wwPDB X-ray Structure Validation Summary Report (i)

Aug 19, 2023 – 09:43 PM EDT

PDB ID	:	2GVZ
Title	:	Crystal Structure of Complex of Gs- with The Catalytic Domains of Mammalian Adenylyl Cyclase: Complex with MANT-ATP and Mn
Authors	:	Mou, T.-C.; Sprang, S.R.
Deposited on	:	2006-05-03
Resolution	:	3.27 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:

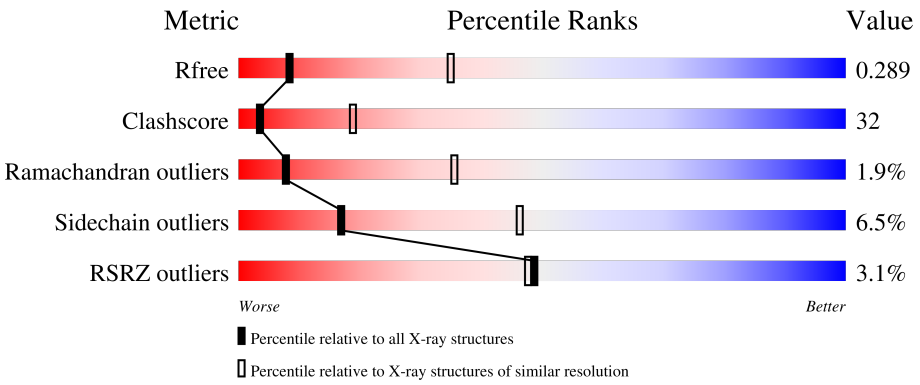
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.27 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	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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	225	4%; 37%, 41%, 6%, 16%
2	B	212	2%; 41%, 45%, •, 11%
3	C	394	2%; 37%, 44%, •, 16%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 5751 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 Adenylate cyclase type 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	189	1476	929	259	271	17	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	356	MET	-	initiating methionine	UNP P30803
A	357	HIS	-	expression tag	UNP P30803
A	358	HIS	-	expression tag	UNP P30803
A	359	HIS	-	expression tag	UNP P30803
A	360	HIS	-	expression tag	UNP P30803
A	361	HIS	-	expression tag	UNP P30803
A	362	HIS	-	expression tag	UNP P30803
A	476	MET	VAL	engineered mutation	UNP P30803

- Molecule 2 is a protein called Adenylate cyclase type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	188	1457	930	239	278	10	0	0	0

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s), alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	330	2702	1714	470	505	13	0	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	A	2	2	2	0	0

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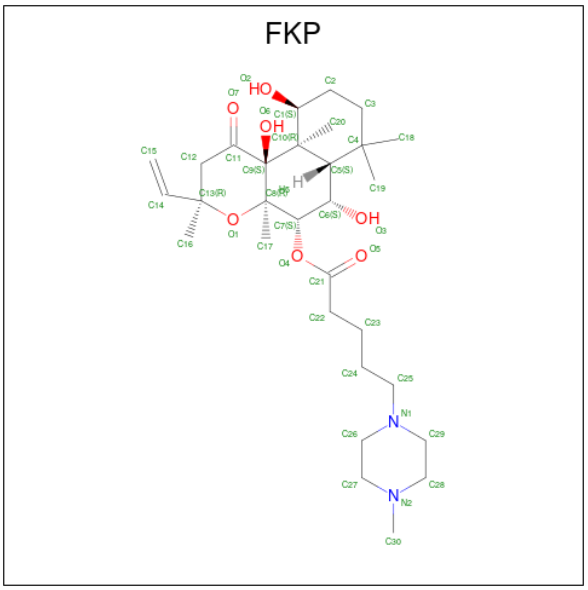
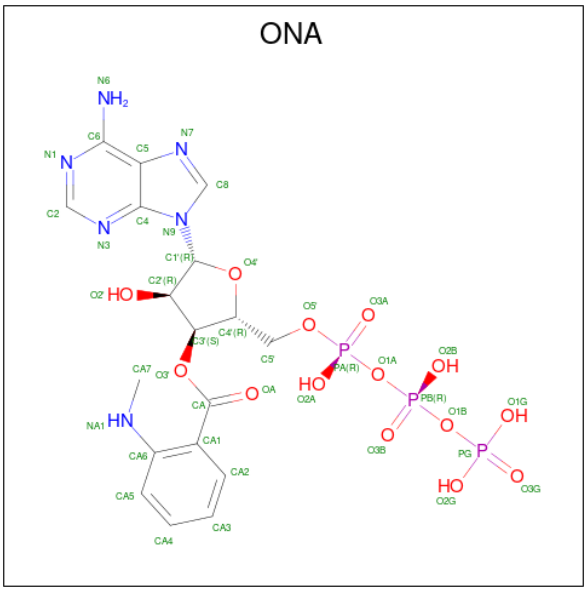
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	C	1	1	1	0	0

- Molecule 5 is METHYLPIPERAZINOFORSKOLIN (three-letter code: FKP) (formula: $C_{30}H_{50}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	39	30	2	7	0	0

- Molecule 6 is 3'-O-[2-(METHYLAMINO)BENZOYL]ADENOSINE 5'-(TETRAHYDROGEN TRIPHOSPHATE) (three-letter code: ONA) (formula: $C_{18}H_{23}N_6O_{14}P_3$).

