



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 07:41 am BST

PDB ID : 2V0N
Title : ACTIVATED RESPONSE REGULATOR PLED IN COMPLEX WITH C-DIGMP AND GTP- ALPHA-S
Authors : Wassmann, P.; Schirmer, T.
Deposited on : 2007-05-15
Resolution : 2.71 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

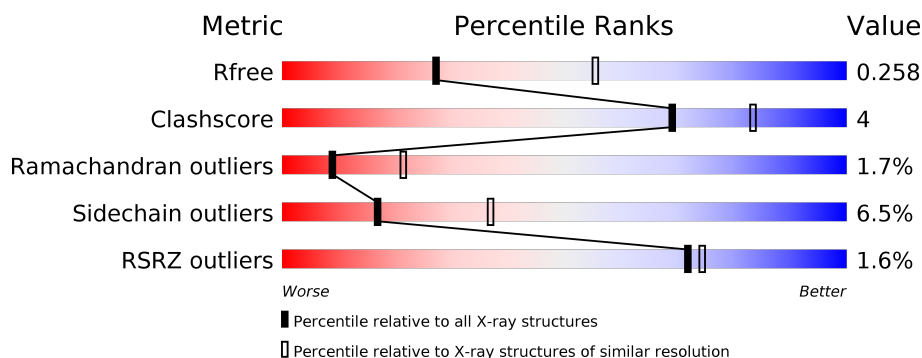
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	<div> <div> <div>0%</div> <div>85%</div> <div>13%</div> <div>2%</div> </div> </div>
1	B	459	<div> <div> <div>2%</div> <div>84%</div> <div>12%</div> <div>2%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	C2E	A	503	X	-	-	-
4	C2E	A	505	X	-	-	-
4	C2E	B	503	X	-	-	-
4	C2E	B	505	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7298 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 RESPONSE REGULATOR PLED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	96	0	0
			3531	2196	654	666	15			
1	B	454	Total	C	N	O	S	97	0	0
			3481	2166	639	661	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	455	HIS	-	expression tag	UNP Q9A5I5
A	456	HIS	-	expression tag	UNP Q9A5I5
A	457	HIS	-	expression tag	UNP Q9A5I5
A	458	HIS	-	expression tag	UNP Q9A5I5
A	459	HIS	-	expression tag	UNP Q9A5I5
A	460	HIS	-	expression tag	UNP Q9A5I5
B	455	HIS	-	expression tag	UNP Q9A5I5
B	456	HIS	-	expression tag	UNP Q9A5I5
B	457	HIS	-	expression tag	UNP Q9A5I5
B	458	HIS	-	expression tag	UNP Q9A5I5
B	459	HIS	-	expression tag	UNP Q9A5I5
B	460	HIS	-	expression tag	UNP Q9A5I5

- Molecule 2 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).

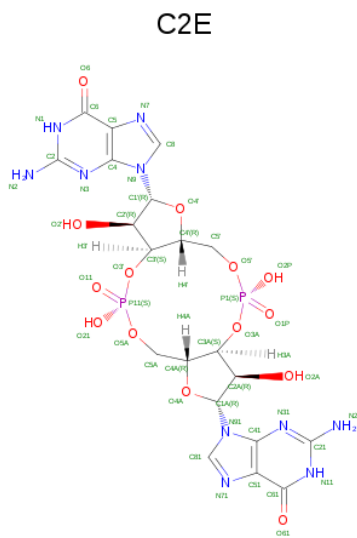


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Be	F	0	0
			4	1	3		
2	B	1	Total	Be	F	0	0
			4	1	3		

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

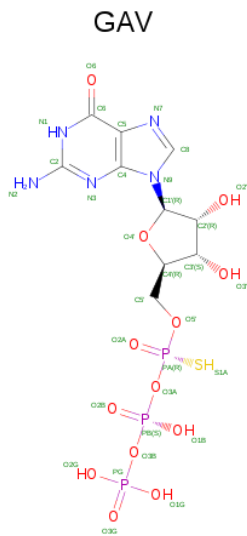
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	3	Total	Mg	0	0
			3	3		

- Molecule 4 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclodecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (three-letter code: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂).



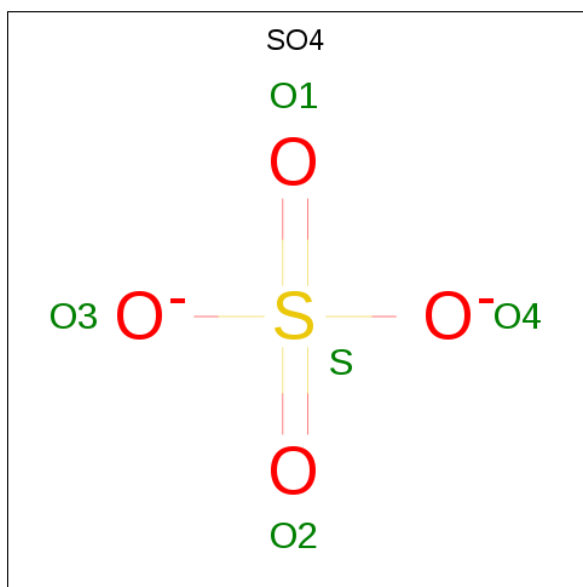
Id	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 46	C 20	N 10	O 14	P 2	0	0
4	A	1	Total 46	C 20	N 10	O 14	P 2	0	0
4	B	1	Total 46	C 20	N 10	O 14	P 2	0	0
4	B	1	Total 46	C 20	N 10	O 14	P 2	0	0

- Molecule 5 is GUANOSINE-5'-RP-ALPHA-THIO-TRIPHOSPHATE (three-letter code: GAV) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3\text{S}$).



