



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2022 – 06:13 PM JST

PDB ID : 6LYO  
Title : Crystal Structure of H296A mutant of Formylglycinamidase Synthetase  
Authors : Sharma, N.; Tanwar, A.S.; Anand, R.  
Deposited on : 2020-02-15  
Resolution : 1.87 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

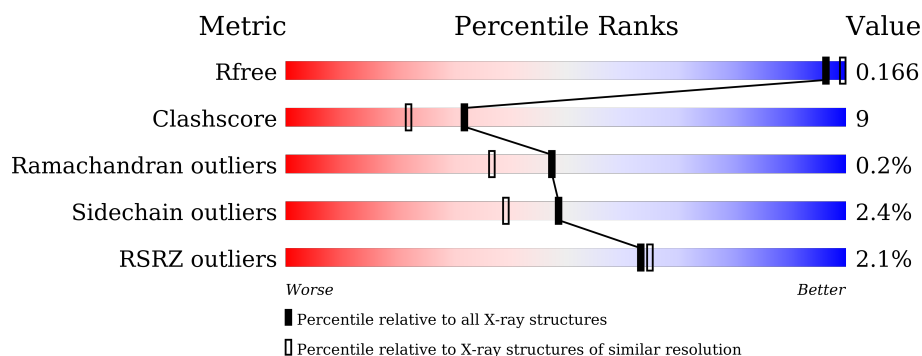
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.87 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	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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>86%</div> <div>12%</div> <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
3	GOL	A	1307	-	-	X	-
3	GOL	A	1311	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	1312	-	X	-	-
3	GOL	A	1313	-	-	X	-
3	GOL	A	1314	-	X	X	-
3	GOL	A	1324	-	-	X	-
3	GOL	A	1325	-	-	X	-
3	GOL	A	1335	-	-	X	-
3	GOL	A	1337	-	-	X	-
3	GOL	A	1339	-	-	X	-
5	SO4	A	1357	-	-	-	X
5	SO4	A	1358	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11690 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.

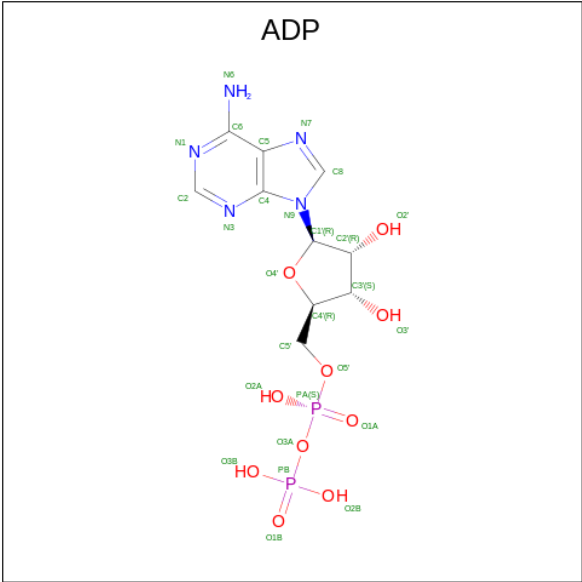
- Molecule 1 is a protein called Phosphoribosylformylglycinamide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1289	Total	C	N	O	S	0	43	0
			10155	6391	1791	1922	51			

There are 10 discrepancies between the modelled and reference sequences:

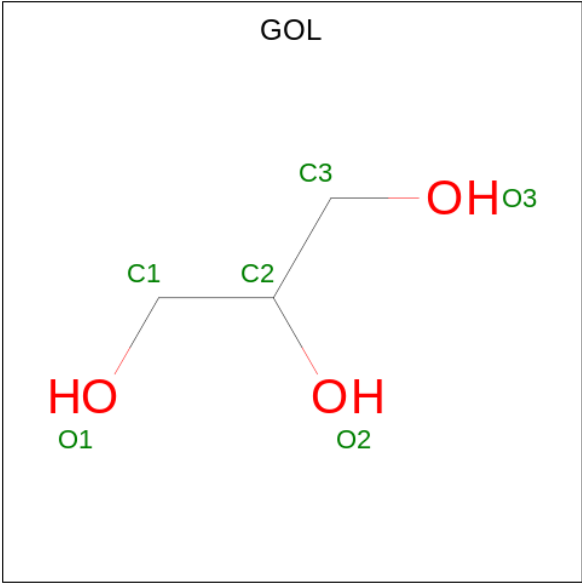
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	SER	-	expression tag	UNP P74881
A	-7	GLY	-	expression tag	UNP P74881
A	-6	LEU	-	expression tag	UNP P74881
A	-5	VAL	-	expression tag	UNP P74881
A	-4	PRO	-	expression tag	UNP P74881
A	-3	ARG	-	expression tag	UNP P74881
A	-2	GLY	-	expression tag	UNP P74881
A	-1	SER	-	expression tag	UNP P74881
A	0	HIS	-	expression tag	UNP P74881
A	296	ALA	HIS	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 GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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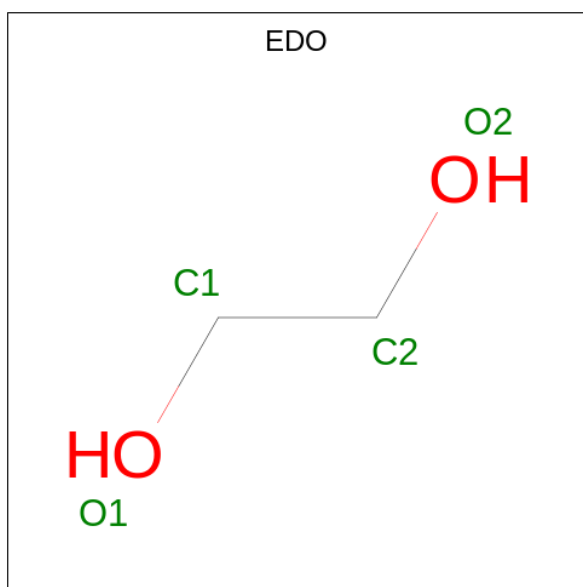
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total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

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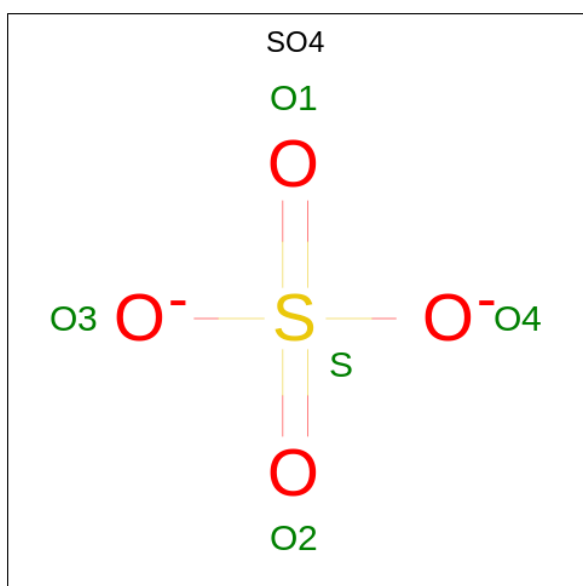
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

