



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2022 – 06:11 PM JST

PDB ID : 6LYL  
Title : Crystal structure of S1052D mutant of Formylglycinamidase synthetase  
Authors : Sharma, N.; Tanwar, A.S.; Anand, R.  
Deposited on : 2020-02-14  
Resolution : 2.10 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](mailto: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.

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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 : 2.26  
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) : 2.26

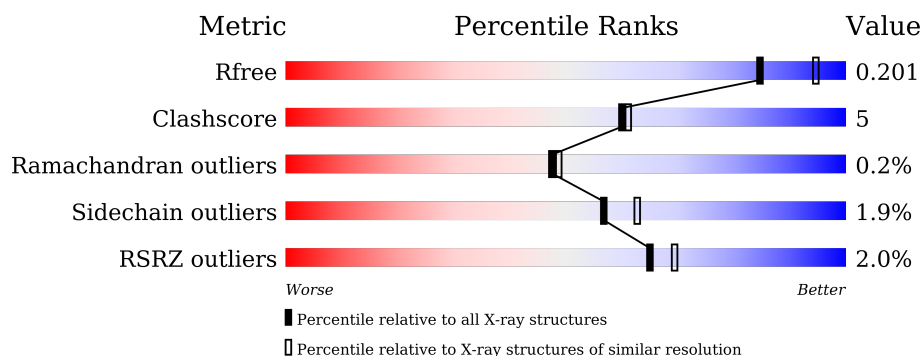
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	1304	<div> <div>2%</div> <div>89%</div> <div>9% ..</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10987 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.

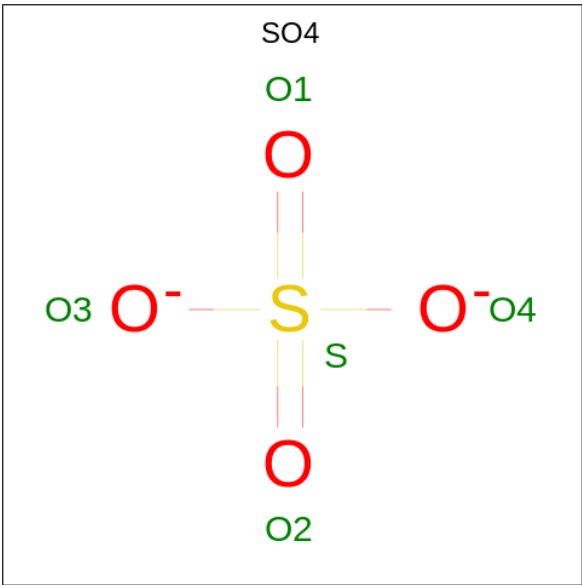
- Molecule 1 is a protein called Phosphoribosylformylglycinamide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1288	Total	C	N	O	S	0	10	0
			9994	6274	1781	1890	49			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ALA	-	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	1052	ASP	SER	engineered mutation	UNP P74881

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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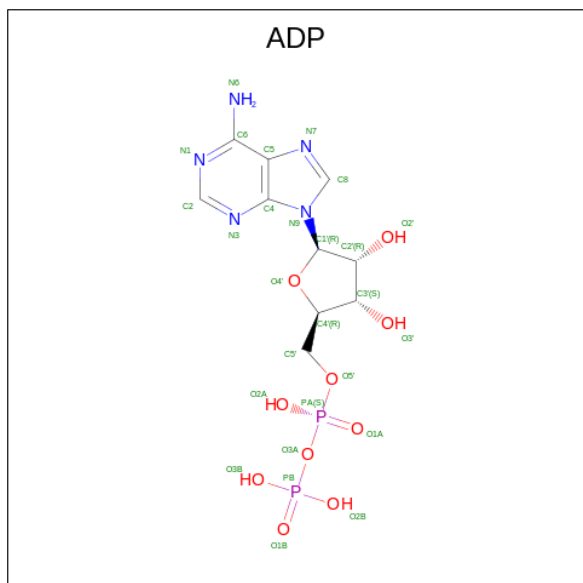
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0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

