wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2023 – 06:03 AM EDT

PDB ID	:	1SXJ
Title	:	Crystal Structure of the Eukaryotic Clamp Loader (Replication Factor C, RFC) Bound to the DNA Sliding Clamp (Proliferating Cell Nuclear Antigen, PCNA)
Authors	:	Bowman, G.D.; O'Donnell, M.; Kuriyan, J.
Deposited on	:	2004-03-30
Resolution	:	2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

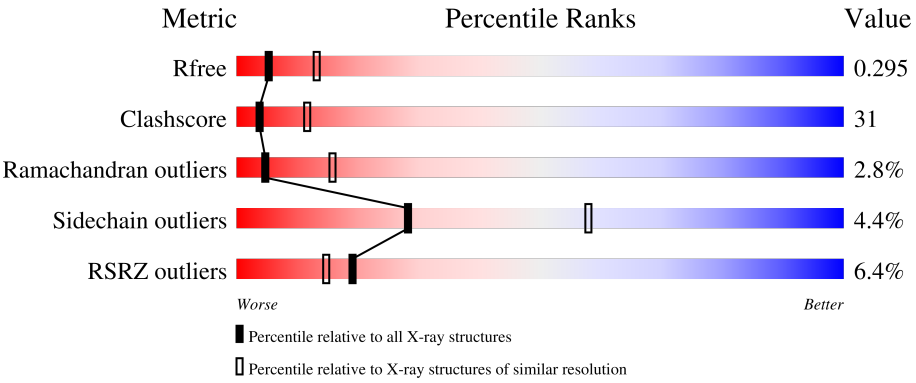
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	516	3% 44% 39% 15%
2	B	323	% 59% 36%
3	C	340	2% 43% 47% 5%
4	D	353	8% 43% 46% 7%

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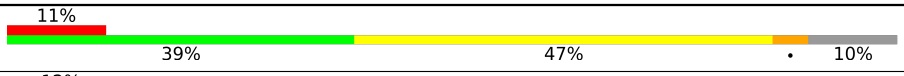
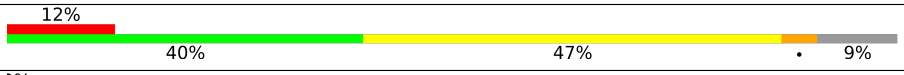
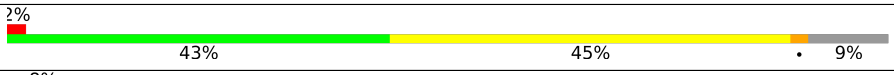
Mol	Chain	Length	Quality of chain
5	E	354	
6	F	283	
6	G	283	
6	H	283	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 19740 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 Activator 1 95 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3345	2110	603	617	15			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	MET	-	expression tag	UNP P38630
A	271	GLY	-	expression tag	UNP P38630
A	272	SER	-	expression tag	UNP P38630
A	273	SER	-	expression tag	UNP P38630
A	274	HIS	-	expression tag	UNP P38630
A	275	HIS	-	expression tag	UNP P38630
A	276	HIS	-	expression tag	UNP P38630
A	277	HIS	-	expression tag	UNP P38630
A	278	HIS	-	expression tag	UNP P38630
A	279	HIS	-	expression tag	UNP P38630
A	280	SER	-	expression tag	UNP P38630
A	281	SER	-	expression tag	UNP P38630
A	282	GLY	-	expression tag	UNP P38630
A	283	LEU	-	expression tag	UNP P38630
A	284	GLU	-	expression tag	UNP P38630
A	285	VAL	-	expression tag	UNP P38630
A	286	LEU	-	expression tag	UNP P38630
A	287	PHE	-	expression tag	UNP P38630
A	288	GLN	-	expression tag	UNP P38630
A	289	GLY	-	expression tag	UNP P38630
A	290	PRO	-	expression tag	UNP P38630
A	291	HIS	-	expression tag	UNP P38630
A	292	MET	-	expression tag	UNP P38630
A	293	ALA	-	expression tag	UNP P38630
A	294	SER	-	expression tag	UNP P38630

- Molecule 2 is a protein called Activator 1 37 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	316	Total	C	N	O	S	0	0	0
			2482	1566	441	462	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	157	GLN	ARG	engineered mutation	UNP P40339

- Molecule 3 is a protein called Activator 1 40 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	322	Total	C	N	O	S	0	0	0
			2544	1604	443	489	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	160	GLN	ARG	engineered mutation	UNP P38629

- Molecule 4 is a protein called Activator 1 41 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	328	Total	C	N	O	S	0	0	0
			2597	1642	446	499	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	183	GLN	ARG	engineered mutation	UNP P40348

- Molecule 5 is a protein called Activator 1 40 kDa subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	317	Total	C	N	O	S	0	0	0
			2495	1582	428	468	17			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	184	GLN	ARG	engineered mutation	UNP P38251

- Molecule 6 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	258	Total	C	N	O	S	Se	0	0	0
			2021	1291	319	401	4	6			
6	G	258	Total	C	N	O	S	Se	5	0	0
			2022	1292	319	400	4	7			
6	H	267	Total	C	N	O	S	Se	0	0	0
			2079	1329	330	409	4	7			

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-24	MSE	-	expression tag	UNP P15873
F	-23	GLY	-	expression tag	UNP P15873
F	-22	SER	-	expression tag	UNP P15873
F	-21	SER	-	expression tag	UNP P15873
F	-20	HIS	-	expression tag	UNP P15873
F	-19	HIS	-	expression tag	UNP P15873
F	-18	HIS	-	expression tag	UNP P15873
F	-17	HIS	-	expression tag	UNP P15873
F	-16	HIS	-	expression tag	UNP P15873
F	-15	HIS	-	expression tag	UNP P15873
F	-14	SER	-	expression tag	UNP P15873
F	-13	SER	-	expression tag	UNP P15873
F	-12	GLY	-	expression tag	UNP P15873
F	-11	LEU	-	expression tag	UNP P15873
F	-10	GLU	-	expression tag	UNP P15873
F	-9	VAL	-	expression tag	UNP P15873
F	-8	LEU	-	expression tag	UNP P15873
F	-7	PHE	-	expression tag	UNP P15873
F	-6	GLN	-	expression tag	UNP P15873
F	-5	GLY	-	expression tag	UNP P15873
F	-4	PRO	-	expression tag	UNP P15873
F	-3	HIS	-	expression tag	UNP P15873
F	-2	MSE	-	expression tag	UNP P15873
F	-1	ALA	-	expression tag	UNP P15873
F	0	SER	-	expression tag	UNP P15873
F	1	MSE	MET	modified residue	UNP P15873
F	70	MSE	MET	modified residue	UNP P15873
F	119	MSE	MET	modified residue	UNP P15873
F	161	MSE	MET	modified residue	UNP P15873
F	188	MSE	MET	modified residue	UNP P15873
F	199	MSE	MET	modified residue	UNP P15873
G	-24	MSE	-	expression tag	UNP P15873
G	-23	GLY	-	expression tag	UNP P15873

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-22	SER	-	expression tag	UNP P15873
G	-21	SER	-	expression tag	UNP P15873
G	-20	HIS	-	expression tag	UNP P15873
G	-19	HIS	-	expression tag	UNP P15873
G	-18	HIS	-	expression tag	UNP P15873
G	-17	HIS	-	expression tag	UNP P15873
G	-16	HIS	-	expression tag	UNP P15873
G	-15	HIS	-	expression tag	UNP P15873
G	-14	SER	-	expression tag	UNP P15873
G	-13	SER	-	expression tag	UNP P15873
G	-12	GLY	-	expression tag	UNP P15873
G	-11	LEU	-	expression tag	UNP P15873
G	-10	GLU	-	expression tag	UNP P15873
G	-9	VAL	-	expression tag	UNP P15873
G	-8	LEU	-	expression tag	UNP P15873
G	-7	PHE	-	expression tag	UNP P15873
G	-6	GLN	-	expression tag	UNP P15873
G	-5	GLY	-	expression tag	UNP P15873
G	-4	PRO	-	expression tag	UNP P15873
G	-3	HIS	-	expression tag	UNP P15873
G	-2	MSE	-	expression tag	UNP P15873
G	-1	ALA	-	expression tag	UNP P15873
G	0	SER	-	expression tag	UNP P15873
G	1	MSE	MET	modified residue	UNP P15873
G	70	MSE	MET	modified residue	UNP P15873
G	119	MSE	MET	modified residue	UNP P15873
G	161	MSE	MET	modified residue	UNP P15873
G	188	MSE	MET	modified residue	UNP P15873
G	199	MSE	MET	modified residue	UNP P15873
H	-24	MSE	-	expression tag	UNP P15873
H	-23	GLY	-	expression tag	UNP P15873
H	-22	SER	-	expression tag	UNP P15873
H	-21	SER	-	expression tag	UNP P15873
H	-20	HIS	-	expression tag	UNP P15873
H	-19	HIS	-	expression tag	UNP P15873
H	-18	HIS	-	expression tag	UNP P15873
H	-17	HIS	-	expression tag	UNP P15873
H	-16	HIS	-	expression tag	UNP P15873
H	-15	HIS	-	expression tag	UNP P15873
H	-14	SER	-	expression tag	UNP P15873
H	-13	SER	-	expression tag	UNP P15873
H	-12	GLY	-	expression tag	UNP P15873

