Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 02:41 am GMT

PDB ID	:	4CKB
Title	:	Vaccinia virus capping enzyme complexed with GTP and SAH
Authors	:	Kyrieleis, O.J.P.; Chang, J.; de la Pena, M.; Shuman, S.; Cusack, S.
Deposited on	:	2014-01-02
Resolution	:	2.80 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:

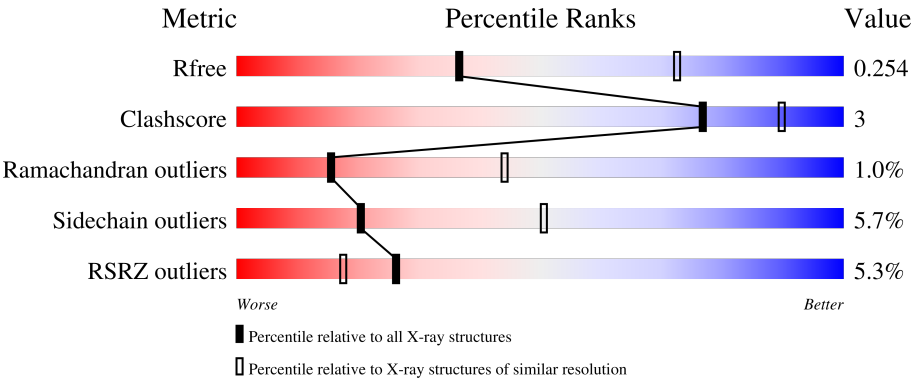
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	844	7% 83% 11%
1	D	844	3% 83% 12%
2	B	287	2% 89% 10%
2	E	287	7% 88% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17863 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.

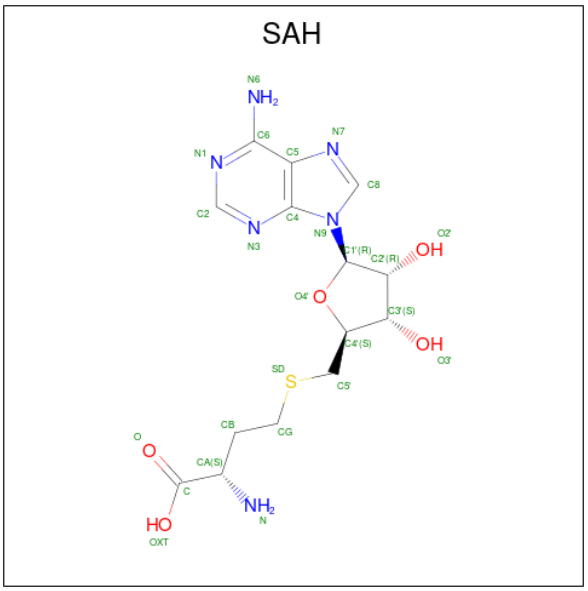
- Molecule 1 is a protein called MRNA-CAPPING ENZYME CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	809	Total	C	N	O	S	0	0	0
			6536	4210	1074	1233	19			
1	D	814	Total	C	N	O	S	0	0	0
			6578	4239	1080	1240	19			

- Molecule 2 is a protein called MRNA-CAPPING ENZYME REGULATORY SUBUNIT.

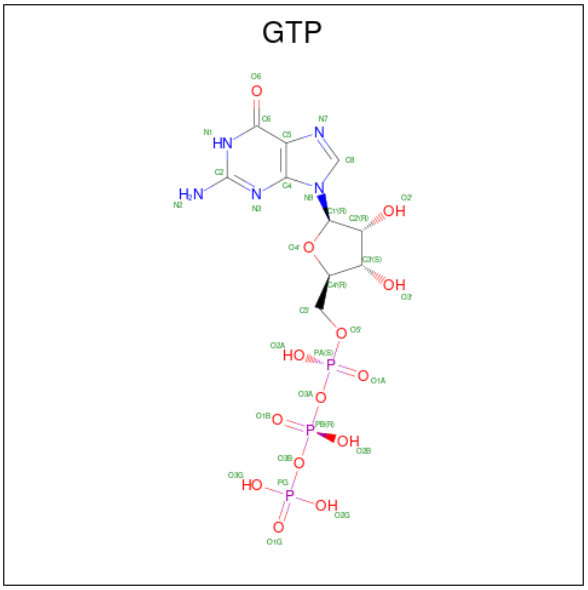
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	284	Total	C	N	O	S	0	0	0
			2320	1492	385	430	13			
2	E	284	Total	C	N	O	S	0	0	0
			2320	1492	385	430	13			

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is water.

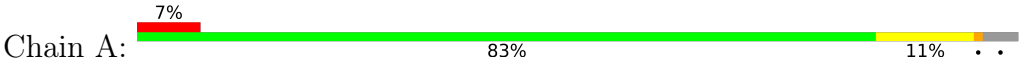
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	4	Total	O	0	0
			4	4		
5	D	10	Total	O	0	0
			10	10		
5	E	2	Total	O	0	0
			2	2		

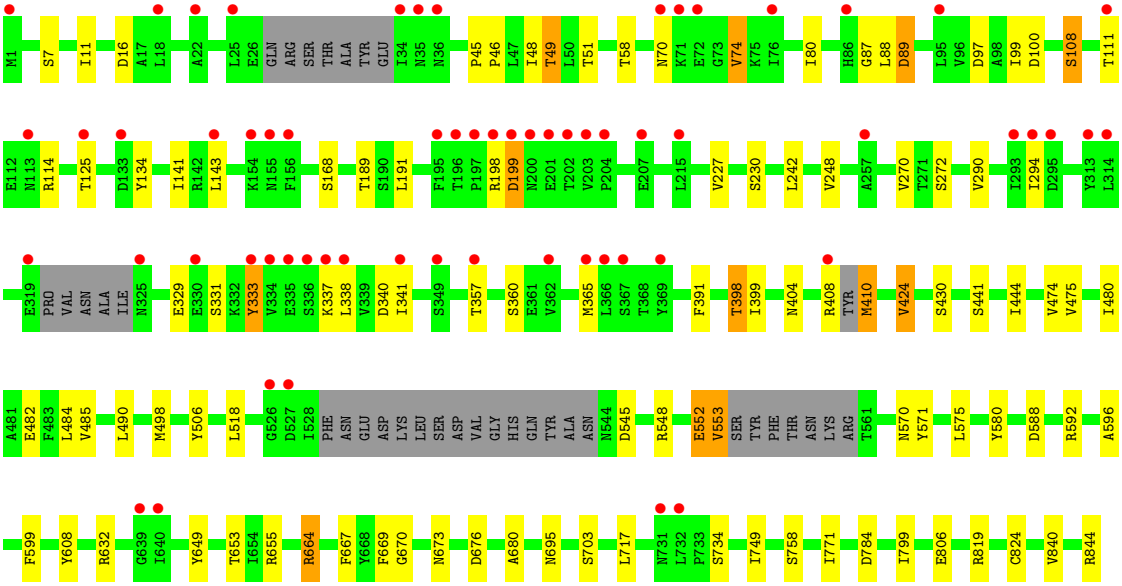
3 Residue-property plots (i)

