wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 12:51 pm BST

PDB ID	:	4LGY
Title	:	Importance of Hydrophobic Cavities in Allosteric Regulation of Formylglycinamide Synthetase: Insight from Xenon Trapping and Statistical Coupling Analysis
Authors	:	Tanwar, A.S.; Goyal, V.D.; Choudhary, D.; Panjikar, S.; Anand, R.
Deposited on	:	2013-06-30
Resolution	:	1.48 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 following versions of software and data (see references (1)) were used in the production of this report:

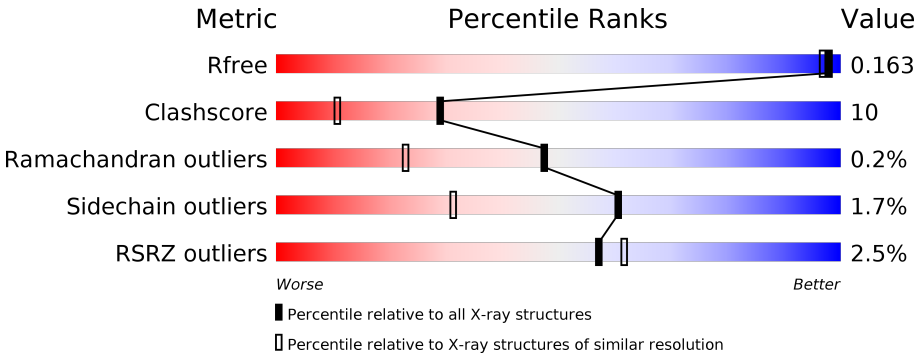
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.48 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	4690 (1.50-1.46)
Clashscore	141614	4955 (1.50-1.46)
Ramachandran outliers	138981	4846 (1.50-1.46)
Sidechain outliers	138945	4844 (1.50-1.46)
RSRZ outliers	127900	4614 (1.50-1.46)

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 <=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	1305	2% 75% 21%

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
5	ACT	A	1324	-	-	X	-
5	ACT	A	1326	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	1327	-	-	X	-
6	GOL	A	1329	-	-	X	-
6	GOL	A	1330	-	X	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11923 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.

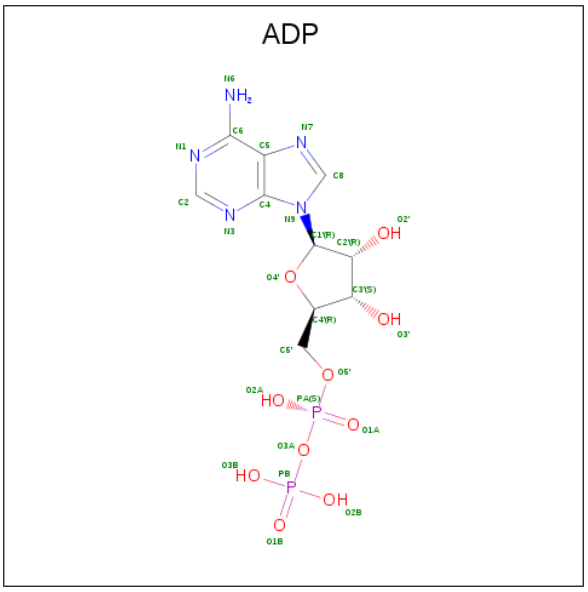
- Molecule 1 is a protein called Phosphoribosylformylglycinamidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1288	Total	C	N	O	S	0	46	0
			10142	6393	1782	1914	53			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	EXPRESSION TAG	UNP P74881
A	-8	ASP	-	EXPRESSION TAG	UNP P74881
A	-7	GLY	-	EXPRESSION TAG	UNP P74881
A	-6	LEU	-	EXPRESSION TAG	UNP P74881
A	-5	VAL	-	EXPRESSION TAG	UNP P74881
A	-4	PRO	-	EXPRESSION TAG	UNP P74881
A	-3	ARG	-	EXPRESSION TAG	UNP P74881
A	-2	GLY	-	EXPRESSION TAG	UNP P74881
A	-1	SER	-	EXPRESSION TAG	UNP P74881
A	0	HIS	-	EXPRESSION TAG	UNP P74881
A	209	TRP	PHE	ENGINEERED MUTATION	UNP P74881