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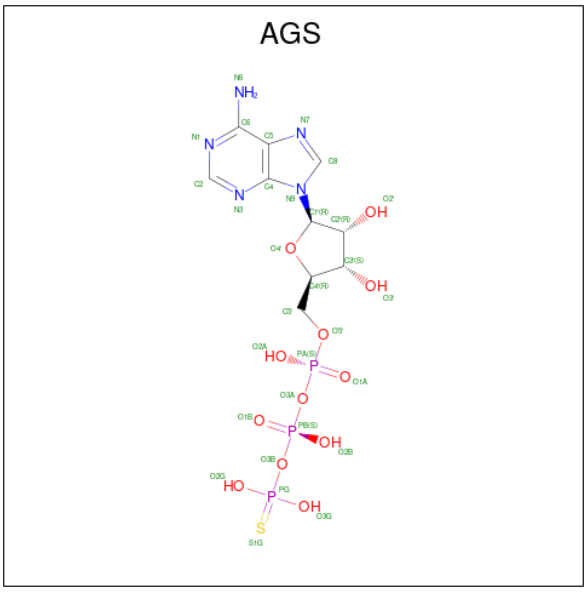
Chain	Residue	Modelled	Actual	Comment	Reference
H	-11	LEU	-	expression tag	UNP P15873
H	-10	GLU	-	expression tag	UNP P15873
H	-9	VAL	-	expression tag	UNP P15873
H	-8	LEU	-	expression tag	UNP P15873
H	-7	PHE	-	expression tag	UNP P15873
H	-6	GLN	-	expression tag	UNP P15873
H	-5	GLY	-	expression tag	UNP P15873
H	-4	PRO	-	expression tag	UNP P15873
H	-3	HIS	-	expression tag	UNP P15873
H	-2	MSE	-	expression tag	UNP P15873
H	-1	ALA	-	expression tag	UNP P15873
H	0	SER	-	expression tag	UNP P15873
H	1	MSE	MET	modified residue	UNP P15873
H	70	MSE	MET	modified residue	UNP P15873
H	119	MSE	MET	modified residue	UNP P15873
H	161	MSE	MET	modified residue	UNP P15873
H	188	MSE	MET	modified residue	UNP P15873
H	199	MSE	MET	modified residue	UNP P15873

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

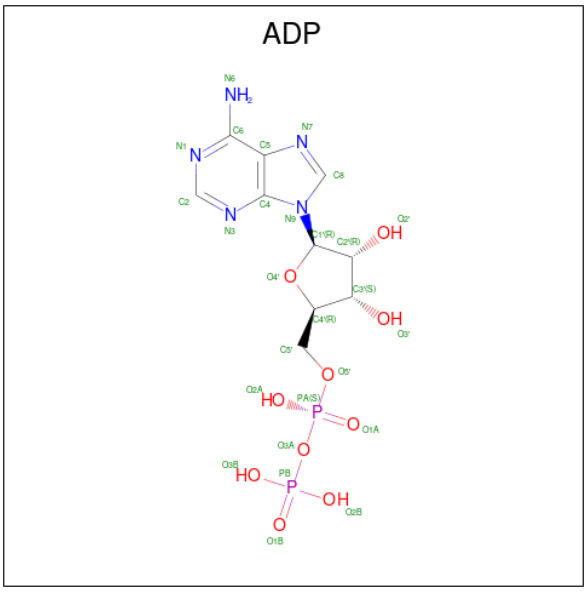
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0

- Molecule 8 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
8	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
8	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
8	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
8	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



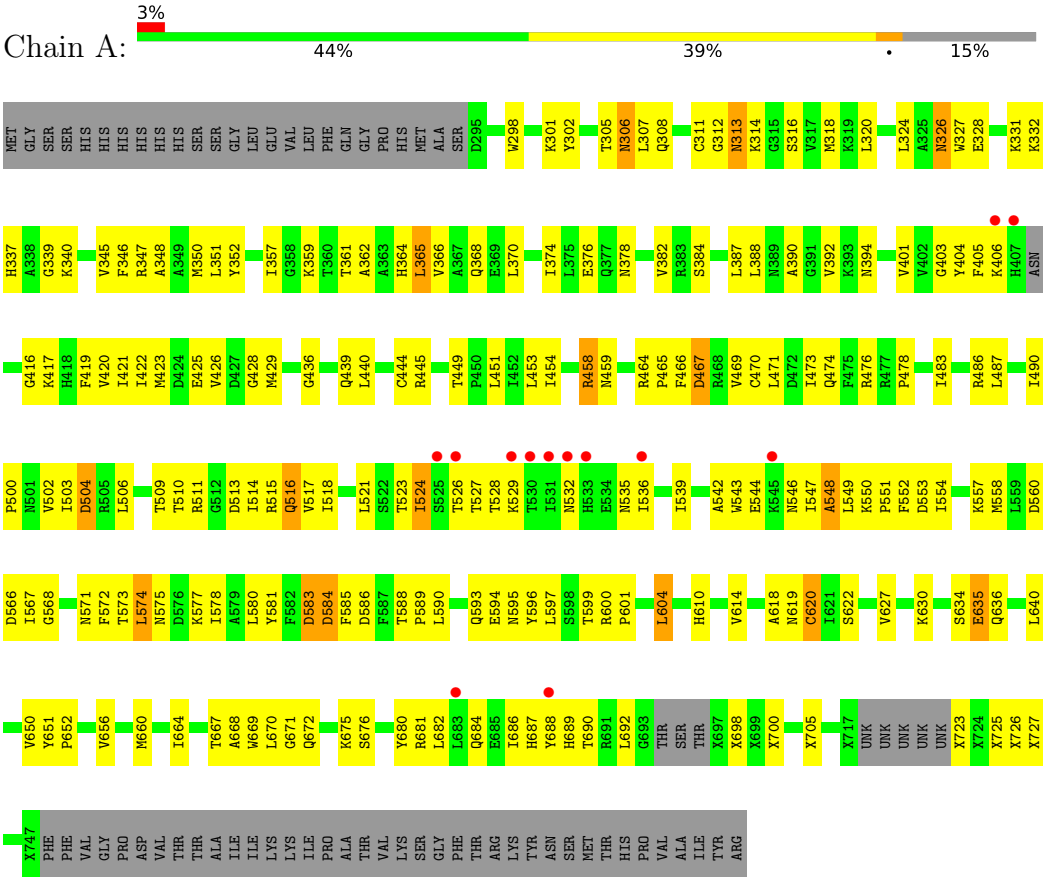
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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.

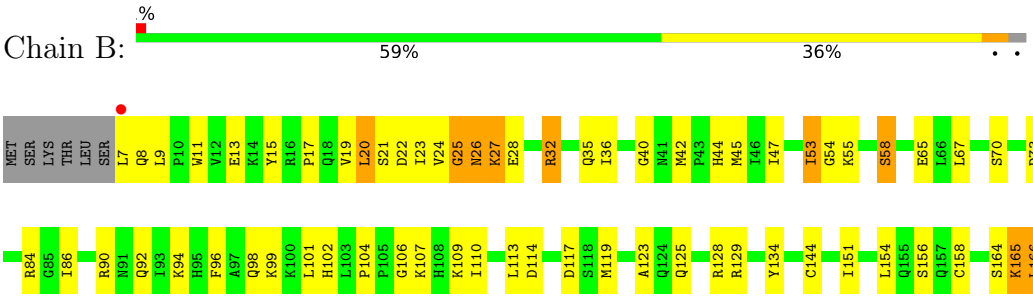
• Molecule 1: Activator 1 95 kDa subunit

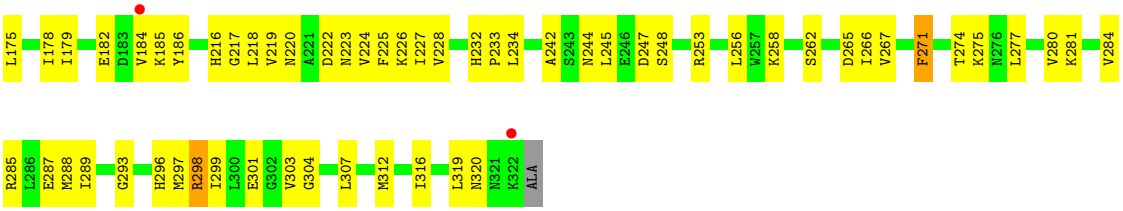
Chain A:

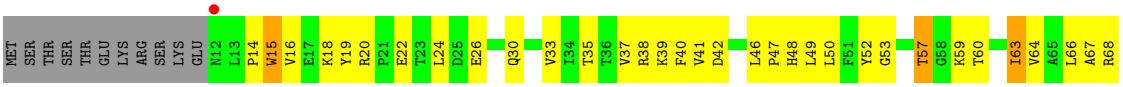


• Molecule 2: Activator 1 37 kDa subunit

Chain B:

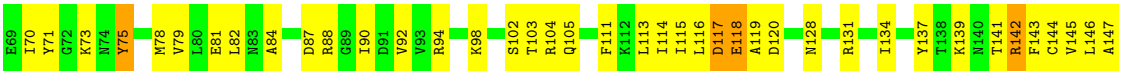


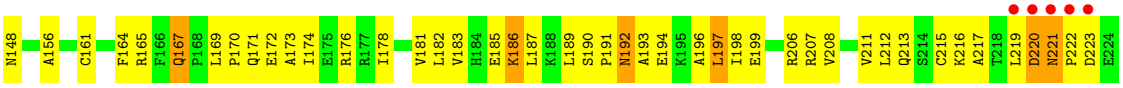


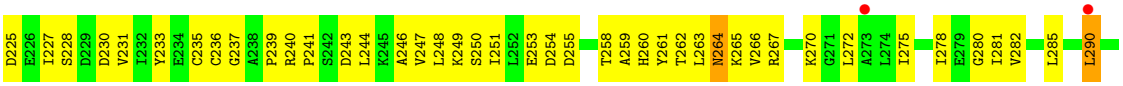


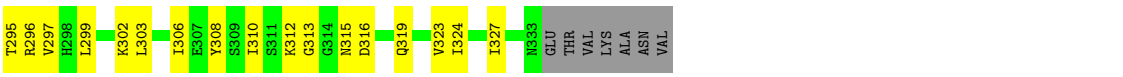
• Molecule 3: Activator 1 40 kDa subunit

Chain C:



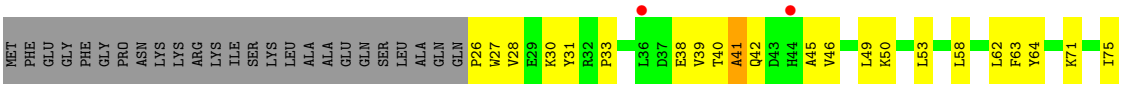


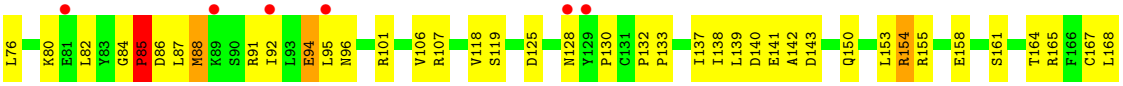


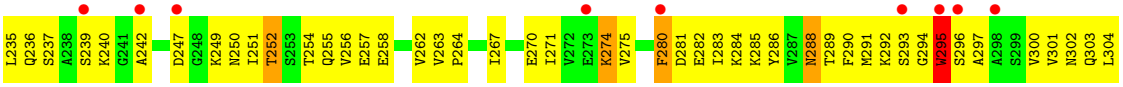


• Molecule 4: Activator 1 41 kDa subunit

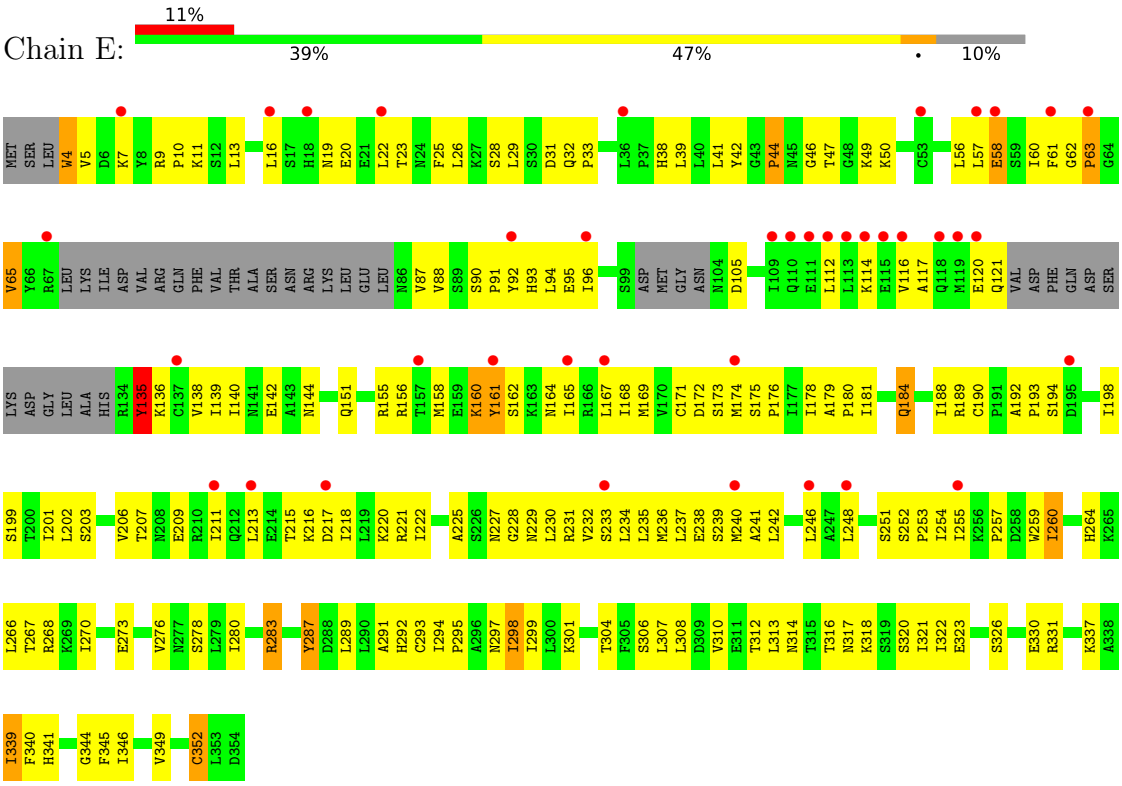
Chain D:



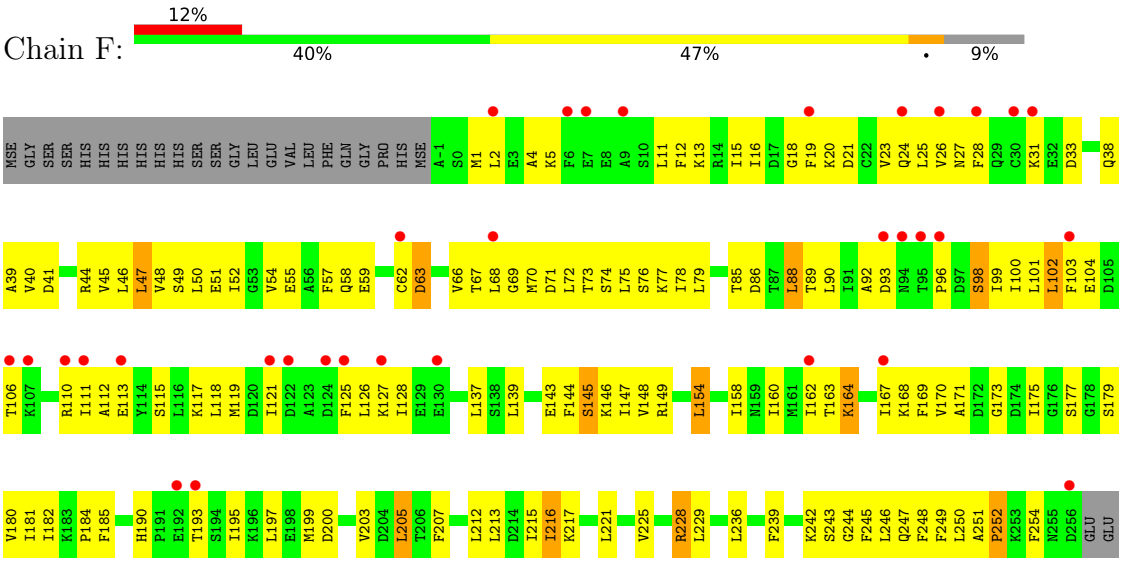




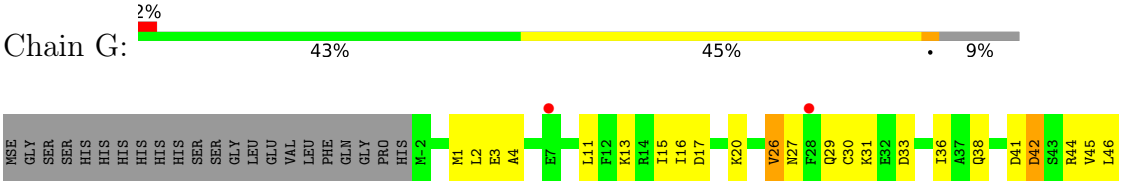
• Molecule 5: Activator 1 40 kDa subunit