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

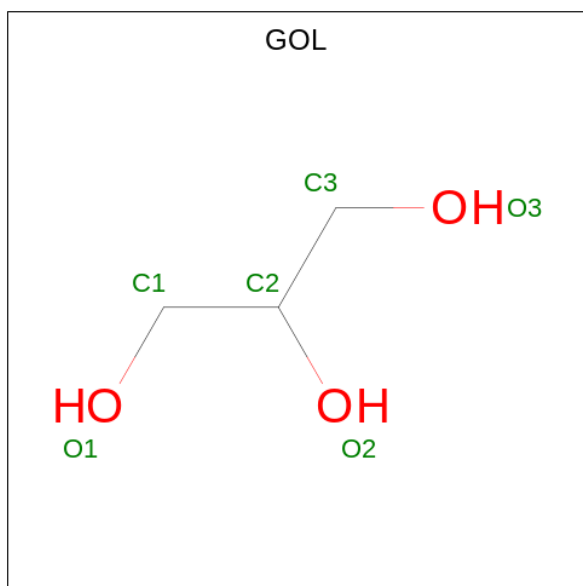
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

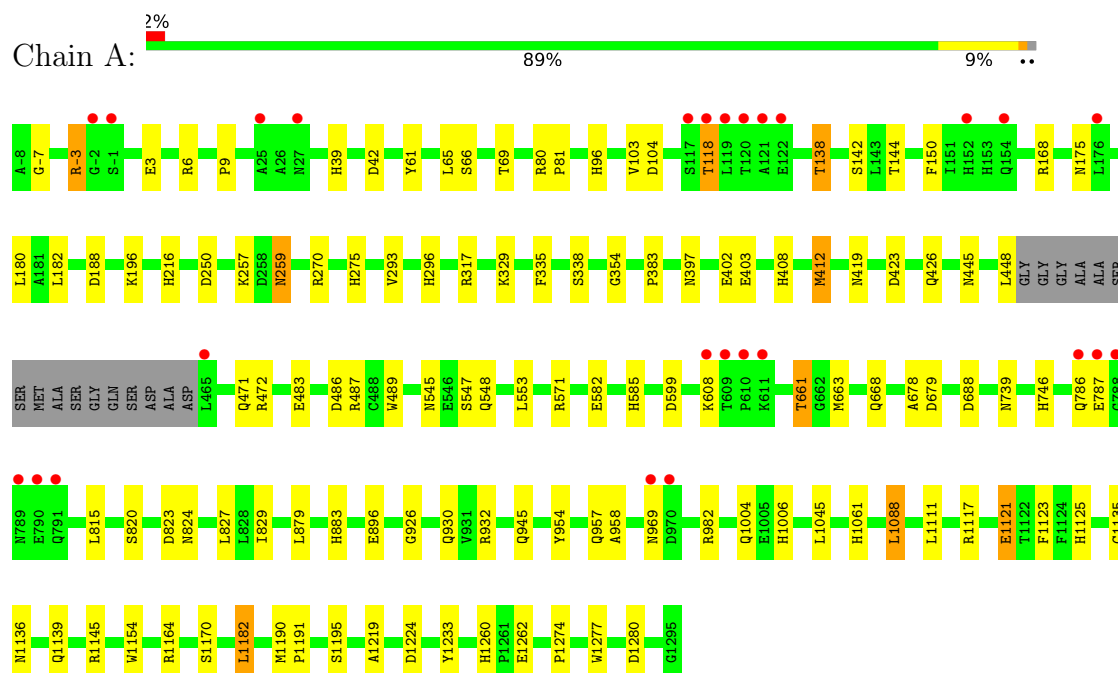
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	786	Total	O	0	0
			786	786		

### 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: Phosphoribosylformylglycinamidine synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.19Å 146.19Å 141.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.85 – 2.10 35.38 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.85-2.10) 98.8 (35.38-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.78 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.153 , 0.192 0.165 , 0.201	Depositor DCC
$R_{free}$ test set	4837 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.017 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10987	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.92	1/10191 (0.0%)	0.93	4/13835 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1121	GLU	CD-OE2	-5.20	1.20	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	1224	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	932	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	423	ASP	CB-CG-OD1	5.18	122.96	118.30

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	9994	0	9771	92	0
2	A	115	0	0	0	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	27	0	12	1	0
5	A	54	0	72	1	0
6	A	8	0	12	0	0
7	A	786	0	0	26	0
All	All	10987	0	9867	93	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 5.

