



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2026 – 08:10 PM EDT

PDB ID : 11GY / pdb_000011gy
Title : Crystal structure of selective inhibitor 16 bound at the active site of CDK1
Authors : Murray, J.M.; Oh, A.; Kiefer, J.R.; Verma, V.A.; Grandner, J.M.; Parr, B.T.
Deposited on : 2026-02-23
Resolution : 2.40 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

A user guide is available at

<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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

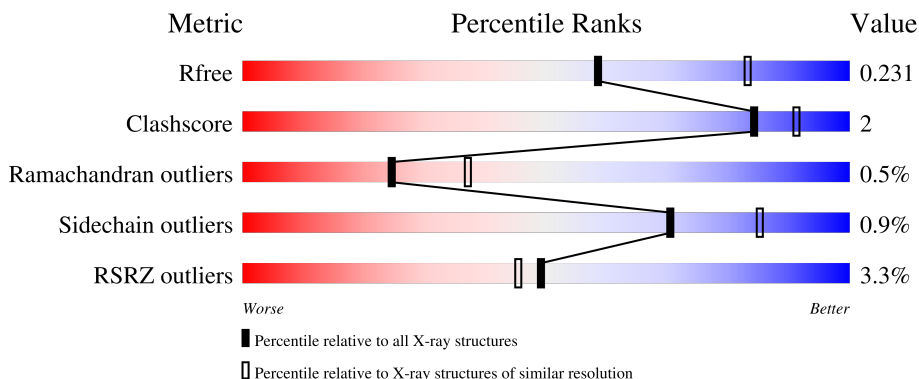
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 ≥ 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	316	 4% 84% 7% 9%
2	B	273	 3% 95%
3	C	80	 2% 90% 5% 5%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 5521 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 Cyclin-dependent kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	289	2330	1503	391	427	1	8	0	1	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P06493
A	-17	HIS	-	expression tag	UNP P06493
A	-16	HIS	-	expression tag	UNP P06493
A	-15	HIS	-	expression tag	UNP P06493
A	-14	HIS	-	expression tag	UNP P06493
A	-13	HIS	-	expression tag	UNP P06493
A	-12	HIS	-	expression tag	UNP P06493
A	-11	GLY	-	expression tag	UNP P06493
A	-10	GLU	-	expression tag	UNP P06493
A	-9	ASN	-	expression tag	UNP P06493
A	-8	LEU	-	expression tag	UNP P06493
A	-7	TYR	-	expression tag	UNP P06493
A	-6	PHE	-	expression tag	UNP P06493
A	-5	GLN	-	expression tag	UNP P06493
A	-4	GLY	-	expression tag	UNP P06493
A	-3	SER	-	expression tag	UNP P06493
A	-2	LEU	-	expression tag	UNP P06493
A	-1	GLY	-	expression tag	UNP P06493
A	0	SER	-	expression tag	UNP P06493

- Molecule 2 is a protein called G2/mitotic-specific cyclin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	270	2168	1396	366	388	18	0	1	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	160	GLY	-	expression tag	UNP P14635
B	161	SER	-	expression tag	UNP P14635
B	162	HIS	-	expression tag	UNP P14635
B	163	MET	-	expression tag	UNP P14635
B	166	SER	CYS	conflict	UNP P14635
B	237	SER	CYS	conflict	UNP P14635
B	349	SER	CYS	conflict	UNP P14635

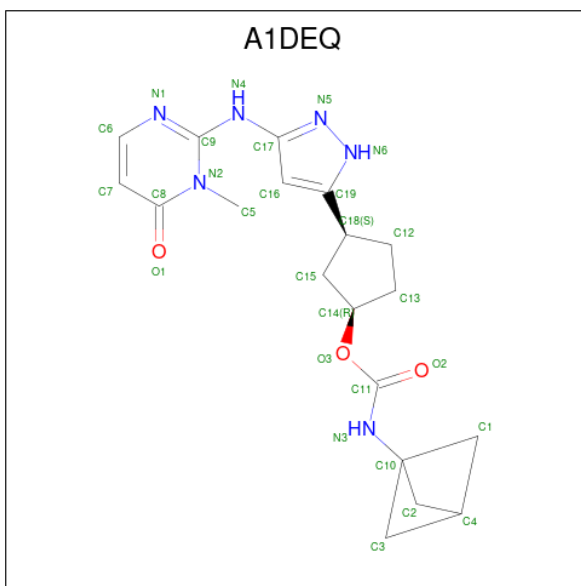
- Molecule 3 is a protein called Cyclin-dependent kinases regulatory subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	76	640	414	110	113	3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