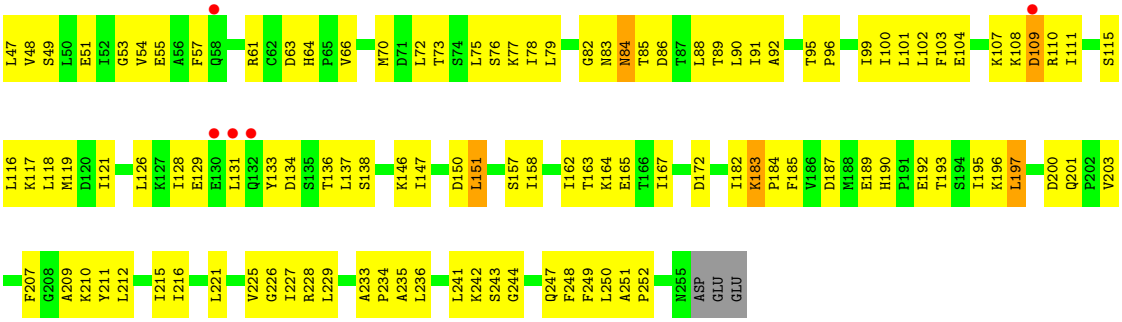


• Molecule 6: Proliferating cell nuclear antigen



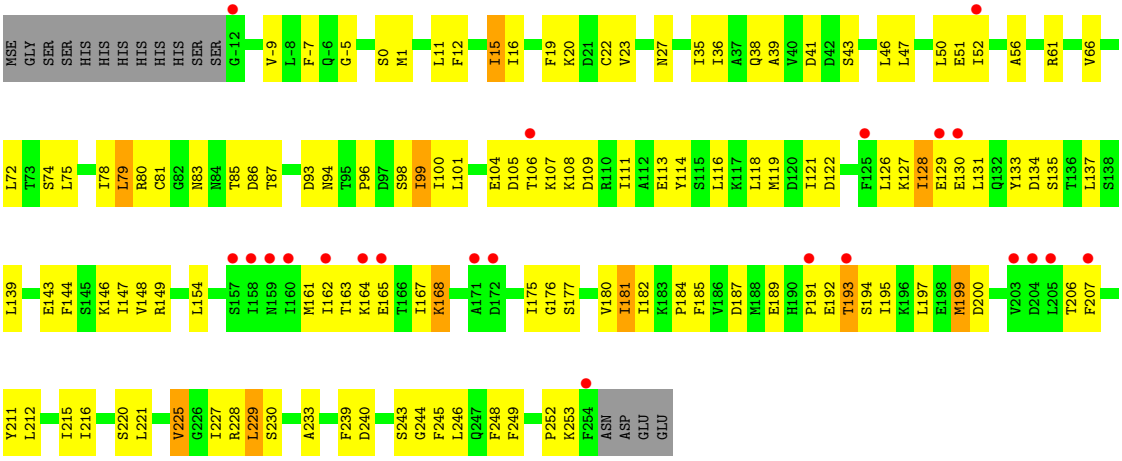
• Molecule 6: Proliferating cell nuclear antigen





• Molecule 6: Proliferating cell nuclear antigen

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.21Å 110.48Å 268.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 2.85 48.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.81-2.85) 94.8 (48.81-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.306 0.241 , 0.295	Depositor DCC
R_{free} test set	6077 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å^2)	72.9	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 51.2	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	0.93	EDS
Total number of atoms	19740	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: ADP, 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	0.31	0/3173	0.59	0/4283
2	B	0.32	0/2517	0.58	0/3394
3	C	0.30	0/2584	0.56	0/3497
4	D	0.27	0/2642	0.53	0/3573
5	E	0.27	0/2529	0.52	0/3416
6	F	0.30	0/2045	0.55	0/2749
6	G	0.31	0/2046	0.56	0/2749
6	H	0.31	0/2105	0.56	0/2828
All	All	0.30	0/19641	0.56	0/26489

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3345	0	3207	210	0
2	B	2482	0	2572	132	0
3	C	2544	0	2573	171	0
4	D	2597	0	2627	183	0
5	E	2495	0	2598	216	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	2021	0	2036	159	0
6	G	2022	0	2044	122	0
6	H	2079	0	2083	126	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	31	0	12	1	0
8	B	31	0	12	2	0
8	C	31	0	12	2	0
8	D	31	0	12	2	0
9	E	27	0	12	3	0
All	All	19740	0	19800	1225	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 31.

The worst 5 of 1225 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:523:THR:HG21	1:A:547:ILE:HG21	1.30	1.09
4:D:138:ILE:HG22	4:D:167:CYS:HB3	1.39	1.04
3:C:221:ASN:HB2	3:C:222:PRO:HD3	1.33	1.03
5:E:39:LEU:HD21	5:E:41:LEU:HG	1.41	1.01
4:D:41:ALA:HB1	4:D:192:LEU:HD22	1.41	1.01

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	391/516 (76%)	324 (83%)	55 (14%)	12 (3%)	4 14
2	B	314/323 (97%)	279 (89%)	32 (10%)	3 (1%)	15 40
3	C	320/340 (94%)	257 (80%)	53 (17%)	10 (3%)	4 14
4	D	326/353 (92%)	268 (82%)	43 (13%)	15 (5%)	2 7
5	E	309/354 (87%)	244 (79%)	57 (18%)	8 (3%)	5 17
6	F	256/283 (90%)	216 (84%)	32 (12%)	8 (3%)	4 14
6	G	256/283 (90%)	219 (86%)	31 (12%)	6 (2%)	6 20
6	H	265/283 (94%)	224 (84%)	34 (13%)	7 (3%)	5 17
All	All	2437/2735 (89%)	2031 (83%)	337 (14%)	69 (3%)	5 16

5 of 69 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	ASP
1	A	584	ASP
2	B	25	GLY
2	B	27	LYS
4	D	41	ALA

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	340/400 (85%)	320 (94%)	20 (6%)	19 45
2	B	277/283 (98%)	263 (95%)	14 (5%)	24 52
3	C	279/296 (94%)	266 (95%)	13 (5%)	26 56
4	D	292/312 (94%)	282 (97%)	10 (3%)	37 67
5	E	290/324 (90%)	280 (97%)	10 (3%)	37 67
6	F	231/246 (94%)	224 (97%)	7 (3%)	41 72
6	G	232/246 (94%)	221 (95%)	11 (5%)	26 56
6	H	235/246 (96%)	224 (95%)	11 (5%)	26 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2176/2353 (92%)	2080 (96%)	96 (4%)	28 58

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	4	TRP
6	F	185	PHE
5	E	63	PRO
5	E	339	ILE
6	G	20	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	128	ASN
6	H	24	GLN
4	D	340	HIS
6	G	247	GLN
6	F	247	GLN

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
8	AGS	B	802	7	26,33,33	2.01	4 (15%)	26,52,52	1.34	3 (11%)
8	AGS	A	801	7	26,33,33	2.12	5 (19%)	26,52,52	1.52	3 (11%)
8	AGS	D	804	7	26,33,33	2.02	5 (19%)	26,52,52	1.50	4 (15%)
9	ADP	E	805	-	24,29,29	1.74	6 (25%)	29,45,45	1.36	4 (13%)
8	AGS	C	803	7	26,33,33	2.20	4 (15%)	26,52,52	1.46	4 (15%)

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
8	AGS	B	802	7	-	5/17/38/38	0/3/3/3
8	AGS	A	801	7	-	3/17/38/38	0/3/3/3
8	AGS	D	804	7	-	2/17/38/38	0/3/3/3
9	ADP	E	805	-	-	4/12/32/32	0/3/3/3
8	AGS	C	803	7	-	3/17/38/38	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	803	AGS	PG-S1G	-9.44	1.70	1.90
8	A	801	AGS	PG-S1G	-8.97	1.71	1.90
8	B	802	AGS	PG-S1G	-8.45	1.72	1.90
8	D	804	AGS	PG-S1G	-7.94	1.73	1.90
9	E	805	ADP	C2-N3	3.65	1.38	1.32