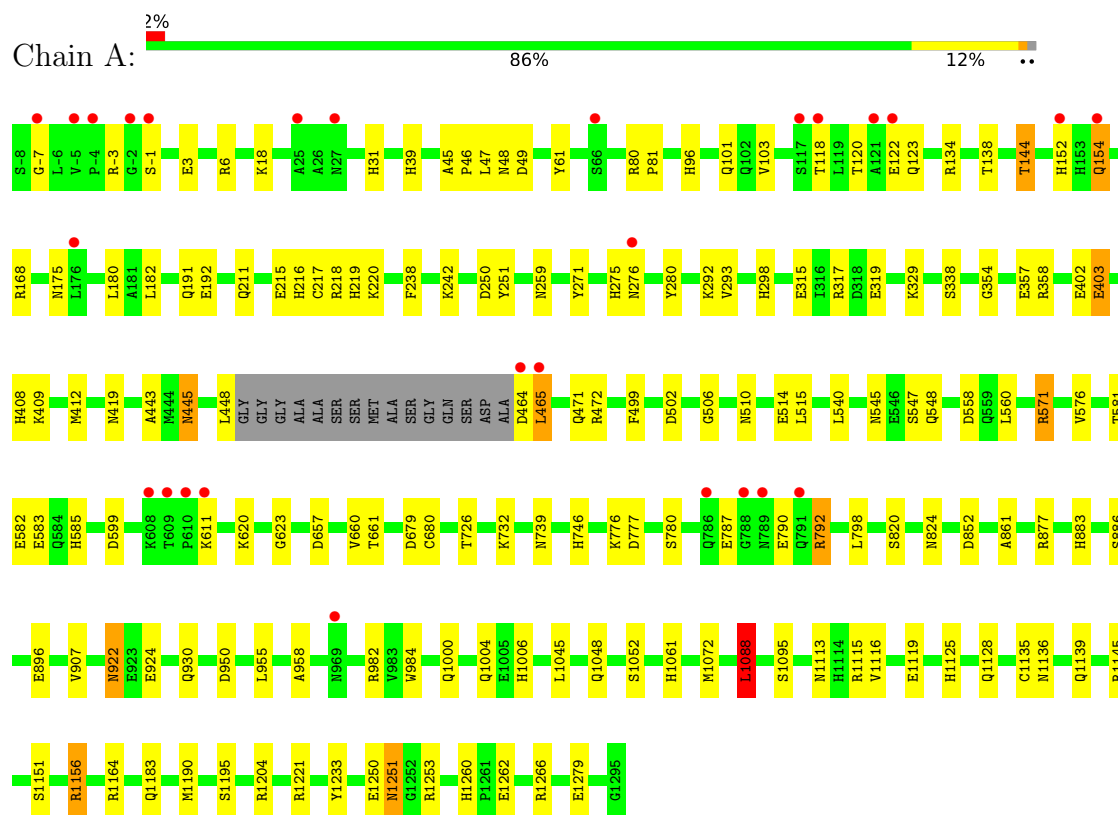
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1175	Total	O	0	0
			1175	1175		

### 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: Phosphoribosylformylglycinamide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.29Å 146.29Å 140.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.88 – 1.87 31.45 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.88-1.87) 99.7 (31.45-1.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.79 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.125 , 0.158 0.139 , 0.166	Depositor DCC
$R_{free}$ test set	6697 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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

### 5.1 Standard geometry

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

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	1.08	6/10462 (0.1%)	1.01	11/14202 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1119	GLU	CD-OE2	-7.08	1.17	1.25
1	A	403	GLU	CD-OE1	-6.96	1.18	1.25
1	A	1119	GLU	CD-OE1	-5.45	1.19	1.25
1	A	1250	GLU	CD-OE2	-5.27	1.19	1.25
1	A	1088[A]	LEU	CA-C	5.17	1.66	1.52
1	A	1088[B]	LEU	CA-C	5.17	1.66	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	A	1156	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	A	6	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	A	502	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	358	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	792	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	1088[A]	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	1088[B]	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	358	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	1266	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	558	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10155	0	10027	163	0
2	A	27	0	12	0	0
3	A	222	0	292	75	0
4	A	8	0	12	1	0
5	A	100	0	0	1	0
6	A	3	0	0	0	0
7	A	1175	0	0	54	0
All	All	11690	0	10343	185	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 9.