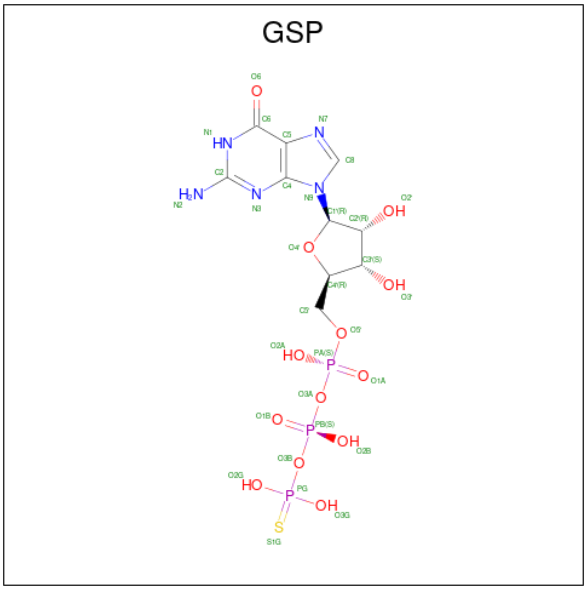


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	41	18	6	14	3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
7	C	1	1	1	0	0

- Molecule 8 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: $C_{10}H_{16}N_5O_{13}P_3S$).



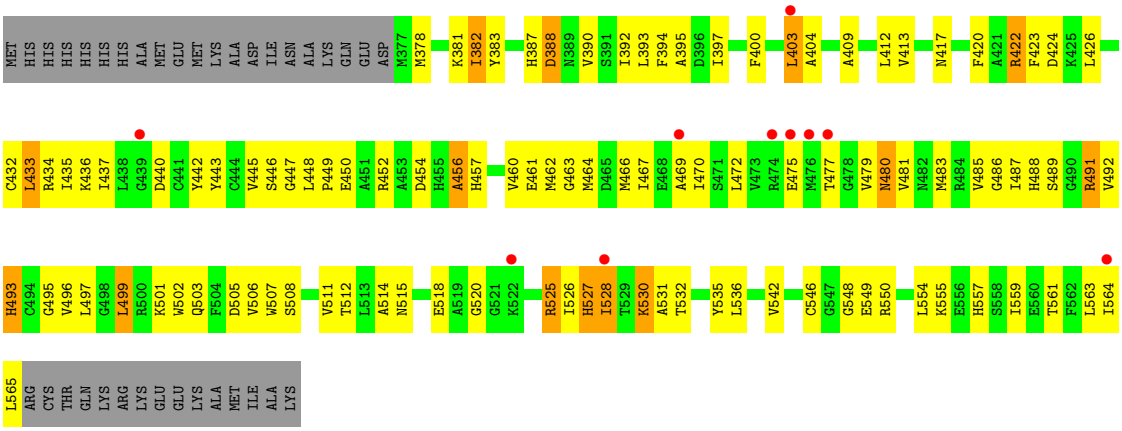
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
8	C	1	32	10	5	13	3	1	0	0

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.

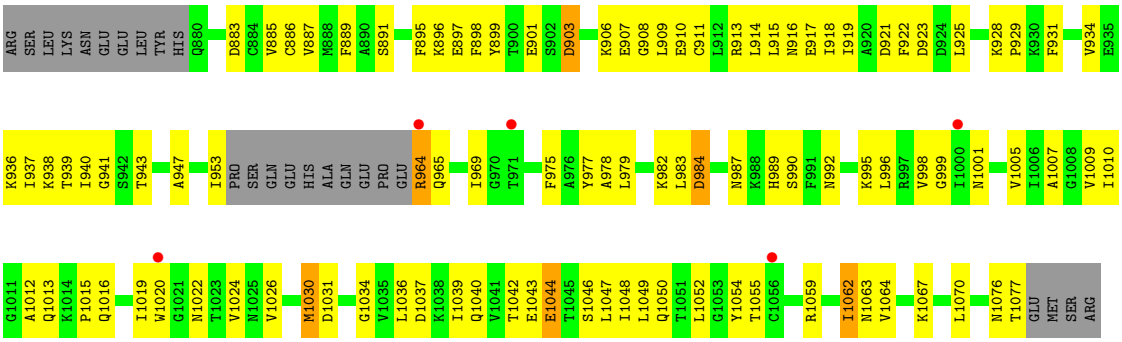
• Molecule 1: Adenylate cyclase type 5

Chain A:



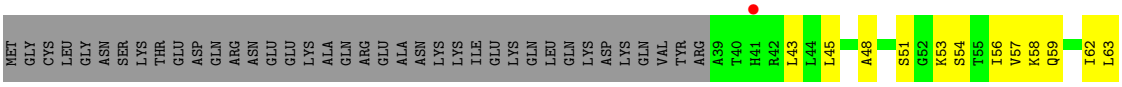
• Molecule 2: Adenylate cyclase type 2

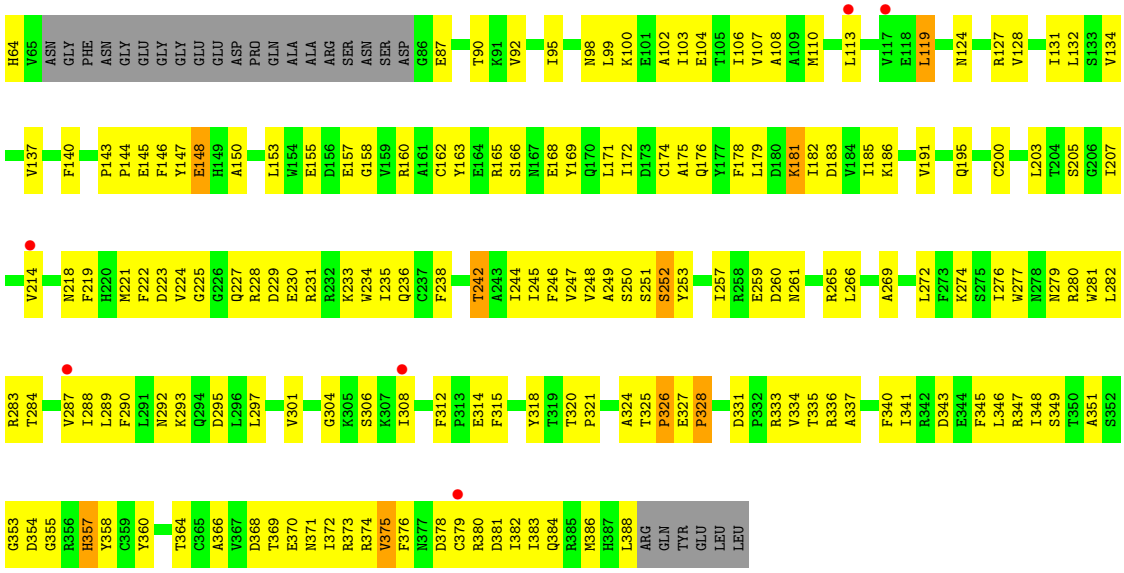
Chain B:



• Molecule 3: Guanine nucleotide-binding protein G(s), alpha subunit

Chain C:




H64 V65 ASN GLY PHE ASN GLY GLU GLY GLY GLU GLU ASP PRO GLN ALA ALA ARG SER ASN SER ASP G86 E87 T90 K91 V92 I95 N98 L99 K100 E101 A102 I103 E104 T105 I106 V107 A108 A109 M110 L113 V117 E118 L119 N124 R127 V128 I131 L132 S133 V134
V137 F140 P143 P144 E145 F146 Y147 E148 H149 A150 L153 W154 E155 D156 E157 G158 V159 R160 A161 C162 Y163 E164 R165 S166 N167 E168 Y169 Q170 L171 I172 D173 C174 A175 Q176 Y177 F178 L179 D180 K181 I182 D183 V184 I185 K186 V191 Q195 C200 L203 T204 S205 G206 I207
V214 N218 F219 H220 M221 F222 D223 V224 G225 G226 Q227 R228 D229 E230 R231 R232 K233 W234 I235 Q236 C237 F238 T242 A243 I244 I245 F246 V247 V248 A249 S250 S251 S252 Y253 I257 R258 E259 D260 N261 R265 L266 A269 L272 F273 K274 S275 I276 W277 N278 N279 R280 W281 L282
R283 T284 V287 I288 L289 F290 L291 N292 K293 Q294 D295 L296 L297 V301 G304 K305 S306 K307 I308 F312 P313 E314 F315 Y318 T319 T320 P321 A324 T325 P326 E327 P328 D331 P332 R333 V334 T335 R336 A337 F340 I341 R342 D343 E344 F345 L346 R347 I348 S349 T350 A351 S352
G353 D354 G355 R356 H357 Y358 C359 Y360 T364 C365 A366 V367 D368 T369 E370 N371 I372 R373 R374 V375 F376 N377 D378 C379 R380 D381 I382 I383 Q384 R385 M386 H387 L388 ARG GLN TYR GLU LEU LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.80Å 132.10Å 69.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.97 – 3.27 44.74 – 3.27	Depositor EDS
% Data completeness (in resolution range)	85.8 (14.97-3.27) 76.4 (44.74-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 3.25Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.275 , 0.330 0.240 , 0.289	Depositor DCC
R_{free} test set	774 reflections (5.32%)	wwPDB-VP
Wilson B-factor (Å^2)	55.9	Xtriage
Anisotropy	1.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 75.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	5751	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FKP, GSP, MN, CL, ONA