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	801	AGS	C1'-N9-C4	4.98	135.40	126.64
8	D	804	AGS	C1'-N9-C4	4.52	134.58	126.64
9	E	805	ADP	C1'-N9-C4	4.38	134.34	126.64
8	C	803	AGS	C1'-N9-C4	4.18	133.98	126.64
8	B	802	AGS	C1'-N9-C4	3.95	133.59	126.64

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	801	AGS	C5'-O5'-PA-O1A
8	B	802	AGS	C5'-O5'-PA-O1A
8	C	803	AGS	C5'-O5'-PA-O1A
9	E	805	ADP	C5'-O5'-PA-O1A
9	E	805	ADP	O4'-C4'-C5'-O5'

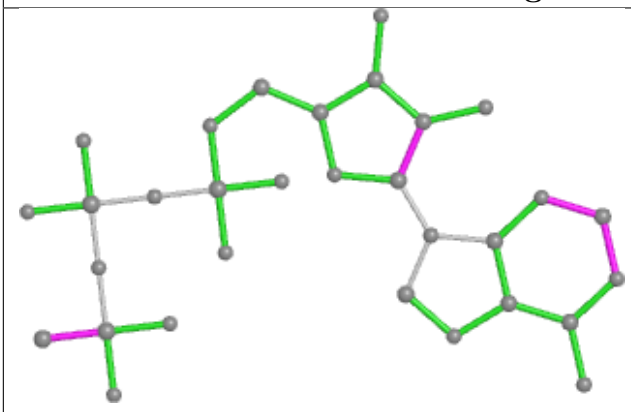
There are no ring outliers.

5 monomers are involved in 10 short contacts:

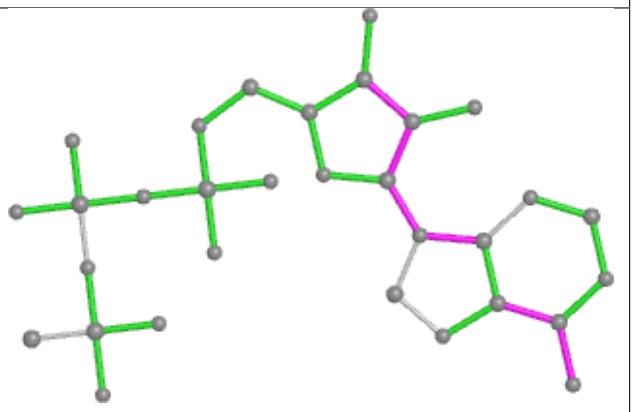
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	802	AGS	2	0
8	A	801	AGS	1	0
8	D	804	AGS	2	0
9	E	805	ADP	3	0
8	C	803	AGS	2	0

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.

