



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 19, 2023 – 04:24 PM JST

PDB ID : 6LYK  
Title : Crystal Structure of R1263A mutant of Formylglycinamide Synthetase  
Authors : Sharma, N.; Tanwar, A.S.; Anand, R.  
Deposited on : 2020-02-14  
Resolution : 1.70 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](mailto:validation@mail.wwpdb.org)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

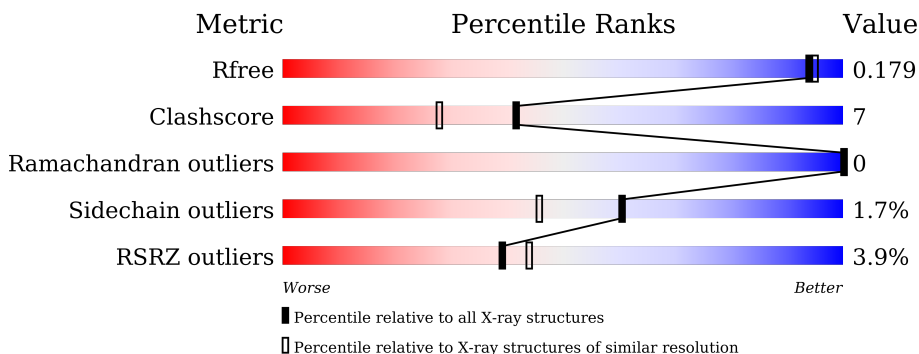
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1305	

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
2	EDO	A	1602	-	-	X	-
2	EDO	A	1613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1616	-	-	-	X
7	SO4	A	1639	-	-	-	X
8	GOL	A	1647	-	-	X	-
8	GOL	A	1651	-	X	-	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12144 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
			Total	C	N	O	S			
1	A	1293	10360	6544	1822	1938	56	0	75	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	expression tag	UNP P74881
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	1263	ALA	ARG	engineered mutation	UNP P74881

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



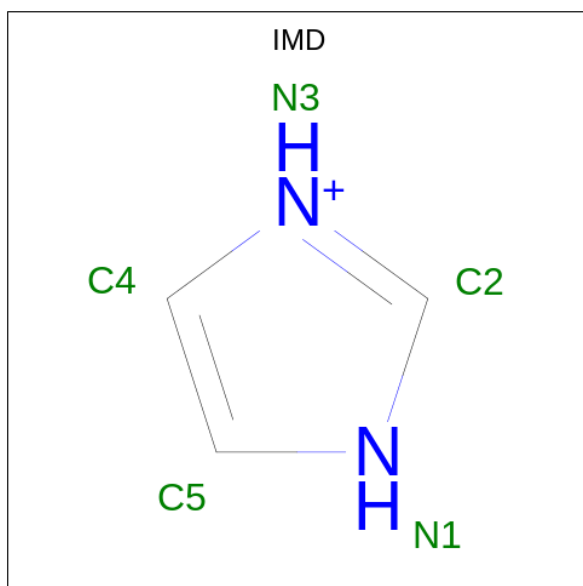
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0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

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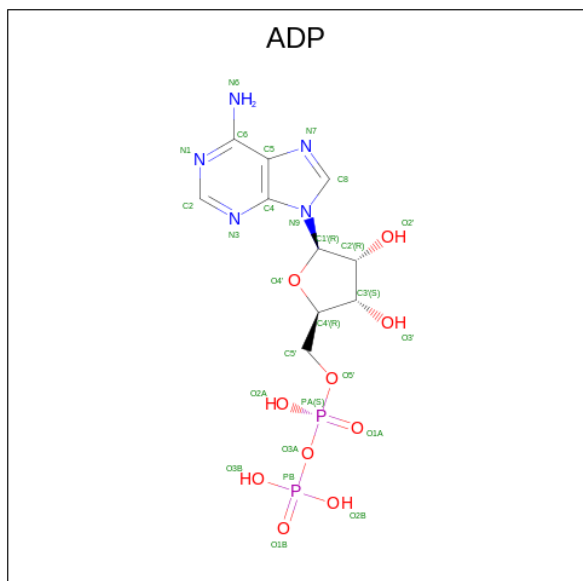
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