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: MRNA-CAPPING ENZYME CATALYTIC SUBUNIT

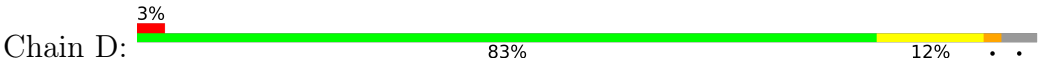
Chain A:

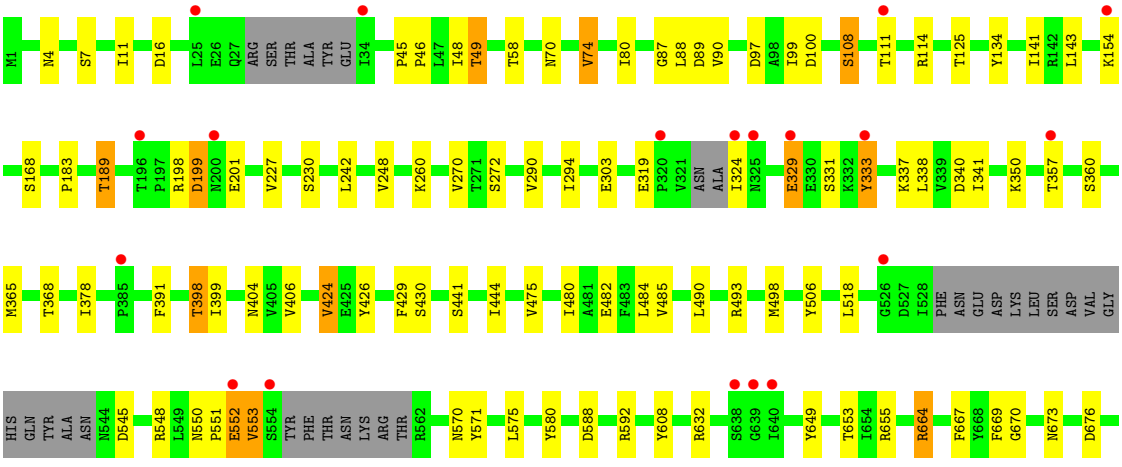


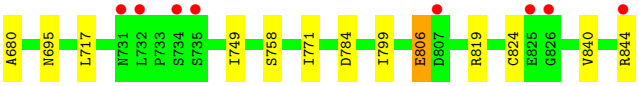


• Molecule 1: MRNA-CAPPING ENZYME CATALYTIC SUBUNIT

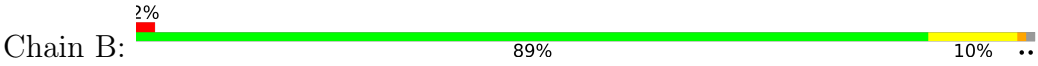
Chain D:

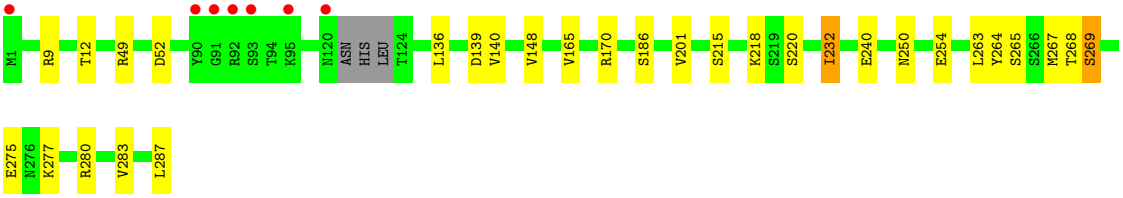




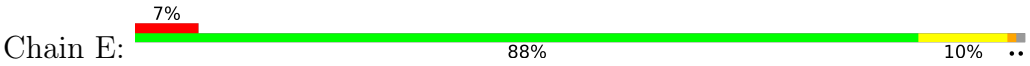


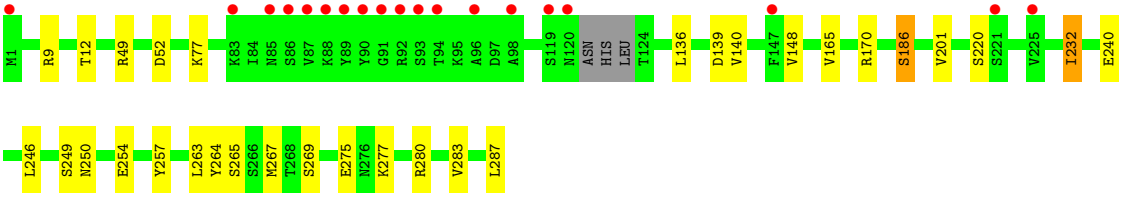
• Molecule 2: MRNA-CAPPING ENZYME REGULATORY SUBUNIT





• Molecule 2: MRNA-CAPPING ENZYME REGULATORY SUBUNIT





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.34Å 197.73Å 61.11Å 90.13° 109.27° 94.05°	Depositor
Resolution (Å)	49.20 – 2.80 48.47 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.20-2.80) 96.6 (48.47-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.209 , 0.255 0.210 , 0.254	Depositor DCC
R_{free} test set	3184 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.024 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17863	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: GTP, SAH

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	0.36	0/6664	0.57	0/9006
1	D	0.39	0/6709	0.58	0/9070
2	B	0.41	0/2365	0.59	0/3189
2	E	0.35	0/2365	0.55	0/3189
All	All	0.38	0/18103	0.57	0/24454

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	6536	0	6623	41	0
1	D	6578	0	6666	51	0
2	B	2320	0	2363	8	0
2	E	2320	0	2363	9	0
3	A	26	0	19	1	0
3	D	26	0	19	1	0
4	D	32	0	12	8	0
5	A	9	0	0	0	0
5	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	10	0	0	0	0
5	E	2	0	0	0	0
All	All	17863	0	18065	108	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 3.

