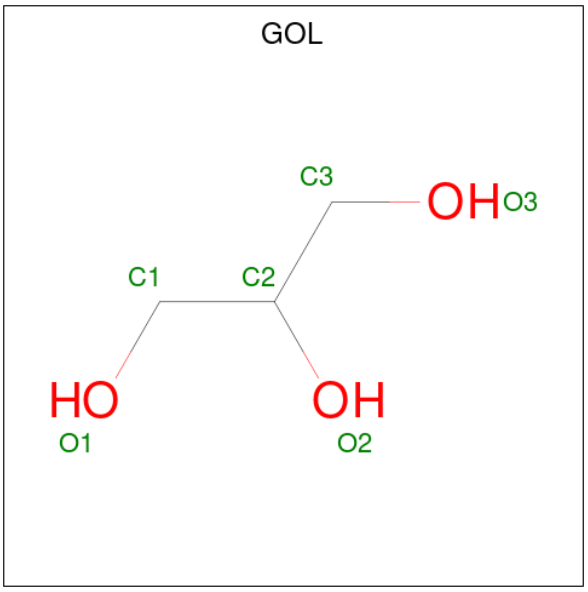


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

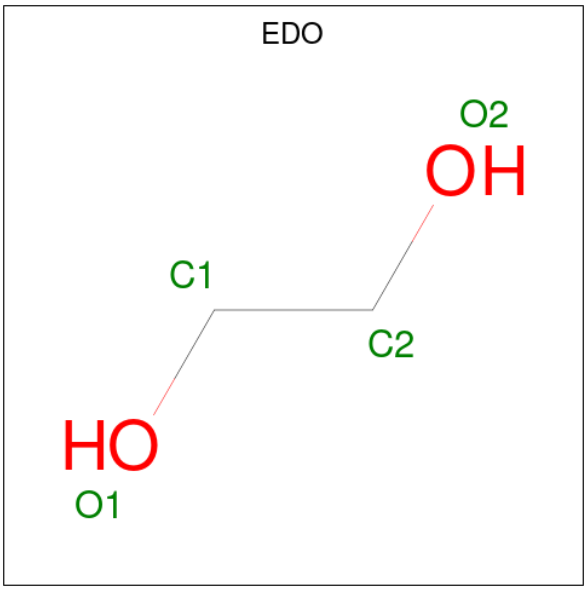
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

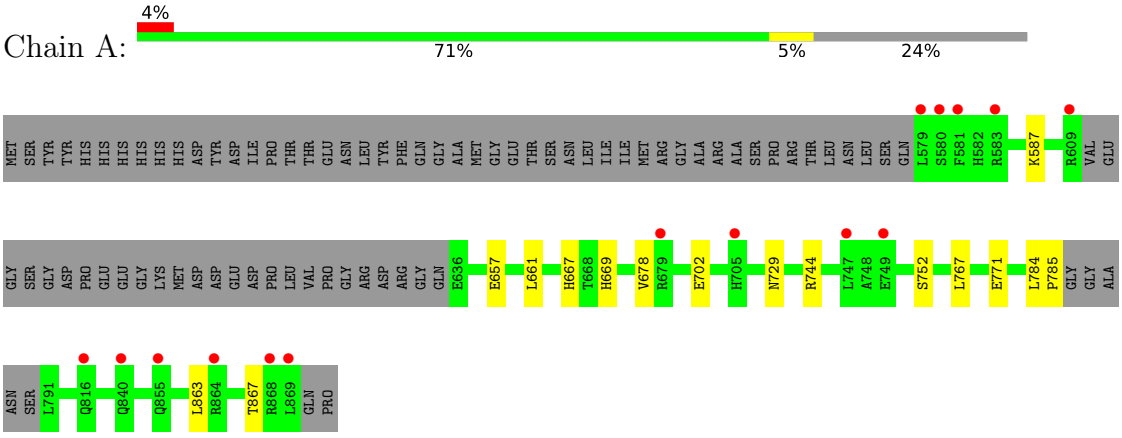
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	156	Total O 156 156	0	0
6	B	142	Total O 142 142	0	0

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.