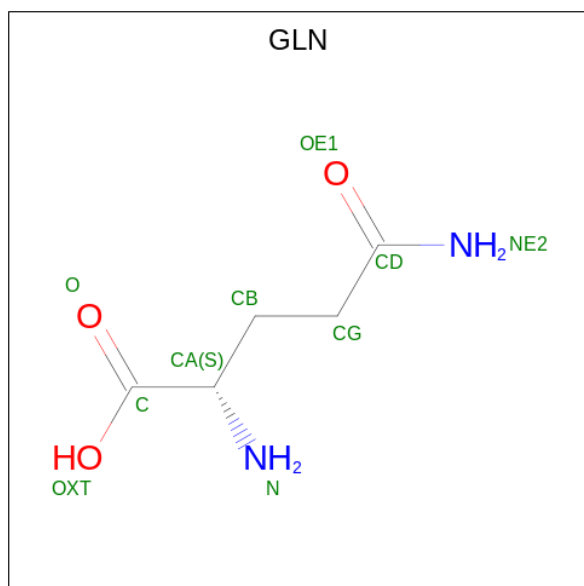
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			5	3	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	10	5	2	3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	4	4	4	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	1
			10	8	2		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

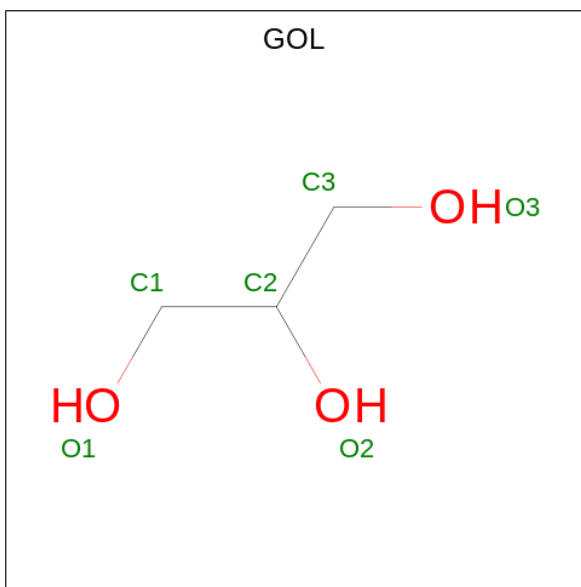
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	1
			12	6	6		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 12 6 6	0	1
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0
8	A	1	Total C O 6 3 3	0	0