All (108) 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:655:ARG:NH2	3:D:1845:SAH:N7	2.31	0.79
1:D:378:ILE:HD13	4:D:1846:GTP:C6	2.20	0.76
1:A:655:ARG:NH2	3:A:1845:SAH:N7	2.33	0.76
1:D:45:PRO:HD2	1:D:189:THR:HG22	1.70	0.72
1:D:493:ARG:NH2	4:D:1846:GTP:O2G	2.23	0.71
1:A:45:PRO:HD2	1:A:189:THR:HG22	1.73	0.71
1:D:580:TYR:O	1:D:592:ARG:NH1	2.27	0.68
1:D:46:PRO:O	1:D:49:THR:HB	1.94	0.67
1:A:46:PRO:O	1:A:49:THR:HB	1.95	0.66
1:A:717:LEU:HD13	1:A:749:ILE:CD1	2.27	0.65
1:D:717:LEU:HD13	1:D:749:ILE:CD1	2.27	0.64
1:D:303:GLU:HG3	4:D:1846:GTP:C8	2.32	0.64
1:A:580:TYR:O	1:A:592:ARG:NH1	2.31	0.64
1:D:485:VAL:HG11	1:D:518:LEU:HA	1.82	0.62
1:D:74:VAL:HG12	1:D:108:SER:HB3	1.83	0.61
1:A:74:VAL:HG12	1:A:108:SER:HB3	1.83	0.61
1:D:198:ARG:O	1:D:199:ASP:HB2	2.03	0.59
1:A:485:VAL:HG11	1:A:518:LEU:HA	1.83	0.58
1:D:653:THR:HG21	1:D:655:ARG:CZ	2.33	0.58
1:A:653:THR:HG21	1:A:655:ARG:CZ	2.32	0.58
1:D:324:ILE:HG21	1:D:329:GLU:HB3	1.85	0.58
1:D:338:LEU:HA	1:D:341:ILE:HD11	1.86	0.57
2:E:136:LEU:HD11	2:E:140:VAL:HG11	1.86	0.57
1:A:588:ASP:O	1:A:592:ARG:NH2	2.38	0.56
1:D:350:LYS:NZ	4:D:1846:GTP:N7	2.53	0.56
2:B:136:LEU:HD11	2:B:140:VAL:HG11	1.87	0.56
1:A:338:LEU:HA	1:A:341:ILE:HD11	1.87	0.54
1:D:378:ILE:HD13	4:D:1846:GTP:C5	2.41	0.54
1:D:378:ILE:CD1	4:D:1846:GTP:C5	2.90	0.54
1:D:717:LEU:HD13	1:D:749:ILE:HD11	1.91	0.53
1:D:588:ASP:O	1:D:592:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:571:TYR:CE2	1:D:575:LEU:HD11	2.44	0.52
2:B:52:ASP:HB3	2:B:264:TYR:CE1	2.45	0.52
1:D:806:GLU:HG2	2:E:257:TYR:OH	2.10	0.51
1:A:799:ILE:O	1:A:819:ARG:HD3	2.09	0.51
2:E:263:LEU:HG	2:E:267:MET:HE3	1.92	0.51
1:A:717:LEU:HD13	1:A:749:ILE:HD11	1.91	0.51
1:A:99:ILE:O	1:A:134:TYR:OH	2.29	0.50
1:A:784:ASP:HB3	1:A:840:VAL:HB	1.93	0.50
1:D:99:ILE:O	1:D:134:TYR:OH	2.30	0.50
1:D:552:GLU:O	1:D:553:VAL:HG13	2.13	0.49
2:E:52:ASP:HB3	2:E:264:TYR:CE1	2.48	0.49
1:D:664:ARG:NH1	1:D:667:PHE:O	2.46	0.49
1:D:545:ASP:OD1	1:D:655:ARG:NH1	2.44	0.49
1:A:664:ARG:NH1	1:A:667:PHE:O	2.45	0.49
1:A:571:TYR:CE2	1:A:575:LEU:HD11	2.48	0.48
1:A:408:ARG:O	1:A:410:MET:HA	2.14	0.48
1:D:784:ASP:HB3	1:D:840:VAL:HB	1.95	0.48
2:B:263:LEU:HG	2:B:267:MET:HE3	1.96	0.48
1:D:799:ILE:O	1:D:819:ARG:HD3	2.14	0.47
1:D:608:TYR:OH	1:D:676:ASP:HB2	2.14	0.47
1:A:545:ASP:OD1	1:A:655:ARG:NH1	2.46	0.47
1:A:290:VAL:HG11	1:A:294:ILE:HD11	1.97	0.47
1:D:673:ASN:N	1:D:673:ASN:OD1	2.47	0.47
2:E:250:ASN:O	2:E:254:GLU:HB2	2.15	0.47
1:A:669:PHE:CG	1:A:670:GLY:N	2.83	0.46
1:A:11:ILE:HD12	1:A:227:VAL:HG11	1.98	0.45
1:A:673:ASN:OD1	1:A:673:ASN:N	2.47	0.45
1:A:424:VAL:HG12	1:A:444:ILE:HB	1.99	0.45
1:A:608:TYR:OH	1:A:676:ASP:HB2	2.16	0.45
1:A:398:THR:OG1	1:A:482:GLU:HG3	2.17	0.45
1:D:290:VAL:HG11	1:D:294:ILE:HD11	1.98	0.45
2:E:77:LYS:HG3	2:E:186:SER:OG	2.16	0.45
1:D:669:PHE:CG	1:D:670:GLY:N	2.85	0.45
2:B:268:THR:O	2:B:269:SER:C	2.55	0.44
1:A:45:PRO:CD	1:A:189:THR:HG22	2.45	0.44
1:D:114:ARG:O	1:D:114:ARG:HG3	2.16	0.44
1:D:154:LYS:HA	1:D:198:ARG:CZ	2.48	0.44
1:D:424:VAL:HG12	1:D:444:ILE:HB	1.99	0.44
1:D:398:THR:OG1	1:D:482:GLU:HG3	2.18	0.44
1:D:324:ILE:HD12	1:D:333:TYR:CD2	2.53	0.43
1:A:51:THR:HG23	1:A:474:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ILE:CD1	1:A:506:TYR:CE2	3.02	0.43
1:D:87:GLY:O	1:D:90:VAL:HG23	2.18	0.43
1:D:260:LYS:NZ	4:D:1846:GTP:O4'	2.33	0.43
1:A:552:GLU:O	1:A:553:VAL:HG13	2.19	0.43
1:A:49:THR:HG21	1:A:191:LEU:HD22	2.01	0.42
2:B:250:ASN:O	2:B:254:GLU:HB2	2.19	0.42
1:D:242:LEU:HB2	1:D:391:PHE:HB3	2.00	0.42
1:A:596:ALA:HB1	1:A:599:PHE:CD1	2.54	0.42
1:A:270:VAL:HG12	1:A:294:ILE:HD13	2.01	0.42
1:A:333:TYR:CD1	1:A:333:TYR:C	2.92	0.42
1:A:198:ARG:O	1:A:199:ASP:CB	2.68	0.42
1:D:270:VAL:HG12	1:D:294:ILE:HD13	2.01	0.42
1:D:484:LEU:CD1	1:D:490:LEU:HD21	2.50	0.42
1:A:484:LEU:CD1	1:A:490:LEU:HD21	2.50	0.42
1:D:480:ILE:CD1	1:D:506:TYR:CE2	3.03	0.42
2:E:246:LEU:HA	2:E:249:SER:OG	2.20	0.42
1:A:114:ARG:O	1:A:114:ARG:HG3	2.18	0.41
2:B:283:VAL:HG13	2:B:287:LEU:HD12	2.02	0.41
1:D:183:PRO:HG3	1:D:429:PHE:CG	2.54	0.41
1:A:141:ILE:O	1:A:168:SER:HA	2.20	0.41
1:A:333:TYR:CE1	1:A:337:LYS:HD2	2.55	0.41
1:A:87:GLY:O	1:A:89:ASP:N	2.53	0.41
1:D:333:TYR:CE1	1:D:337:LYS:HD2	2.56	0.41
1:D:45:PRO:CD	1:D:189:THR:HG22	2.43	0.41
1:D:70:ASN:HB2	1:D:74:VAL:HG23	2.02	0.41
1:A:242:LEU:HB2	1:A:391:PHE:HB3	2.01	0.41
1:D:378:ILE:HD13	4:D:1846:GTP:N1	2.34	0.41
1:D:11:ILE:HD12	1:D:227:VAL:HG11	2.03	0.41
2:B:277:LYS:HA	2:B:280:ARG:HD2	2.03	0.41
1:A:70:ASN:HB2	1:A:74:VAL:HG23	2.02	0.40
1:D:141:ILE:O	1:D:168:SER:HA	2.21	0.40
1:D:406:VAL:HG23	1:D:426:TYR:HA	2.03	0.40
2:E:283:VAL:HG13	2:E:287:LEU:HD12	2.04	0.40
2:B:215:SER:O	2:B:218:LYS:HE2	2.21	0.40
1:D:550:ASN:N	1:D:551:PRO:HD3	2.36	0.40
2:E:277:LYS:HA	2:E:280:ARG:HD2	2.02	0.40