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

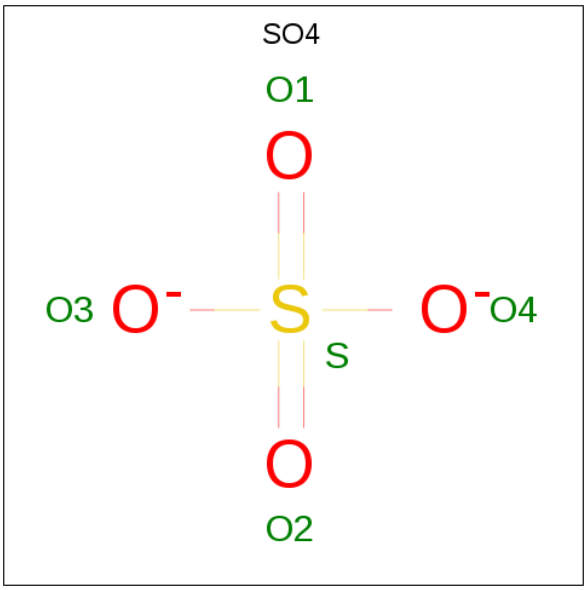


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

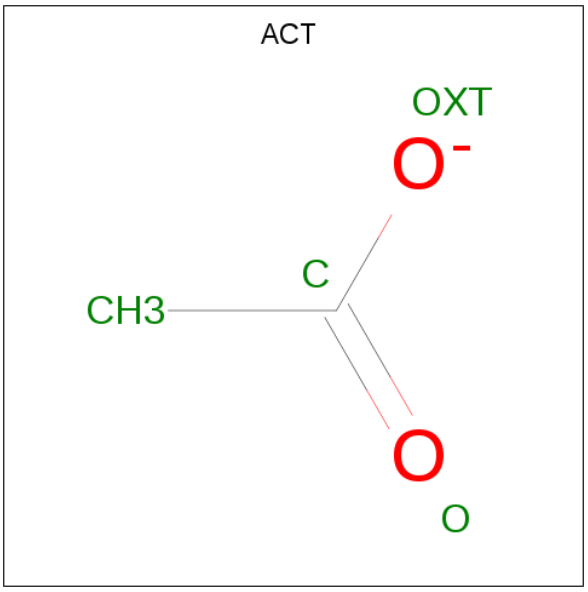
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	Mg	0	0
			7	7		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



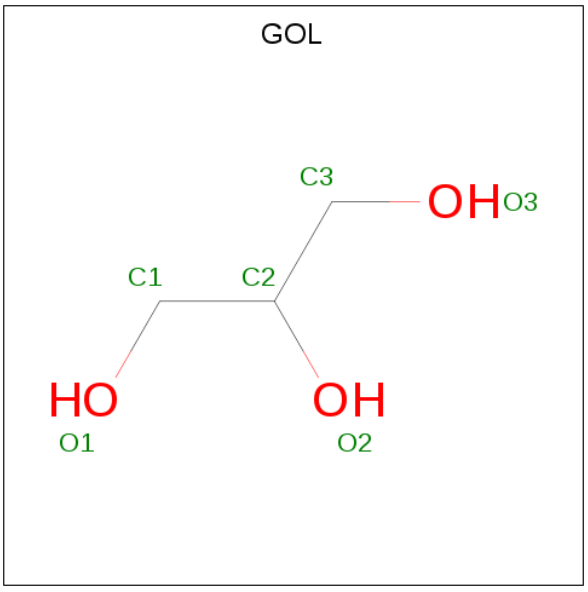
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	6	Total Cl 6 6	0	0

- Molecule 8 is water.