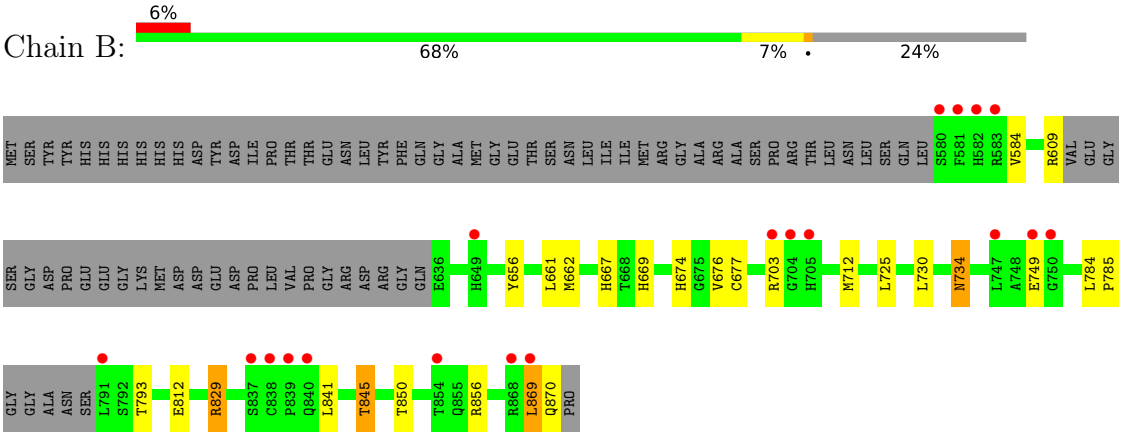
• Molecule 1: Non-receptor tyrosine-protein kinase TYK2

Chain A:



• Molecule 1: Non-receptor tyrosine-protein kinase TYK2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.12Å 47.69Å 112.75Å 90.00° 93.72° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 43.91 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-1.90) 99.2 (43.91-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.181 , 0.218 0.189 , 0.222	Depositor DCC
R_{free} test set	2383 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 56.0	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	0.95	EDS
Total number of atoms	4568	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% 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: GOL, EDO, MG, AGS

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	0.43	0/2117	0.65	0/2871
1	B	0.39	0/2135	0.60	1/2895 (0.0%)
All	All	0.41	0/4252	0.62	1/5766 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	829	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	2067	0	2068	10	0
1	B	2085	0	2086	26	0
2	A	31	0	12	0	0
2	B	31	0	12	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	18	0	24	1	0
4	B	12	0	16	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	18	0	0
5	B	12	0	18	0	0
6	A	156	0	0	3	0
6	B	142	0	0	4	0
All	All	4568	0	4254	36	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 4.