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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O S		
			5	4 1	0	0
6	A	1	Total	O S		
			5	4 1	0	0

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

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

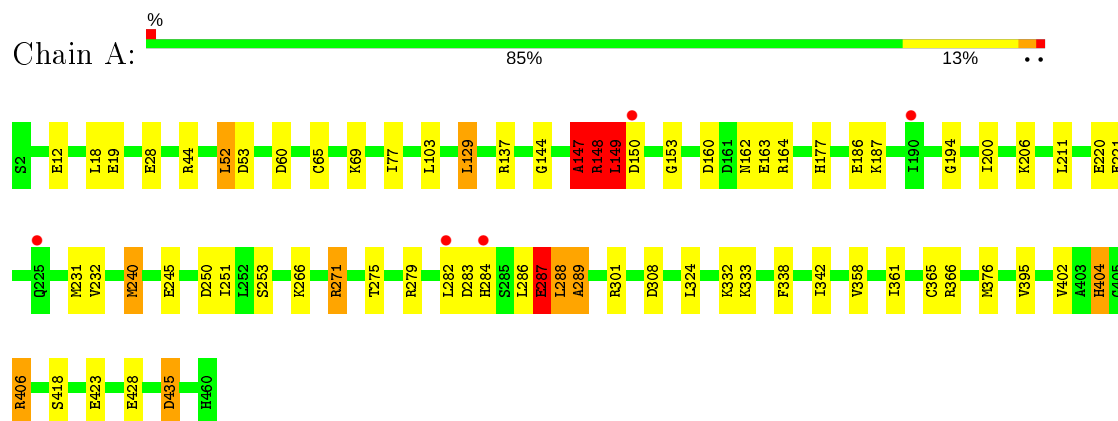
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	8	Total	O		
			8	8	0	0
8	B	6	Total	O		
			6	6	0	0

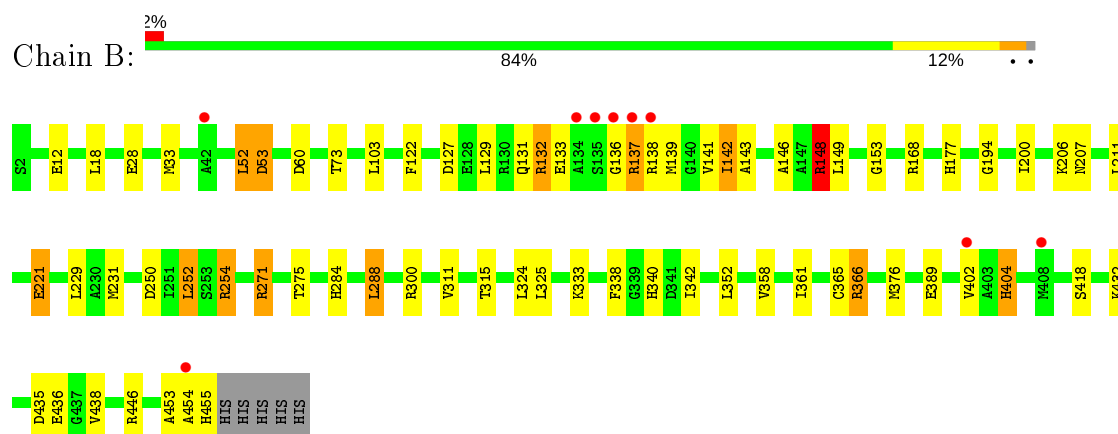
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: RESPONSE REGULATOR PLED



• Molecule 1: RESPONSE REGULATOR PLED



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.97Å 132.56Å 88.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.71 73.56 – 2.71	Depositor EDS
% Data completeness (in resolution range)	94.0 (30.00-2.71) 94.0 (73.56-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.252 0.220 , 0.258	Depositor DCC
R_{free} test set	1971 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7298	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, GAV, BEF, SO4, C2E

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	2.47	24/3580 (0.7%)	3.00	48/4840 (1.0%)
1	B	1.04	12/3524 (0.3%)	0.97	18/4762 (0.4%)
All	All	1.90	36/7104 (0.5%)	2.24	66/9602 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	1
All	All	0	10

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	GLU	CD-OE2	111.38	2.48	1.25
1	A	44	ARG	NE-CZ	-50.31	0.67	1.33
1	A	12	GLU	CG-CD	-33.96	1.01	1.51
1	A	406	ARG	NE-CZ	30.01	1.72	1.33
1	A	206	LYS	CG-CD	-28.49	0.55	1.52

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	NE-CZ-NH2	-110.75	64.93	120.30
1	A	44	ARG	NE-CZ-NH1	94.48	167.54	120.30
1	A	186	GLU	OE1-CD-OE2	-50.93	62.18	123.30
1	A	406	ARG	NE-CZ-NH1	-46.14	97.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	GLU	O-C-N	-45.42	50.03	122.70

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	ALA	Mainchain
1	A	148	ARG	Peptide
1	A	149	LEU	Mainchain,Peptide
1	A	287	GLU	Mainchain,Peptide
1	A	288	LEU	Mainchain

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	3531	0	3586	19	0
1	B	3481	0	3551	30	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
4	A	92	0	44	3	0
4	B	92	0	43	2	0
5	A	32	0	13	0	0
5	B	32	0	13	0	0
6	A	10	0	0	0	0
7	A	1	0	0	0	0
8	A	8	0	0	0	0
8	B	6	0	0	1	0
All	All	7298	0	7250	52	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 52 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:324:LEU:HD13	1:A:376:MET:HE1	1.36	1.02
1:B:324:LEU:HD13	1:B:376:MET:HE1	1.50	0.92
1:B:324:LEU:HD13	1:B:376:MET:CE	2.00	0.92
1:A:324:LEU:HD13	1:A:376:MET:CE	1.99	0.91
1:B:229:LEU:HD13	1:B:250:ASP:HB3	1.68	0.73

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	457/459 (100%)	437 (96%)	13 (3%)	7 (2%)	10	24
1	B	450/459 (98%)	427 (95%)	15 (3%)	8 (2%)	8	20
All	All	907/918 (99%)	864 (95%)	28 (3%)	15 (2%)	9	21