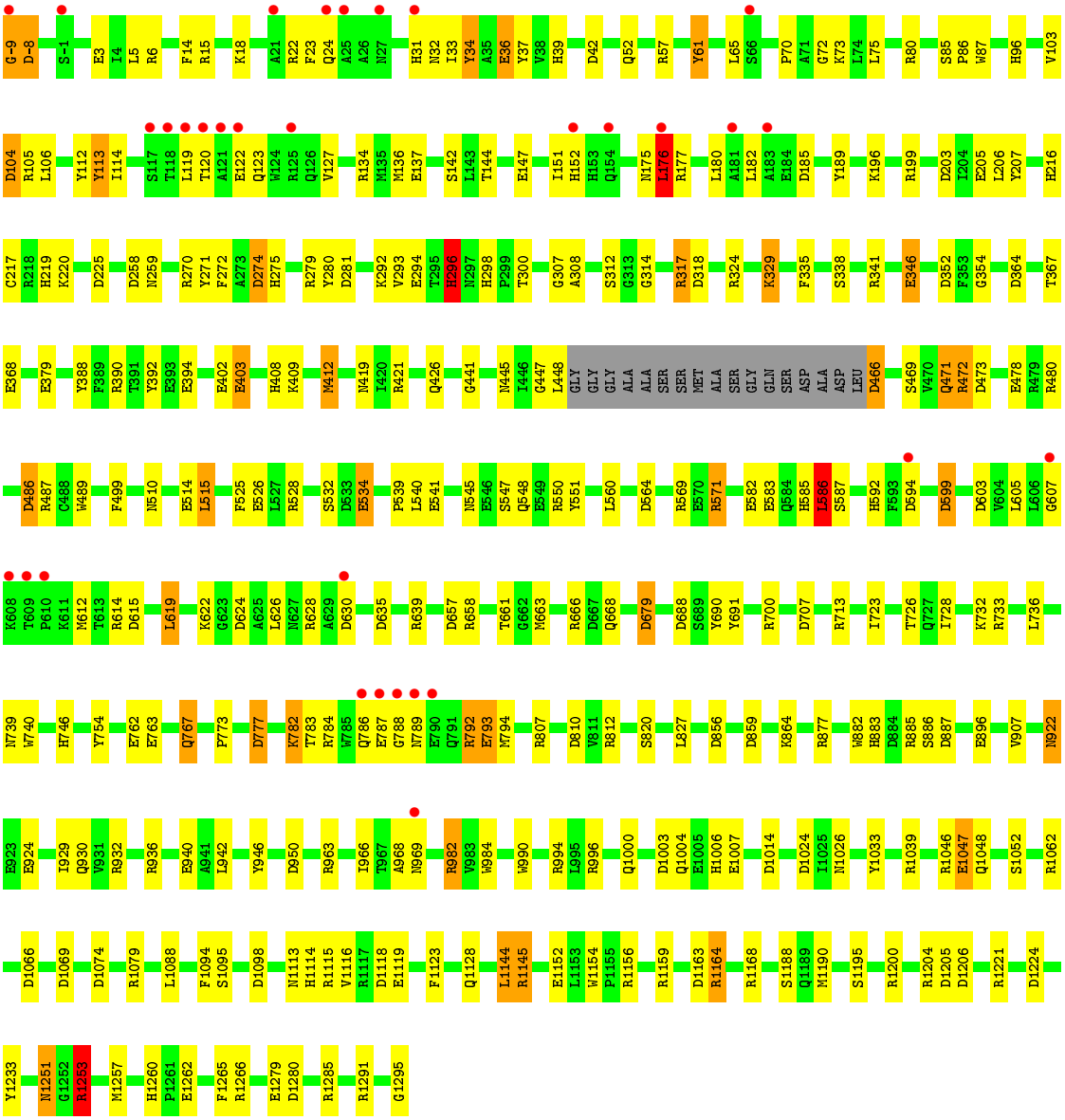
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1610	Total O 1610 1610	0	0

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: Phosphoribosylformylglycinamidine synthase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	146.33Å 146.33Å 140.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.50 – 1.48 27.50 – 1.48	Depositor EDS
% Data completeness (in resolution range)	96.3 (27.50-1.48) 96.3 (27.50-1.48)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.142 , 0.166 0.142 , 0.163	Depositor DCC
R_{free} test set	1114 reflections (0.41%)	wwPDB-VP
Wilson B-factor (Å^2)	10.3	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11923	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ADP, CL, CYG, SO4, ACT

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	1.52	61/10483 (0.6%)	1.69	203/14224 (1.4%)

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	5

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1253	ARG	CZ-NH1	12.30	1.49	1.33
1	A	1253	ARG	CZ-NH2	9.82	1.45	1.33
1	A	1266	ARG	CZ-NH2	9.31	1.45	1.33
1	A	36	GLU	CD-OE1	8.74	1.35	1.25
1	A	1119	GLU	CB-CG	-8.62	1.35	1.52

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1164	ARG	NE-CZ-NH1	26.23	133.42	120.30
1	A	1253	ARG	NE-CZ-NH2	-25.80	107.40	120.30
1	A	994	ARG	NE-CZ-NH1	17.07	128.84	120.30
1	A	713	ARG	NE-CZ-NH2	-16.56	112.02	120.30
1	A	199	ARG	NE-CZ-NH2	-16.55	112.03	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1253	ARG	Sidechain
1	A	296	HIS	Sidechain
1	A	421	ARG	Sidechain
1	A	441	GLY	Mainchain
1	A	788	GLY	Peptide

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	10142	0	10058	184	2
2	A	27	0	12	1	0
3	A	7	0	0	0	0
4	A	95	0	0	1	0
5	A	12	0	9	6	0
6	A	24	0	31	13	2
7	A	6	0	0	0	0
8	A	1610	0	0	88	5
All	All	11923	0	10110	195	5

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 10.