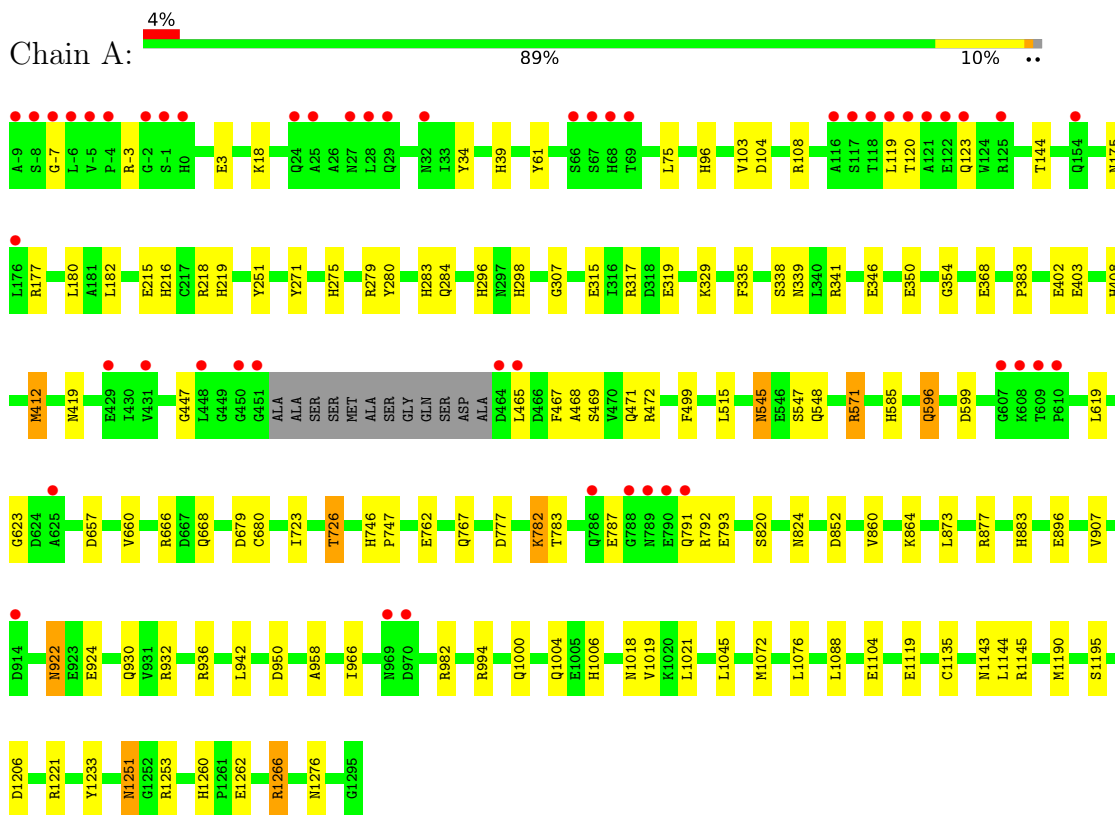
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1474	Total O 1474 1474	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Phosphoribosylformylglycinamide synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.90Å 146.90Å 141.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.74 – 1.70 39.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.74-1.70) 99.8 (39.74-1.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.152 , 0.177 0.158 , 0.179	Depositor DCC
$R_{free}$ test set	9442 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.4	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12144	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: IMD, MG, EDO, SO4, ADP, GOL

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	1.07	6/10766 (0.1%)	1.04	9/14603 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1119	GLU	CD-OE2	-7.58	1.17	1.25
1	A	762	GLU	CD-OE2	-5.99	1.19	1.25
1	A	1266[A]	ARG	CA-C	5.67	1.67	1.52
1	A	1266[B]	ARG	CA-C	5.67	1.67	1.52
1	A	412[A]	MET	CA-C	5.20	1.66	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412[A]	MET	CG-SD-CE	6.74	110.98	100.20
1	A	412[B]	MET	CG-SD-CE	6.74	110.98	100.20
1	A	950	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	994	ARG	CG-CD-NE	-6.08	99.04	111.80
1	A	571	ARG	NE-CZ-NH1	6.03	123.31	120.30

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	10360	0	10329	136	0
2	A	60	0	90	8	0
3	A	5	0	5	0	0
4	A	27	0	12	1	0
5	A	10	0	7	2	0
6	A	4	0	0	0	0
7	A	90	0	0	1	0
8	A	114	0	151	22	0
9	A	1474	0	0	56	0
All	All	12144	0	10594	149	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 7.

The worst 5 of 149 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1608:EDO:H11	9:A:2845:HOH:O	1.74	0.84
1:A:75:LEU:HD23	9:A:1736:HOH:O	1.77	0.84
1:A:747:PRO:HA	8:A:1644:GOL:H31	1.58	0.82
1:A:296[B]:HIS:CE1	9:A:1854:HOH:O	2.33	0.82
1:A:820:SER:H	1:A:930:GLN:HE22	1.29	0.80

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	1364/1305 (104%)	1324 (97%)	40 (3%)	0	<b>100</b> <b>100</b>

There are no Ramachandran outliers to report.