All (93) 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:1045[B]:LEU:HD11	1:A:1088[B]:LEU:CD1	1.57	1.32
1:A:1045[B]:LEU:CD1	1:A:1088[B]:LEU:HD11	1.87	1.03
1:A:1045[B]:LEU:HD11	1:A:1088[B]:LEU:HD11	0.94	0.94
1:A:402:GLU:HG2	7:A:2108:HOH:O	1.79	0.81
1:A:820:SER:H	1:A:930:GLN:HE22	1.27	0.81
1:A:608:LYS:CB	7:A:2821:HOH:O	2.29	0.80
1:A:787:GLU:CB	7:A:2812:HOH:O	2.34	0.75
1:A:824:ASN:HD21	1:A:958:ALA:H	1.34	0.74
1:A:1045[B]:LEU:CD1	1:A:1088[B]:LEU:CD1	2.53	0.73
1:A:96:HIS:HE1	1:A:103:VAL:O	1.76	0.69
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.78	0.65
1:A:175:ASN:HD21	1:A:182:LEU:H	1.43	0.65
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.81	0.64
1:A:6:ARG:CB	7:A:2768:HOH:O	2.46	0.63
1:A:445:ASN:OD1	1:A:448:LEU:HD12	1.98	0.62
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.83	0.62
1:A:1045[B]:LEU:HD11	1:A:1088[B]:LEU:HD12	1.75	0.60
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.65	0.60
1:A:397:ASN:HB2	7:A:2108:HOH:O	2.00	0.60
1:A:545:ASN:HD22	1:A:547:SER:H	1.50	0.59
1:A:-3:ARG:HD3	1:A:42:ASP:OD1	2.03	0.57
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.88	0.57
1:A:354:GLY:O	1:A:408:HIS:HE1	1.87	0.57
1:A:471:GLN:HE21	1:A:472:ARG:H	1.52	0.57
1:A:402:GLU:CG	7:A:2108:HOH:O	2.45	0.56
1:A:80:ARG:HA	1:A:138:THR:HG22	1.86	0.56
1:A:275:HIS:HD2	7:A:2842:HOH:O	1.87	0.56
1:A:335:PHE:CE1	1:A:412[B]:MET:CE	2.88	0.56
1:A:329:LYS:HG3	7:A:2379:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088[B]:LEU:HD23	1:A:1088[B]:LEU:O	2.08	0.54
1:A:69[A]:THR:HG22	7:A:2743:HOH:O	2.08	0.54
1:A:827:LEU:HD23	1:A:954:TYR:HA	1.90	0.53
1:A:663:MET:HE3	7:A:2866:HOH:O	2.07	0.53
1:A:329:LYS:NZ	1:A:419:ASN:HD21	2.07	0.53
1:A:1111:LEU:HA	1:A:1117:ARG:HG3	1.92	0.52
1:A:815:LEU:HD21	1:A:879:LEU:O	2.09	0.52
1:A:335:PHE:CE1	1:A:412[B]:MET:HE1	2.45	0.51
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.75	0.51
1:A:820:SER:N	1:A:930:GLN:HE22	2.04	0.51
1:A:969:ASN:ND2	7:A:2116:HOH:O	2.43	0.51
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.94	0.50
1:A:81:PRO:HD3	1:A:138:THR:HG21	1.93	0.49
1:A:329:LYS:CG	7:A:2379:HOH:O	2.60	0.49
1:A:335:PHE:CE1	1:A:412[B]:MET:HE2	2.46	0.49