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	797/844 (94%)	750 (94%)	40 (5%)	7 (1%)	17	46
1	D	804/844 (95%)	753 (94%)	43 (5%)	8 (1%)	15	44
2	B	280/287 (98%)	263 (94%)	14 (5%)	3 (1%)	14	41
2	E	280/287 (98%)	262 (94%)	15 (5%)	3 (1%)	14	41
All	All	2161/2262 (96%)	2028 (94%)	112 (5%)	21 (1%)	15	44

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	199	ASP
1	A	88	LEU
1	A	734	SER
2	B	148	VAL
2	B	269	SER
1	D	88	LEU
1	D	553	VAL
2	E	148	VAL
2	E	269	SER
1	A	89	ASP
1	A	199	ASP
2	B	232	ILE
1	A	680	ALA
1	D	89	ASP
1	D	680	ALA
2	E	232	ILE
1	D	319	GLU
1	D	552	GLU
1	A	552	GLU
1	A	248	VAL
1	D	248	VAL

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	743/774 (96%)	699 (94%)	44 (6%)	19	49
1	D	748/774 (97%)	703 (94%)	45 (6%)	19	48
2	B	269/272 (99%)	256 (95%)	13 (5%)	25	58
2	E	269/272 (99%)	256 (95%)	13 (5%)	25	58
All	All	2029/2092 (97%)	1914 (94%)	115 (6%)	20	50

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	16	ASP
1	A	48	ILE
1	A	49	THR
1	A	58	THR
1	A	74	VAL
1	A	80	ILE
1	A	97	ASP
1	A	100	ASP
1	A	108	SER
1	A	111	THR
1	A	125	THR
1	A	143	LEU
1	A	230	SER
1	A	272	SER
1	A	329	GLU
1	A	331	SER
1	A	333	TYR
1	A	340	ASP
1	A	357	THR
1	A	360	SER
1	A	365	MET
1	A	398	THR
1	A	399	ILE

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Mol	Chain	Res	Type
1	A	404	ASN
1	A	410	MET
1	A	424	VAL
1	A	430	SER
1	A	441	SER
1	A	475	VAL
1	A	498	MET
1	A	548	ARG
1	A	553	VAL
1	A	570	ASN
1	A	632	ARG
1	A	649	TYR
1	A	664	ARG
1	A	695	ASN
1	A	703	SER
1	A	758	SER
1	A	771	ILE
1	A	806	GLU
1	A	824	CYS
1	A	844	ARG
2	B	9	ARG
2	B	12	THR
2	B	49	ARG
2	B	139	ASP
2	B	165	VAL
2	B	170	ARG
2	B	186	SER
2	B	201	VAL
2	B	220	SER
2	B	232	ILE
2	B	240	GLU
2	B	265	SER
2	B	275	GLU
1	D	4	ASN
1	D	7	SER
1	D	16	ASP
1	D	48	ILE
1	D	49	THR
1	D	58	THR
1	D	74	VAL
1	D	80	ILE
1	D	97	ASP

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Mol	Chain	Res	Type
1	D	100	ASP
1	D	108	SER
1	D	111	THR
1	D	125	THR
1	D	143	LEU
1	D	189	THR
1	D	201	GLU
1	D	230	SER
1	D	272	SER
1	D	329	GLU
1	D	331	SER
1	D	333	TYR
1	D	340	ASP
1	D	357	THR
1	D	360	SER
1	D	365	MET
1	D	368	THR
1	D	398	THR
1	D	399	ILE
1	D	404	ASN
1	D	424	VAL
1	D	430	SER
1	D	441	SER
1	D	475	VAL
1	D	498	MET
1	D	548	ARG
1	D	570	ASN
1	D	632	ARG
1	D	649	TYR
1	D	664	ARG
1	D	695	ASN
1	D	758	SER
1	D	771	ILE
1	D	806	GLU
1	D	824	CYS
1	D	844	ARG
2	E	9	ARG
2	E	12	THR
2	E	49	ARG
2	E	139	ASP
2	E	165	VAL
2	E	170	ARG

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Mol	Chain	Res	Type
2	E	186	SER
2	E	201	VAL
2	E	220	SER
2	E	232	ILE
2	E	240	GLU
2	E	265	SER
2	E	275	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