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	ALA
1	A	149	LEU
1	A	289	ALA
1	B	143	ALA
1	B	149	LEU

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	374/374 (100%)	353 (94%)	21 (6%)	21	43
1	B	369/374 (99%)	342 (93%)	27 (7%)	14	31
All	All	743/748 (99%)	695 (94%)	48 (6%)	17	37

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	LEU
1	B	129	LEU
1	B	404	HIS
1	B	33	MET
1	B	73	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	207	ASN
1	B	335	ASN
1	B	280	ASN
1	A	280	ASN
1	B	293	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	C2E	B	505	-	44,52,52	0.65	0	54,82,82	2.17	19 (35%)
5	GAV	A	600	3	24,34,34	1.17	2 (8%)	31,54,54	1.92	7 (22%)
6	SO4	A	1470	-	4,4,4	0.18	0	6,6,6	0.21	0
2	BEF	B	501	1,3	0,3,3	0.00	-	-	-	-
4	C2E	A	503	-	44,52,52	0.77	1 (2%)	54,82,82	1.99	20 (37%)
2	BEF	A	501	1,3	0,3,3	0.00	-	-	-	-
4	C2E	A	505	-	44,52,52	0.59	0	54,82,82	2.18	22 (40%)
6	SO4	A	1471	-	4,4,4	0.19	0	6,6,6	0.18	0
4	C2E	B	503	-	44,52,52	0.63	0	54,82,82	2.24	22 (40%)
5	GAV	B	600	3	24,34,34	1.08	2 (8%)	31,54,54	1.51	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C2E	B	505	-	2/2/10/10	9/22/62/62	0/6/7/7
5	GAV	A	600	3	-	2/14/38/38	0/3/3/3
5	GAV	B	600	3	-	3/14/38/38	0/3/3/3
4	C2E	A	503	-	1/1/10/10	4/22/62/62	0/6/7/7
4	C2E	B	503	-	2/2/10/10	7/22/62/62	0/6/7/7
4	C2E	A	505	-	2/2/10/10	13/22/62/62	0/6/7/7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	GAV	C6-N1	3.25	1.38	1.33
5	A	600	GAV	PA-O5'	3.13	1.62	1.57
5	B	600	GAV	PA-O5'	2.52	1.61	1.57
5	B	600	GAV	C6-N1	2.28	1.37	1.33
4	A	503	C2E	C21-N11	-2.19	1.31	1.35

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	GAV	N3-C2-N1	-5.71	119.60	127.22
5	A	600	GAV	C2-N3-C4	5.40	121.52	115.36
4	A	505	C2E	C2-N3-C4	4.81	120.85	115.36
5	B	600	GAV	N3-C2-N1	-4.75	120.88	127.22
4	B	505	C2E	O4'-C1'-C2'	-4.72	100.03	106.93

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	505	C2E	C4'
4	B	505	C2E	C4A
4	A	505	C2E	C4'
4	A	505	C2E	C4A
4	A	503	C2E	C4'

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	505	C2E	C5'-O5'-P1-O2P
4	B	505	C2E	C5'-O5'-P1-O1P
4	B	505	C2E	C5'-O5'-P1-O3A
4	B	505	C2E	C3'-C4'-C5'-O5'
4	B	505	C2E	C3A-C4A-C5A-O5A

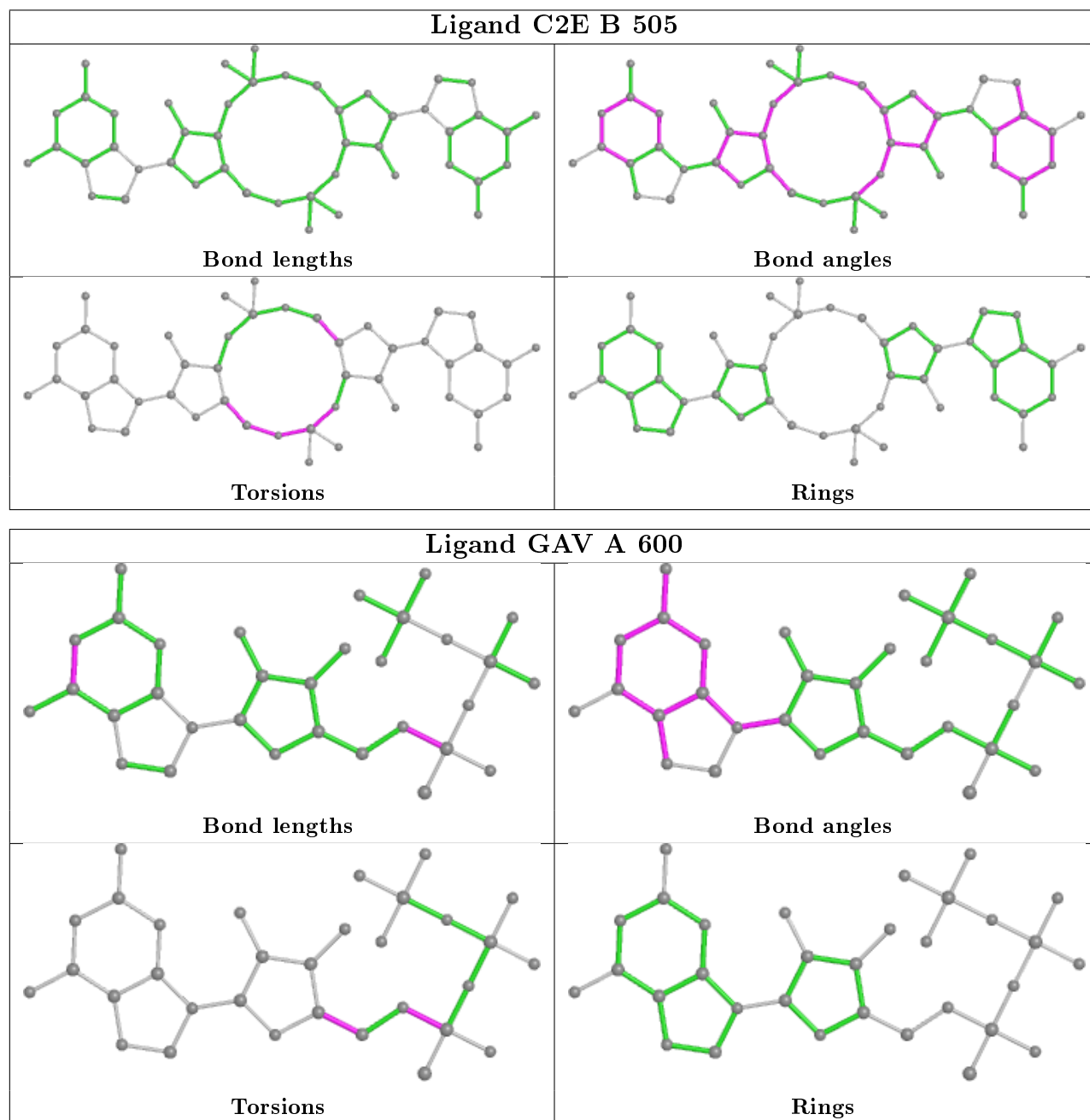
There are no ring outliers.