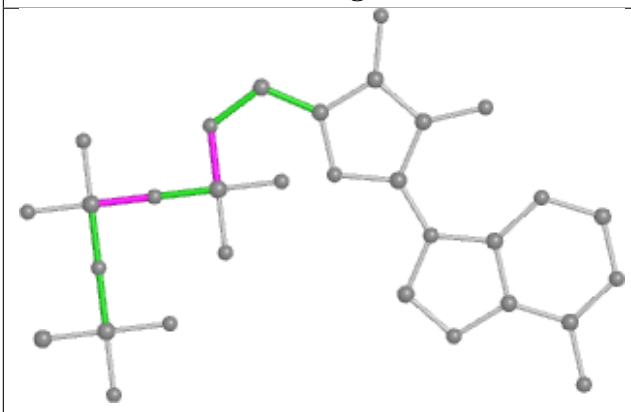
Ligand AGS B 802



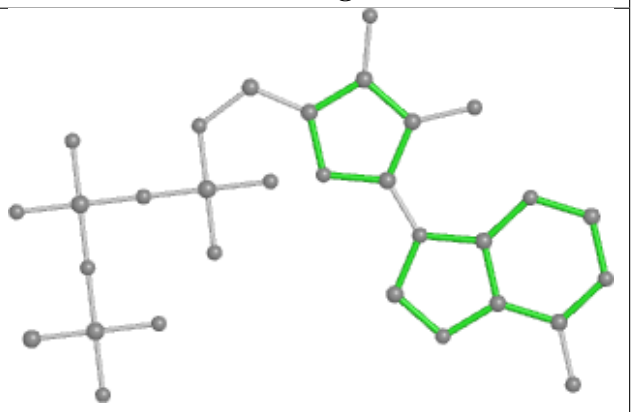
Bond lengths



Bond angles

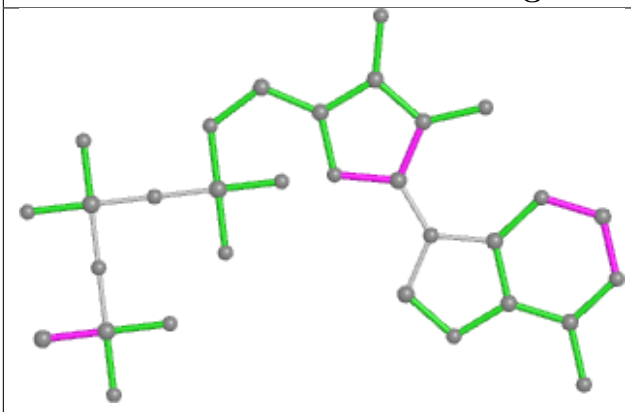


Torsions

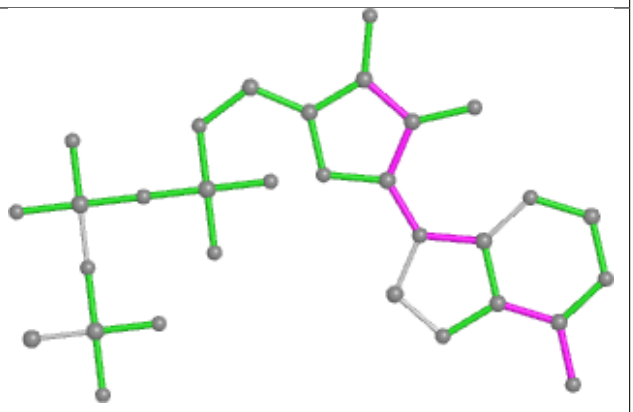


Rings

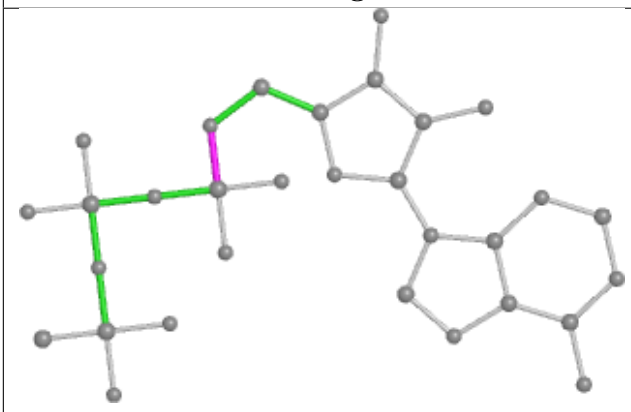
Ligand AGS A 801



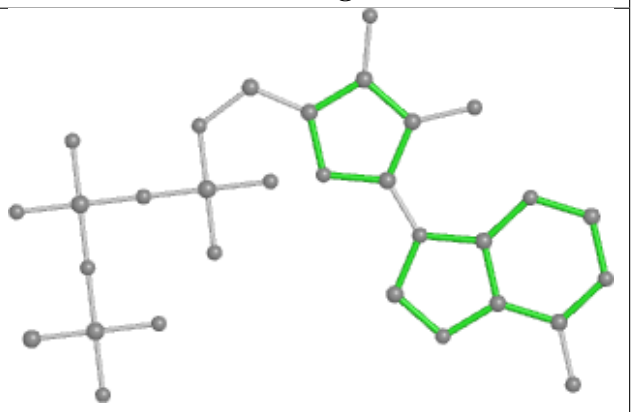
Bond lengths



Bond angles

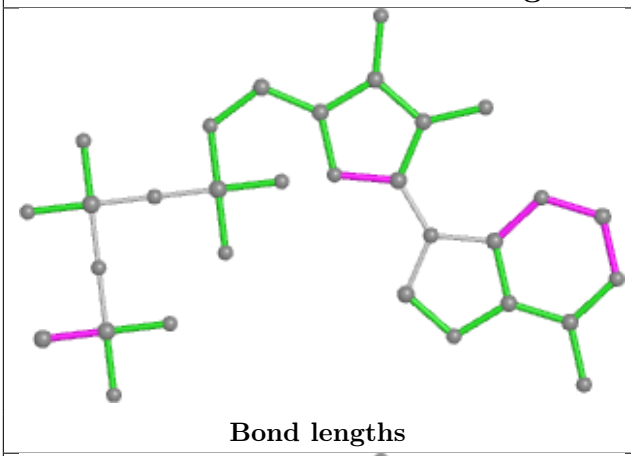


Torsions

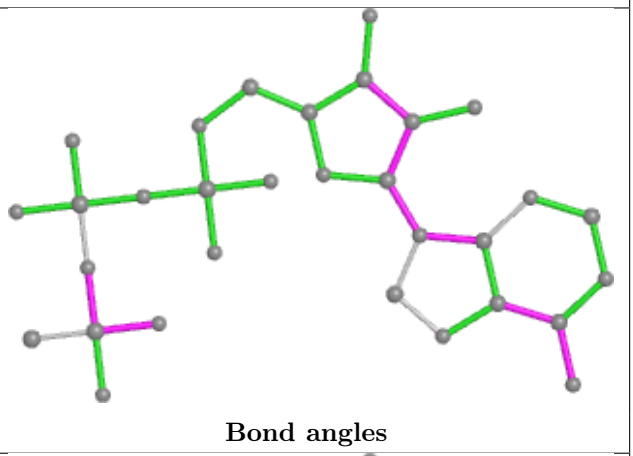


Rings

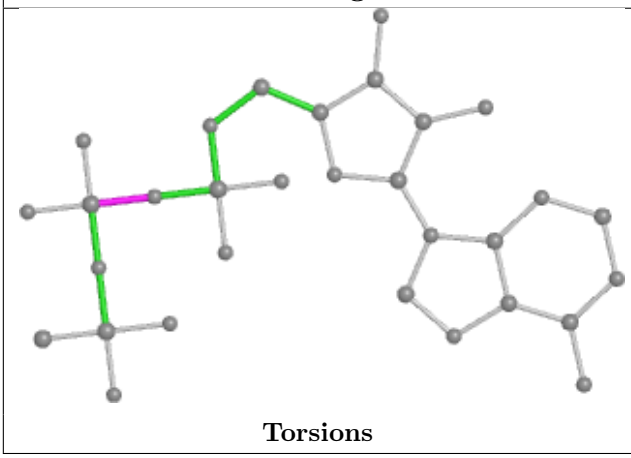
Ligand AGS D 804



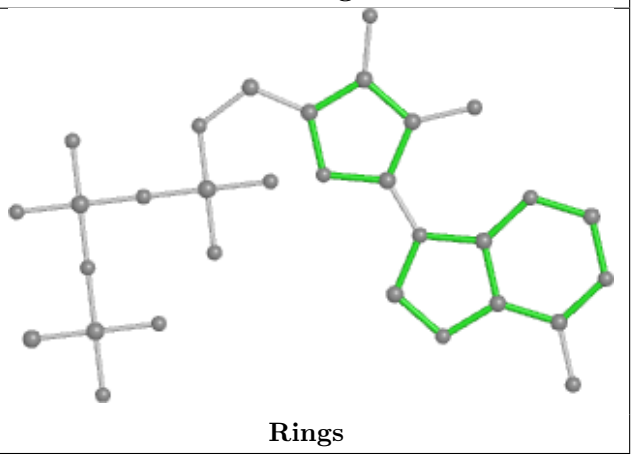
Bond lengths



Bond angles

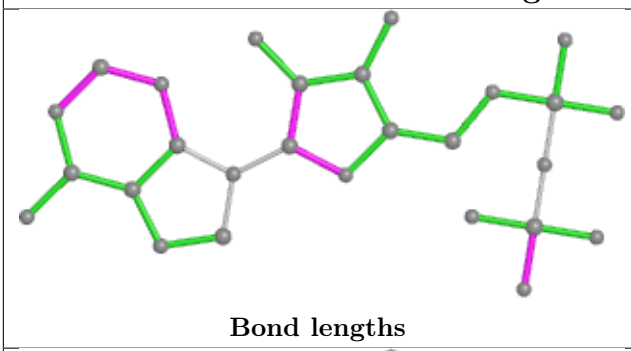


Torsions

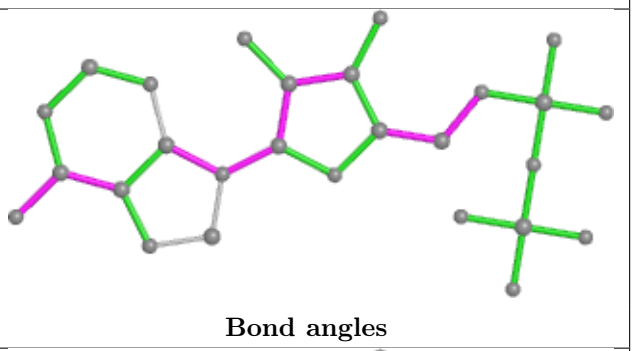


Rings

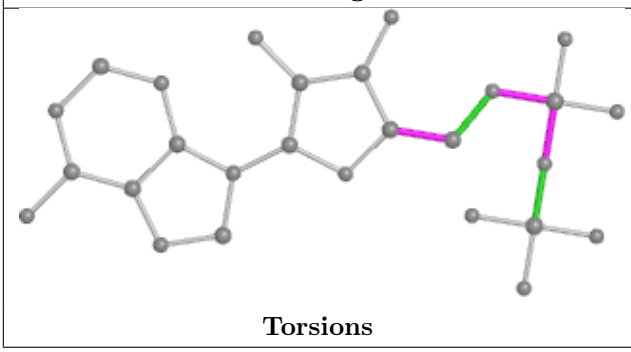
Ligand ADP E 805



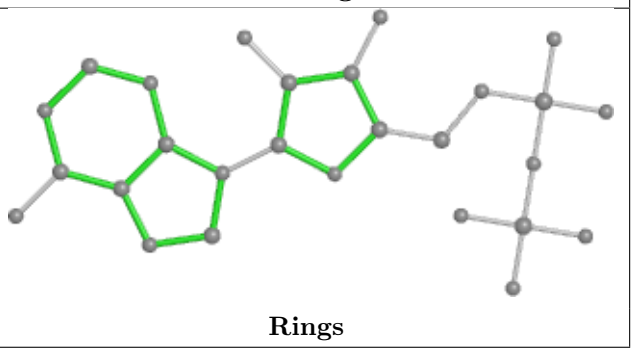
Bond lengths



Bond angles

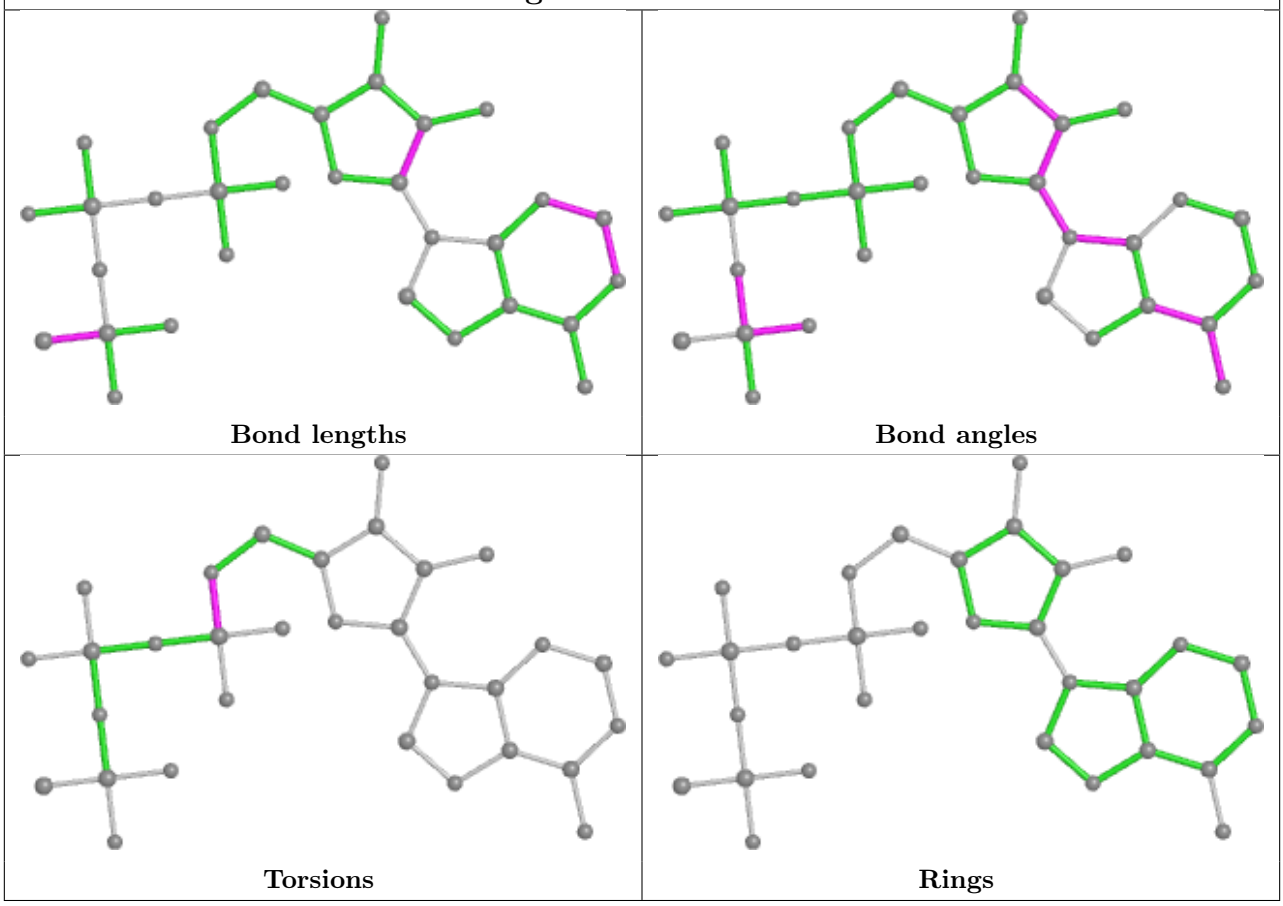


Torsions



Rings

Ligand AGS C 803



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	395/516 (76%)	0.06	14 (3%) 44 38	37, 72, 130, 181	0
2	B	316/323 (97%)	-0.09	3 (0%) 84 84	32, 60, 99, 142	0
3	C	322/340 (94%)	0.05	8 (2%) 57 54	33, 76, 126, 178	0
4	D	328/353 (92%)	0.44	30 (9%) 9 6	53, 105, 167, 187	0