3 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	$\#\|Z\| > 2$
3	SAH	A	1845	-	24,28,28	0.99	2 (8%)	25,40,40	1.43	3 (12%)
4	GTP	D	1846	-	26,34,34	0.88	0	32,54,54	1.23	4 (12%)
3	SAH	D	1845	-	24,28,28	1.02	2 (8%)	25,40,40	1.45	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	A	1845	-	-	1/11/31/31	0/3/3/3
4	GTP	D	1846	-	-	6/18/38/38	0/3/3/3
3	SAH	D	1845	-	-	1/11/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1845	SAH	C5-C4	2.41	1.47	1.40
3	A	1845	SAH	C5-C4	2.20	1.46	1.40
3	A	1845	SAH	OXT-C	-2.10	1.23	1.30
3	D	1845	SAH	OXT-C	-2.02	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1845	SAH	N3-C2-N1	-3.86	122.65	128.68
3	A	1845	SAH	N3-C2-N1	-3.76	122.80	128.68
4	D	1846	GTP	C3'-C2'-C1'	3.00	105.49	100.98
3	D	1845	SAH	OXT-C-O	-2.98	117.32	124.09
4	D	1846	GTP	PB-O3B-PG	-2.92	122.82	132.83
4	D	1846	GTP	C8-N7-C5	2.61	107.96	102.99
3	D	1845	SAH	OXT-C-CA	2.47	121.79	113.38
4	D	1846	GTP	C5-C6-N1	2.39	118.17	113.95
3	D	1845	SAH	C4-C5-N7	-2.37	106.93	109.40
3	A	1845	SAH	CB-CG-SD	-2.28	108.20	113.31
3	A	1845	SAH	OXT-C-O	-2.22	119.06	124.09
3	D	1845	SAH	C2-N1-C6	2.04	122.25	118.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1846	GTP	C5'-O5'-PA-O1A
4	D	1846	GTP	C5'-O5'-PA-O2A
4	D	1846	GTP	C4'-C5'-O5'-PA
4	D	1846	GTP	PG-O3B-PB-O1B
3	D	1845	SAH	CB-CG-SD-C5'

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Mol	Chain	Res	Type	Atoms
4	D	1846	GTP	PB-O3A-PA-O2A
3	A	1845	SAH	CB-CG-SD-C5'
4	D	1846	GTP	C5'-O5'-PA-O3A

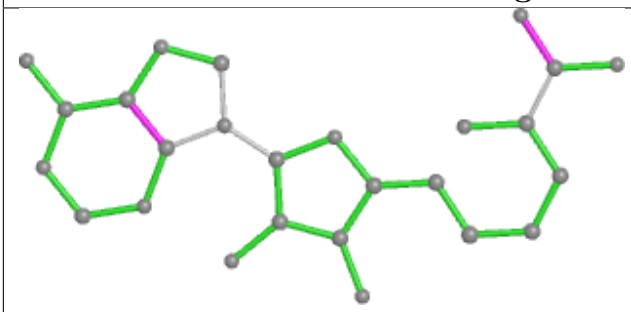
There are no ring outliers.

3 monomers are involved in 10 short contacts:

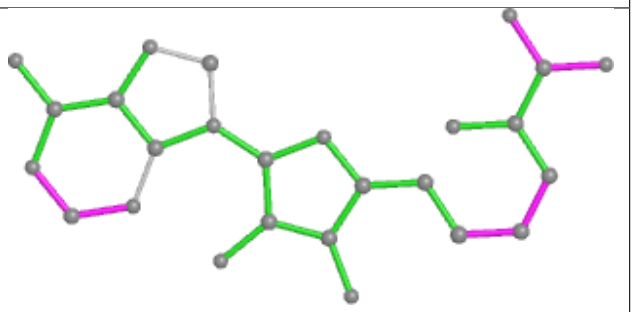
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1845	SAH	1	0
4	D	1846	GTP	8	0
3	D	1845	SAH	1	0

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.