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	0.42	0/1504	0.71	2/2027 (0.1%)
2	B	0.56	0/1481	0.67	0/1999
3	C	0.50	0/2759	0.68	0/3733
All	All	0.50	0/5744	0.69	2/7759 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	525	ARG	N-CA-C	-8.39	88.34	111.00
1	A	388	ASP	N-CA-C	7.44	131.10	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1476	0	1450	120	0
2	B	1457	0	1463	96	0
3	C	2702	0	2650	172	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
5	A	39	0	50	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	41	0	19	2	0
7	C	1	0	0	1	0
8	C	32	0	12	1	0
All	All	5751	0	5644	365	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 32.

The worst 5 of 365 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)
2:B:925:LEU:HG	2:B:982:LYS:HZ2	1.23	1.00
3:C:231:ARG:HH21	3:C:272:LEU:HD22	1.26	0.98
3:C:63:LEU:HD13	3:C:373:ARG:HE	1.31	0.94
5:A:1:FKP:H173	5:A:1:FKP:H201	1.51	0.90
3:C:119:LEU:H	3:C:119:LEU:HD12	1.37	0.88

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	187/225 (83%)	153 (82%)	30 (16%)	4 (2%)	7 33
2	B	184/212 (87%)	156 (85%)	26 (14%)	2 (1%)	14 46
3	C	326/394 (83%)	270 (83%)	49 (15%)	7 (2%)	7 33
All	All	697/831 (84%)	579 (83%)	105 (15%)	13 (2%)	8 35

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	351	ALA
1	A	382	ILE
1	A	456	ALA
1	A	479	VAL
1	A	480	ASN

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	158/189 (84%)	145 (92%)	13 (8%)	11	36
2	B	161/184 (88%)	150 (93%)	11 (7%)	16	44
3	C	297/351 (85%)	281 (95%)	16 (5%)	22	53
All	All	616/724 (85%)	576 (94%)	40 (6%)	17	46

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	200	CYS
3	C	328	PRO
3	C	218	ASN
3	C	314	GLU
3	C	357	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	371	ASN
3	C	220	HIS
2	B	1013	GLN
3	C	213	GLN
2	B	1002	HIS

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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
5	FKP	A	1	-	39,42,42	2.59	16 (41%)	49,68,68	2.50	17 (34%)
6	ONA	A	100	4	37,44,44	3.87	16 (43%)	46,67,67	2.33	15 (32%)
8	GSP	C	395	4	26,34,34	1.59	6 (23%)	27,54,54	1.71	4 (14%)

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
5	FKP	A	1	-	-	11/14/97/97	0/4/4/4
6	ONA	A	100	4	-	6/28/48/48	0/4/4/4
8	GSP	C	395	4	-	3/17/38/38	0/3/3/3

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	100	ONA	CA5-CA6	11.61	1.59	1.39
6	A	100	ONA	CA4-CA5	9.84	1.59	1.38
6	A	100	ONA	CA3-CA2	8.54	1.56	1.38
6	A	100	ONA	OA-CA	7.95	1.44	1.22
6	A	100	ONA	CA3-CA4	7.22	1.57	1.38

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1	FKP	C19-C4-C18	-10.86	91.89	107.89
6	A	100	ONA	N3-C2-N1	-6.86	117.95	128.68
6	A	100	ONA	PB-O1B-PG	-5.66	113.41	132.83
8	C	395	GSP	O6-C6-N1	5.49	127.14	120.65
6	A	100	ONA	C3'-O3'-CA	5.41	125.88	117.21

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1	FKP	C6-C7-O4-C21
5	A	1	FKP	C16-C13-C14-C15
5	A	1	FKP	C22-C21-O4-C7
6	A	100	ONA	O4'-C4'-C5'-O5'
5	A	1	FKP	O5-C21-O4-C7

There are no ring outliers.