1:A:216:HIS:HD2	7:A:2144:HOH:O	1.96	0.49
1:A:259:ASN:HB2	7:A:2460:HOH:O	2.11	0.49
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.11	0.48
1:A:80:ARG:HD3	7:A:2114:HOH:O	2.13	0.48
1:A:1045[B]:LEU:HD21	1:A:1088[B]:LEU:HD12	1.95	0.48
1:A:338:SER:OG	1:A:408:HIS:HD2	1.96	0.48
1:A:957:GLN:HB3	7:A:2104:HOH:O	2.13	0.48
1:A:1006:HIS:HE1	7:A:2362:HOH:O	1.95	0.48
1:A:168:ARG:NH1	1:A:188:ASP:OD1	2.45	0.48
1:A:96:HIS:CE1	1:A:103:VAL:O	2.64	0.47
1:A:329:LYS:O	1:A:383:PRO:HD2	2.14	0.47
1:A:257:LYS:NZ	1:A:426:GLN:OE1	2.40	0.47
1:A:1088[A]:LEU:HD12	1:A:1123:PHE:CE2	2.50	0.47
1:A:1006:HIS:HD2	7:A:2428:HOH:O	1.98	0.46
1:A:1136:ASN:HA	1:A:1139:GLN:OE1	2.15	0.46
1:A:661:THR:HG21	7:A:2379:HOH:O	2.15	0.46
1:A:1121:GLU:O	1:A:1125:HIS:HD2	1.99	0.46
1:A:1260:HIS:CD2	1:A:1262:GLU:OE2	2.67	0.46
1:A:142:SER:HB3	1:A:144:THR:HG22	1.99	0.45
1:A:270:ARG:HD3	7:A:2229:HOH:O	2.17	0.45
1:A:1280:ASP:OD2	7:A:2101:HOH:O	2.20	0.45
1:A:-3:ARG:HD2	1:A:150:PHE:HB2	1.99	0.44
1:A:175:ASN:ND2	1:A:182:LEU:H	2.13	0.44
1:A:1164:ARG:HD3	7:A:2125:HOH:O	2.16	0.44
1:A:142:SER:CB	1:A:144:THR:HG22	2.48	0.44
1:A:1004:GLN:HE21	1:A:1233:TYR:H	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.16	0.44
1:A:403:GLU:OE1	1:A:746:HIS:HE1	2.00	0.44
1:A:486:ASP:HA	1:A:489:TRP:NE1	2.34	0.43
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.66	0.43
1:A:668:GLN:HA	1:A:678:ALA:HB3	2.00	0.43
1:A:1045[B]:LEU:HD11	1:A:1088[B]:LEU:CG	2.39	0.43
1:A:823:ASP:HB3	7:A:2774:HOH:O	2.18	0.43
1:A:1121:GLU:O	1:A:1125:HIS:CD2	2.72	0.43
1:A:1061:HIS:HD2	7:A:2463:HOH:O	2.00	0.42
1:A:412[A]:MET:SD	1:A:412[A]:MET:C	2.98	0.42
1:A:1088[A]:LEU:HD12	1:A:1123:PHE:CD2	2.54	0.42
5:A:2031:GOL:O1	7:A:2102:HOH:O	2.21	0.42
1:A:81:PRO:CD	1:A:138:THR:HG21	2.49	0.42
1:A:1170:SER:O	1:A:1191:PRO:HA	2.20	0.42
1:A:1274:PRO:HD2	1:A:1277:TRP:CE2	2.55	0.42
1:A:-7:GLY:O	1:A:3:GLU:HA	2.20	0.41
1:A:483:GLU:O	1:A:487:ARG:HG2	2.20	0.41
1:A:829:ILE:O	1:A:926:GLY:HA3	2.21	0.41
1:A:1182:LEU:HD23	1:A:1219:ALA:HB1	2.03	0.41
1:A:957:GLN:CD	7:A:2104:HOH:O	2.58	0.41
1:A:1145:ARG:HD3	1:A:1154:TRP:HB2	2.02	0.41
1:A:9:PRO:HB2	1:A:65:LEU:HB2	2.04	0.40
1:A:668:GLN:HG2	4:A:2008:ADP:H1'	2.02	0.40