All (185) 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:950:ASP:HB3	3:A:1339:GOL:O1	1.50	1.08
1:A:192:GLU:OE2	3:A:1331:GOL:H12	1.52	1.08
1:A:402:GLU:HG2	7:A:2375:HOH:O	1.54	1.06
1:A:251:TYR:H	3:A:1313:GOL:H12	1.20	1.02
3:A:1332:GOL:H12	7:A:2275:HOH:O	1.63	0.98
1:A:950:ASP:HA	3:A:1339:GOL:H11	1.46	0.96
1:A:1145:ARG:HH12	3:A:1325:GOL:H11	1.27	0.95
1:A:49:ASP:H	3:A:1335:GOL:H31	1.34	0.93
1:A:1253:ARG:HH21	3:A:1311:GOL:H12	1.36	0.90
1:A:251:TYR:H	3:A:1313:GOL:C1	1.87	0.87
1:A:409:LYS:NZ	3:A:1324:GOL:H12	1.90	0.86
1:A:-1:SER:HA	7:A:2396:HOH:O	1.75	0.85
1:A:1052:SER:HB3	7:A:1555:HOH:O	1.79	0.82
1:A:776:LYS:HE3	3:A:1329:GOL:O2	1.80	0.81
1:A:820:SER:H	1:A:930:GLN:HE22	1.29	0.80
1:A:824:ASN:HD21	1:A:958:ALA:H	1.28	0.78
1:A:583:GLU:H	3:A:1307:GOL:H32	1.49	0.77
1:A:49:ASP:H	3:A:1335:GOL:C3	1.97	0.77
1:A:298:HIS:CD2	3:A:1324:GOL:H11	2.20	0.77
1:A:215:GLU:HA	7:A:1415:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:HD21	1:A:182:LEU:H	1.33	0.76
1:A:877[B]:ARG:HH11	1:A:877[B]:ARG:HG3	1.51	0.75
3:A:1308:GOL:H32	7:A:1820:HOH:O	1.87	0.75
1:A:1113:ASN:HD22	1:A:1116:VAL:H	1.36	0.74
1:A:96:HIS:HE1	1:A:103:VAL:O	1.72	0.73
1:A:679:ASP:OD2	1:A:883:HIS:HD2	1.74	0.71
3:A:1337:GOL:H2	7:A:1550:HOH:O	1.91	0.71
1:A:39:HIS:HE1	1:A:61:TYR:OH	1.74	0.71
1:A:1145:ARG:HH12	3:A:1325:GOL:C1	2.03	0.71
1:A:680:CYS:SG	1:A:726[B]:THR:HG21	2.31	0.70
1:A:1253:ARG:HH21	3:A:1311:GOL:C1	2.03	0.70
1:A:583:GLU:H	3:A:1307:GOL:C3	2.04	0.70
1:A:582:GLU:H	3:A:1307:GOL:C1	2.05	0.69
1:A:582:GLU:H	3:A:1307:GOL:H12	1.56	0.69
1:A:175:ASN:HD22	1:A:180:LEU:HB2	1.56	0.69
1:A:1145:ARG:HB3	7:A:2113:HOH:O	1.93	0.68
1:A:409:LYS:HZ2	3:A:1324:GOL:H12	1.58	0.68
1:A:403:GLU:OE1	1:A:746:HIS:HE1	1.77	0.68
1:A:1000:GLN:NE2	7:A:1402:HOH:O	2.25	0.68
1:A:1128:GLN:HG3	7:A:2445:HOH:O	1.94	0.68
1:A:657[B]:ASP:OD2	1:A:660:VAL:HG12	1.95	0.67
1:A:409:LYS:HZ1	3:A:1324:GOL:H12	1.57	0.67
1:A:545:ASN:HD22	1:A:547:SER:H	1.44	0.66
1:A:877[B]:ARG:HG3	1:A:877[B]:ARG:NH1	2.11	0.66
1:A:922:ASN:HD22	1:A:924:GLU:H	1.42	0.66
3:A:1309:GOL:O2	3:A:1337:GOL:H32	1.97	0.65
3:A:1314:GOL:H11	7:A:1419:HOH:O	1.96	0.65
3:A:1329:GOL:H31	7:A:1871:HOH:O	1.97	0.63
1:A:950:ASP:HA	3:A:1339:GOL:C1	2.27	0.63
1:A:49:ASP:N	3:A:1335:GOL:H31	2.11	0.63
1:A:329:LYS:HG3	7:A:1479:HOH:O	2.00	0.62
1:A:571:ARG:HA	3:A:1317:GOL:H12	1.81	0.62
1:A:787:GLU:HB2	1:A:792:ARG:HG3	1.80	0.61
3:A:1308:GOL:C3	7:A:1820:HOH:O	2.44	0.61
1:A:950:ASP:CA	3:A:1339:GOL:H11	2.26	0.61
1:A:1260:HIS:HD2	1:A:1262:GLU:OE2	1.83	0.61
1:A:883:HIS:HE1	1:A:896:GLU:OE1	1.84	0.60
1:A:219:HIS:N	7:A:1415:HOH:O	2.34	0.60
1:A:276:ASN:HB2	7:A:1575:HOH:O	2.01	0.60
1:A:1145:ARG:HH22	3:A:1325:GOL:H2	1.66	0.60
1:A:251:TYR:N	3:A:1313:GOL:H12	2.05	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:ALA:HB3	7:A:2009:HOH:O	2.02	0.60
1:A:238:PHE:CZ	1:A:242:LYS:HE3	2.37	0.59
3:A:1314:GOL:H32	7:A:2406:HOH:O	2.01	0.59
1:A:219:HIS:HE1	7:A:1421:HOH:O	1.86	0.59
1:A:732:LYS:HD2	7:A:1975:HOH:O	2.01	0.58
1:A:154:GLN:HE21	1:A:154:GLN:HA	1.69	0.58
1:A:1145:ARG:NH1	3:A:1325:GOL:H11	2.10	0.58
1:A:1221:ARG:HE	3:A:1314:GOL:H12	1.70	0.57
1:A:409:LYS:HZ2	3:A:1324:GOL:C1	2.17	0.57
1:A:787:GLU:CB	1:A:792:ARG:HG3	2.34	0.57
3:A:1334:GOL:C3	7:A:2425:HOH:O	2.52	0.57
1:A:1251:ASN:HB3	3:A:1311:GOL:H31	1.85	0.57
1:A:582:GLU:N	3:A:1307:GOL:H32	2.18	0.57
1:A:275:HIS:HD2	7:A:2489:HOH:O	1.88	0.57
1:A:80:ARG:HA	1:A:138[B]:THR:HG23	1.87	0.56
3:A:1326:GOL:H11	7:A:2395:HOH:O	2.05	0.56
1:A:-7:GLY:O	1:A:3:GLU:HA	2.06	0.56
1:A:219:HIS:N	7:A:1416:HOH:O	2.37	0.56
1:A:354:GLY:O	1:A:408:HIS:HE1	1.89	0.56
1:A:780:SER:OG	3:A:1324:GOL:H32	2.05	0.56
1:A:445:ASN:ND2	1:A:448[A]:LEU:HD12	2.20	0.55
1:A:1251:ASN:HD22	1:A:1253:ARG:H	1.53	0.55
1:A:402:GLU:CG	7:A:2375:HOH:O	2.32	0.55
3:A:1332:GOL:H32	7:A:1556:HOH:O	2.06	0.55
1:A:471:GLN:HE21	1:A:472:ARG:H	1.52	0.55
1:A:499:PHE:CD2	1:A:515[B]:LEU:CD1	2.90	0.55
1:A:216:HIS:HD2	7:A:1819:HOH:O	1.89	0.54
1:A:1045[B]:LEU:HD11	1:A:1088[B]:LEU:HD13	1.89	0.54
1:A:238:PHE:CE2	1:A:242:LYS:HE3	2.43	0.54
1:A:1045[B]:LEU:CD1	1:A:1088[B]:LEU:HD13	2.37	0.54
1:A:907[B]:VAL:HG23	1:A:955:LEU:HB3	1.89	0.54
1:A:1183:GLN:HG3	7:A:2546:HOH:O	2.08	0.54
1:A:950:ASP:CB	3:A:1339:GOL:O1	2.41	0.54
1:A:219:HIS:HD2	1:A:777:ASP:OD1	1.91	0.54
1:A:1125:HIS:NE2	3:A:1333:GOL:H31	2.24	0.53
1:A:218[B]:ARG:HD3	1:A:220:LYS:HE3	1.90	0.53
1:A:-7:GLY:O	1:A:3:GLU:HG3	2.09	0.53
1:A:1251:ASN:ND2	1:A:1253:ARG:H	2.07	0.53
1:A:1204:ARG:HH11	3:A:1325:GOL:C2	2.22	0.53
1:A:576:VAL:HG12	3:A:1323:GOL:H32	1.91	0.52
3:A:1334:GOL:H32	7:A:2425:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:HB2	3:A:1335:GOL:H31	1.92	0.51
1:A:134:ARG:HD2	1:A:464:ASP:N	2.25	0.51
1:A:499:PHE:CD2	1:A:515[B]:LEU:HD12	2.45	0.51
1:A:1006:HIS:HD2	7:A:1900:HOH:O	1.93	0.51
1:A:585:HIS:HE1	1:A:599:ASP:OD1	1.94	0.51
1:A:317:ARG:HH22	1:A:548:GLN:NE2	2.09	0.50
1:A:298:HIS:CG	3:A:1324:GOL:H11	2.46	0.50
1:A:1004:GLN:NE2	1:A:1233:TYR:H	2.10	0.50
1:A:1253:ARG:NH2	3:A:1311:GOL:H12	2.17	0.50
1:A:746:HIS:HD2	3:A:1312:GOL:O2	1.94	0.50
1:A:510[A]:ASN:OD1	1:A:514:GLU:OE2	2.30	0.49
1:A:219:HIS:CD2	1:A:777:ASP:OD1	2.65	0.49
1:A:317:ARG:HH22	1:A:548:GLN:HE22	1.60	0.49
1:A:292[B]:LYS:HZ1	3:A:1329:GOL:H32	1.77	0.49
1:A:950:ASP:HB3	3:A:1339:GOL:C1	2.39	0.49
3:A:1326:GOL:C1	7:A:2395:HOH:O	2.61	0.49
1:A:144[B]:THR:OG1	7:A:1401:HOH:O	2.20	0.49
3:A:1334:GOL:H31	7:A:2425:HOH:O	2.10	0.49
1:A:293:VAL:HB	1:A:739:ASN:HD21	1.78	0.49
3:A:1335:GOL:H11	7:A:2292:HOH:O	2.13	0.48
1:A:329:LYS:NZ	1:A:419:ASN:HD21	2.12	0.48
1:A:861:ALA:N	3:A:1308:GOL:O3	2.43	0.48
3:A:1321:GOL:H2	7:A:1880:HOH:O	2.13	0.48
1:A:218[A]:ARG:N	7:A:1416:HOH:O	2.47	0.48
1:A:820:SER:N	1:A:930:GLN:HE22	2.07	0.48
1:A:211[B]:GLN:CD	1:A:506:GLY:HA2	2.35	0.47
1:A:581:THR:HA	3:A:1307:GOL:H12	1.95	0.46
3:A:1314:GOL:C3	7:A:2406:HOH:O	2.62	0.46
1:A:1113:ASN:ND2	1:A:1116:VAL:H	2.09	0.46
1:A:81:PRO:HD3	1:A:138[A]:THR:HG21	1.97	0.46
1:A:798:LEU:HD13	7:A:1924:HOH:O	2.14	0.46
1:A:1145:ARG:HD2	1:A:1151:SER:O	2.16	0.46
3:A:1313:GOL:H11	7:A:2118:HOH:O	2.14	0.46
1:A:39:HIS:HD2	7:A:1776:HOH:O	1.99	0.46
1:A:217[A]:CYS:C	7:A:1416:HOH:O	2.53	0.45
1:A:1006:HIS:HE1	7:A:1892:HOH:O	1.98	0.45
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.19	0.45
1:A:623:GLY:HA3	1:A:852[B]:ASP:HA	1.98	0.45
1:A:338:SER:OG	1:A:408:HIS:HD2	1.99	0.45
1:A:271:TYR:CZ	1:A:280:TYR:HB3	2.51	0.45
1:A:583:GLU:N	3:A:1307:GOL:H32	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:HIS:CD2	7:A:2316:HOH:O	2.69	0.45
1:A:582:GLU:N	3:A:1307:GOL:H12	2.27	0.45
1:A:31:HIS:HB2	4:A:1340:EDO:O2	2.17	0.44
1:A:984:TRP:HE1	3:A:1332:GOL:H32	1.82	0.44
1:A:329:LYS:CG	7:A:1479:HOH:O	2.60	0.44
1:A:1260:HIS:HE1	7:A:1870:HOH:O	2.00	0.44
1:A:217[B]:CYS:C	7:A:1416:HOH:O	2.54	0.44
1:A:298:HIS:CD2	3:A:1324:GOL:C1	2.96	0.44
1:A:1072[B]:MET:HA	1:A:1072[B]:MET:HE2	2.00	0.44
1:A:448[B]:LEU:HD23	1:A:448[B]:LEU:HA	1.75	0.44
1:A:571:ARG:HA	3:A:1317:GOL:C1	2.46	0.44
1:A:154:GLN:HG2	3:A:1310:GOL:O2	2.17	0.44
1:A:1113:ASN:HD21	1:A:1115:ARG:HB3	1.82	0.44
1:A:540:LEU:C	1:A:540:LEU:HD23	2.38	0.43
1:A:39:HIS:CE1	1:A:61:TYR:OH	2.63	0.43
1:A:120:THR:H	1:A:123:GLN:HE21	1.66	0.43
1:A:216:HIS:HE1	5:A:1351:SO4:O1	2.01	0.43
3:A:1311:GOL:H11	7:A:1764:HOH:O	2.18	0.43
1:A:950:ASP:CA	3:A:1339:GOL:C1	2.95	0.43
3:A:1335:GOL:C1	7:A:2292:HOH:O	2.67	0.43
1:A:1061:HIS:HD2	7:A:1886:HOH:O	2.01	0.43
1:A:443:ALA:HB2	7:A:1518:HOH:O	2.18	0.43
3:A:1309:GOL:C1	3:A:1337:GOL:H32	2.49	0.42
1:A:1136:ASN:HA	1:A:1139:GLN:OE1	2.20	0.42
1:A:80:ARG:HA	1:A:81:PRO:HD3	1.99	0.42
1:A:218[A]:ARG:O	1:A:218[A]:ARG:CG	2.66	0.42
1:A:315:GLU:OE2	1:A:319:GLU:OE2	2.37	0.42
1:A:680:CYS:SG	1:A:726[B]:THR:CG2	3.06	0.42
1:A:1048:GLN:O	1:A:1095:SER:HA	2.18	0.42
1:A:1164:ARG:HD3	7:A:1471:HOH:O	2.18	0.41
1:A:45:ALA:HB1	1:A:46:PRO:HD2	2.02	0.41
1:A:218[B]:ARG:HD3	1:A:220:LYS:CE	2.51	0.41
1:A:585:HIS:HD2	7:A:2346:HOH:O	2.04	0.41
3:A:1309:GOL:C2	3:A:1337:GOL:H32	2.50	0.41
1:A:877[B]:ARG:NH1	7:A:1405:HOH:O	2.27	0.41
1:A:1156:ARG:HG3	3:A:1325:GOL:H12	2.03	0.41
1:A:168:ARG:HG3	1:A:191[B]:GLN:NE2	2.36	0.41
1:A:357:GLU:HB3	7:A:2239:HOH:O	2.20	0.41
1:A:576:VAL:CG1	3:A:1323:GOL:H32	2.50	0.41
1:A:545:ASN:ND2	1:A:547:SER:H	2.17	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1326/1304 (102%)	1289 (97%)	34 (3%)	3 (0%)	47	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	465	LEU
1	A	661	THR
1	A	886	SER