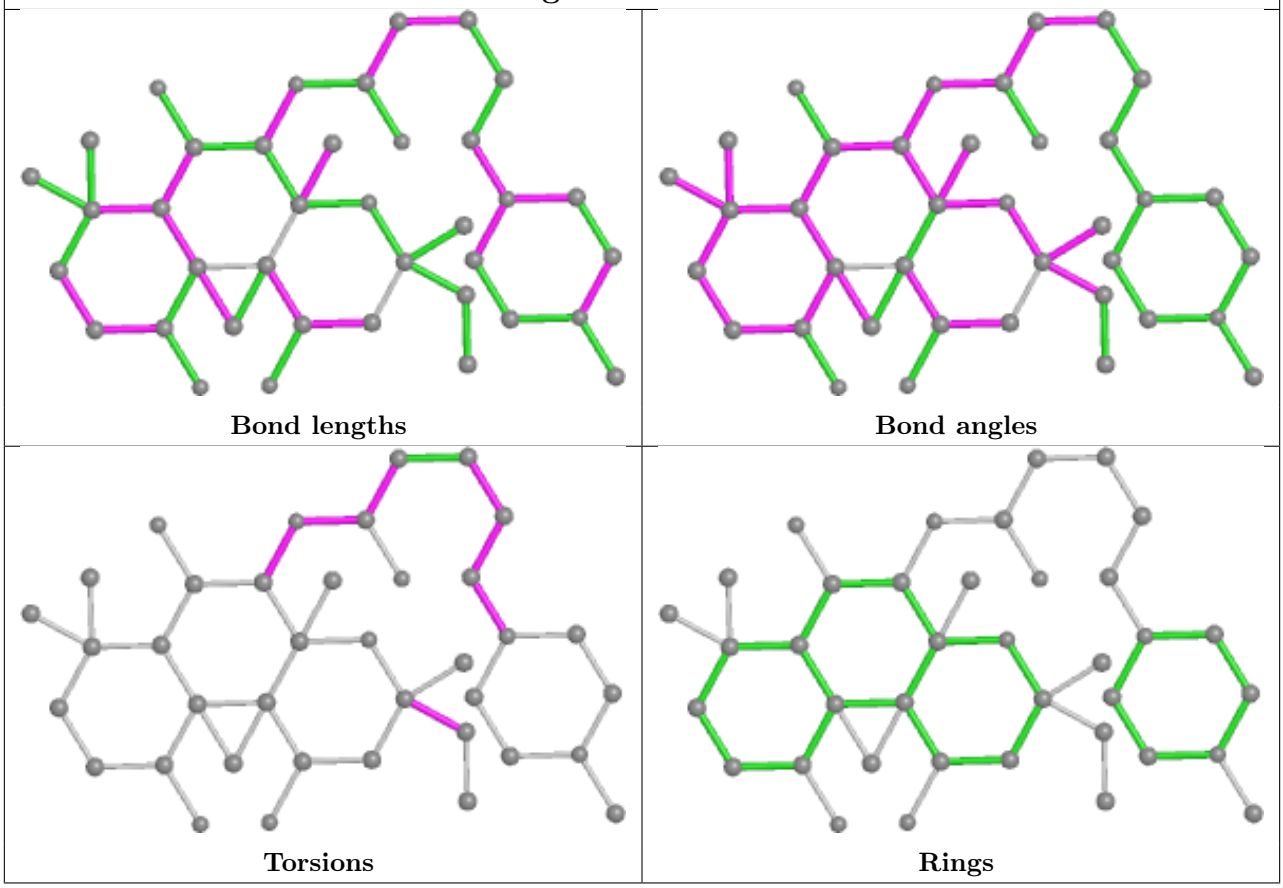
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	FKP	6	0
6	A	100	ONA	2	0
8	C	395	GSP	1	0

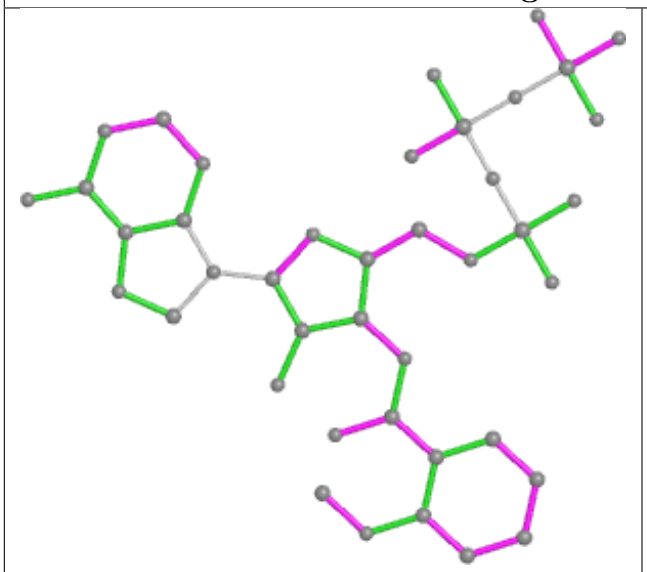
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