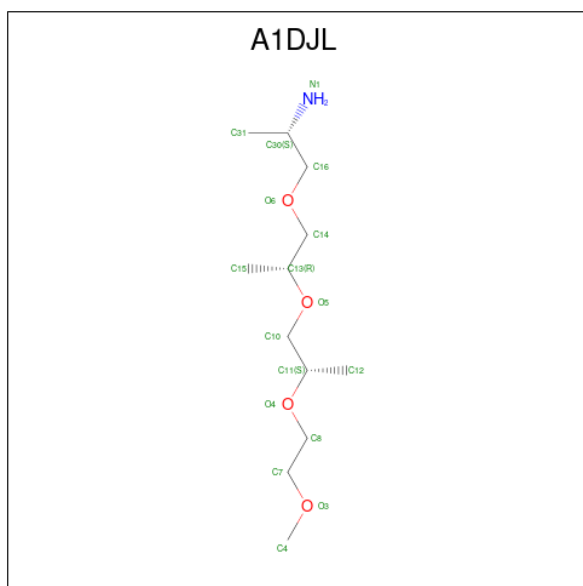
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP P33552
C	1	SER	-	expression tag	UNP P33552

- Molecule 4 is (1R,3S)-3-{3-[(1-methyl-6-oxo-1,6-dihydropyrimidin-2-yl)amino]-1H-pyrazol-5-yl}cyclopentyl bicyclo[1.1.1]pentan-1-ylcarbamate (CCD ID: A1DEQ) (formula: C₁₉H₂₄N₆O₃) (labeled as "Ligand of Interest" by depositor).



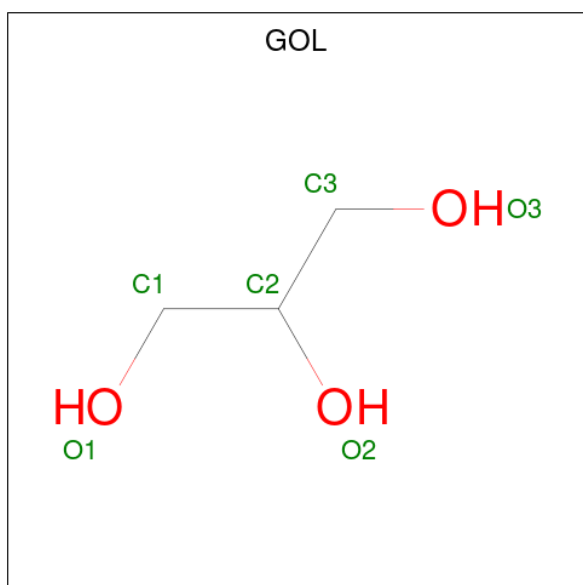
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	28	19	6	3	0	0

- Molecule 5 is (6S,9R,13S)-6,9-dimethyl-2,5,8,11-tetraoxatetradecan-13-amine (CCD ID: A1DJL) (formula: C₁₂H₂₇NO₄).



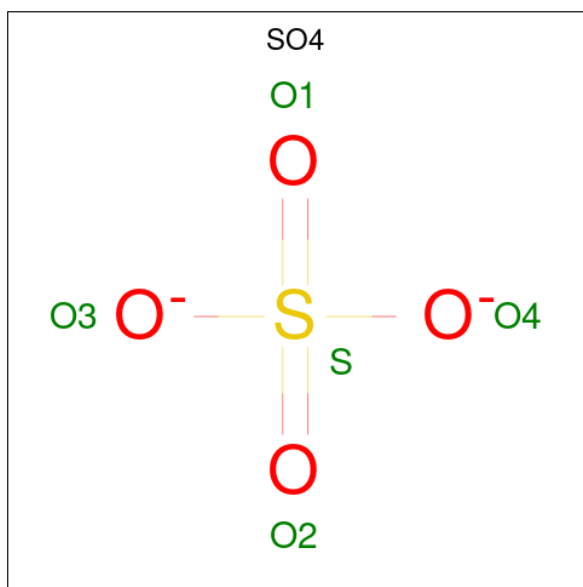
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	17	12	1	4	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