### 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	1103/1041 (106%)	1082 (98%)	21 (2%)	57 41

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1144[B]	LEU
1	A	1195[A]	SER
1	A	1276	ASN
1	A	1195[B]	SER
1	A	1190[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1006	HIS
1	A	1276	ASN
1	A	1018	ASN
1	A	1189	GLN
1	A	408	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 59 ligands modelled in this entry, 4 are monoatomic - leaving 55 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
7	SO4	A	1637	-	4,4,4	0.59	0	6,6,6	0.74	0
8	GOL	A	1644	-	5,5,5	0.37	0	5,5,5	0.62	0
2	EDO	A	1601	-	3,3,3	0.58	0	2,2,2	1.01	0
8	GOL	A	1641[A]	-	5,5,5	1.05	0	5,5,5	0.63	0
8	GOL	A	1643	-	5,5,5	0.72	0	5,5,5	1.00	0
2	EDO	A	1602	-	3,3,3	0.43	0	2,2,2	1.31	0
7	SO4	A	1625	-	4,4,4	0.28	0	6,6,6	0.91	0
7	SO4	A	1633[A]	-	4,4,4	0.28	0	6,6,6	0.36	0
7	SO4	A	1623	-	4,4,4	0.14	0	6,6,6	1.02	0
8	GOL	A	1647	-	5,5,5	2.63	2 (40%)	5,5,5	3.13	2 (40%)
7	SO4	A	1636	-	4,4,4	0.42	0	6,6,6	0.69	0
8	GOL	A	1648	-	5,5,5	1.20	1 (20%)	5,5,5	1.49	0
2	EDO	A	1614	-	3,3,3	0.77	0	2,2,2	0.67	0
8	GOL	A	1651	-	5,5,5	2.52	3 (60%)	5,5,5	5.01	4 (80%)
2	EDO	A	1615	-	3,3,3	0.63	0	2,2,2	0.25	0
8	GOL	A	1652	-	5,5,5	0.61	0	5,5,5	0.89	0
2	EDO	A	1604	-	3,3,3	0.59	0	2,2,2	0.68	0
8	GOL	A	1649[A]	-	5,5,5	0.60	0	5,5,5	1.92	2 (40%)
8	GOL	A	1653	-	5,5,5	0.68	0	5,5,5	1.43	0
2	EDO	A	1608	-	3,3,3	0.57	0	2,2,2	0.37	0
2	EDO	A	1607	-	3,3,3	0.94	0	2,2,2	0.46	0
2	EDO	A	1612	-	3,3,3	0.37	0	2,2,2	1.53	0
7	SO4	A	1624	-	4,4,4	0.64	0	6,6,6	0.56	0
7	SO4	A	1626	-	4,4,4	0.33	0	6,6,6	1.20	0
2	EDO	A	1616	-	3,3,3	0.67	0	2,2,2	0.14	0
7	SO4	A	1632	-	4,4,4	1.04	0	6,6,6	0.90	0
2	EDO	A	1610	-	3,3,3	0.50	0	2,2,2	1.00	0
8	GOL	A	1645	-	5,5,5	1.12	0	5,5,5	1.19	0
2	EDO	A	1613	-	3,3,3	0.58	0	2,2,2	0.10	0
7	SO4	A	1635	-	4,4,4	0.70	0	6,6,6	0.42	0
7	SO4	A	1627	-	4,4,4	0.36	0	6,6,6	1.25	1 (16%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	IMD	A	1611	-	3,5,5	0.40	0	4,5,5	0.76	0
7	SO4	A	1639	-	4,4,4	0.49	0	6,6,6	0.32	0
2	EDO	A	1603	-	3,3,3	0.30	0	2,2,2	0.73	0
7	SO4	A	1634	-	4,4,4	0.78	0	6,6,6	0.83	0
4	ADP	A	1617	6	24,29,29	1.33	2 (8%)	29,45,45	1.19	2 (6%)
8	GOL	A	1654	-	5,5,5	0.21	0	5,5,5	0.29	0