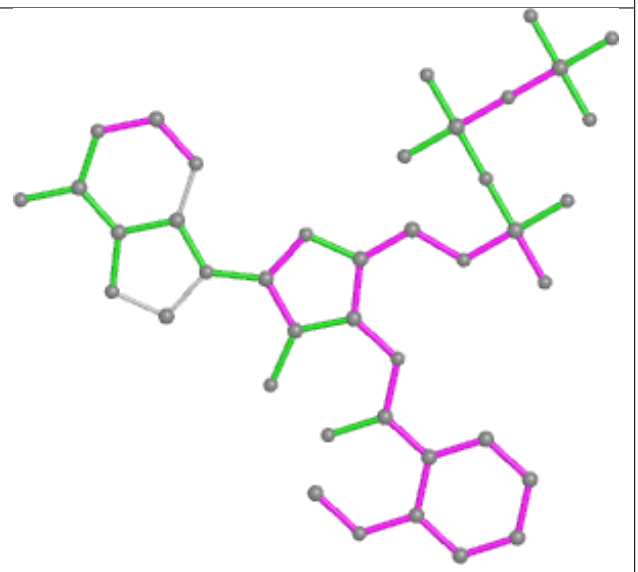
Ligand FKP A 1



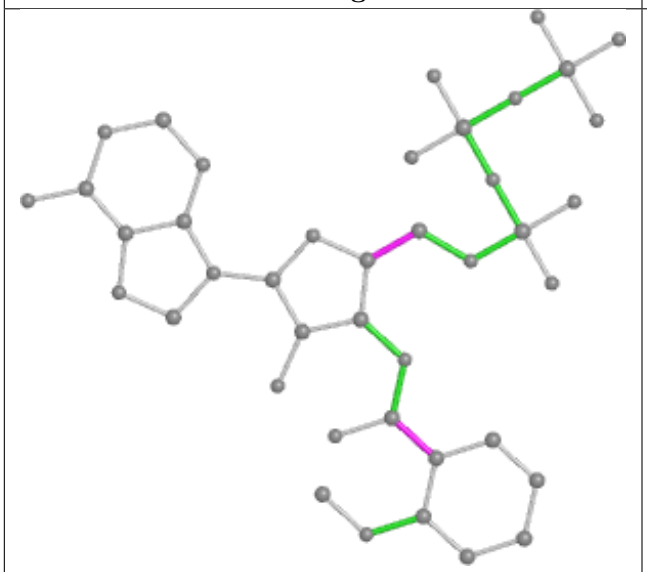
Ligand ONA A 100



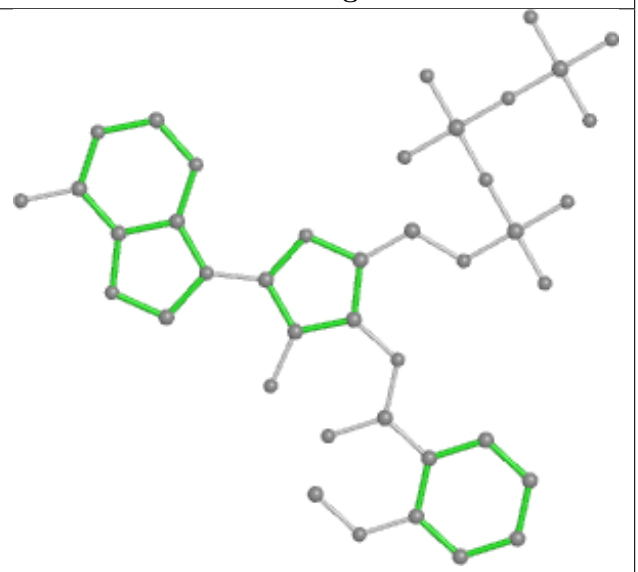
Bond lengths



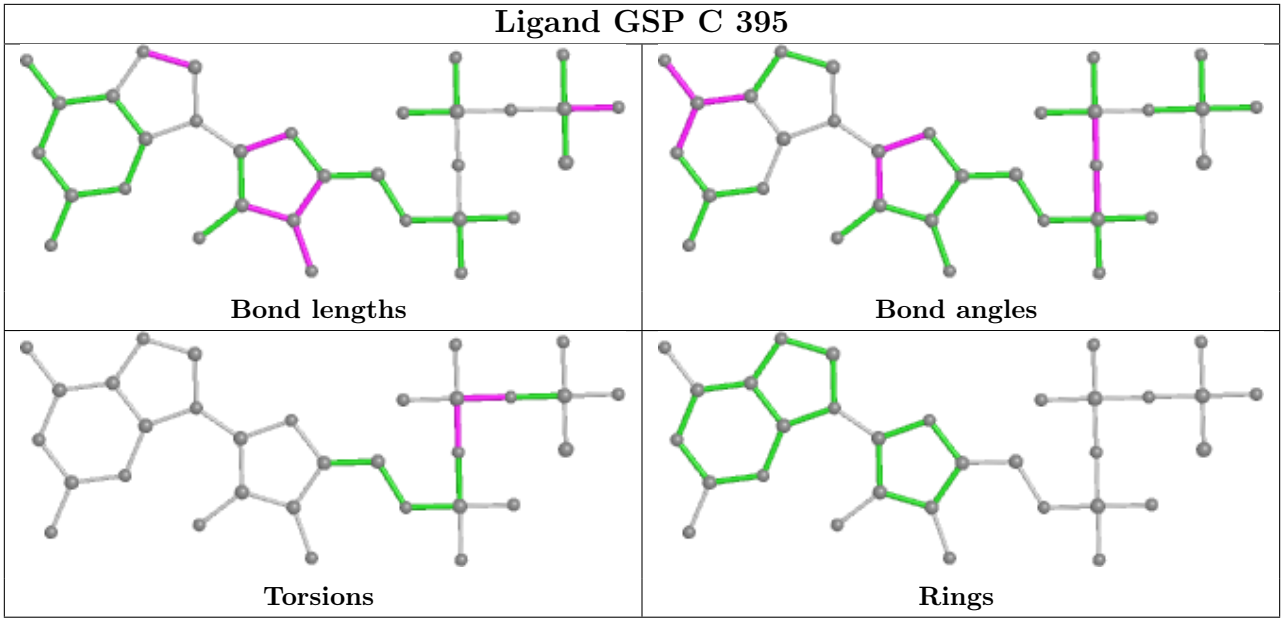
Bond angles



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	189/225 (84%)	0.36	10 (5%)	26	25	30, 87, 99, 116	0
2	B	188/212 (88%)	0.15	5 (2%)	54	52	13, 49, 96, 98	0
3	C	330/394 (83%)	0.10	7 (2%)	63	61	19, 55, 93, 100	0
All	All	707/831 (85%)	0.18	22 (3%)	49	48	13, 59, 97, 116	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	477	THR	8.8