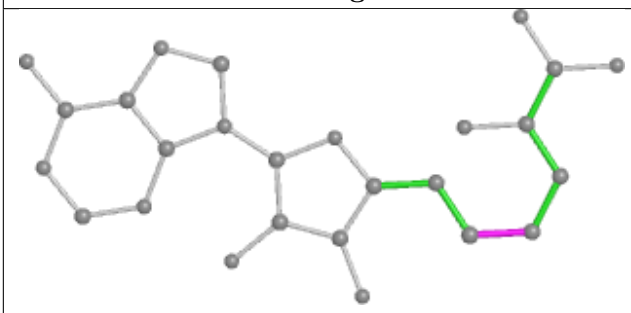
Ligand SAH A 1845



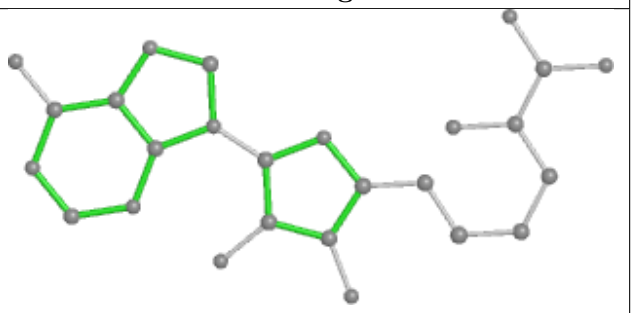
Bond lengths



Bond angles

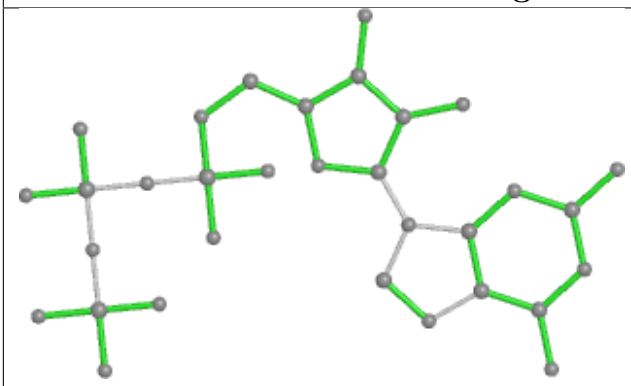


Torsions

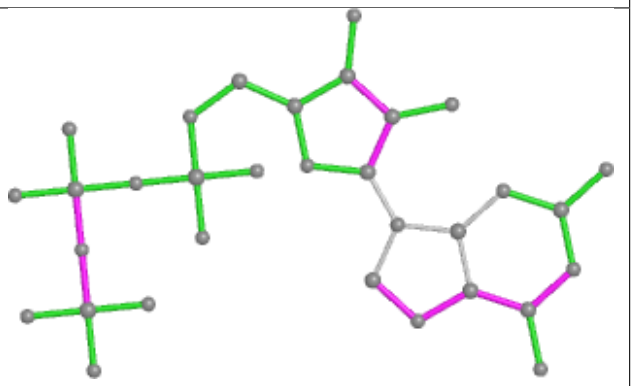


Rings

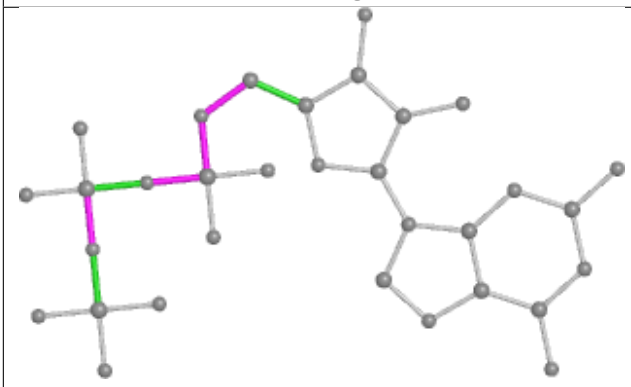
Ligand GTP D 1846



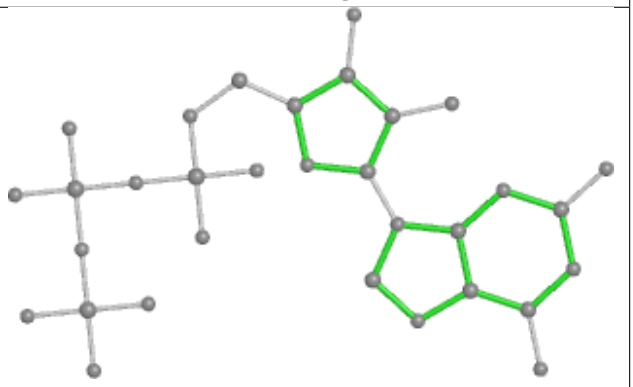
Bond lengths



Bond angles

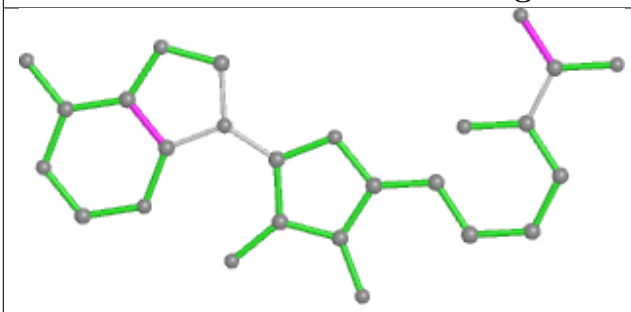


Torsions

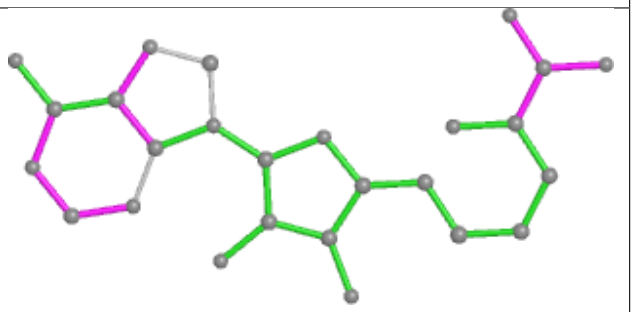


Rings

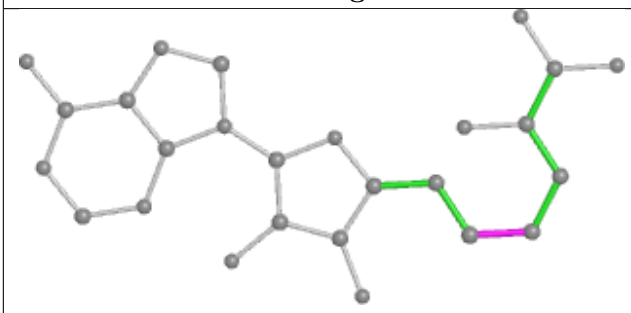
Ligand SAH D 1845



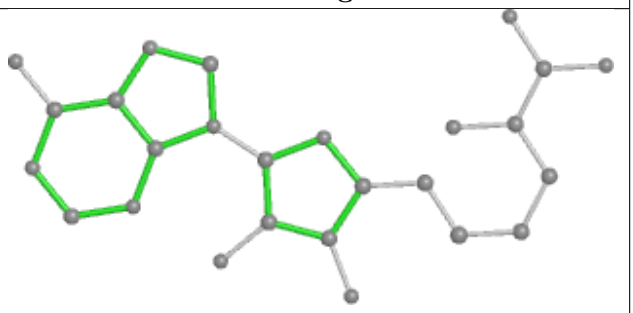
Bond lengths



Bond angles



Torsions



Rings

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	809/844 (95%)	0.39	63 (7%) 13 7	41, 83, 120, 142	0
1	D	814/844 (96%)	0.21	27 (3%) 46 36	41, 68, 109, 155	0
2	B	284/287 (98%)	-0.06	7 (2%) 57 47	37, 56, 94, 139	0
2	E	284/287 (98%)	0.48	19 (6%) 17 10	56, 87, 149, 195	0
All	All	2191/2262 (96%)	0.28	116 (5%) 26 17	37, 73, 121, 195	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	90	TYR	8.4
2	E	89	TYR	6.4
2	E	91	GLY	6.3
2	E	93	SER	5.9
1	D	731	ASN	5.3
1	D	640	ILE	5.2
1	A	640	ILE	5.2
1	D	324	ILE	5.1
1	A	294	ILE	5.0
2	E	1	MET	4.8
2	B	93	SER	4.5
1	D	639	GLY	4.5
2	E	87	VAL	4.3
1	A	203	VAL	4.2
1	A	526	GLY	4.2
1	A	200	ASN	4.1
1	A	199	ASP	4.1
2	E	85	ASN	4.0
1	D	200	ASN	3.9
2	E	120	ASN	3.9
2	E	96	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	357	THR	3.9
2	B	90	TYR	3.8
1	D	325	ASN	3.7
2	B	95	LYS	3.5
1	D	735	SER	3.4
1	A	319	GLU	3.4
2	E	92	ARG	3.4
1	A	198	ARG	3.4
2	E	119	SER	3.3
2	E	147	PHE	3.3
1	A	25	LEU	3.3
2	E	94	THR	3.1
2	E	86	SER	3.1
1	A	204	PRO	3.1
1	D	554	SER	3.1
1	A	202	THR	3.1
1	A	333	TYR	3.1