There are no symmetry-related clashes.

## 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	1293/1304 (99%)	1256 (97%)	35 (3%)	2 (0%)	47 49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	THR
1	A	661	THR

### 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	1037/1040 (100%)	1015 (98%)	22 (2%)	53	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ARG
1	A	66	SER
1	A	104	ASP
1	A	118	THR
1	A	138	THR
1	A	196	LYS
1	A	250	ASP
1	A	259	ASN
1	A	296	HIS
1	A	412[A]	MET
1	A	412[B]	MET
1	A	553	LEU
1	A	571	ARG
1	A	582	GLU
1	A	786	GLN
1	A	945	GLN
1	A	982	ARG
1	A	1088[A]	LEU
1	A	1088[B]	LEU
1	A	1182	LEU
1	A	1190	MET
1	A	1195	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	96	HIS
1	A	175	ASN
1	A	216	HIS
1	A	219	HIS
1	A	233	GLN
1	A	243	ASN
1	A	275	HIS
1	A	296	HIS
1	A	298	HIS
1	A	408	HIS
1	A	419	ASN
1	A	471	GLN
1	A	545	ASN
1	A	548	GLN
1	A	585	HIS
1	A	674	GLN
1	A	739	ASN
1	A	746	HIS
1	A	791	GLN
1	A	818	GLN
1	A	824	ASN
1	A	883	HIS
1	A	906	GLN
1	A	930	GLN
1	A	969	ASN
1	A	993	GLN
1	A	1000	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1018	ASN
1	A	1026	ASN
1	A	1061	HIS
1	A	1125	HIS
1	A	1161	HIS
1	A	1189	GLN
1	A	1260	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	2.32	3 (33%)	6,17,19	1.44	1 (16%)

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	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	CYG	CG1-CD1	4.88	1.55	1.50
1	A	1135	CYG	OE2-CD1	3.52	1.26	1.21
1	A	1135	CYG	CD1-SG	-3.21	1.68	1.76

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	CYG	CB1-CG1-CD1	-2.92	105.86	112.33

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 3 are monoatomic - leaving 35 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	$\# Z  > 2$
2	SO4	A	2014	-	4,4,4	0.89	0	6,6,6	0.96	0
5	GOL	A	2028	-	5,5,5	0.92	0	5,5,5	1.28	1 (20%)
2	SO4	A	2021	-	4,4,4	0.64	0	6,6,6	0.63	0
5	GOL	A	2029	-	5,5,5	0.60	0	5,5,5	0.65	0
2	SO4	A	2013	-	4,4,4	0.19	0	6,6,6	0.56	0
2	SO4	A	2004	-	4,4,4	0.49	0	6,6,6	0.73	0
5	GOL	A	2034	-	5,5,5	0.72	0	5,5,5	1.59	2 (40%)
2	SO4	A	2012	-	4,4,4	0.24	0	6,6,6	1.00	0
2	SO4	A	2011	-	4,4,4	0.76	0	6,6,6	1.00	0
2	SO4	A	2022	-	4,4,4	0.49	0	6,6,6	0.81	0
5	GOL	A	2030	-	5,5,5	1.36	0	5,5,5	1.17	0
5	GOL	A	2031	-	5,5,5	0.81	0	5,5,5	1.54	1 (20%)
5	GOL	A	2033	-	5,5,5	1.22	0	5,5,5	1.23	0
5	GOL	A	2032	-	5,5,5	0.34	0	5,5,5	1.71	1 (20%)
2	SO4	A	2020	-	4,4,4	0.67	0	6,6,6	0.58	0
5	GOL	A	2027	-	5,5,5	0.73	0	5,5,5	0.95	0
2	SO4	A	2035	-	4,4,4	0.53	0	6,6,6	1.33	1 (16%)
4	ADP	A	2008	3	24,29,29	0.80	0	29,45,45	1.21	5 (17%)
2	SO4	A	2010	-	4,4,4	0.36	0	6,6,6	0.50	0
5	GOL	A	2026	-	5,5,5	1.36	0	5,5,5	1.18	0
2	SO4	A	2019	-	4,4,4	0.45	0	6,6,6	0.80	0
6	EDO	A	2038	-	3,3,3	0.39	0	2,2,2	0.73	0
2	SO4	A	2036	-	4,4,4	0.35	0	6,6,6	0.75	0
2	SO4	A	2017	-	4,4,4	0.27	0	6,6,6	0.58	0
2	SO4	A	2009	-	4,4,4	0.52	0	6,6,6	0.76	0
2	SO4	A	2003	-	4,4,4	0.37	0	6,6,6	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	2025	-	4,4,4	0.52	0	6,6,6	0.70	0
2	SO4	A	2015	-	4,4,4	0.40	0	6,6,6	0.61	0
2	SO4	A	2016	-	4,4,4	0.55	0	6,6,6	0.80	0
2	SO4	A	2023	-	4,4,4	0.45	0	6,6,6	0.27	0
6	EDO	A	2037	-	3,3,3	0.53	0	2,2,2	0.37	0
2	SO4	A	2001	-	4,4,4	0.51	0	6,6,6	0.37	0
2	SO4	A	2024	-	4,4,4	0.46	0	6,6,6	0.33	0
2	SO4	A	2002	-	4,4,4	1.02	0	6,6,6	1.29	1 (16%)
2	SO4	A	2018	-	4,4,4	0.37	0	6,6,6	0.65	0