### 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	1072/1040 (103%)	1043 (97%)	29 (3%)	44	34

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	ARG
1	A	18	LYS
1	A	47	LEU
1	A	101	GLN
1	A	118	THR
1	A	122	GLU
1	A	144[A]	THR
1	A	144[B]	THR

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Mol	Chain	Res	Type
1	A	154	GLN
1	A	250	ASP
1	A	259[A]	ASN
1	A	259[B]	ASN
1	A	412	MET
1	A	445	ASN
1	A	465	LEU
1	A	560	LEU
1	A	571	ARG
1	A	611	LYS
1	A	620	LYS
1	A	790	GLU
1	A	922	ASN
1	A	982	ARG
1	A	1088[A]	LEU
1	A	1088[B]	LEU
1	A	1190	MET
1	A	1195	SER
1	A	1251	ASN
1	A	1279[A]	GLU
1	A	1279[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	96	HIS
1	A	101	GLN
1	A	123	GLN
1	A	154	GLN
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	298	HIS
1	A	408	HIS
1	A	419	ASN
1	A	445	ASN
1	A	471	GLN
1	A	545	ASN

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Mol	Chain	Res	Type
1	A	548	GLN
1	A	585	HIS
1	A	674	GLN
1	A	739	ASN
1	A	746	HIS
1	A	786	GLN
1	A	791	GLN
1	A	818	GLN
1	A	824	ASN
1	A	883	HIS
1	A	922	ASN
1	A	930	GLN
1	A	993	GLN
1	A	1004	GLN
1	A	1006	HIS
1	A	1018	ASN
1	A	1026	ASN
1	A	1061	HIS
1	A	1113	ASN
1	A	1189	GLN
1	A	1251	ASN
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	2.29	4 (44%)	6,17,19	4.66	4 (66%)

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	-	0/10/16/18	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1135	CYG	CG1-CD1	4.72	1.55	1.50
1	A	1135	CYG	OE2-CD1	3.20	1.26	1.21
1	A	1135	CYG	CD1-SG	2.90	1.83	1.76
1	A	1135	CYG	CB-CA	-2.00	1.48	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1135	CYG	OE2-CD1-CG1	-8.57	113.86	123.99
1	A	1135	CYG	CG1-CD1-SG	5.09	119.38	113.46
1	A	1135	CYG	CB1-CG1-CD1	-4.67	101.98	112.33
1	A	1135	CYG	OE2-CD1-SG	2.78	126.23	122.61

There are no chirality outliers.