2	B	1	MET	3.0
1	A	369	TYR	3.0
1	A	341	ILE	3.0
1	A	125	THR	3.0
1	A	357	THR	2.9
1	A	36	ASN	2.9
1	A	334	VAL	2.9
1	A	527	ASP	2.9
1	A	295	ASP	2.8
1	D	25	LEU	2.8
1	A	197	PRO	2.8
1	A	330	GLU	2.7
1	A	362	VAL	2.7
1	A	86	HIS	2.7
1	A	111	THR	2.7
2	B	120	ASN	2.7
1	A	133	ASP	2.7
1	A	293	ILE	2.6
2	E	225	VAL	2.6
1	A	22	ALA	2.6
1	A	155	ASN	2.6
1	D	154	LYS	2.6
1	A	113	ASN	2.6
1	D	34	ILE	2.5
1	A	366	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	71	LYS	2.5
1	A	154	LYS	2.5
1	A	70	ASN	2.5
1	A	95	LEU	2.5
1	A	18	LEU	2.5
1	A	72	GLU	2.5
1	A	408	ARG	2.5
1	A	196	THR	2.5
2	E	83	LYS	2.5
1	D	638	SER	2.5
1	A	325	ASN	2.5
1	A	731	ASN	2.5
1	A	207	GLU	2.4
1	A	1	MET	2.4
1	D	844	ARG	2.4
1	D	825	GLU	2.4
1	A	201	GLU	2.4
1	D	552	GLU	2.4
1	D	329	GLU	2.3
1	D	807	ASP	2.3
1	A	367	SER	2.3
1	A	338	LEU	2.3
1	A	365	MET	2.2
1	D	320	PRO	2.2
1	A	313	TYR	2.2
1	A	314	LEU	2.2
1	A	156	PHE	2.2
1	A	349	SER	2.2
1	D	826	GLY	2.2
1	A	143	LEU	2.2
1	A	195	PHE	2.2
2	B	92	ARG	2.2
2	E	88	LYS	2.2
1	A	76	ILE	2.2
1	A	335	GLU	2.2
1	A	639	GLY	2.1
1	A	337	LYS	2.1
2	E	221	SER	2.1
1	D	333	TYR	2.1
1	A	336	SER	2.1
1	A	732	LEU	2.1
2	B	91	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	385	PRO	2.1
1	D	111	THR	2.1
2	E	98	ALA	2.1
1	D	734	SER	2.1
1	A	35	ASN	2.1
1	A	215	LEU	2.0
1	A	257	ALA	2.0
1	D	732	LEU	2.0
1	D	526	GLY	2.0
1	D	196	THR	2.0
1	A	34	ILE	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)

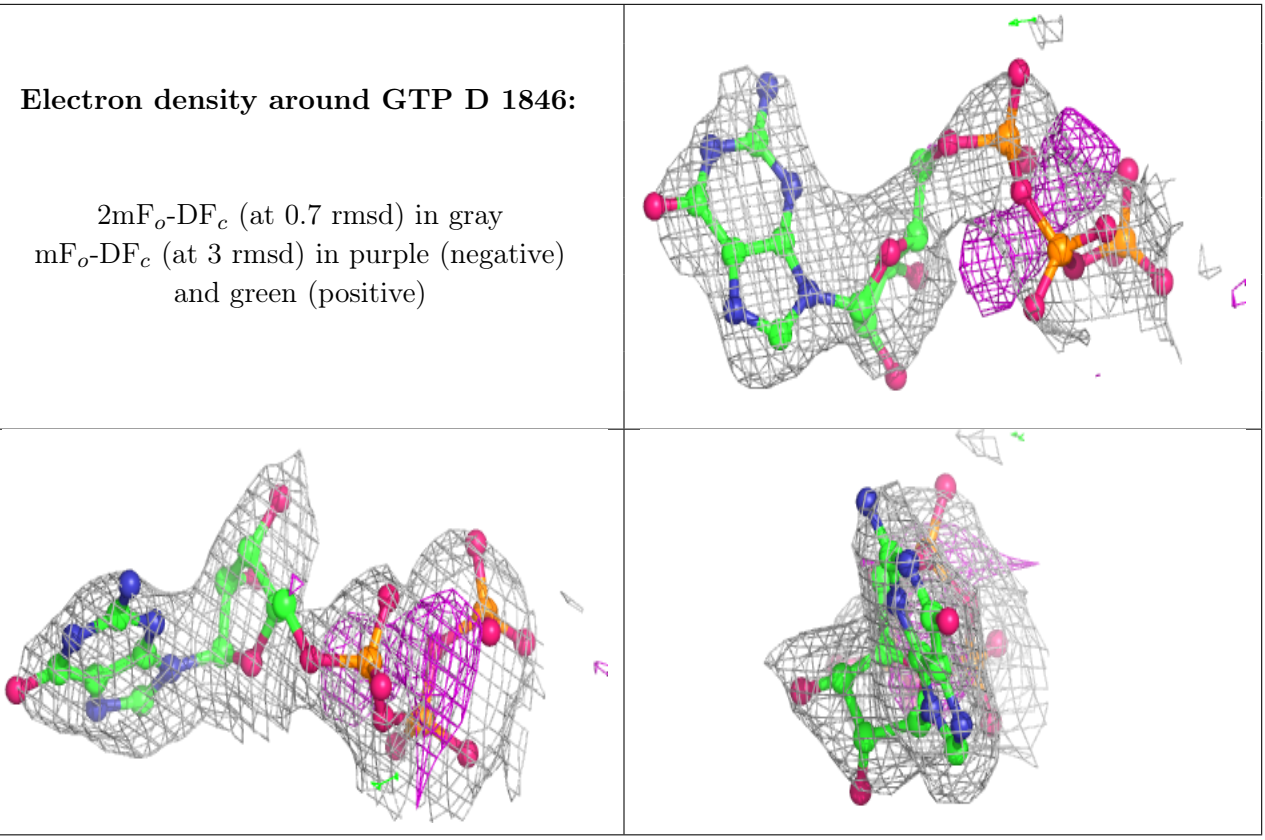
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GTP	D	1846	32/32	0.89	0.23	89,100,133,138	0
3	SAH	D	1845	26/26	0.95	0.17	58,61,67,69	0
3	SAH	A	1845	26/26	0.97	0.16	49,51,52,53	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.