8	GOL	A	1655	-	5,5,5	0.69	0	5,5,5	0.95	0
8	GOL	A	1641[B]	-	5,5,5	0.52	0	5,5,5	0.75	0
8	GOL	A	1642	-	5,5,5	1.57	1 (20%)	5,5,5	1.59	1 (20%)
5	GLN	A	1618	-	8,9,9	0.64	0	10,11,11	1.07	1 (10%)
8	GOL	A	1656	-	5,5,5	0.52	0	5,5,5	1.26	1 (20%)
2	EDO	A	1605	-	3,3,3	0.76	0	2,2,2	0.55	0
7	SO4	A	1638	-	4,4,4	0.52	0	6,6,6	0.38	0
7	SO4	A	1633[B]	-	4,4,4	0.25	0	6,6,6	1.12	1 (16%)
7	SO4	A	1629	-	4,4,4	0.63	0	6,6,6	1.09	0
8	GOL	A	1650	-	5,5,5	0.37	0	5,5,5	0.69	0
7	SO4	A	1630	-	4,4,4	0.51	0	6,6,6	0.80	0
7	SO4	A	1631	-	4,4,4	0.57	0	6,6,6	0.61	0
8	GOL	A	1640	-	5,5,5	0.95	0	5,5,5	1.24	1 (20%)
8	GOL	A	1646	-	5,5,5	1.00	0	5,5,5	0.54	0
2	EDO	A	1609	-	3,3,3	0.45	0	2,2,2	0.48	0
8	GOL	A	1649[B]	-	5,5,5	0.51	0	5,5,5	0.48	0
2	EDO	A	1606	-	3,3,3	0.30	0	2,2,2	0.42	0
7	SO4	A	1628	-	4,4,4	0.61	0	6,6,6	0.23	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	1644	-	-	2/4/4/4	-
2	EDO	A	1601	-	-	1/1/1/1	-
8	GOL	A	1641[A]	-	-	0/4/4/4	-
8	GOL	A	1643	-	-	0/4/4/4	-
2	EDO	A	1602	-	-	1/1/1/1	-
8	GOL	A	1647	-	-	1/4/4/4	-
8	GOL	A	1648	-	-	2/4/4/4	-
2	EDO	A	1614	-	-	1/1/1/1	-
8	GOL	A	1651	-	-	2/4/4/4	-
2	EDO	A	1615	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	1652	-	-	0/4/4/4	-
2	EDO	A	1604	-	-	1/1/1/1	-
8	GOL	A	1649[A]	-	-	0/4/4/4	-
8	GOL	A	1653	-	-	2/4/4/4	-
2	EDO	A	1608	-	-	1/1/1/1	-
2	EDO	A	1607	-	-	1/1/1/1	-
2	EDO	A	1612	-	-	0/1/1/1	-
2	EDO	A	1616	-	-	1/1/1/1	-
2	EDO	A	1610	-	-	1/1/1/1	-
8	GOL	A	1645	-	-	0/4/4/4	-
2	EDO	A	1613	-	-	1/1/1/1	-
3	IMD	A	1611	-	-	-	0/1/1/1
2	EDO	A	1603	-	-	0/1/1/1	-
4	ADP	A	1617	6	-	1/12/32/32	0/3/3/3
8	GOL	A	1654	-	-	3/4/4/4	-
8	GOL	A	1655	-	-	3/4/4/4	-
8	GOL	A	1641[B]	-	-	0/4/4/4	-
8	GOL	A	1642	-	-	0/4/4/4	-
5	GLN	A	1618	-	-	1/9/9/9	-
8	GOL	A	1656	-	-	2/4/4/4	-
2	EDO	A	1605	-	-	1/1/1/1	-
8	GOL	A	1650	-	-	2/4/4/4	-
8	GOL	A	1640	-	-	1/4/4/4	-
8	GOL	A	1646	-	-	0/4/4/4	-
2	EDO	A	1609	-	-	0/1/1/1	-
8	GOL	A	1649[B]	-	-	2/4/4/4	-
2	EDO	A	1606	-	-	1/1/1/1	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1647	GOL	O2-C2	5.08	1.58	1.43
8	A	1651	GOL	O2-C2	4.02	1.55	1.43
4	A	1617	ADP	C2'-C1'	3.39	1.58	1.53
4	A	1617	ADP	C2-N3	3.39	1.37	1.32
8	A	1642	GOL	O1-C1	-3.14	1.29	1.42