4 monomers are involved in 5 short contacts:

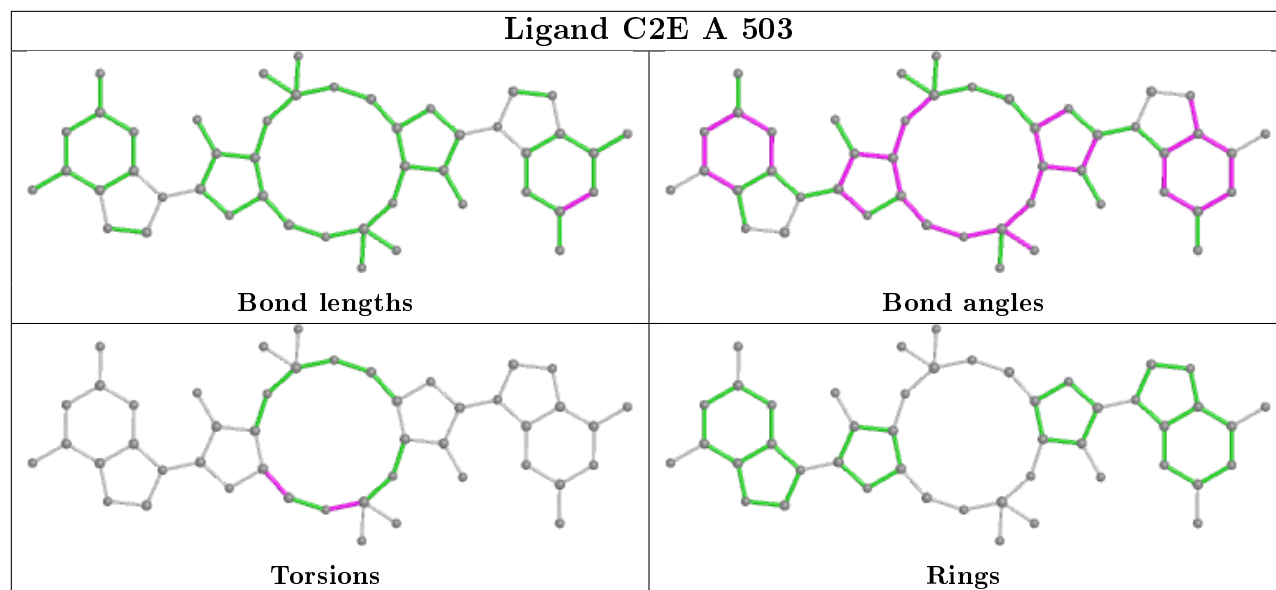
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	505	C2E	1	0
4	A	503	C2E	1	0
4	A	505	C2E	2	0
4	B	503	C2E	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

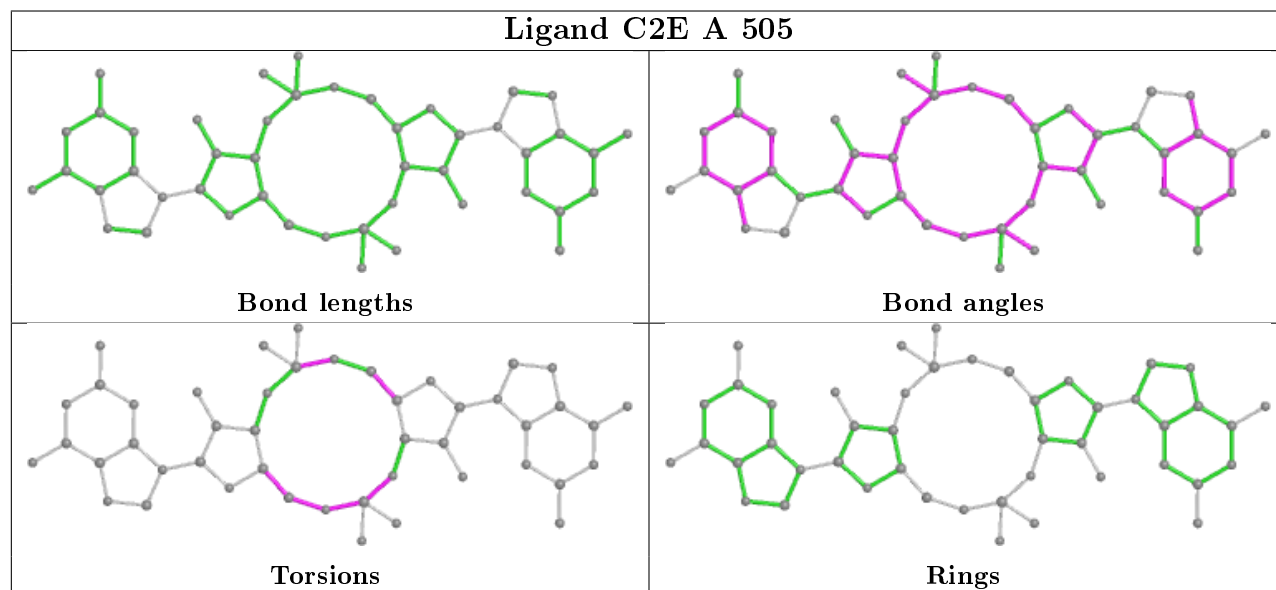
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