The worst 5 of 195 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:630:ASP:HB3	8:A:2645:HOH:O	1.35	1.26
1:A:335:PHE:HE1	1:A:412[B]:MET:CE	1.50	1.25
1:A:75[A]:LEU:HD23	8:A:2652:HOH:O	1.30	1.24
1:A:346[B]:GLU:OE1	8:A:2503:HOH:O	1.55	1.22
1:A:402:GLU:HG2	8:A:2533:HOH:O	1.36	1.22

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1329:GOL:O2	8:A:2019:HOH:O[6_554]	1.69	0.51
8:A:2885:HOH:O	8:A:2964:HOH:O[5_555]	1.83	0.37
6:A:1329:GOL:C2	8:A:2019:HOH:O[6_554]	1.92	0.28
1:A:196:LYS:CE	8:A:2769:HOH:O[3_445]	2.02	0.18
1:A:-8:ASP:OD1	8:A:1684:HOH:O[4_444]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	1330/1305 (102%)	1300 (98%)	28 (2%)	2 (0%)	47 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	661	THR
1	A	886	SER

5.3.2 Protein sidechains

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	1077/1041 (104%)	1057 (98%)	20 (2%)	57 26

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	A	471	GLN
1	A	982	ARG
1	A	412[A]	MET
1	A	412[B]	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	471	GLN
1	A	674	GLN
1	A	1113	ASN
1	A	545	ASN
1	A	548	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	CYG	A	1135	1	9,14,15	2.62	6 (66%)	6,17,19	3.23	3 (50%)

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
1	CYG	A	1135	1	-	1/10/16/18	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	CYG	CG1-CD1	4.66	1.55	1.50
1	A	1135	CYG	OE2-CD1	3.37	1.26	1.21
1	A	1135	CYG	CD1-SG	3.11	1.83	1.76
1	A	1135	CYG	CA1-N1	3.00	1.53	1.47
1	A	1135	CYG	CB-SG	2.32	1.86	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1135	CYG	CB1-CG1-CD1	-5.93	99.18	112.33
1	A	1135	CYG	OE2-CD1-CG1	-4.13	119.11	123.99
1	A	1135	CYG	CG1-CD1-SG	3.19	117.17	113.46

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1135	CYG	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 40 ligands modelled in this entry, 13 are monoatomic - leaving 27 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	ACT	A	1324	-	1,3,3	3.75	1 (100%)	0,3,3	0.00	-
4	SO4	A	1320	-	4,4,4	0.43	0	6,6,6	1.28	0
4	SO4	A	1321	-	4,4,4	0.50	0	6,6,6	1.13	0
5	ACT	A	1325	-	1,3,3	3.03	1 (100%)	0,3,3	0.00	-
4	SO4	A	1322	-	4,4,4	0.34	0	6,6,6	0.90	0
4	SO4	A	1314	-	4,4,4	0.84	0	6,6,6	0.76	0
4	SO4	A	1306	-	4,4,4	0.50	0	6,6,6	0.73	0
4	SO4	A	1305	-	4,4,4	0.73	0	6,6,6	1.12	1 (16%)
4	SO4	A	1323	-	4,4,4	0.90	0	6,6,6	1.75	2 (33%)
4	SO4	A	1311	-	4,4,4	0.74	0	6,6,6	1.48	2 (33%)
4	SO4	A	1319	-	4,4,4	0.89	0	6,6,6	1.41	0
6	GOL	A	1328	-	5,5,5	1.38	0	5,5,5	0.76	0
4	SO4	A	1315	-	4,4,4	1.18	0	6,6,6	0.77	0
4	SO4	A	1318	-	4,4,4	0.88	0	6,6,6	1.09	0
4	SO4	A	1312	-	4,4,4	0.80	0	6,6,6	0.52	0
4	SO4	A	1313	-	4,4,4	0.94	0	6,6,6	0.65	0
4	SO4	A	1317	-	4,4,4	0.51	0	6,6,6	1.09	0
4	SO4	A	1310	-	4,4,4	0.50	0	6,6,6	0.96	0
4	SO4	A	1308	-	4,4,4	0.65	0	6,6,6	1.02	0
6	GOL	A	1327	-	5,5,5	0.70	0	5,5,5	1.54	1 (20%)
4	SO4	A	1307	-	4,4,4	0.80	0	6,6,6	2.06	3 (50%)
6	GOL	A	1330	-	5,5,5	1.75	1 (20%)	5,5,5	1.53	2 (40%)
4	SO4	A	1316	-	4,4,4	0.73	0	6,6,6	0.57	0
5	ACT	A	1326	-	1,3,3	7.60	1 (100%)	0,3,3	0.00	-
4	SO4	A	1309	-	4,4,4	0.41	0	6,6,6	0.44	0
6	GOL	A	1329	-	5,5,5	0.94	0	5,5,5	1.58	1 (20%)
2	ADP	A	1301	3	24,29,29	1.35	1 (4%)	29,45,45	0.97	1 (3%)