5	E	317/354 (89%)	0.65	39 (12%) 4 2	45, 113, 154, 181	0
6	F	252/283 (89%)	0.59	33 (13%) 3 2	48, 107, 154, 179	0
6	G	251/283 (88%)	0.09	7 (2%) 53 48	42, 77, 136, 165	0
6	H	260/283 (91%)	0.39	22 (8%) 10 7	44, 92, 148, 169	0
All	All	2441/2735 (89%)	0.26	156 (6%) 19 15	32, 85, 149, 187	0

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	122	ASP	11.8
6	H	158	ILE	8.2
1	A	533	HIS	6.0
6	F	193	THR	5.8
4	D	216	VAL	5.8

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

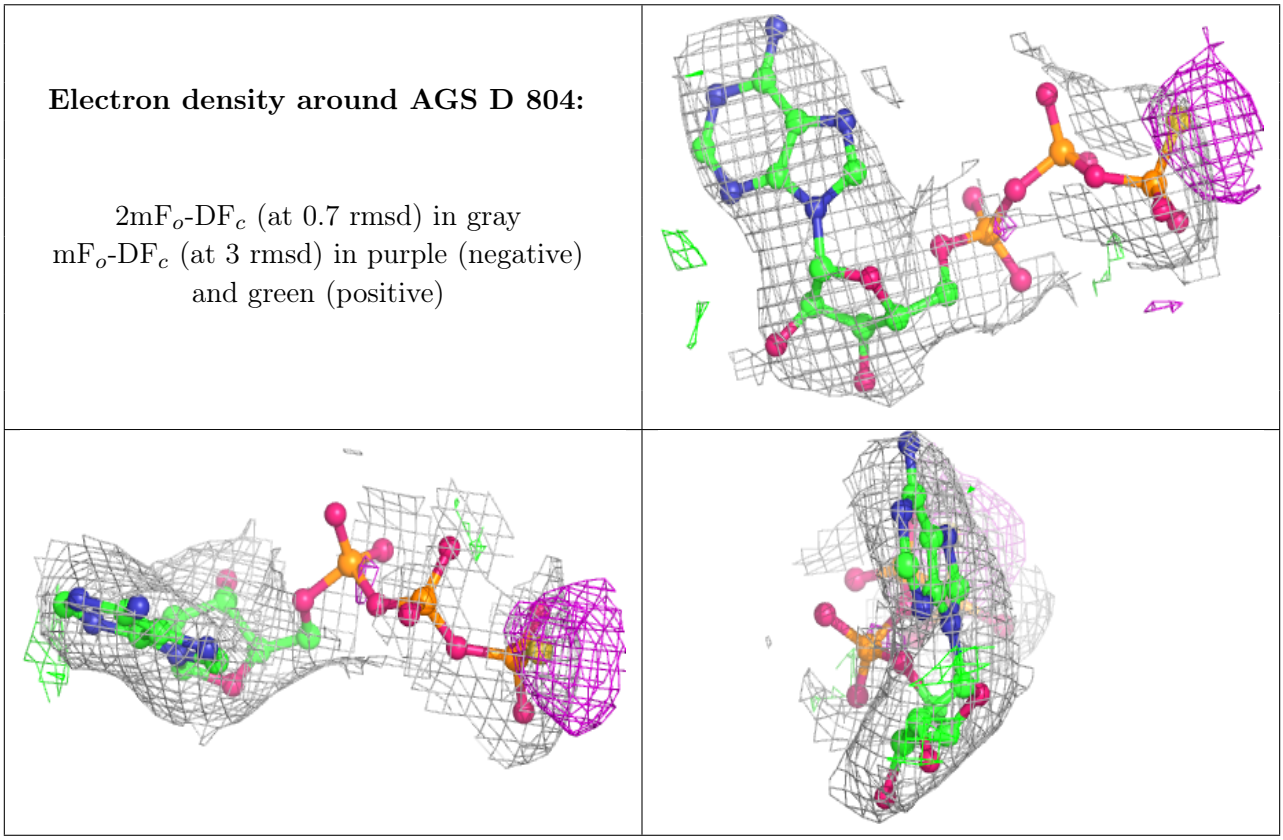
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	B	812	1/1	0.82	0.30	48,48,48,48	0
7	MG	A	811	1/1	0.89	0.43	56,56,56,56	0
7	MG	D	814	1/1	0.93	0.17	66,66,66,66	0
8	AGS	D	804	31/31	0.93	0.16	86,86,86,86	0
9	ADP	E	805	27/27	0.93	0.15	93,93,93,93	0
7	MG	C	813	1/1	0.94	0.30	40,40,40,40	0
8	AGS	B	802	31/31	0.94	0.18	51,51,51,51	0
8	AGS	A	801	31/31	0.96	0.17	51,51,51,51	0
8	AGS	C	803	31/31	0.96	0.18	50,50,50,50	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.

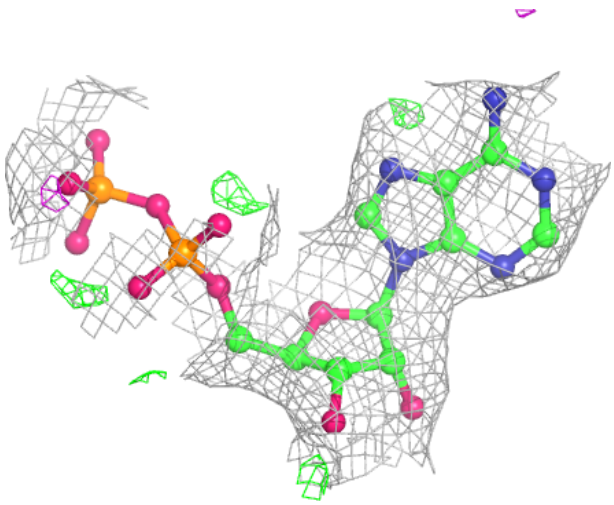
Electron density around AGS D 804:

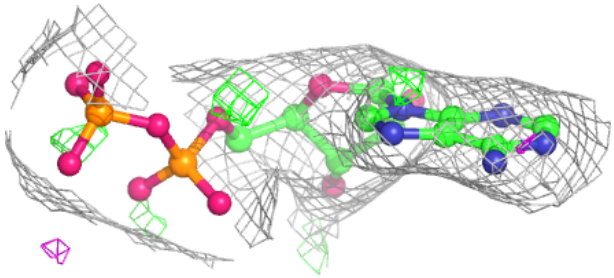
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