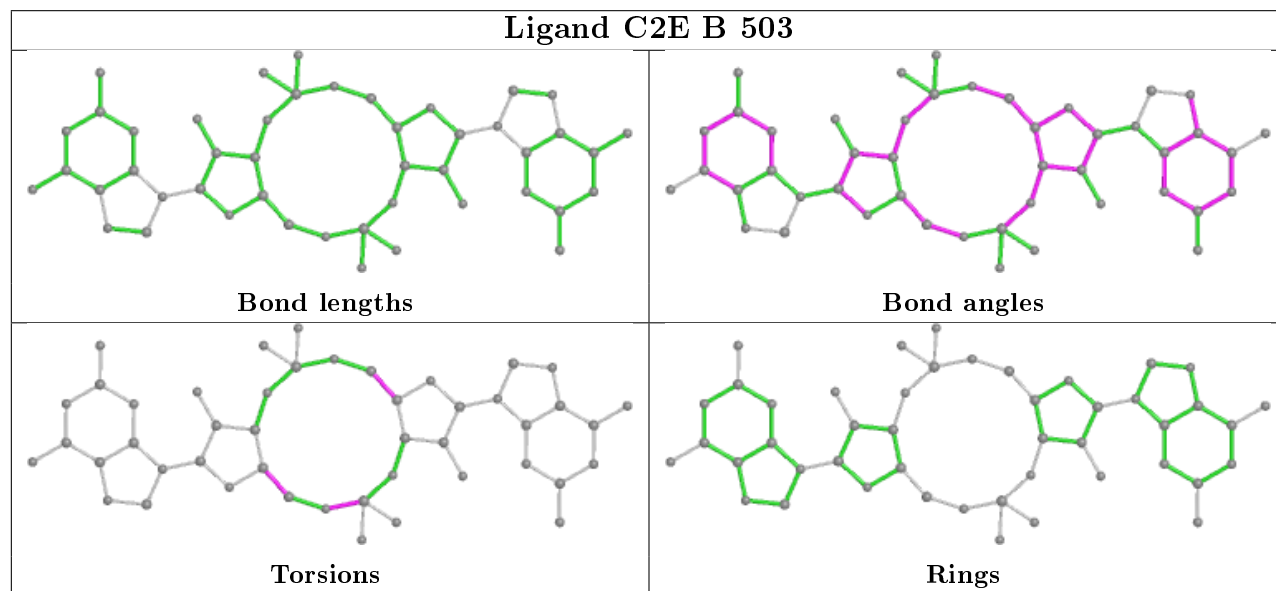
Ligand C2E A 503

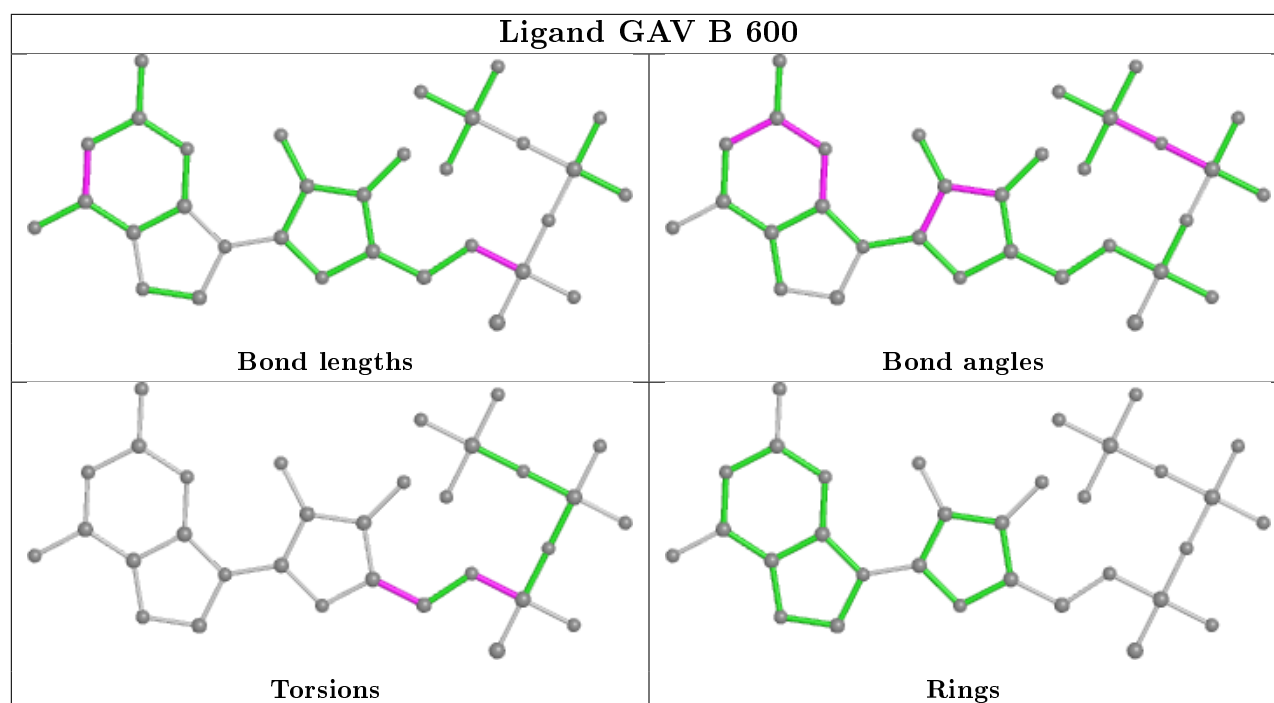


Ligand C2E A 505



Ligand C2E B 503





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	138:ARG	C	139:MET	N	2.39
1	B	148:ARG	C	149:LEU	N	1.81
1	A	147:ALA	C	148:ARG	N	1.06
1	A	287:GLU	C	288:LEU	N	1.02