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
6	GOL	A	1329	-	-	3/4/4/4	-
2	ADP	A	1301	3	-	1/12/32/32	0/3/3/3
6	GOL	A	1327	-	-	0/4/4/4	-
6	GOL	A	1328	-	-	0/4/4/4	-
6	GOL	A	1330	-	-	3/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1326	ACT	CH3-C	7.60	1.58	1.48
5	A	1324	ACT	CH3-C	3.75	1.53	1.48
2	A	1301	ADP	C2-N1	3.73	1.40	1.33
6	A	1330	GOL	O2-C2	3.48	1.53	1.43
5	A	1325	ACT	CH3-C	3.03	1.52	1.48

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1329	GOL	O2-C2-C3	3.00	122.35	109.12
6	A	1327	GOL	O2-C2-C1	2.89	121.85	109.12
4	A	1307	SO4	O4-S-O1	2.89	124.37	109.31
4	A	1323	SO4	O4-S-O3	2.79	120.98	109.06
4	A	1307	SO4	O3-S-O2	-2.57	95.88	109.31

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1330	GOL	O1-C1-C2-C3
6	A	1329	GOL	C1-C2-C3-O3
6	A	1329	GOL	O2-C2-C3-O3
6	A	1330	GOL	O1-C1-C2-O2
6	A	1329	GOL	O1-C1-C2-O2

There are no ring outliers.

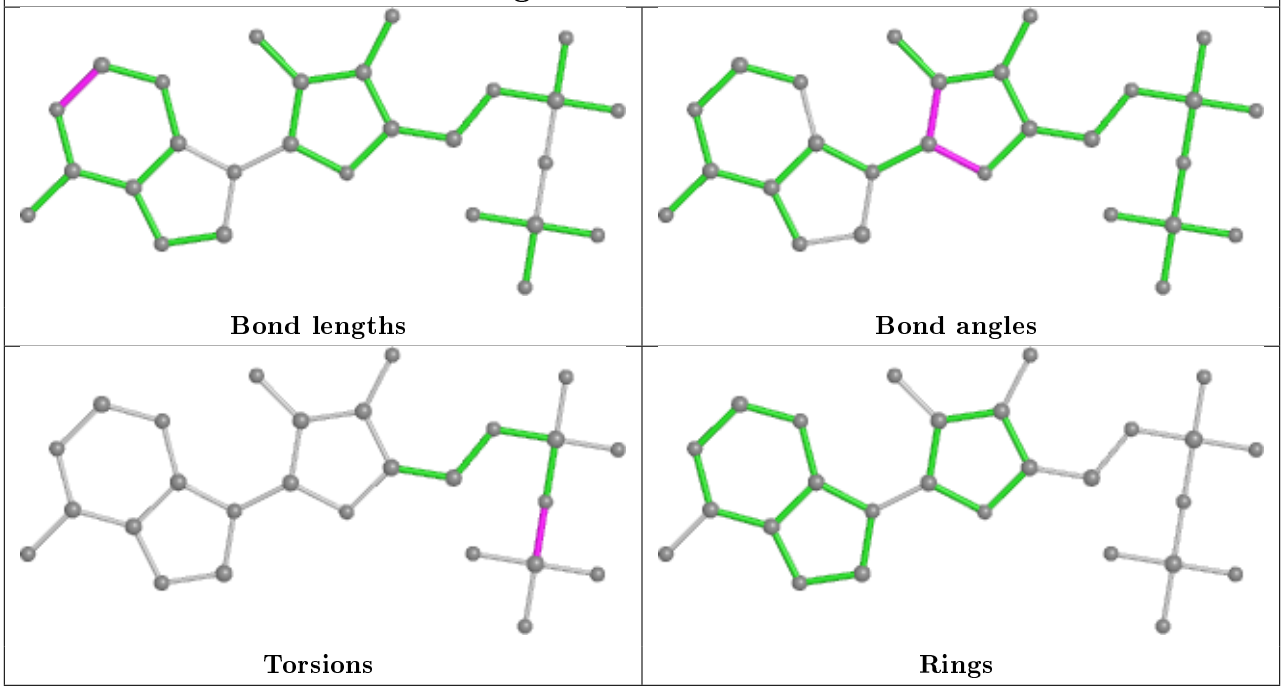
8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1324	ACT	3	0
5	A	1325	ACT	1	0
4	A	1322	SO4	1	0
6	A	1327	GOL	5	0
6	A	1330	GOL	6	0
5	A	1326	ACT	2	0
6	A	1329	GOL	2	2
2	A	1301	ADP	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 ADP A 1301