All (36) 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:B:661[B]:LEU:CD1	1:B:662[B]:MET:HE3	1.85	1.06
1:B:661[B]:LEU:HD12	1:B:662[B]:MET:HE3	1.38	1.04
1:B:661[B]:LEU:CD1	1:B:662[B]:MET:CE	2.48	0.90
1:A:667:HIS:HD2	1:A:669:HIS:H	1.30	0.80
1:B:674:HIS:O	4:B:903:GOL:H2	1.83	0.78
1:B:667:HIS:HD2	1:B:669:HIS:H	1.34	0.72
1:A:667:HIS:CD2	1:A:669:HIS:H	2.15	0.62
1:B:661[B]:LEU:HD13	1:B:662[B]:MET:CE	2.29	0.62
1:B:584:VAL:HG22	1:B:677:CYS:HB2	1.81	0.61
1:A:767:LEU:HB3	1:A:771:GLU:HG3	1.82	0.61
1:B:667:HIS:CD2	1:B:669:HIS:H	2.17	0.60
1:B:661[B]:LEU:HD13	1:B:662[B]:MET:HE3	1.82	0.59
1:A:678:VAL:CG1	6:A:1001:HOH:O	2.50	0.58
1:B:661[B]:LEU:HD13	1:B:661[B]:LEU:C	2.28	0.54
1:B:661[B]:LEU:HD21	1:B:730:LEU:HD13	1.90	0.53
1:B:845:THR:CG2	6:B:1022:HOH:O	2.57	0.52
1:B:656:TYR:CE1	1:B:676:VAL:HG11	2.44	0.52
1:A:784:LEU:HB3	1:A:785:PRO:HD3	1.94	0.49
1:B:674:HIS:O	4:B:903:GOL:C2	2.58	0.48
1:B:850[A]:THR:HG22	1:B:856:ARG:HG2	1.95	0.48
1:A:744:ARG:NH2	6:A:1003:HOH:O	2.46	0.47
1:B:734:ASN:ND2	6:B:1002:HOH:O	2.45	0.47
1:A:863:LEU:O	1:A:867:THR:HG23	2.14	0.47
1:B:784:LEU:HB3	1:B:785:PRO:HD3	1.97	0.47
1:B:661[B]:LEU:CD1	1:B:662[B]:MET:HE2	2.43	0.46
1:A:657:GLU:O	1:A:661:LEU:HD13	2.16	0.45
1:B:661[B]:LEU:O	1:B:661[B]:LEU:HD22	2.15	0.45
1:B:712:MET:HE1	1:B:869:LEU:HD12	1.99	0.44
1:B:703:ARG:NH1	1:B:812:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661[B]:LEU:HD13	1:B:662[B]:MET:HE2	1.99	0.43
1:B:845:THR:HG22	6:B:1022:HOH:O	2.18	0.43
1:A:678:VAL:HG13	6:A:1121:HOH:O	2.18	0.43
1:B:661[B]:LEU:HD21	1:B:730:LEU:HD22	1.99	0.43
1:B:829:ARG:NH2	6:B:1001:HOH:O	2.42	0.42
1:A:702:GLU:CD	4:A:907:GOL:H2	2.40	0.41
1:B:712:MET:CE	1:B:869:LEU:HD12	2.51	0.41

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	255/342 (75%)	251 (98%)	4 (2%)	0	100	100
1	B	257/342 (75%)	251 (98%)	6 (2%)	0	100	100
All	All	512/684 (75%)	502 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	228/295 (77%)	225 (99%)	3 (1%)	69	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	230/295 (78%)	221 (96%)	9 (4%)	32 23
All	All	458/590 (78%)	446 (97%)	12 (3%)	46 39