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	456/459 (99%)	0.32	5 (1%) 80 82	23, 42, 51, 83	23 (5%)
1	B	444/459 (96%)	0.36	9 (2%) 65 67	25, 42, 53, 80	10 (2%)
All	All	900/918 (98%)	0.34	14 (1%) 72 74	23, 42, 52, 83	33 (3%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	137	ARG	3.9
1	A	284	HIS	3.5
1	B	138	ARG	3.2
1	B	134	ALA	2.8
1	B	136	GLY	2.5

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](#)

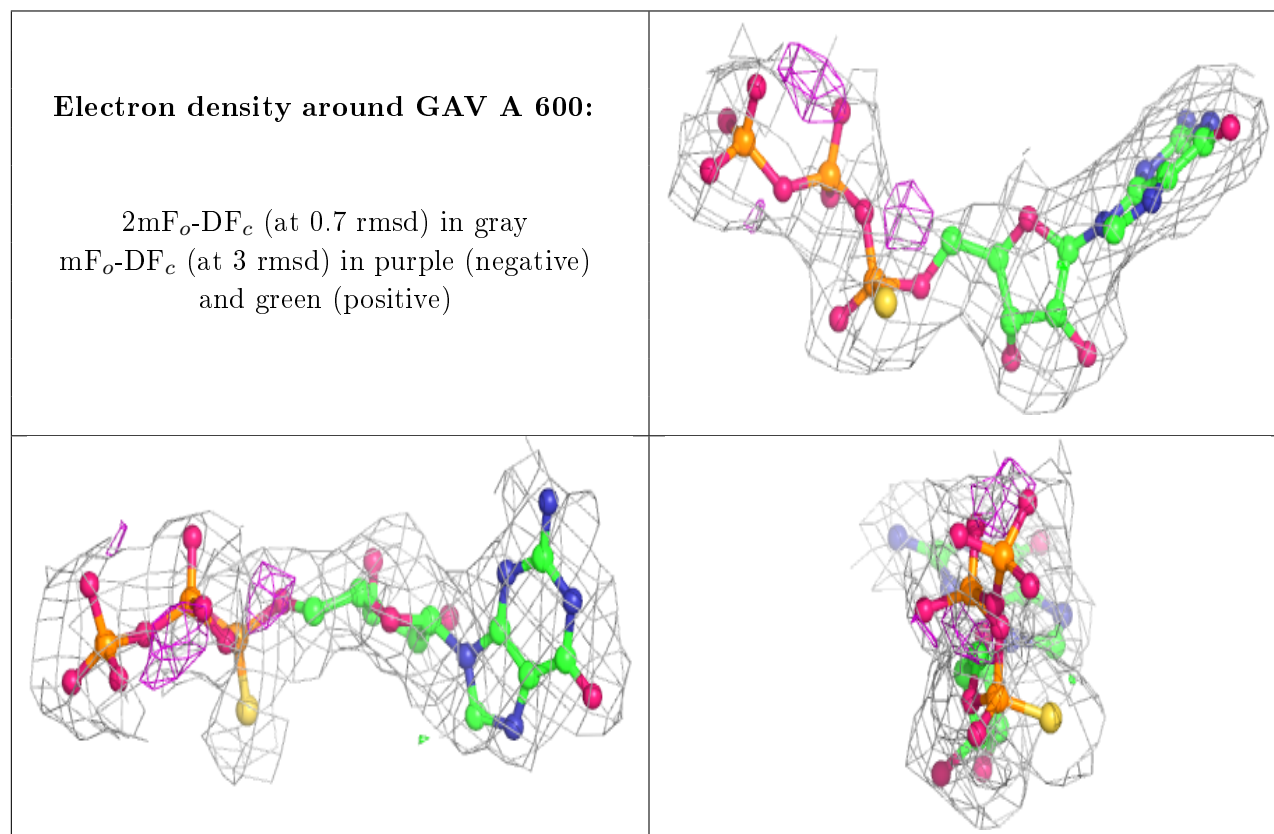
There are no carbohydrates in this entry.

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.