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1651	GOL	O2-C2-C1	-6.14	82.09	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1651	GOL	O2-C2-C3	6.12	136.08	109.12
8	A	1647	GOL	O3-C3-C2	6.01	139.00	110.20
8	A	1651	GOL	O3-C3-C2	5.55	136.83	110.20
8	A	1651	GOL	O1-C1-C2	4.24	130.53	110.20

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1644	GOL	O1-C1-C2-O2
8	A	1644	GOL	O1-C1-C2-C3
8	A	1648	GOL	O1-C1-C2-C3
8	A	1649[B]	GOL	C1-C2-C3-O3
8	A	1651	GOL	C1-C2-C3-O3

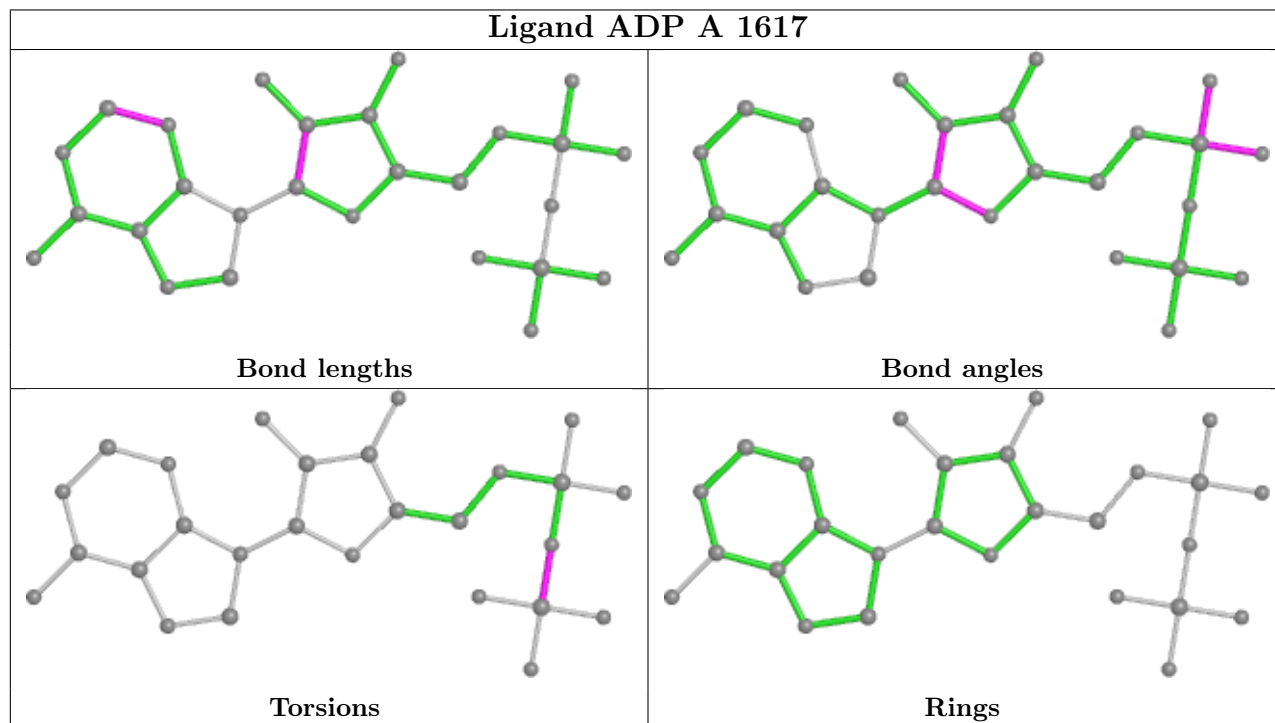
There are no ring outliers.

16 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1644	GOL	3	0
2	A	1601	EDO	1	0
2	A	1602	EDO	4	0
8	A	1647	GOL	7	0
8	A	1651	GOL	2	0
8	A	1653	GOL	3	0
2	A	1608	EDO	1	0
2	A	1610	EDO	2	0
4	A	1617	ADP	1	0
8	A	1654	GOL	1	0
8	A	1655	GOL	2	0
8	A	1642	GOL	2	0
5	A	1618	GLN	2	0
8	A	1656	GOL	1	0
7	A	1633[B]	SO4	1	0
8	A	1650	GOL	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1293/1305 (99%)	0.29	50 (3%) 39 44	12, 17, 37, 68	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-5	VAL	5.5
1	A	-4	PRO	5.3
1	A	789	ASN	5.0
1	A	-7	GLY	4.9
1	A	118	THR	4.9

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	EDO	A	1615	4/4	0.47	0.24	67,69,78,83	0
2	EDO	A	1614	4/4	0.68	0.36	58,60,60,72	0