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	587	LYS
1	A	729	ASN
1	A	752	SER
1	B	609	ARG
1	B	725	LEU
1	B	734	ASN
1	B	749	GLU
1	B	793	THR
1	B	841	LEU
1	B	845	THR
1	B	869	LEU
1	B	870	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	602	ASN
1	A	667	HIS
1	B	667	HIS
1	B	734	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	GOL	A	906	-	5,5,5	0.38	0	5,5,5	0.31	0
4	GOL	B	903	-	5,5,5	0.35	0	5,5,5	0.68	0
2	AGS	A	901	3	26,33,33	1.60	2 (7%)	26,52,52	1.56	5 (19%)
5	EDO	A	904	-	3,3,3	0.49	0	2,2,2	0.32	0
5	EDO	A	908	-	3,3,3	0.45	0	2,2,2	0.38	0
2	AGS	B	901	3	26,33,33	1.52	3 (11%)	26,52,52	1.38	2 (7%)
5	EDO	B	904	-	3,3,3	0.53	0	2,2,2	0.25	0
5	EDO	B	906	-	3,3,3	0.38	0	2,2,2	0.26	0
4	GOL	A	907	-	5,5,5	0.21	0	5,5,5	0.35	0
5	EDO	B	905	-	3,3,3	0.49	0	2,2,2	0.42	0
5	EDO	A	905	-	3,3,3	0.56	0	2,2,2	0.10	0
4	GOL	B	907	-	5,5,5	0.28	0	5,5,5	0.12	0
4	GOL	A	903	-	5,5,5	0.28	0	5,5,5	0.21	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
4	GOL	A	906	-	-	0/4/4/4	-
4	GOL	B	903	-	-	4/4/4/4	-
2	AGS	A	901	3	-	0/17/38/38	0/3/3/3
5	EDO	A	904	-	-	1/1/1/1	-
5	EDO	A	908	-	-	0/1/1/1	-
2	AGS	B	901	3	-	2/17/38/38	0/3/3/3
5	EDO	B	904	-	-	0/1/1/1	-
5	EDO	B	906	-	-	1/1/1/1	-
4	GOL	A	907	-	-	3/4/4/4	-
5	EDO	B	905	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	905	-	-	1/1/1/1	-
4	GOL	B	907	-	-	0/4/4/4	-
4	GOL	A	903	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	AGS	PG-S1G	6.27	2.04	1.90
2	B	901	AGS	PG-S1G	5.94	2.03	1.90
2	B	901	AGS	C5-C4	2.37	1.47	1.40
2	A	901	AGS	C5-C4	2.18	1.46	1.40
2	B	901	AGS	O4'-C1'	2.12	1.44	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	901	AGS	N3-C2-N1	-4.26	122.03	128.68
2	B	901	AGS	N3-C2-N1	-3.68	122.92	128.68
2	A	901	AGS	N6-C6-N1	2.96	124.72	118.57
2	B	901	AGS	C1'-N9-C4	-2.83	121.68	126.64
2	A	901	AGS	C1'-N9-C4	-2.39	122.45	126.64
2	A	901	AGS	C2-N1-C6	2.34	122.76	118.75
2	A	901	AGS	C5-C6-N6	-2.26	116.91	120.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	903	GOL	O1-C1-C2-C3
4	B	903	GOL	O1-C1-C2-O2
4	A	903	GOL	O1-C1-C2-C3
4	A	907	GOL	C1-C2-C3-O3
4	B	903	GOL	C1-C2-C3-O3
2	B	901	AGS	PG-O3B-PB-O1B
5	A	904	EDO	O1-C1-C2-O2
5	A	905	EDO	O1-C1-C2-O2
5	B	906	EDO	O1-C1-C2-O2
5	B	905	EDO	O1-C1-C2-O2
4	A	907	GOL	O2-C2-C3-O3
2	B	901	AGS	PG-O3B-PB-O2B
4	B	903	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	907	GOL	O1-C1-C2-O2

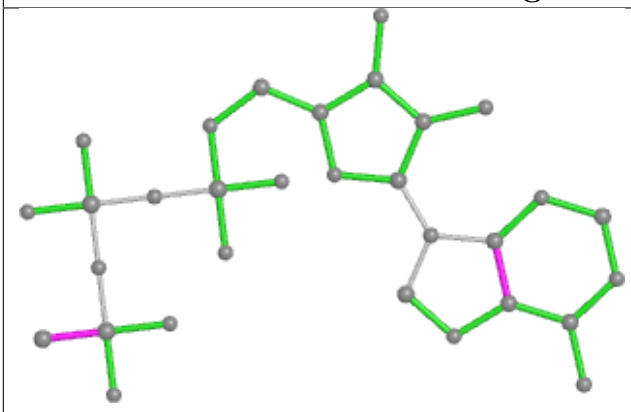
There are no ring outliers.

2 monomers are involved in 3 short contacts:

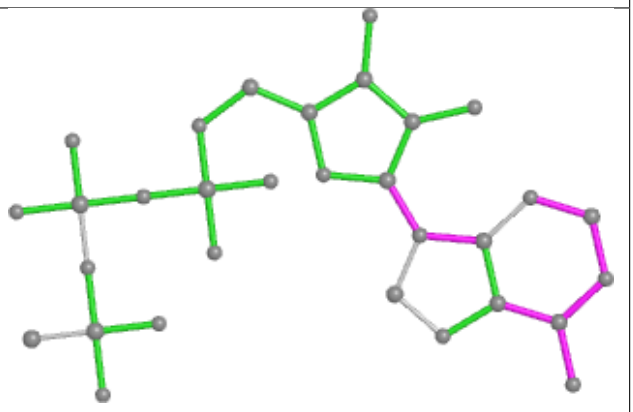
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	GOL	2	0
4	A	907	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