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	1287/1305 (98%)	-0.20	32 (2%) 57 61	5, 10, 26, 68	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	789	ASN	6.0
1	A	120	THR	4.2
1	A	119	LEU	4.1
1	A	788	GLY	4.1
1	A	118	THR	4.0

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

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
1	CYG	A	1135	15/16	0.99	0.05	5,6,8,11	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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,

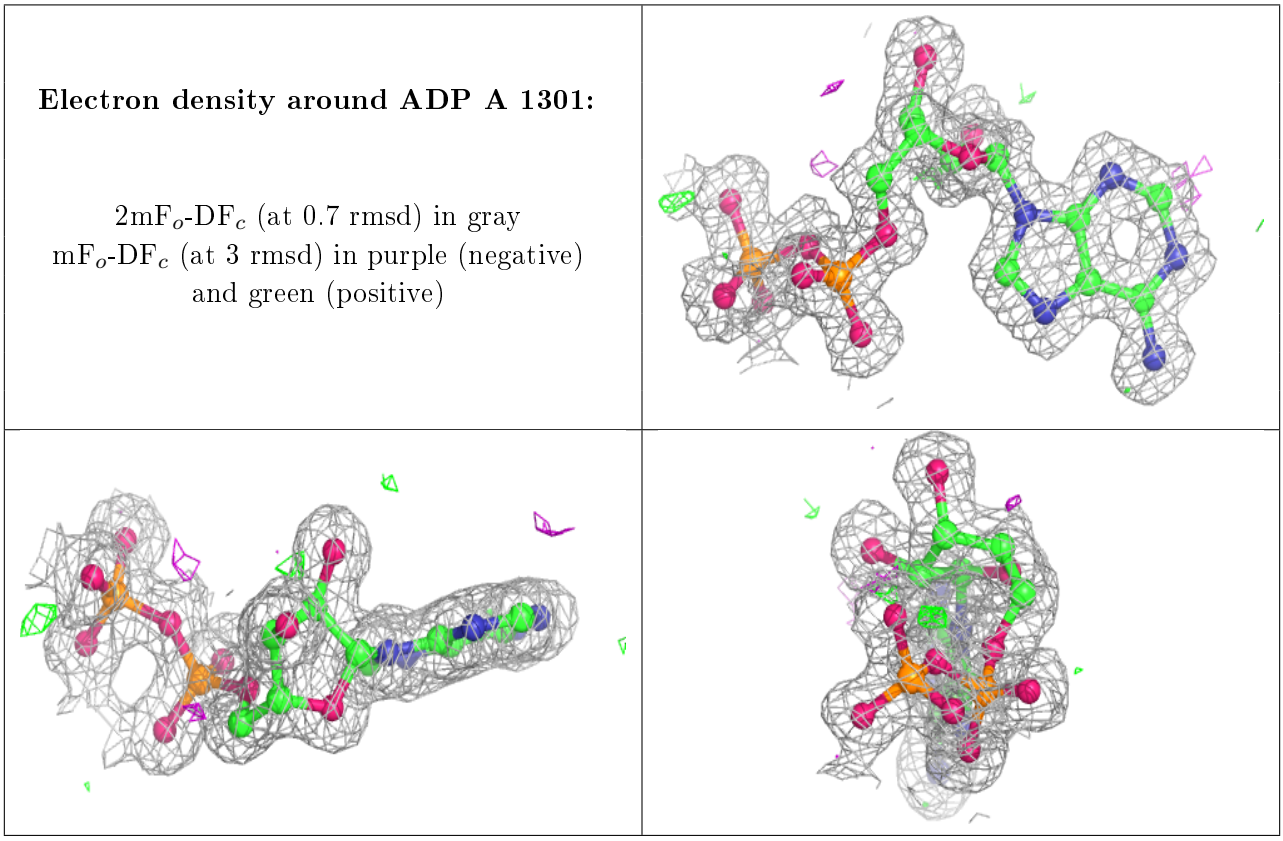
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	1339	1/1	0.79	0.22	39,39,39,39	0
7	CL	A	1334	1/1	0.81	0.13	46,46,46,46	0
6	GOL	A	1327	6/6	0.81	0.24	16,24,48,51	0
4	SO4	A	1323	5/5	0.82	0.19	15,22,28,29	5
5	ACT	A	1324	4/4	0.84	0.17	22,29,30,44	0
7	CL	A	1336	1/1	0.84	0.13	35,35,35,35	1
6	GOL	A	1330	6/6	0.85	0.25	29,33,37,49	0
5	ACT	A	1325	4/4	0.89	0.16	35,45,48,63	0
5	ACT	A	1326	4/4	0.89	0.18	19,21,31,38	0
4	SO4	A	1318	5/5	0.90	0.21	42,43,60,68	0
3	MG	A	1337	1/1	0.90	0.11	27,27,27,27	0
4	SO4	A	1322	5/5	0.90	0.18	37,38,40,42	5
4	SO4	A	1314	5/5	0.91	0.15	21,25,32,35	5
6	GOL	A	1329	6/6	0.91	0.16	22,26,34,52	0
4	SO4	A	1315	5/5	0.92	0.14	12,13,21,22	5