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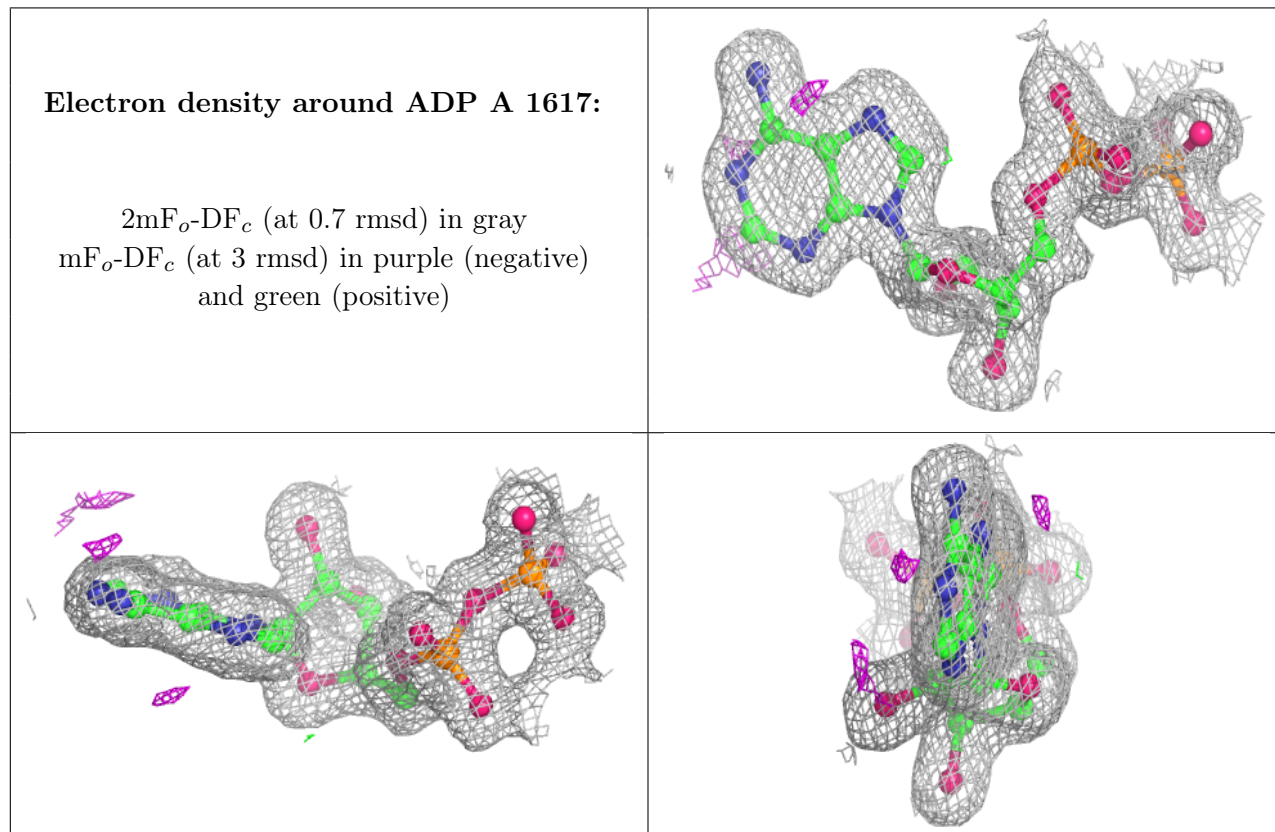
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	A	1607	4/4	0.68	0.23	42,43,50,51	0
8	GOL	A	1655	6/6	0.68	0.30	49,53,57,65	0
2	EDO	A	1610	4/4	0.71	0.18	40,48,49,49	0
8	GOL	A	1653	6/6	0.72	0.18	37,43,49,50	0
2	EDO	A	1613	4/4	0.74	0.40	56,59,70,72	0
2	EDO	A	1616	4/4	0.75	0.40	46,46,51,56	0
8	GOL	A	1649[A]	6/6	0.76	0.34	21,30,33,35	6
8	GOL	A	1649[B]	6/6	0.76	0.34	30,35,37,39	6
8	GOL	A	1650	6/6	0.76	0.16	44,45,51,51	0
7	SO4	A	1639	5/5	0.76	0.45	88,99,114,128	0
8	GOL	A	1646	6/6	0.76	0.15	33,37,41,42	0
8	GOL	A	1656	6/6	0.77	0.28	44,51,55,64	0
8	GOL	A	1652	6/6	0.78	0.17	30,51,55,62	0
8	GOL	A	1647	6/6	0.78	0.20	28,34,43,46	0
8	GOL	A	1644	6/6	0.79	0.25	24,37,42,47	1
8	GOL	A	1645	6/6	0.80	0.16	31,35,40,40	0
2	EDO	A	1601	4/4	0.80	0.12	52,55,55,56	0
8	GOL	A	1654	6/6	0.82	0.28	46,59,60,81	0
7	SO4	A	1637	5/5	0.84	0.31	55,65,80,86	0
2	EDO	A	1604	4/4	0.84	0.14	33,38,40,43	0
8	GOL	A	1651	6/6	0.85	0.17	27,32,36,36	0
8	GOL	A	1641[B]	6/6	0.86	0.15	21,29,32,33	6
8	GOL	A	1641[A]	6/6	0.86	0.15	20,25,26,27	6
3	IMD	A	1611	5/5	0.87	0.25	46,55,58,65	0
8	GOL	A	1643	6/6	0.87	0.15	21,25,27,30	1
2	EDO	A	1609	4/4	0.87	0.21	47,63,64,64	0
2	EDO	A	1606	4/4	0.88	0.13	46,48,52,58	0
8	GOL	A	1640	6/6	0.89	0.15	19,22,29,31	0