1	A	475	GLU	5.2
1	A	476	MET	4.2
2	B	1056	CYS	3.4
3	C	117	VAL	3.2

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)

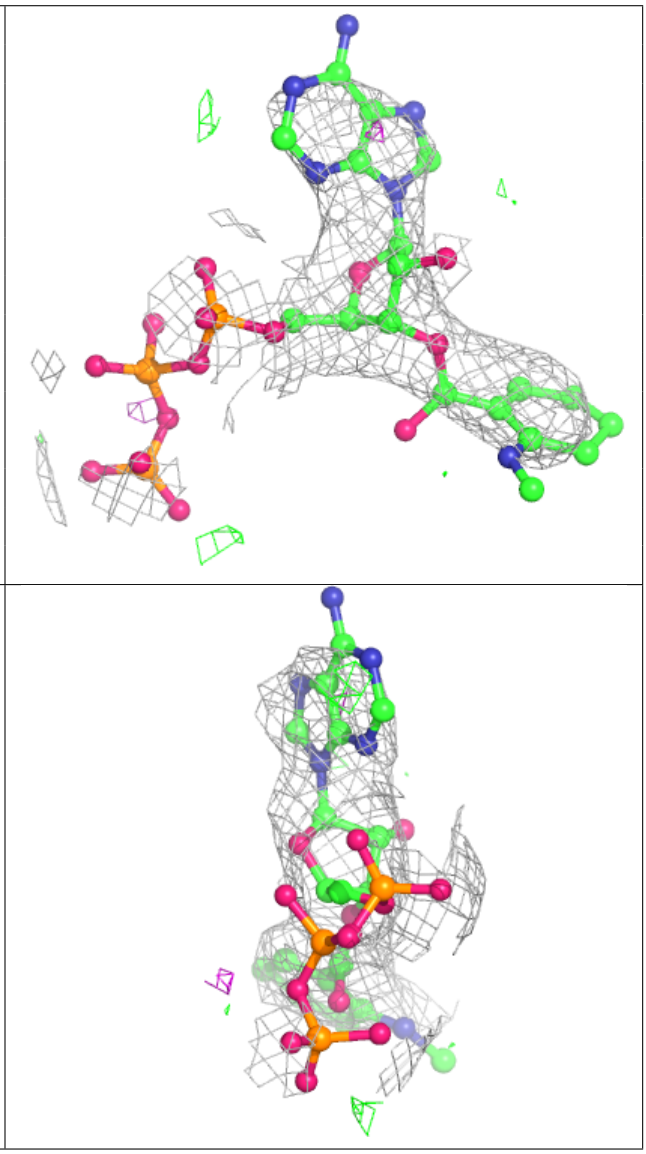
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ONA	A	100	41/41	0.84	0.34	53,88,97,100	0
5	FKP	A	1	39/39	0.92	0.30	13,23,87,89	0
4	MN	A	581	1/1	0.93	0.23	64,64,64,64	0
4	MN	A	582	1/1	0.95	0.14	31,31,31,31	0
4	MN	C	396	1/1	0.95	0.12	17,17,17,17	0
7	CL	C	397	1/1	0.95	0.86	59,59,59,59	0
8	GSP	C	395	32/32	0.96	0.19	31,41,73,76	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.