3	MG	A	1340	1/1	0.92	0.17	26,26,26,26	0
3	MG	A	1338	1/1	0.92	0.20	31,31,31,31	0
7	CL	A	1331	1/1	0.94	0.15	52,52,52,52	0
7	CL	A	1332	1/1	0.94	0.15	31,31,31,31	1
4	SO4	A	1321	5/5	0.94	0.19	44,48,50,52	0
6	GOL	A	1328	6/6	0.95	0.11	12,15,19,22	0
4	SO4	A	1305	5/5	0.95	0.12	20,24,26,28	5
7	CL	A	1333	1/1	0.96	0.06	23,23,23,23	1
7	CL	A	1335	1/1	0.96	0.14	20,20,20,20	1
4	SO4	A	1310	5/5	0.97	0.16	21,22,24,30	5
4	SO4	A	1308	5/5	0.97	0.10	17,18,20,25	5
4	SO4	A	1306	5/5	0.97	0.08	9,13,14,19	5
4	SO4	A	1319	5/5	0.97	0.09	19,20,26,29	0
4	SO4	A	1307	5/5	0.98	0.11	16,20,29,32	0
4	SO4	A	1316	5/5	0.98	0.21	22,29,34,34	5
4	SO4	A	1313	5/5	0.98	0.08	8,12,14,15	5
4	SO4	A	1309	5/5	0.98	0.10	17,18,23,28	0
4	SO4	A	1320	5/5	0.98	0.11	17,19,20,25	5
4	SO4	A	1311	5/5	0.99	0.06	14,15,21,22	0
4	SO4	A	1317	5/5	0.99	0.13	20,21,28,28	5
4	SO4	A	1312	5/5	0.99	0.07	14,15,16,20	0
3	MG	A	1303	1/1	0.99	0.05	7,7,7,7	0
2	ADP	A	1301	27/27	0.99	0.05	5,6,7,8	0
3	MG	A	1302	1/1	1.00	0.04	5,5,5,5	0
3	MG	A	1304	1/1	1.00	0.05	6,6,6,6	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 ADP A 1301:

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



6.5 Other polymers

There are no such residues in this entry.