There are no torsion outliers.

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 63 ligands modelled in this entry, 3 are monoatomic - leaving 60 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	$\# Z  > 2$
3	GOL	A	1327	-	5,5,5	0.36	0	5,5,5	0.36	0
3	GOL	A	1318	-	5,5,5	0.71	0	5,5,5	0.74	0
5	SO4	A	1353	-	4,4,4	0.39	0	6,6,6	0.35	0
3	GOL	A	1309	-	5,5,5	0.68	0	5,5,5	0.91	0
3	GOL	A	1303	-	5,5,5	0.51	0	5,5,5	1.25	0
5	SO4	A	1346	-	4,4,4	0.95	0	6,6,6	1.59	1 (16%)
5	SO4	A	1352	-	4,4,4	0.80	0	6,6,6	0.33	0
5	SO4	A	1348	-	4,4,4	0.33	0	6,6,6	0.43	0
3	GOL	A	1306	-	5,5,5	0.99	0	5,5,5	0.80	0
3	GOL	A	1325	-	5,5,5	0.52	0	5,5,5	0.98	0
3	GOL	A	1322	-	5,5,5	0.54	0	5,5,5	1.15	1 (20%)
5	SO4	A	1345	-	4,4,4	0.19	0	6,6,6	0.66	0
4	EDO	A	1340	-	3,3,3	0.40	0	2,2,2	0.32	0
4	EDO	A	1338	-	3,3,3	0.29	0	2,2,2	0.96	0
3	GOL	A	1317	-	5,5,5	0.71	0	5,5,5	0.54	0
5	SO4	A	1354	-	4,4,4	0.53	0	6,6,6	0.33	0
3	GOL	A	1331	-	5,5,5	0.43	0	5,5,5	0.34	0
3	GOL	A	1312	-	5,5,5	1.51	1 (20%)	5,5,5	2.30	2 (40%)
3	GOL	A	1334	-	5,5,5	0.41	0	5,5,5	0.96	0
3	GOL	A	1326	-	5,5,5	0.90	0	5,5,5	1.05	0
3	GOL	A	1323	-	5,5,5	0.21	0	5,5,5	0.58	0
5	SO4	A	1351	-	4,4,4	0.77	0	6,6,6	1.31	0
3	GOL	A	1336	-	5,5,5	0.41	0	5,5,5	0.99	0
5	SO4	A	1349	-	4,4,4	0.54	0	6,6,6	0.88	0
3	GOL	A	1319	-	5,5,5	0.57	0	5,5,5	0.57	0
3	GOL	A	1310	-	5,5,5	0.76	0	5,5,5	0.85	0
3	GOL	A	1314	-	5,5,5	1.55	1 (20%)	5,5,5	2.87	2 (40%)
3	GOL	A	1320	-	5,5,5	0.29	0	5,5,5	1.16	1 (20%)
3	GOL	A	1333	-	5,5,5	0.27	0	5,5,5	1.18	0
3	GOL	A	1302	-	5,5,5	0.83	0	5,5,5	0.65	0
2	ADP	A	1301	6	24,29,29	0.98	2 (8%)	29,45,45	1.09	4 (13%)
3	GOL	A	1332	-	5,5,5	0.75	0	5,5,5	1.27	1 (20%)
3	GOL	A	1315	-	5,5,5	0.67	0	5,5,5	1.16	0
3	GOL	A	1339	-	5,5,5	0.29	0	5,5,5	0.97	0
3	GOL	A	1308	-	5,5,5	1.21	1 (20%)	5,5,5	1.42	1 (20%)
3	GOL	A	1305	-	5,5,5	1.05	0	5,5,5	1.62	1 (20%)
3	GOL	A	1329	-	5,5,5	0.36	0	5,5,5	0.51	0
5	SO4	A	1341	-	4,4,4	0.57	0	6,6,6	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	1313	-	5,5,5	0.48	0	5,5,5	0.71	0
3	GOL	A	1321	-	5,5,5	0.85	0	5,5,5	1.18	0
5	SO4	A	1360	-	4,4,4	0.61	0	6,6,6	1.03	0
5	SO4	A	1355	-	4,4,4	0.45	0	6,6,6	0.56	0
5	SO4	A	1357	-	4,4,4	0.54	0	6,6,6	0.27	0
5	SO4	A	1343	-	4,4,4	0.72	0	6,6,6	1.55	2 (33%)
3	GOL	A	1328	-	5,5,5	0.84	0	5,5,5	0.98	0
3	GOL	A	1311	-	5,5,5	0.53	0	5,5,5	1.05	0
5	SO4	A	1342	-	4,4,4	0.39	0	6,6,6	0.84	0
3	GOL	A	1335	-	5,5,5	0.62	0	5,5,5	0.76	0
3	GOL	A	1337	-	5,5,5	0.39	0	5,5,5	0.76	0
3	GOL	A	1307	-	5,5,5	0.47	0	5,5,5	0.57	0
5	SO4	A	1350	-	4,4,4	0.64	0	6,6,6	0.72	0
3	GOL	A	1316	-	5,5,5	0.64	0	5,5,5	1.21	0
3	GOL	A	1330	-	5,5,5	0.68	0	5,5,5	1.19	1 (20%)
5	SO4	A	1356	-	4,4,4	0.58	0	6,6,6	0.48	0
5	SO4	A	1358	-	4,4,4	0.52	0	6,6,6	0.64	0
5	SO4	A	1347	-	4,4,4	1.06	0	6,6,6	1.17	1 (16%)
3	GOL	A	1304	-	5,5,5	1.14	0	5,5,5	1.33	0
5	SO4	A	1359	-	4,4,4	0.47	0	6,6,6	0.28	0
3	GOL	A	1324	-	5,5,5	0.39	0	5,5,5	0.72	0
5	SO4	A	1344	-	4,4,4	0.60	0	6,6,6	1.28	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
3	GOL	A	1327	-	-	0/4/4/4	-
3	GOL	A	1318	-	-	2/4/4/4	-
3	GOL	A	1309	-	-	0/4/4/4	-
3	GOL	A	1303	-	-	2/4/4/4	-
3	GOL	A	1306	-	-	0/4/4/4	-
3	GOL	A	1325	-	-	0/4/4/4	-
3	GOL	A	1322	-	-	2/4/4/4	-
4	EDO	A	1340	-	-	1/1/1/1	-
4	EDO	A	1338	-	-	1/1/1/1	-
3	GOL	A	1317	-	-	2/4/4/4	-
3	GOL	A	1331	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1312	-	-	3/4/4/4	-
3	GOL	A	1334	-	-	4/4/4/4	-
3	GOL	A	1326	-	-	2/4/4/4	-
3	GOL	A	1323	-	-	2/4/4/4	-
3	GOL	A	1336	-	-	1/4/4/4	-
3	GOL	A	1319	-	-	0/4/4/4	-
3	GOL	A	1310	-	-	2/4/4/4	-
3	GOL	A	1314	-	-	4/4/4/4	-
3	GOL	A	1320	-	-	2/4/4/4	-
3	GOL	A	1333	-	-	3/4/4/4	-
3	GOL	A	1302	-	-	0/4/4/4	-
2	ADP	A	1301	6	-	2/12/32/32	0/3/3/3
3	GOL	A	1332	-	-	2/4/4/4	-
3	GOL	A	1315	-	-	4/4/4/4	-
3	GOL	A	1339	-	-	2/4/4/4	-
3	GOL	A	1308	-	-	3/4/4/4	-
3	GOL	A	1305	-	-	2/4/4/4	-
3	GOL	A	1329	-	-	0/4/4/4	-
3	GOL	A	1313	-	-	2/4/4/4	-
3	GOL	A	1321	-	-	4/4/4/4	-
3	GOL	A	1328	-	-	4/4/4/4	-
3	GOL	A	1311	-	-	2/4/4/4	-
3	GOL	A	1335	-	-	0/4/4/4	-
3	GOL	A	1337	-	-	3/4/4/4	-
3	GOL	A	1307	-	-	3/4/4/4	-
3	GOL	A	1316	-	-	1/4/4/4	-
3	GOL	A	1330	-	-	2/4/4/4	-
3	GOL	A	1304	-	-	2/4/4/4	-
3	GOL	A	1324	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	ADP	O4'-C1'	2.71	1.44	1.41
2	A	1301	ADP	O3'-C3'	2.48	1.48	1.43
3	A	1312	GOL	O1-C1	2.36	1.52	1.42
3	A	1314	GOL	O3-C3	2.07	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1308	GOL	O1-C1	-2.02	1.33	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1314	GOL	O3-C3-C2	5.64	137.26	110.20
3	A	1312	GOL	O2-C2-C1	4.01	126.77	109.12
5	A	1346	SO4	O3-S-O1	2.87	124.28	109.31
3	A	1305	GOL	O2-C2-C1	-2.58	97.77	109.12
2	A	1301	ADP	O3B-PB-O2B	2.56	117.42	107.64
3	A	1312	GOL	O1-C1-C2	2.56	122.46	110.20
5	A	1344	SO4	O4-S-O1	2.55	122.63	109.31
2	A	1301	ADP	O2A-PA-O1A	2.49	124.53	112.24
3	A	1314	GOL	O1-C1-C2	2.48	122.11	110.20
3	A	1322	GOL	O3-C3-C2	2.42	121.81	110.20
3	A	1330	GOL	O3-C3-C2	2.41	121.76	110.20
3	A	1308	GOL	O2-C2-C3	2.39	119.64	109.12
2	A	1301	ADP	PA-O3A-PB	-2.29	124.98	132.83
5	A	1343	SO4	O3-S-O2	2.28	121.20	109.31
2	A	1301	ADP	N6-C6-N1	2.25	123.25	118.57
5	A	1343	SO4	O3-S-O1	-2.23	97.66	109.31
3	A	1320	GOL	C3-C2-C1	-2.17	103.29	111.70
3	A	1332	GOL	O3-C3-C2	2.13	120.42	110.20
5	A	1347	SO4	O3-S-O1	2.01	119.78	109.31