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	GOL	A	2028	-	-	3/4/4/4	-
5	GOL	A	2026	-	-	1/4/4/4	-
6	EDO	A	2038	-	-	1/1/1/1	-
5	GOL	A	2029	-	-	4/4/4/4	-
5	GOL	A	2032	-	-	2/4/4/4	-
5	GOL	A	2034	-	-	2/4/4/4	-
5	GOL	A	2027	-	-	2/4/4/4	-
6	EDO	A	2037	-	-	0/1/1/1	-
4	ADP	A	2008	3	-	2/12/32/32	0/3/3/3
5	GOL	A	2030	-	-	3/4/4/4	-
5	GOL	A	2031	-	-	3/4/4/4	-
5	GOL	A	2033	-	-	0/4/4/4	-

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2032	GOL	O3-C3-C2	-3.08	95.44	110.20
2	A	2002	SO4	O4-S-O1	2.76	123.73	109.31
2	A	2035	SO4	O3-S-O1	2.57	122.70	109.31
5	A	2028	GOL	O2-C2-C3	2.53	120.27	109.12
5	A	2031	GOL	O2-C2-C3	2.50	120.14	109.12
4	A	2008	ADP	N6-C6-N1	2.46	123.67	118.57
4	A	2008	ADP	O2A-PA-O1A	2.40	124.13	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2008	ADP	PA-O3A-PB	-2.40	124.61	132.83
4	A	2008	ADP	C5-C6-N6	-2.38	116.74	120.35
5	A	2034	GOL	O2-C2-C3	-2.36	98.74	109.12
5	A	2034	GOL	C3-C2-C1	2.28	120.58	111.70
4	A	2008	ADP	O3B-PB-O2B	2.20	116.04	107.64

There are no chirality outliers.

All (23) torsion outliers are listed below:

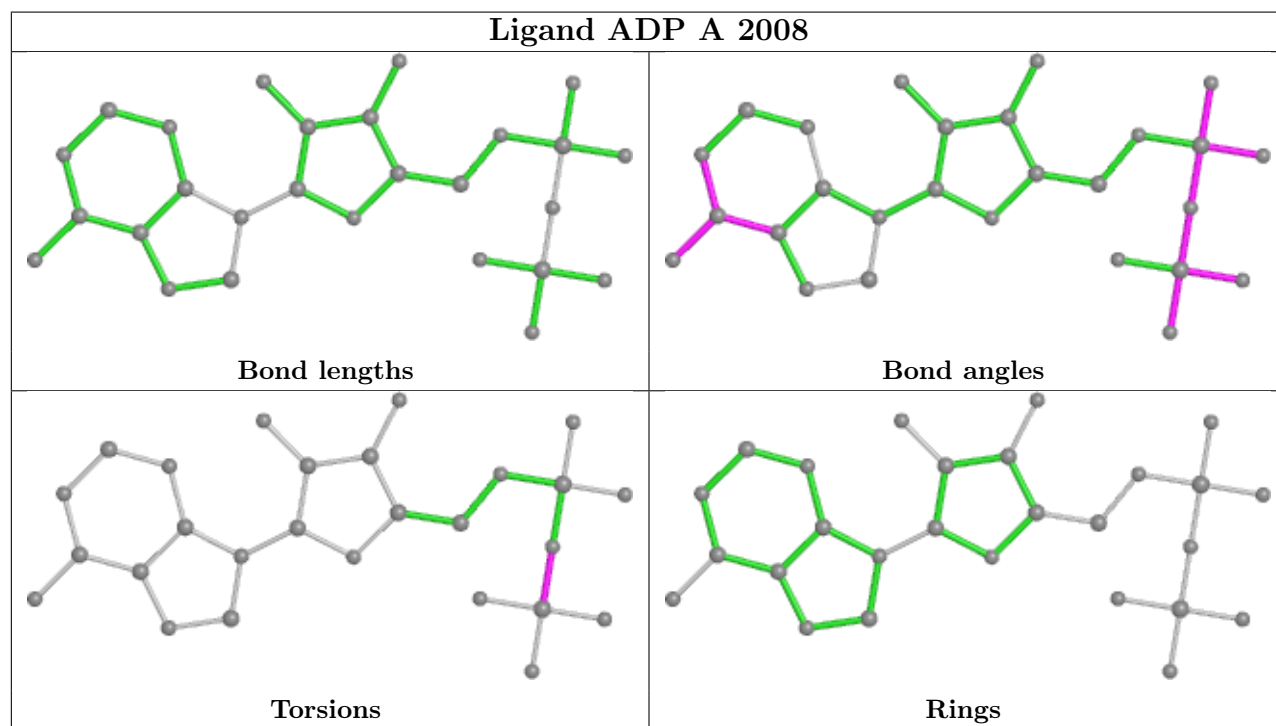
Mol	Chain	Res	Type	Atoms
4	A	2008	ADP	PA-O3A-PB-O2B
5	A	2028	GOL	C1-C2-C3-O3
5	A	2029	GOL	O1-C1-C2-C3
5	A	2030	GOL	O1-C1-C2-C3
5	A	2030	GOL	C1-C2-C3-O3
5	A	2031	GOL	O1-C1-C2-C3
5	A	2031	GOL	C1-C2-C3-O3
5	A	2032	GOL	C1-C2-C3-O3
5	A	2034	GOL	C1-C2-C3-O3
6	A	2038	EDO	O1-C1-C2-O2
5	A	2028	GOL	O2-C2-C3-O3
5	A	2029	GOL	O2-C2-C3-O3
5	A	2027	GOL	C1-C2-C3-O3
5	A	2029	GOL	C1-C2-C3-O3
5	A	2027	GOL	O2-C2-C3-O3
5	A	2029	GOL	O1-C1-C2-O2
5	A	2030	GOL	O2-C2-C3-O3
5	A	2031	GOL	O2-C2-C3-O3
5	A	2034	GOL	O2-C2-C3-O3
4	A	2008	ADP	PA-O3A-PB-O3B
5	A	2032	GOL	O2-C2-C3-O3
5	A	2028	GOL	O1-C1-C2-C3
5	A	2026	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2031	GOL	1	0
4	A	2008	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 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.



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1287/1304 (98%)	-0.39	26 (2%) 65 69	18, 26, 48, 76	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	118	THR	4.7
1	A	788	GLY	4.5
1	A	789	ASN	4.1
1	A	608	LYS	3.7
1	A	152	HIS	3.6
1	A	786	GLN	3.5
1	A	609	THR	3.2
1	A	117	SER	3.2
1	A	119	LEU	3.1
1	A	176	LEU	3.0
1	A	465	LEU	3.0
1	A	610	PRO	3.0
1	A	25	ALA	2.9
1	A	121	ALA	2.9
1	A	-1	SER	2.9
1	A	790	GLU	2.6
1	A	969	ASN	2.5
1	A	154	GLN	2.5
1	A	122	GLU	2.3
1	A	791	GLN	2.3
1	A	120	THR	2.3
1	A	611	LYS	2.3
1	A	787	GLU	2.3
1	A	-2	GLY	2.2
1	A	27	ASN	2.0
1	A	970	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
1	CYG	A	1135	15/16	0.97	0.09	21,25,37,38	0