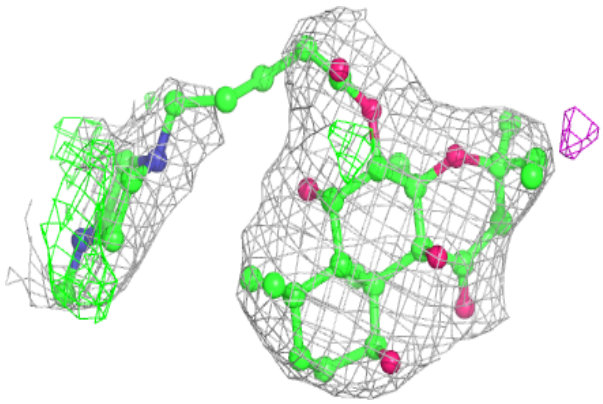
Electron density around ONA A 100:

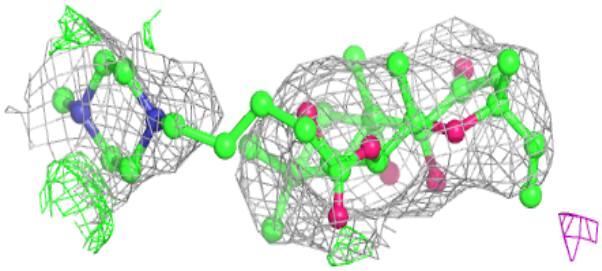
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

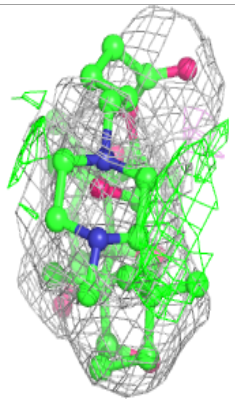


Electron density around FKP A 1:

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

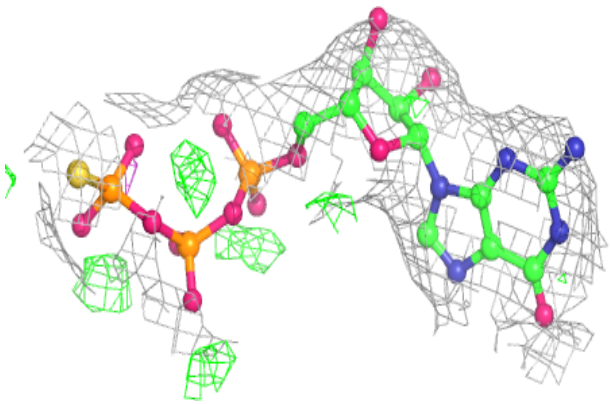


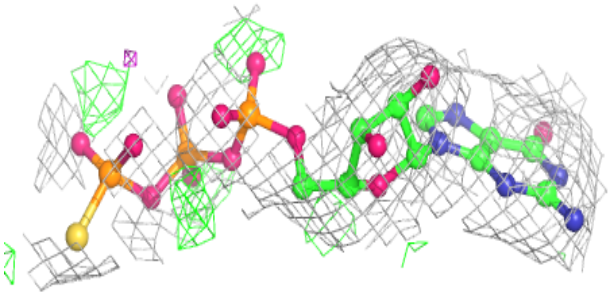


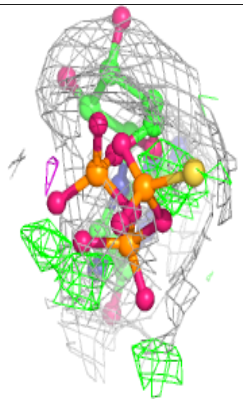


Electron density around GSP C 395:

$2mF_o$-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.