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	ADP	PA-O3A-PB-O2B
3	A	1307	GOL	C1-C2-C3-O3
3	A	1308	GOL	C1-C2-C3-O3
3	A	1310	GOL	C1-C2-C3-O3
3	A	1311	GOL	O1-C1-C2-C3
3	A	1312	GOL	O1-C1-C2-C3
3	A	1313	GOL	C1-C2-C3-O3
3	A	1314	GOL	O1-C1-C2-O2
3	A	1314	GOL	O1-C1-C2-C3
3	A	1314	GOL	C1-C2-C3-O3
3	A	1314	GOL	O2-C2-C3-O3
3	A	1315	GOL	O1-C1-C2-C3
3	A	1318	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	1320	GOL	C1-C2-C3-O3
3	A	1321	GOL	O1-C1-C2-C3
3	A	1323	GOL	O1-C1-C2-C3
3	A	1324	GOL	O1-C1-C2-C3
3	A	1326	GOL	O1-C1-C2-C3
3	A	1328	GOL	C1-C2-C3-O3
3	A	1331	GOL	O1-C1-C2-O2
3	A	1331	GOL	O1-C1-C2-C3
3	A	1332	GOL	C1-C2-C3-O3
3	A	1333	GOL	O1-C1-C2-C3
3	A	1334	GOL	O1-C1-C2-C3
3	A	1337	GOL	O1-C1-C2-C3
3	A	1339	GOL	O1-C1-C2-O2
3	A	1339	GOL	O1-C1-C2-C3
3	A	1307	GOL	O2-C2-C3-O3
3	A	1310	GOL	O2-C2-C3-O3
3	A	1311	GOL	O1-C1-C2-O2
3	A	1313	GOL	O2-C2-C3-O3
3	A	1318	GOL	O1-C1-C2-O2
3	A	1323	GOL	O1-C1-C2-O2
3	A	1328	GOL	O1-C1-C2-O2
3	A	1333	GOL	O1-C1-C2-O2
3	A	1303	GOL	C1-C2-C3-O3
3	A	1304	GOL	C1-C2-C3-O3
3	A	1305	GOL	O1-C1-C2-C3
3	A	1308	GOL	O1-C1-C2-C3
3	A	1317	GOL	C1-C2-C3-O3
3	A	1321	GOL	C1-C2-C3-O3
3	A	1322	GOL	O1-C1-C2-C3
3	A	1328	GOL	O1-C1-C2-C3
3	A	1330	GOL	O1-C1-C2-C3
3	A	1331	GOL	C1-C2-C3-O3
3	A	1334	GOL	C1-C2-C3-O3
3	A	1336	GOL	O1-C1-C2-C3
3	A	1337	GOL	C1-C2-C3-O3
3	A	1308	GOL	O2-C2-C3-O3
3	A	1315	GOL	O1-C1-C2-O2
3	A	1321	GOL	O2-C2-C3-O3
3	A	1324	GOL	O1-C1-C2-O2
3	A	1328	GOL	O2-C2-C3-O3
3	A	1332	GOL	O2-C2-C3-O3
3	A	1337	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	1340	EDO	O1-C1-C2-O2
3	A	1303	GOL	O2-C2-C3-O3
3	A	1312	GOL	O1-C1-C2-O2
3	A	1312	GOL	O2-C2-C3-O3
3	A	1320	GOL	O2-C2-C3-O3
3	A	1321	GOL	O1-C1-C2-O2
3	A	1333	GOL	O2-C2-C3-O3
3	A	1334	GOL	O1-C1-C2-O2
3	A	1322	GOL	O1-C1-C2-O2
3	A	1334	GOL	O2-C2-C3-O3
4	A	1338	EDO	O1-C1-C2-O2
3	A	1305	GOL	O1-C1-C2-O2
3	A	1307	GOL	O1-C1-C2-O2
3	A	1315	GOL	O2-C2-C3-O3
3	A	1317	GOL	O2-C2-C3-O3
3	A	1331	GOL	O2-C2-C3-O3
3	A	1315	GOL	C1-C2-C3-O3
3	A	1316	GOL	O1-C1-C2-C3
2	A	1301	ADP	PA-O3A-PB-O3B
3	A	1326	GOL	O1-C1-C2-O2
3	A	1330	GOL	O1-C1-C2-O2
3	A	1304	GOL	O1-C1-C2-C3

There are no ring outliers.