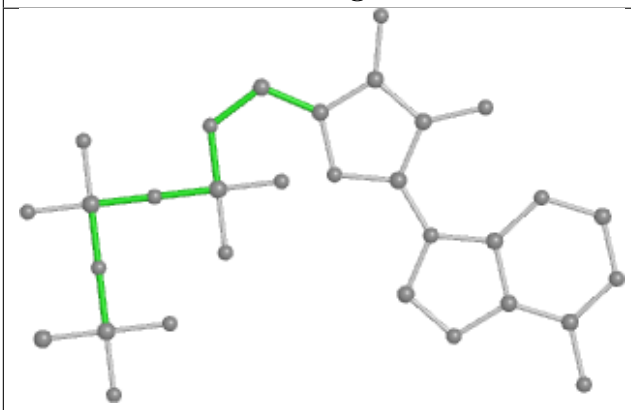
Ligand AGS A 901



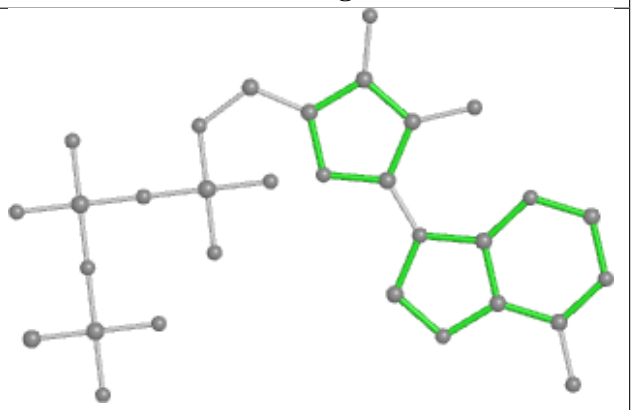
Bond lengths



Bond angles

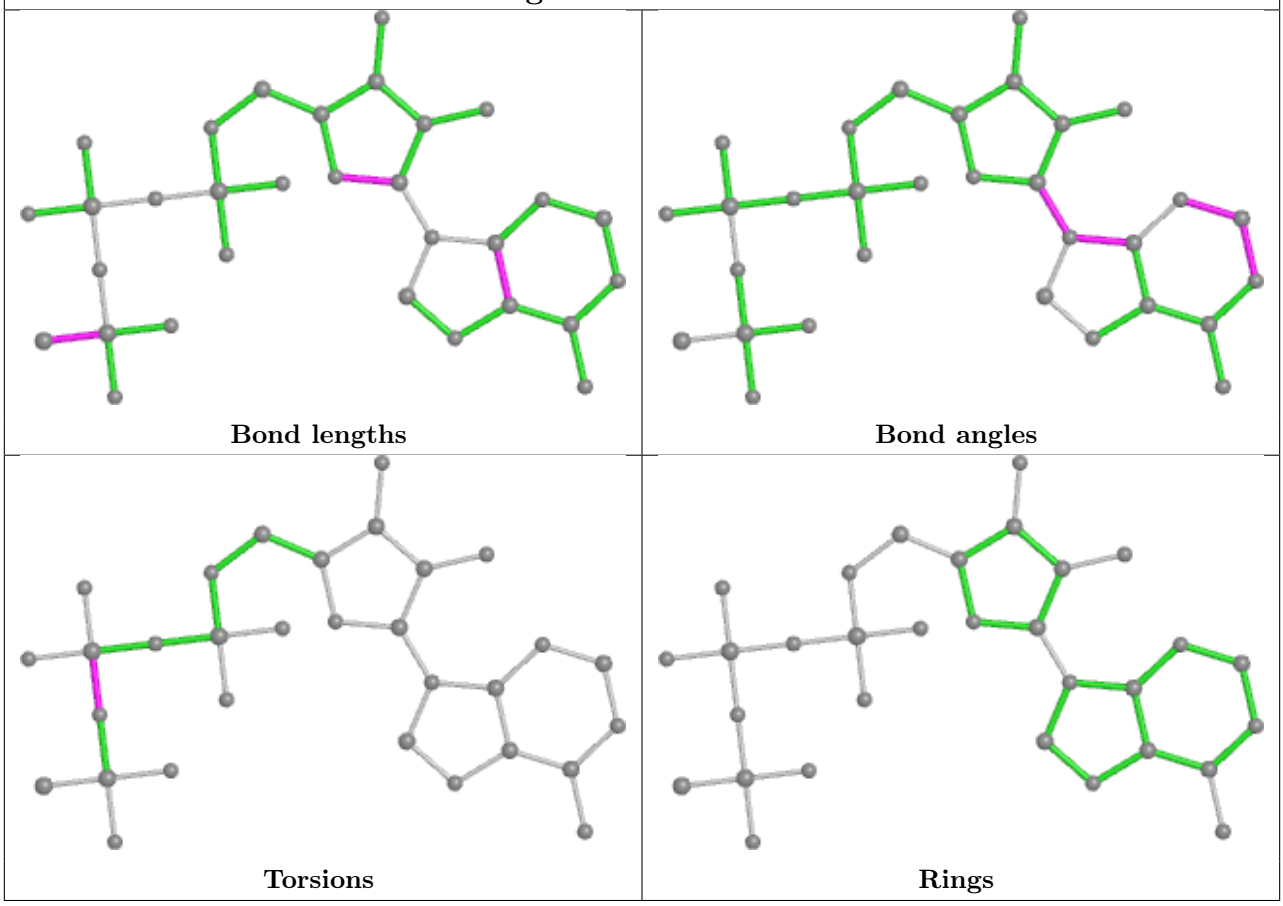


Torsions



Rings

Ligand AGS B 901



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	260/342 (76%)	0.29	15 (5%)	23	25	11, 22, 46, 63	0
1	B	260/342 (76%)	0.40	19 (7%)	15	16	14, 24, 52, 65	0
All	All	520/684 (76%)	0.34	34 (6%)	18	21	11, 23, 49, 65	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	581	PHE	4.9
1	B	839	PRO	4.8
1	B	840	GLN	4.5
1	A	579	LEU	4.4
1	B	749	GLU	4.3
1	B	747	LEU	3.8
1	A	749	GLU	3.7
1	B	583	ARG	3.6
1	B	791	LEU	3.6
1	B	838	CYS	3.4
1	A	581	PHE	3.4
1	A	679	ARG	3.1
1	B	869	LEU	3.1
1	B	837	SER	2.9
1	A	747	LEU	2.9
1	A	583	ARG	2.9
1	B	750	GLY	2.8
1	B	868	ARG	2.6
1	A	864	ARG	2.5
1	A	609	ARG	2.5
1	A	705	HIS	2.5
1	A	580	SER	2.5
1	B	649	HIS	2.4