8	GOL	A	1642	6/6	0.89	0.24	24,33,43,43	0
2	EDO	A	1608	4/4	0.90	0.17	32,39,41,48	0
7	SO4	A	1634	5/5	0.90	0.30	34,39,43,45	1
8	GOL	A	1648	6/6	0.90	0.16	18,22,29,37	0
7	SO4	A	1636	5/5	0.90	0.28	70,71,85,85	0
2	EDO	A	1602	4/4	0.91	0.21	33,37,42,43	0
2	EDO	A	1612	4/4	0.92	0.13	34,44,51,54	0
7	SO4	A	1635	5/5	0.92	0.36	45,47,50,55	1
7	SO4	A	1632	5/5	0.92	0.14	21,27,30,39	1
7	SO4	A	1638	5/5	0.93	0.27	57,67,79,80	0
2	EDO	A	1603	4/4	0.93	0.21	24,37,47,50	0
2	EDO	A	1605	4/4	0.93	0.10	37,42,45,52	0
7	SO4	A	1633[A]	5/5	0.95	0.13	35,37,42,44	5
7	SO4	A	1633[B]	5/5	0.95	0.13	27,28,31,33	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GLN	A	1618	10/10	0.95	0.11	12,13,16,16	2
7	SO4	A	1629	5/5	0.97	0.07	25,28,35,37	1
7	SO4	A	1631	5/5	0.97	0.22	36,36,47,48	0
4	ADP	A	1617	27/27	0.97	0.09	11,12,14,14	0
6	MG	A	1622	1/1	0.97	0.11	31,31,31,31	0
7	SO4	A	1625	5/5	0.97	0.11	28,32,40,45	1
7	SO4	A	1628	5/5	0.97	0.18	29,34,40,41	0
7	SO4	A	1630	5/5	0.98	0.21	33,35,44,44	0
7	SO4	A	1626	5/5	0.98	0.09	26,26,37,42	1
7	SO4	A	1627	5/5	0.98	0.16	24,24,29,32	1
7	SO4	A	1624	5/5	0.99	0.09	22,24,25,29	0
6	MG	A	1619	1/1	0.99	0.07	13,13,13,13	0
7	SO4	A	1623	5/5	0.99	0.07	16,19,21,24	1
6	MG	A	1620	1/1	1.00	0.07	13,13,13,13	0
6	MG	A	1621	1/1	1.00	0.07	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.