## 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	2030	6/6	0.64	0.18	46,53,56,57	0
6	EDO	A	2038	4/4	0.68	0.21	51,55,61,65	0
5	GOL	A	2033	6/6	0.69	0.22	46,49,56,58	0
5	GOL	A	2032	6/6	0.76	0.25	43,52,58,61	0
5	GOL	A	2029	6/6	0.81	0.17	45,49,53,54	0
2	SO4	A	2001	5/5	0.82	0.25	94,94,104,106	0
5	GOL	A	2034	6/6	0.86	0.14	45,51,53,55	0
5	GOL	A	2028	6/6	0.87	0.15	30,43,46,47	0
6	EDO	A	2037	4/4	0.89	0.28	47,51,53,56	0
5	GOL	A	2031	6/6	0.89	0.20	43,52,58,59	0
5	GOL	A	2026	6/6	0.90	0.10	24,34,36,37	0
2	SO4	A	2036	5/5	0.91	0.33	82,82,93,104	0
2	SO4	A	2025	5/5	0.92	0.21	59,60,70,81	0
2	SO4	A	2022	5/5	0.92	0.28	64,75,77,79	0
2	SO4	A	2018	5/5	0.93	0.23	70,71,76,82	0
2	SO4	A	2024	5/5	0.93	0.42	86,87,95,96	0
2	SO4	A	2021	5/5	0.94	0.21	55,60,69,69	0
2	SO4	A	2023	5/5	0.95	0.38	67,74,79,81	0
2	SO4	A	2019	5/5	0.95	0.18	54,56,59,67	0
2	SO4	A	2014	5/5	0.96	0.21	34,35,47,58	0
2	SO4	A	2020	5/5	0.97	0.26	50,59,63,67	0

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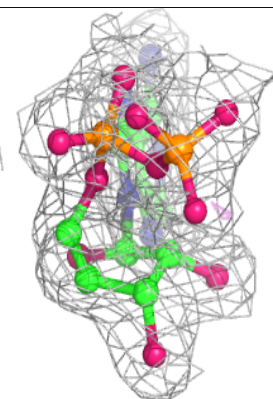
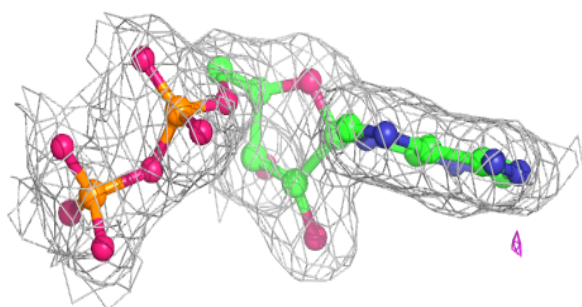
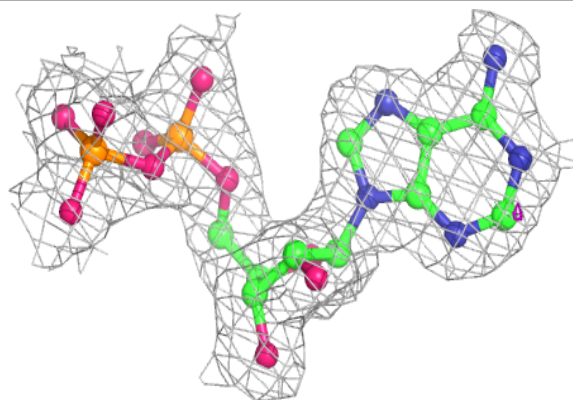
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	2035	5/5	0.97	0.17	42,45,47,48	0
2	SO4	A	2016	5/5	0.97	0.12	40,50,55,58	0
2	SO4	A	2017	5/5	0.97	0.24	54,57,63,66	0
5	GOL	A	2027	6/6	0.97	0.13	24,31,33,42	0
2	SO4	A	2004	5/5	0.97	0.10	47,51,52,55	0
2	SO4	A	2015	5/5	0.97	0.25	36,46,51,52	0
2	SO4	A	2013	5/5	0.98	0.17	46,50,54,64	0
2	SO4	A	2002	5/5	0.98	0.06	28,32,40,41	0
2	SO4	A	2011	5/5	0.99	0.09	28,34,38,38	0
2	SO4	A	2012	5/5	0.99	0.10	36,39,46,47	0
3	MG	A	2006	1/1	0.99	0.11	21,21,21,21	0
3	MG	A	2007	1/1	0.99	0.09	19,19,19,19	0
4	ADP	A	2008	27/27	0.99	0.09	17,20,22,23	0
2	SO4	A	2003	5/5	0.99	0.07	35,39,42,48	0
2	SO4	A	2009	5/5	0.99	0.06	27,31,34,36	0
2	SO4	A	2010	5/5	0.99	0.06	33,36,43,44	0
3	MG	A	2005	1/1	1.00	0.07	18,18,18,18	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 2008:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.