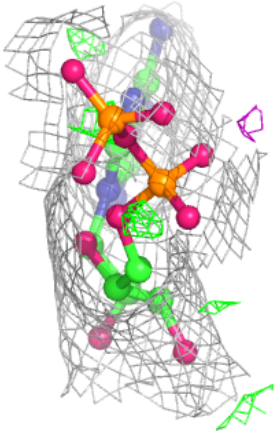


Electron density around ADP E 805:

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

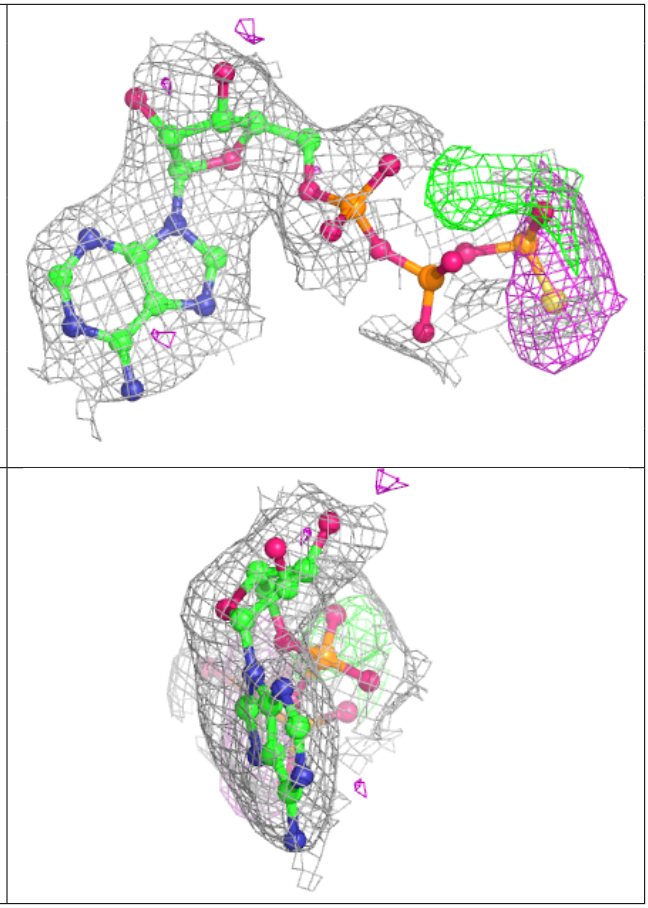


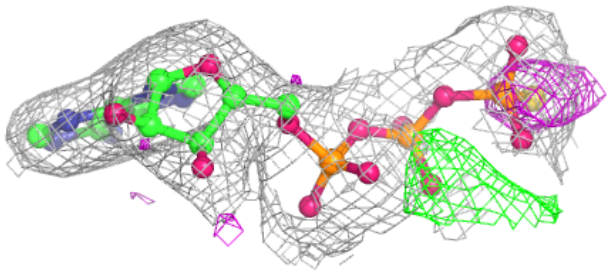




Electron density around AGS B 802:

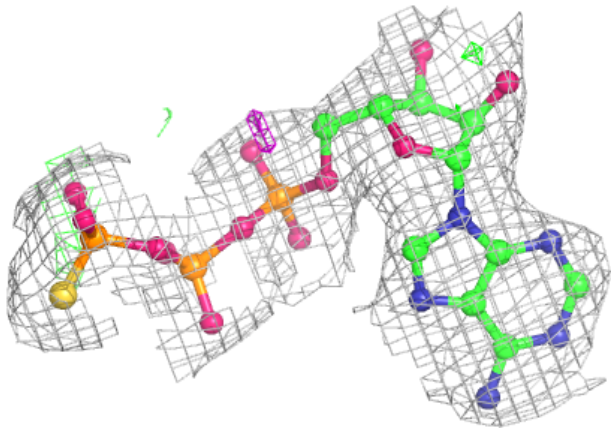
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

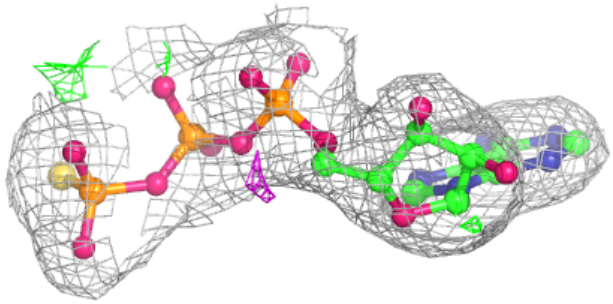


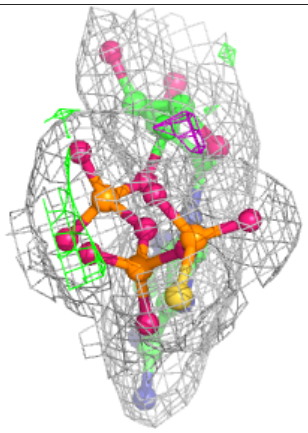


Electron density around AGS A 801:

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

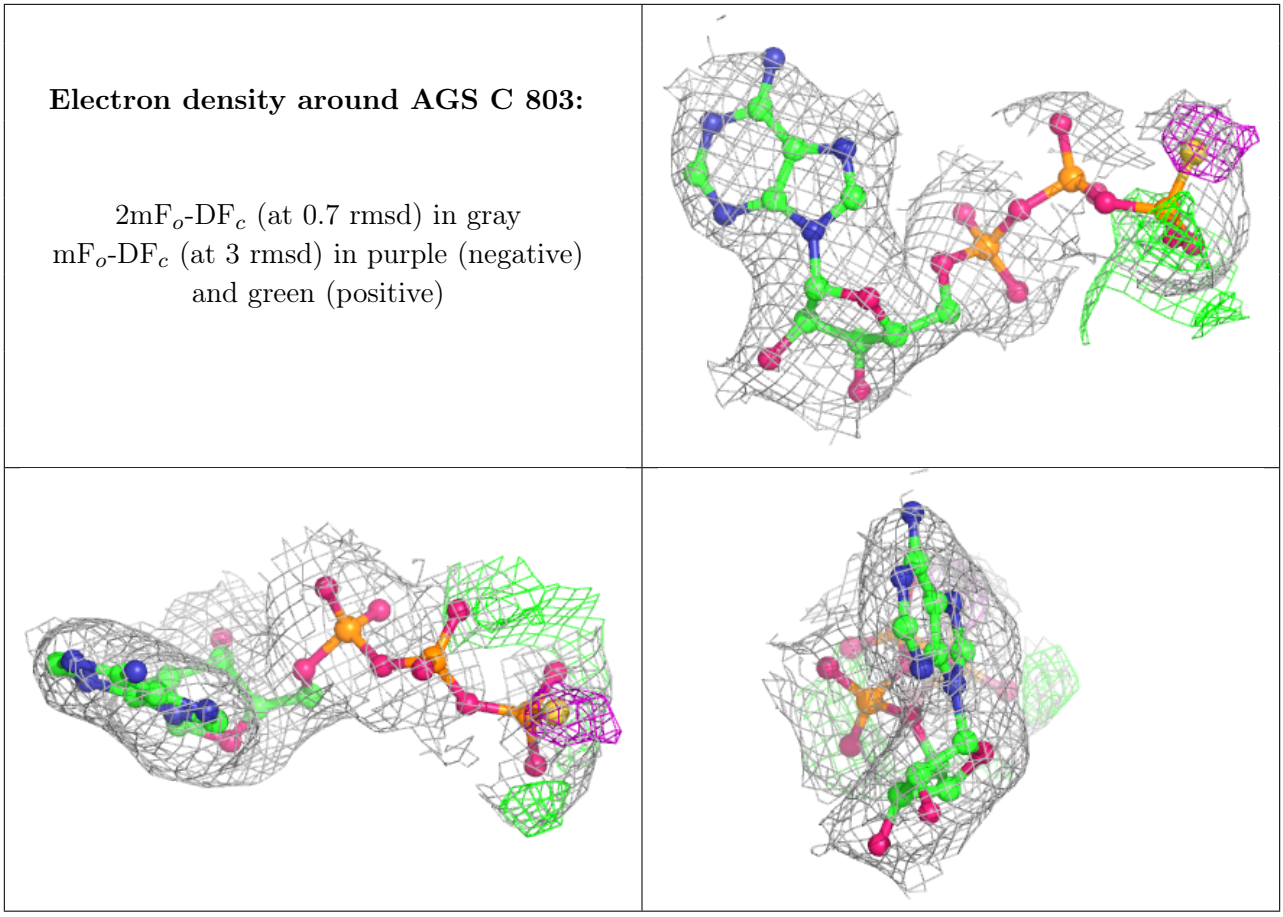






Electron density around AGS C 803:

$2mF_o$-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.