24 monomers are involved in 77 short contacts:

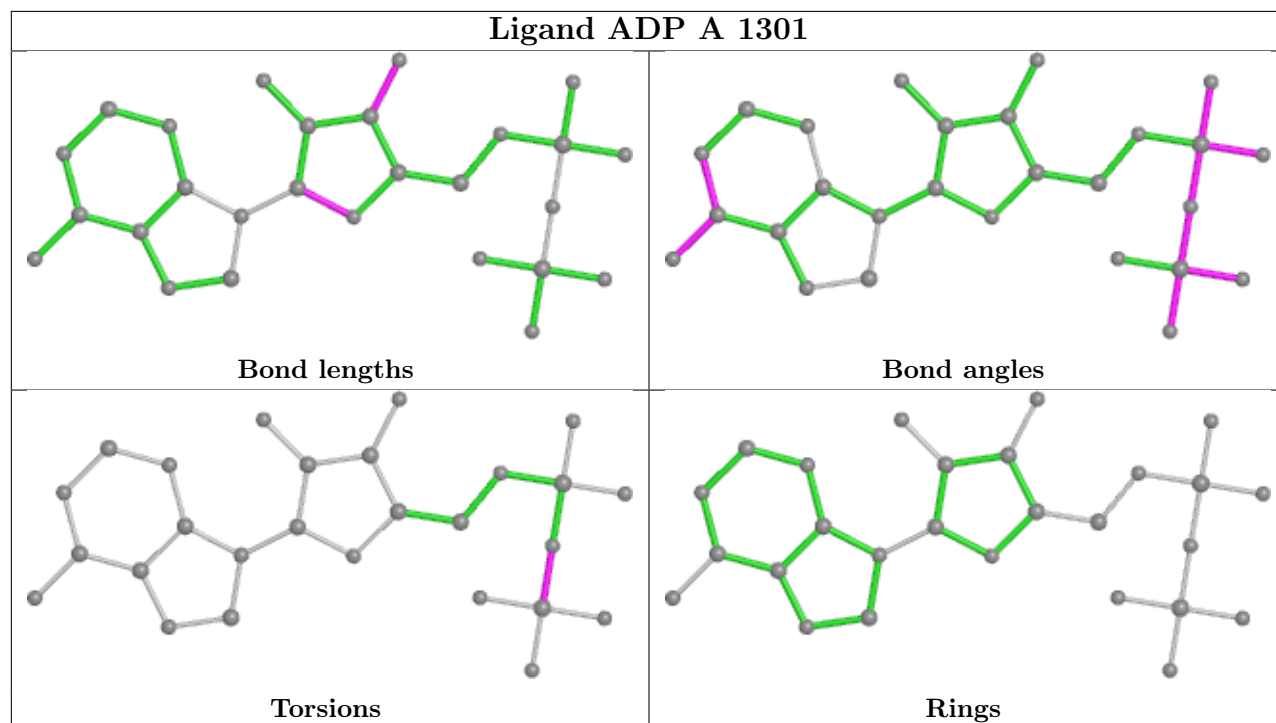
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1309	GOL	3	0
3	A	1325	GOL	6	0
4	A	1340	EDO	1	0
3	A	1317	GOL	2	0
3	A	1331	GOL	1	0
3	A	1312	GOL	1	0
3	A	1334	GOL	3	0
3	A	1326	GOL	2	0
3	A	1323	GOL	2	0
5	A	1351	SO4	1	0
3	A	1310	GOL	1	0
3	A	1314	GOL	4	0
3	A	1333	GOL	1	0
3	A	1332	GOL	3	0
3	A	1339	GOL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1308	GOL	3	0
3	A	1329	GOL	3	0
3	A	1313	GOL	4	0
3	A	1321	GOL	1	0
3	A	1311	GOL	5	0
3	A	1335	GOL	6	0
3	A	1337	GOL	4	0
3	A	1307	GOL	8	0
3	A	1324	GOL	8	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	1288/1304 (98%)	-0.42	27 (2%) 63 65	11, 17, 38, 84	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	464	ASP	6.4
1	A	789	ASN	6.0
1	A	118	THR	4.5
1	A	465	LEU	4.0
1	A	117	SER	3.7
1	A	-4	PRO	3.7
1	A	-2	GLY	3.6
1	A	609	THR	3.5
1	A	-1	SER	3.3
1	A	-5	VAL	3.2
1	A	610	PRO	3.2
1	A	27	ASN	3.0
1	A	176	LEU	3.0
1	A	788	GLY	3.0
1	A	152	HIS	2.9
1	A	786	GLN	2.7
1	A	122	GLU	2.6
1	A	66	SER	2.6
1	A	608	LYS	2.6
1	A	154	GLN	2.6
1	A	25	ALA	2.3
1	A	121	ALA	2.3
1	A	276	ASN	2.3
1	A	791	GLN	2.3
1	A	969	ASN	2.2
1	A	-7	GLY	2.1
1	A	611	LYS	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(Å <sup>2</sup> )	Q<0.9
1	CYG	A	1135	15/16	0.98	0.08	10,12,15,20	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(Å <sup>2</sup> )	Q<0.9
3	GOL	A	1323	6/6	0.61	0.26	56,67,71,72	0
3	GOL	A	1327	6/6	0.67	0.23	56,60,62,66	0
3	GOL	A	1329	6/6	0.72	0.18	49,57,62,63	0
3	GOL	A	1337	6/6	0.72	0.33	46,48,56,64	0
5	SO4	A	1358	5/5	0.72	0.40	68,73,97,98	0
3	GOL	A	1311	6/6	0.74	0.22	45,50,54,55	0
3	GOL	A	1320	6/6	0.76	0.40	60,62,63,70	0
5	SO4	A	1357	5/5	0.77	0.40	69,72,95,100	0
3	GOL	A	1326	6/6	0.77	0.26	48,51,53,53	0
3	GOL	A	1333	6/6	0.78	0.30	38,55,60,61	0
3	GOL	A	1322	6/6	0.80	0.20	47,50,55,57	0
3	GOL	A	1325	6/6	0.81	0.15	55,60,66,67	0
3	GOL	A	1339	6/6	0.81	0.36	46,51,57,65	0
3	GOL	A	1324	6/6	0.82	0.17	47,61,66,68	0
4	EDO	A	1340	4/4	0.83	0.13	56,57,57,59	0
3	GOL	A	1307	6/6	0.84	0.24	32,35,53,54	0
3	GOL	A	1313	6/6	0.84	0.17	38,43,45,52	0
5	SO4	A	1354	5/5	0.85	0.27	74,76,95,97	0
3	GOL	A	1315	6/6	0.85	0.13	31,40,42,43	0
3	GOL	A	1332	6/6	0.85	0.24	38,51,54,57	0
3	GOL	A	1319	6/6	0.86	0.14	43,48,53,54	0