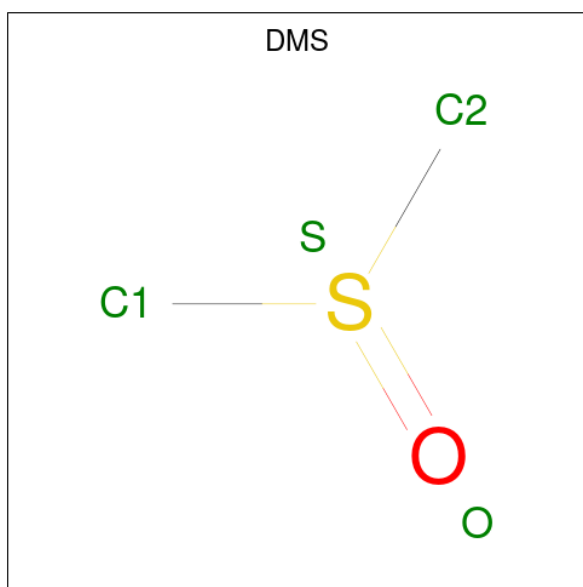
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



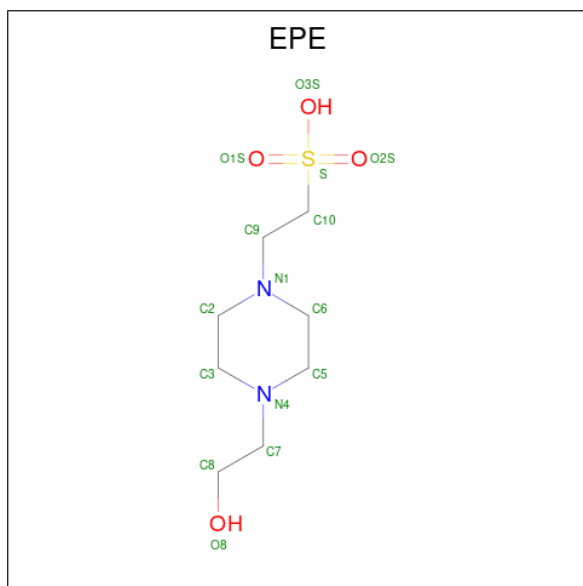
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0

- Molecule 8 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
8	B	1	4	2	1	1	0	0

- Molecule 9 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	15	8	2	4	1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	130	Total 130	O 130	0	0
10	B	118	Total 119	O 119	0	1
10	C	28	Total 28	O 28	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	75.70Å 75.70Å 254.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.60 – 2.40 34.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.1 (34.60-2.40) 94.1 (34.60-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.186 , 0.231 0.189 , 0.231	Depositor DCC
R_{free} test set	1373 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtrriage
Anisotropy	0.471	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5521	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, DMS, TPO, A1DEQ, A1DJL, EPE

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	0.48	0/2375	0.88	0/3213
2	B	0.46	0/2216	0.89	0/2997
3	C	0.47	0/663	0.78	1/903 (0.1%)
All	All	0.47	0/5254	0.87	1/7113 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	14	ASP	CA-CB-CG	6.09	118.69	112.60

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	2330	0	2343	17	0
2	B	2168	0	2206	8	0
3	C	640	0	586	1	0
4	A	28	0	0	0	0
5	A	17	0	0	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	10	0	0	0	0
7	B	15	0	0	0	0
7	C	5	0	0	0	0
8	B	4	0	6	0	0
9	B	15	0	18	0	0
10	A	130	0	0	0	0
10	B	119	0	0	1	0
10	C	28	0	0	0	0
All	All	5521	0	5175	24	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 2.