1	B	705	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	855	GLN	2.4
1	B	703	ARG	2.3
1	B	704	GLY	2.3
1	B	582	HIS	2.3
1	A	869	LEU	2.3
1	A	840	GLN	2.2
1	B	854	THR	2.1
1	A	868	ARG	2.1
1	A	816	GLN	2.0
1	B	580	SER	2.0

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 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
5	EDO	B	905	4/4	0.68	0.25	42,43,43,44	0
4	GOL	A	907	6/6	0.78	0.31	20,20,20,20	0
4	GOL	A	903	6/6	0.82	0.15	51,53,54,55	0
5	EDO	B	904	4/4	0.85	0.23	37,40,40,42	0
4	GOL	A	906	6/6	0.85	0.28	30,37,39,42	0
4	GOL	B	907	6/6	0.87	0.22	47,50,51,51	0
4	GOL	B	903	6/6	0.88	0.28	35,36,39,40	0
5	EDO	A	905	4/4	0.88	0.27	38,38,39,39	0
5	EDO	B	906	4/4	0.89	0.21	34,37,37,39	0
5	EDO	A	904	4/4	0.92	0.09	40,40,40,41	0
5	EDO	A	908	4/4	0.93	0.17	32,34,35,35	0
2	AGS	B	901	31/31	0.98	0.12	16,19,23,25	0
2	AGS	A	901	31/31	0.98	0.11	13,15,19,22	0