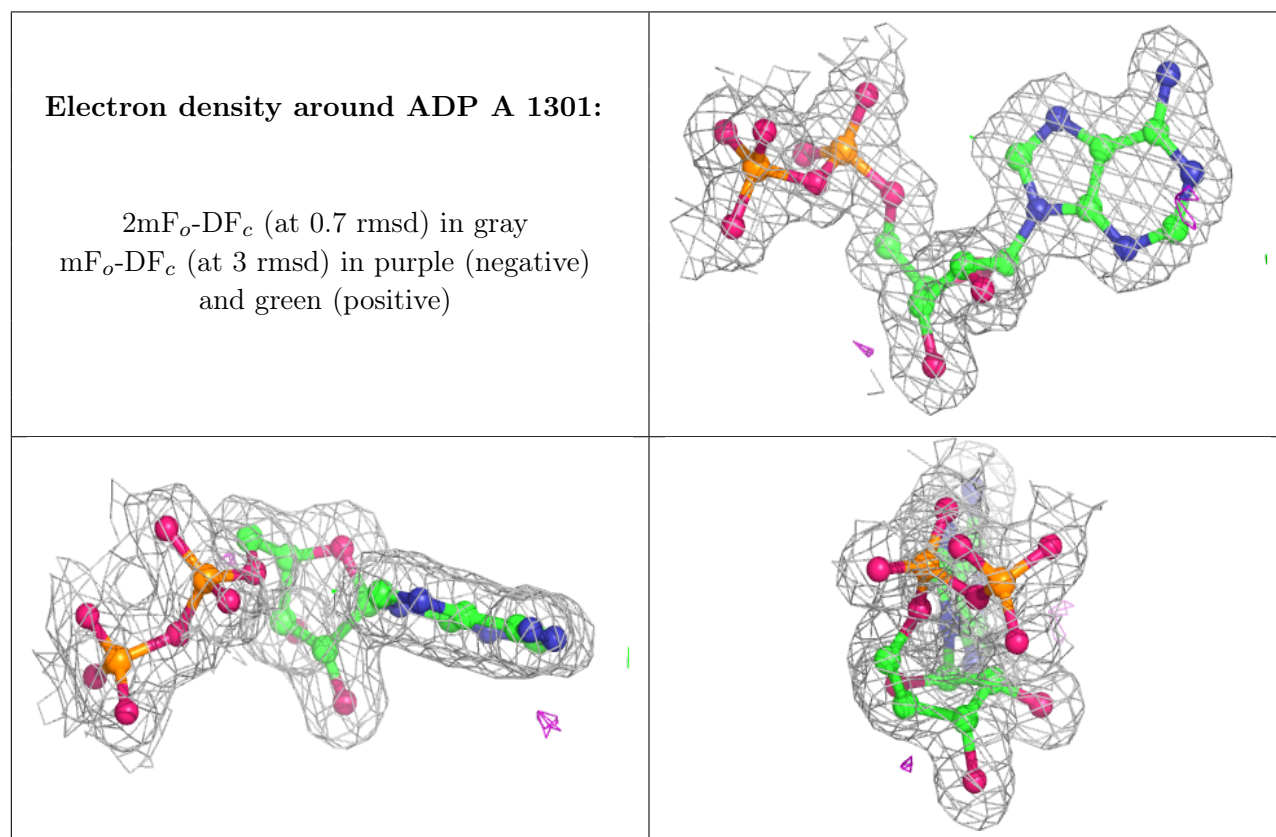
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	1312	6/6	0.87	0.13	33,40,45,46	0
3	GOL	A	1310	6/6	0.88	0.25	45,48,62,77	0
3	GOL	A	1308	6/6	0.88	0.30	24,40,44,46	0
3	GOL	A	1335	6/6	0.89	0.34	49,60,74,77	0
3	GOL	A	1314	6/6	0.89	0.19	27,31,34,35	0
3	GOL	A	1328	6/6	0.89	0.14	26,54,54,56	0
3	GOL	A	1316	6/6	0.89	0.17	32,41,49,49	0
3	GOL	A	1321	6/6	0.89	0.19	28,46,50,50	0
3	GOL	A	1318	6/6	0.89	0.27	38,46,51,52	0
3	GOL	A	1334	6/6	0.89	0.25	30,44,49,59	0
5	SO4	A	1359	5/5	0.89	0.23	60,73,91,92	0
3	GOL	A	1330	6/6	0.90	0.17	36,54,57,57	0
3	GOL	A	1331	6/6	0.90	0.34	51,64,70,78	0
3	GOL	A	1309	6/6	0.90	0.11	26,31,33,35	0
5	SO4	A	1351	5/5	0.90	0.14	31,43,52,54	0
5	SO4	A	1360	5/5	0.90	0.41	68,71,80,85	0
3	GOL	A	1336	6/6	0.91	0.20	31,44,45,47	0
5	SO4	A	1355	5/5	0.91	0.41	61,79,79,80	0
3	GOL	A	1305	6/6	0.92	0.11	24,38,40,41	0
3	GOL	A	1302	6/6	0.93	0.12	30,32,34,35	0
5	SO4	A	1353	5/5	0.93	0.26	74,75,82,86	0
4	EDO	A	1338	4/4	0.93	0.29	43,43,47,50	0
3	GOL	A	1317	6/6	0.93	0.19	34,50,52,62	0
5	SO4	A	1356	5/5	0.94	0.34	66,70,75,85	0
5	SO4	A	1352	5/5	0.95	0.34	38,48,51,54	0
5	SO4	A	1347	5/5	0.95	0.22	22,27,38,38	0
3	GOL	A	1306	6/6	0.95	0.10	21,23,24,27	0
3	GOL	A	1303	6/6	0.96	0.11	14,20,25,32	0
5	SO4	A	1349	5/5	0.96	0.17	32,34,42,49	0
3	GOL	A	1304	6/6	0.96	0.08	17,21,26,29	0
5	SO4	A	1350	5/5	0.97	0.28	45,46,51,54	0
5	SO4	A	1344	5/5	0.98	0.11	30,33,38,42	0
5	SO4	A	1348	5/5	0.98	0.22	38,42,45,49	0
5	SO4	A	1343	5/5	0.99	0.10	29,32,33,42	0
2	ADP	A	1301	27/27	0.99	0.06	10,11,12,12	0
5	SO4	A	1345	5/5	0.99	0.14	26,33,39,40	0
5	SO4	A	1346	5/5	0.99	0.10	24,31,35,40	0
5	SO4	A	1341	5/5	0.99	0.04	18,18,20,22	0
5	SO4	A	1342	5/5	0.99	0.07	23,25,27,29	0
6	MG	A	1362	1/1	0.99	0.06	11,11,11,11	0
6	MG	A	1361	1/1	1.00	0.04	11,11,11,11	0
6	MG	A	1363	1/1	1.00	0.08	12,12,12,12	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.