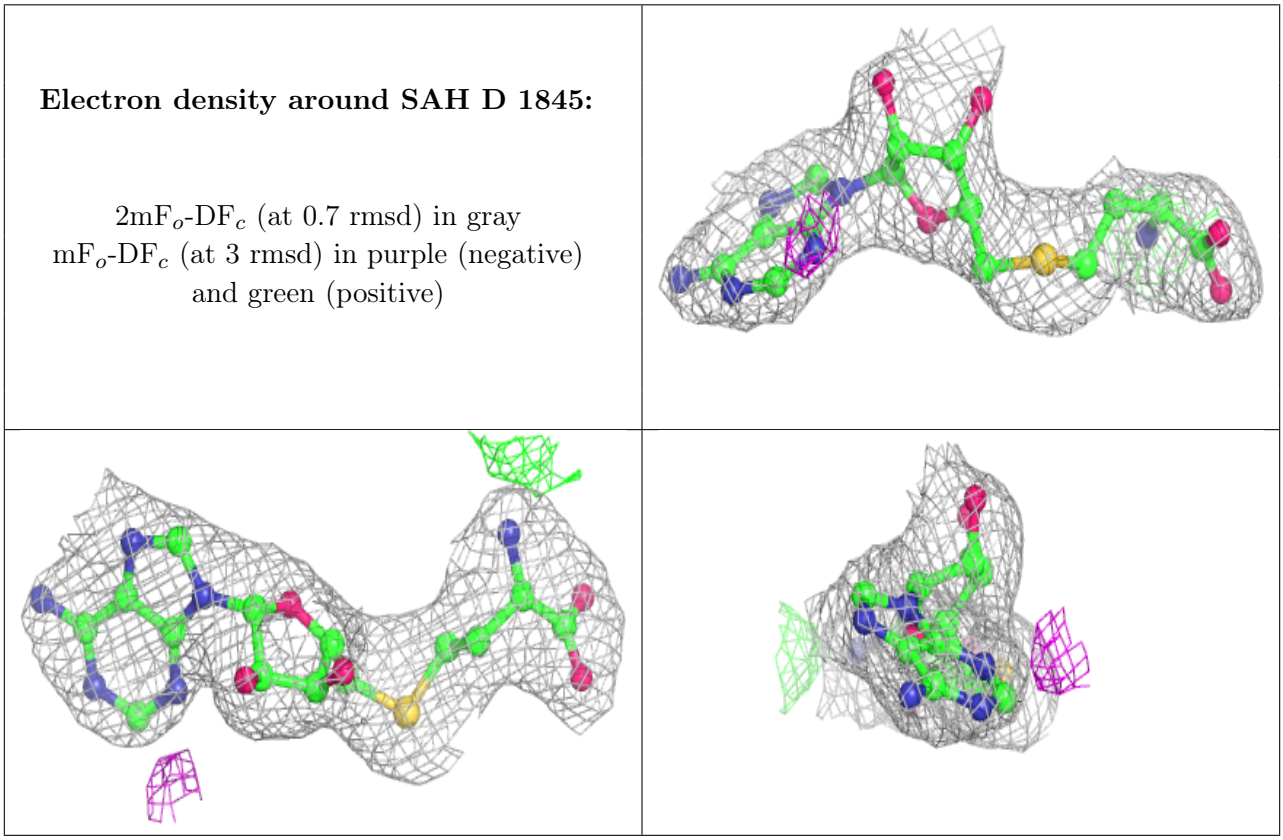
Electron density around GTP D 1846:

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



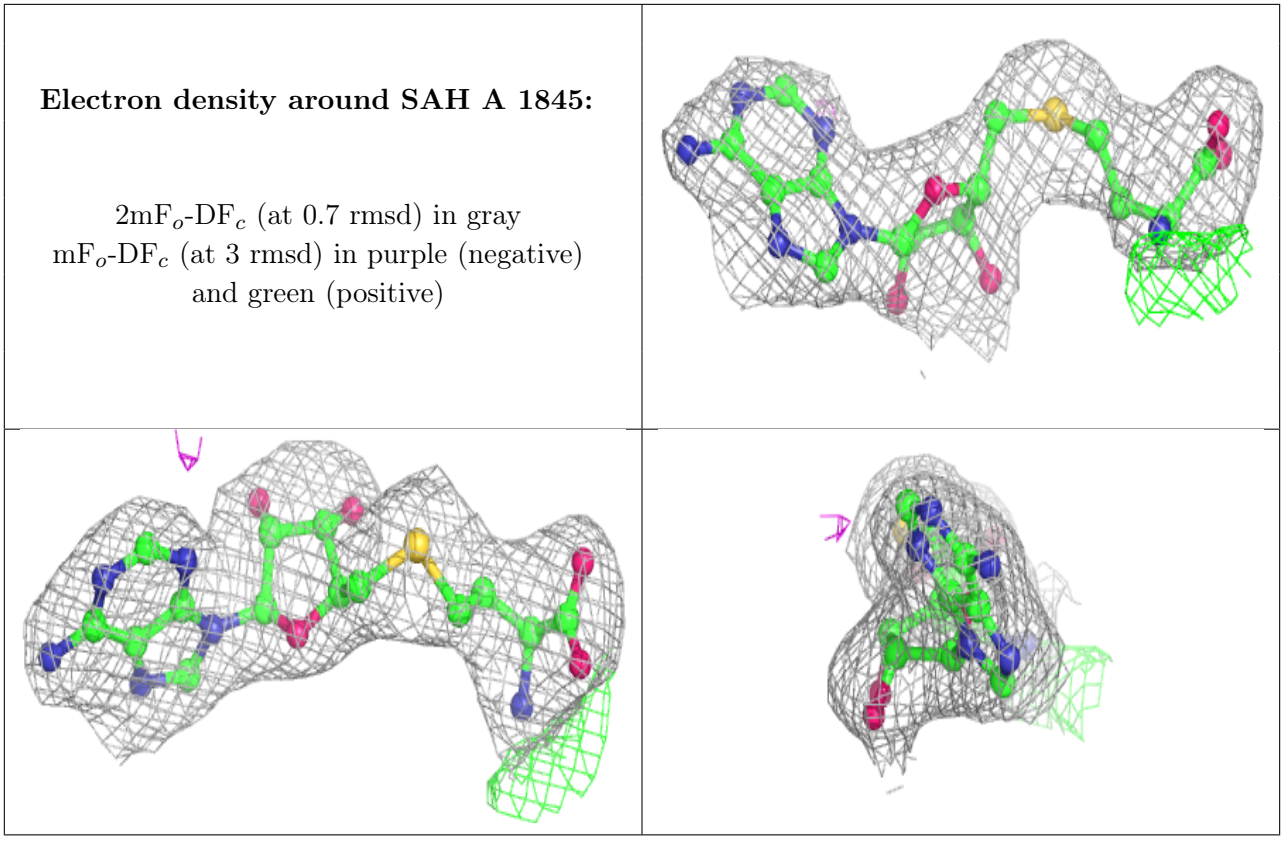
Electron density around SAH D 1845:

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



Electron density around SAH A 1845:

$2mF_o$-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.