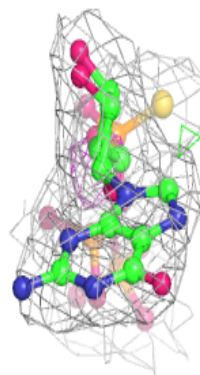
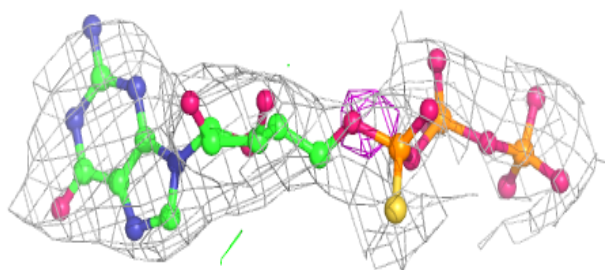
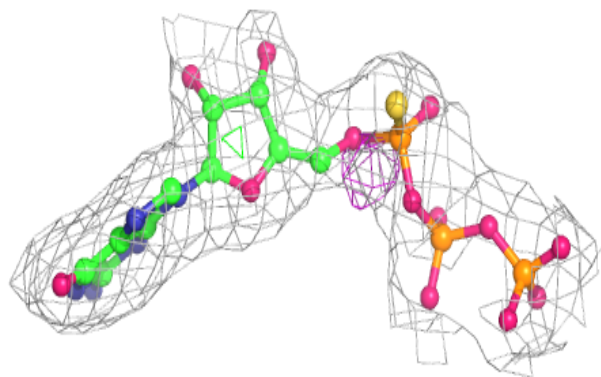
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	602	1/1	0.78	0.16	52,52,52,52	0
3	MG	A	502	1/1	0.82	0.14	37,37,37,37	0
3	MG	A	601	1/1	0.84	0.12	45,45,45,45	0
3	MG	B	601	1/1	0.87	0.06	46,46,46,46	0
6	SO4	A	1471	5/5	0.88	0.29	85,86,88,89	0
5	GAV	A	600	32/32	0.93	0.16	48,60,70,76	0
6	SO4	A	1470	5/5	0.94	0.22	71,76,79,80	0
5	GAV	B	600	32/32	0.94	0.16	33,41,64,70	0
2	BEF	B	501	4/4	0.95	0.11	35,35,39,39	0
7	CL	A	1472	1/1	0.96	0.13	38,38,38,38	0
4	C2E	B	503	46/46	0.96	0.16	37,41,43,44	0
3	MG	B	502	1/1	0.97	0.20	36,36,36,36	0
4	C2E	A	503	46/46	0.97	0.19	37,42,44,45	0
2	BEF	A	501	4/4	0.97	0.12	35,35,39,39	0
4	C2E	B	505	46/46	0.97	0.18	37,41,43,44	0
4	C2E	A	505	46/46	0.97	0.20	37,41,43,45	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.



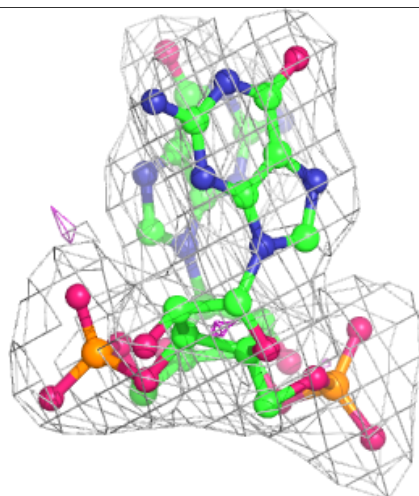
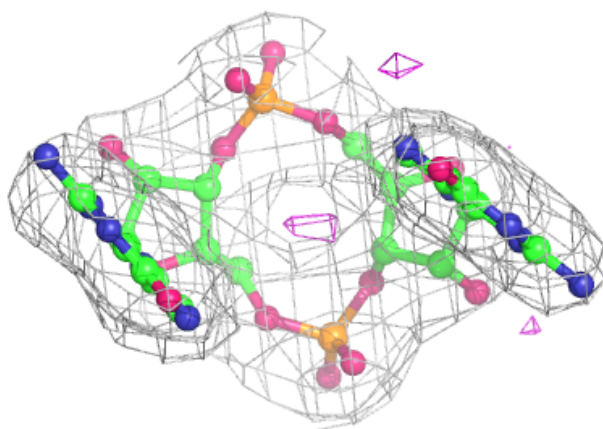
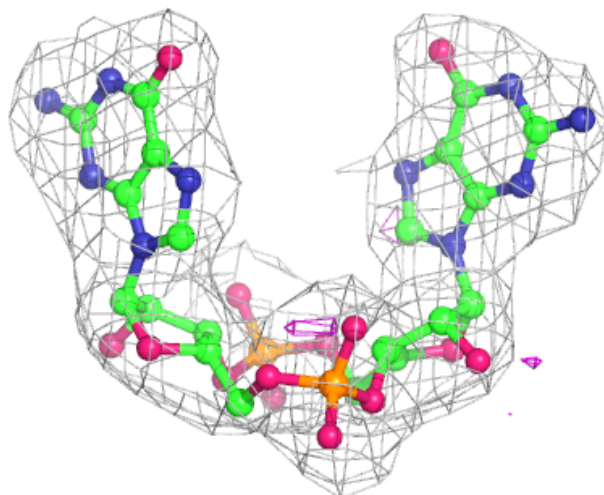
Electron density around GAV B 600:

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



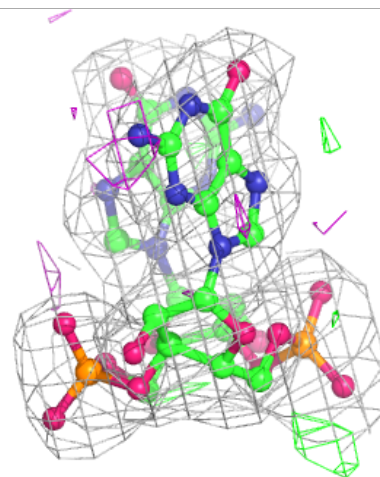
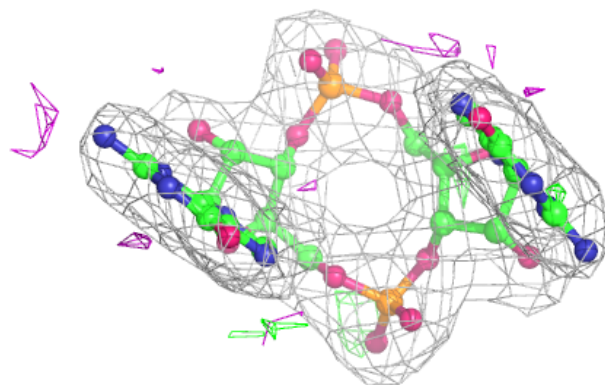
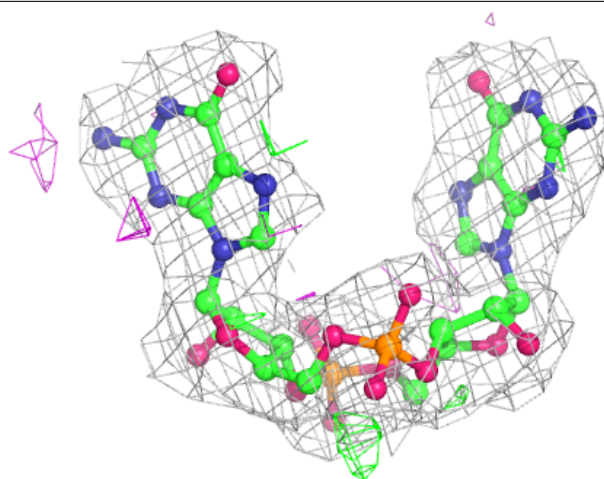
Electron density around C2E B 503:

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



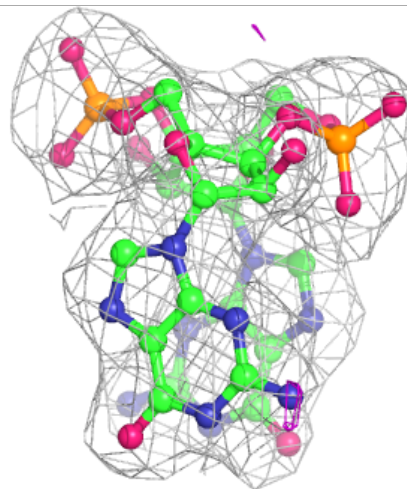
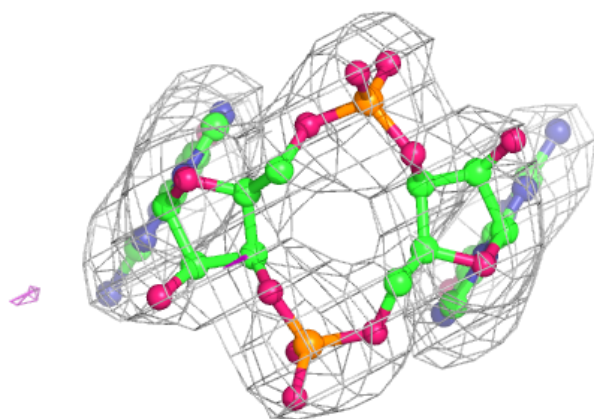
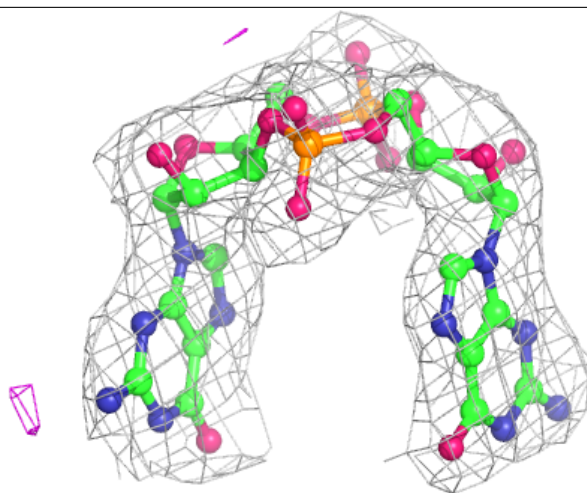
Electron density around C2E A 503:

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



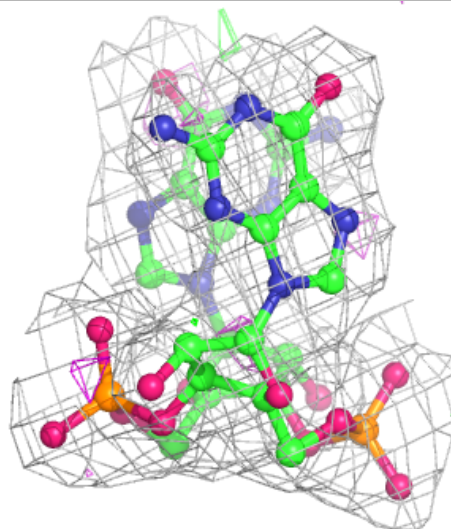
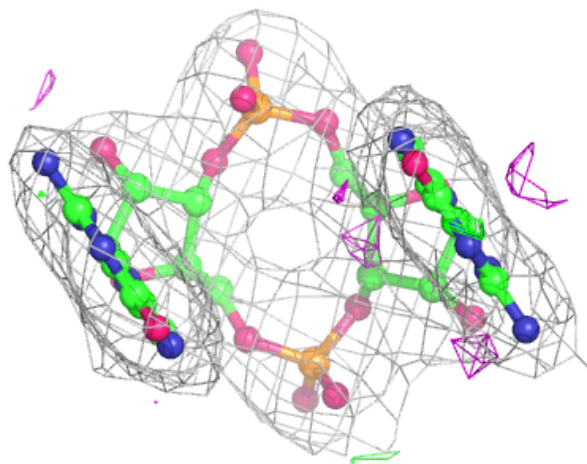
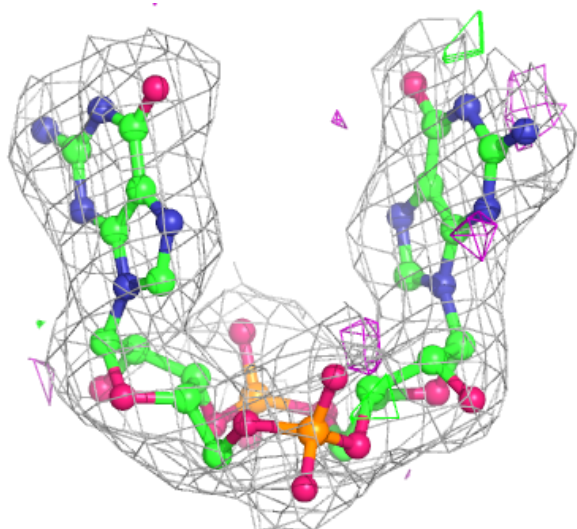
Electron density around C2E B 505:

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



Electron density around C2E A 505:

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.