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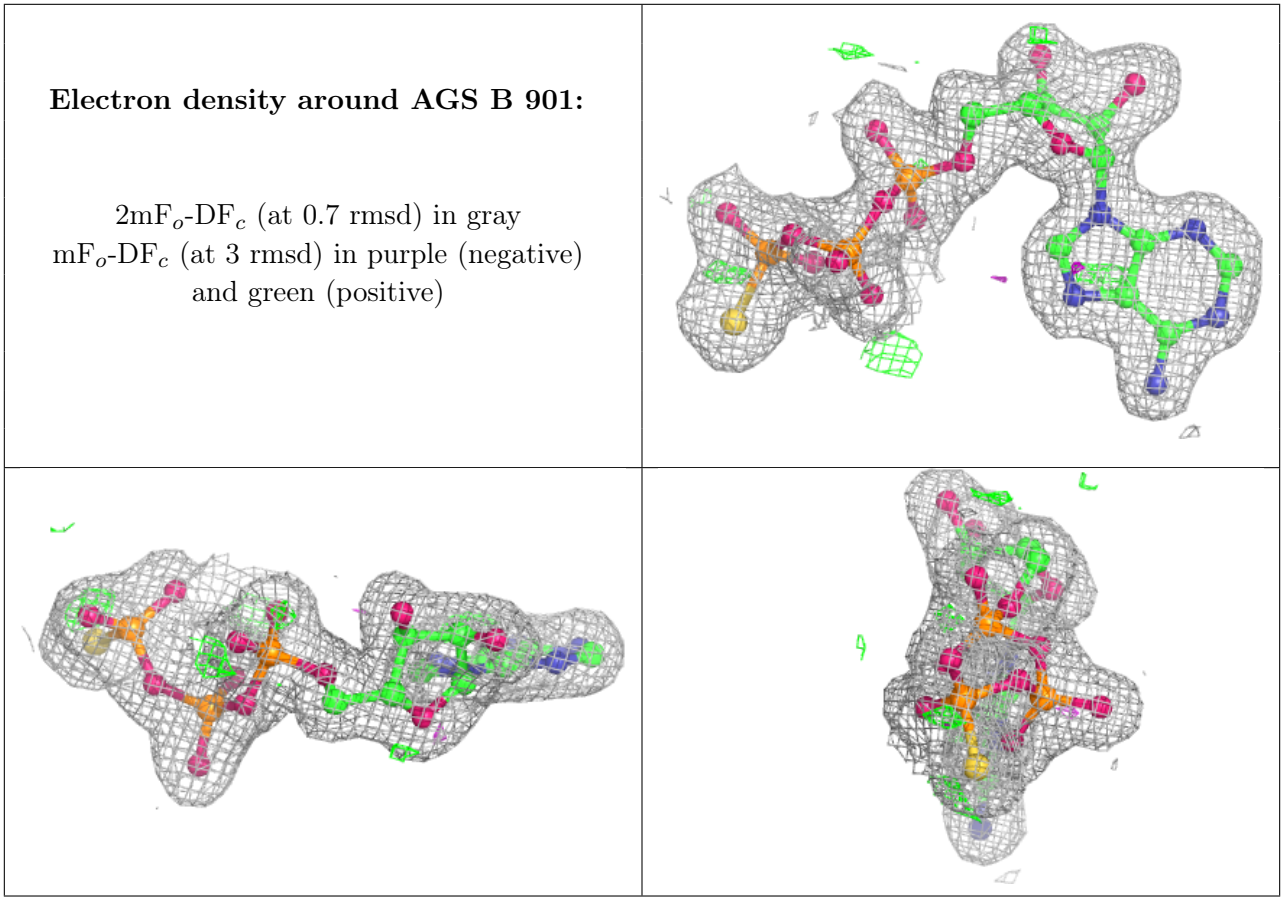
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	902	1/1	0.99	0.17	5,5,5,5	0
3	MG	B	902	1/1	1.00	0.16	8,8,8,8	0

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.

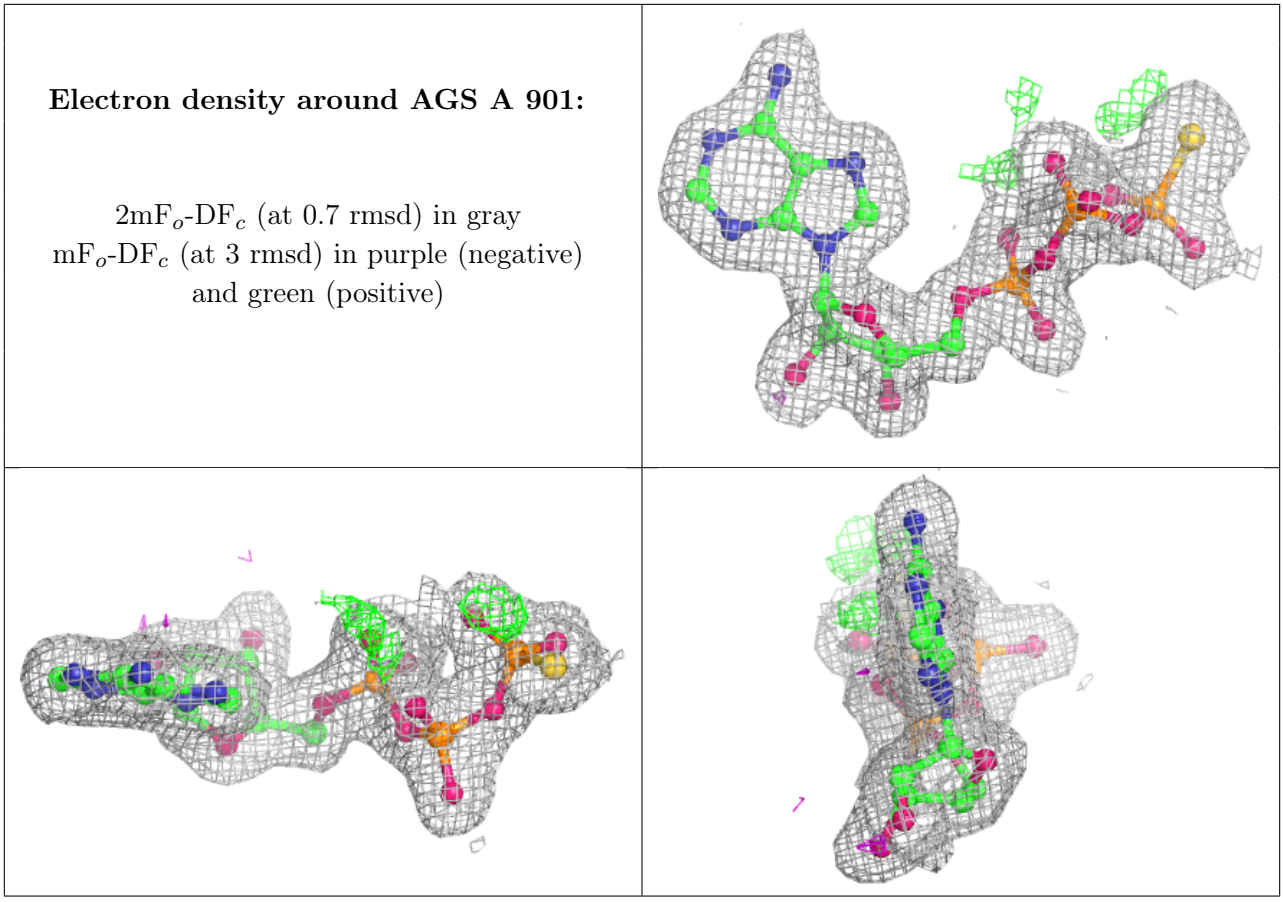
Electron density around AGS B 901:

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



Electron density around AGS A 901:

$2mF_o$-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.