All (24) 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:155:ILE:HB	1:A:156:PRO:HD3	1.46	0.97
1:A:155:ILE:HB	1:A:156:PRO:CD	2.13	0.78
2:B:427:LYS:O	2:B:428:ALA:CB	2.46	0.63
1:A:15:TYR:CE2	1:A:35:ILE:HD12	2.37	0.59
1:A:155:ILE:HD12	1:A:155:ILE:H	1.68	0.58
1:A:158:ARG:HD2	2:B:306:ARG:HH12	1.70	0.57
2:B:220:GLU:OE2	2:B:306:ARG:NH1	2.39	0.54
1:A:183:THR:N	1:A:184:PRO:CD	2.71	0.53
1:A:218:ARG:HG2	1:A:244:TRP:CE2	2.46	0.50
1:A:123:ARG:HD2	1:A:123:ARG:O	2.12	0.50
2:B:427:LYS:O	2:B:428:ALA:HB2	2.14	0.47
1:A:1:MET:HB2	1:A:70:LEU:HD13	1.97	0.47
1:A:120:HIS:CE1	1:A:183:THR:HB	2.49	0.47
1:A:218:ARG:HG2	1:A:244:TRP:CD2	2.50	0.47
3:C:61:GLU:N	3:C:62:PRO:CD	2.79	0.46
1:A:15:TYR:CD2	1:A:47:THR:HG23	2.50	0.46
2:B:305:LEU:HD22	2:B:326:MET:HE2	1.96	0.46
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.99	0.44
1:A:90:TYR:CE2	1:A:100:MET:HE2	2.52	0.44
1:A:155:ILE:H	1:A:155:ILE:CD1	2.29	0.42
1:A:253:VAL:HG11	1:A:256:LEU:HD12	1.99	0.42
1:A:155:ILE:HD11	2:B:303:HIS:O	2.19	0.42
2:B:307:ARG:HG3	10:B:708:HOH:O	2.19	0.42
2:B:201:ARG:O	2:B:205:ILE:HG12	2.20	0.41

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	285/316 (90%)	276 (97%)	8 (3%)	1 (0%)	30	43
2	B	269/273 (98%)	261 (97%)	7 (3%)	1 (0%)	30	43
3	C	74/80 (92%)	70 (95%)	3 (4%)	1 (1%)	9	13
All	All	628/669 (94%)	607 (97%)	18 (3%)	3 (0%)	24	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	VAL
2	B	428	ALA
3	C	75	LYS

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	254/282 (90%)	250 (98%)	4 (2%)	55	76
2	B	236/242 (98%)	235 (100%)	1 (0%)	84	92
3	C	66/76 (87%)	66 (100%)	0	100	100
All	All	556/600 (93%)	551 (99%)	5 (1%)	70	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	71	MET
1	A	155	ILE
1	A	280	MET
2	B	163	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	162	HIS
2	B	279	HIS
3	C	60	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](#)

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	TPO	A	161	1	8,10,11	0.68	0	10,14,16	0.89	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
1	TPO	A	161	1	-	0/9/11/13	-

There are no bond length outliers.

There are no bond angle outliers.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are 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	$\# Z > 2$
7	SO4	B	506	-	4,4,4	0.26	0	6,6,6	0.17	0
7	SO4	A	305	-	4,4,4	0.31	0	6,6,6	0.06	0
6	GOL	A	303	-	5,5,5	0.13	0	5,5,5	0.40	0
7	SO4	C	101	-	4,4,4	0.33	0	6,6,6	0.07	0
9	EPE	B	503	-	15,15,15	0.63	1 (6%)	19,20,20	0.80	1 (5%)
5	A1DJL	A	302	-	16,16,16	1.03	0	18,18,18	0.59	0
7	SO4	B	504	-	4,4,4	0.30	0	6,6,6	0.10	0
4	A1DEQ	A	301	-	29,32,32	3.48	13 (44%)	38,48,48	4.15	15 (39%)
6	GOL	B	501	-	5,5,5	0.12	0	5,5,5	0.29	0
7	SO4	B	505	-	4,4,4	0.30	0	6,6,6	0.10	0
8	DMS	B	502	-	3,3,3	0.24	0	3,3,3	0.12	0
7	SO4	A	304	-	4,4,4	0.31	0	6,6,6	0.11	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
6	GOL	A	303	-	-	1/4/4/4	-
9	EPE	B	503	-	-	2/9/19/19	0/1/1/1
5	A1DJL	A	302	-	-	4/16/16/16	-
4	A1DEQ	A	301	-	-	7/17/41/41	0/6/5/5
6	GOL	B	501	-	-	0/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	A1DEQ	C15-C14	-9.79	1.32	1.52
4	A	301	A1DEQ	C12-C18	-7.59	1.32	1.54
4	A	301	A1DEQ	C11-N3	6.33	1.46	1.35
4	A	301	A1DEQ	C15-C18	5.78	1.68	1.54
4	A	301	A1DEQ	C2-C4	4.47	1.59	1.55
4	A	301	A1DEQ	C8-N2	-4.05	1.32	1.40
4	A	301	A1DEQ	C1-C4	3.77	1.58	1.55
4	A	301	A1DEQ	C17-N4	3.72	1.45	1.39
4	A	301	A1DEQ	O3-C11	3.46	1.41	1.35
4	A	301	A1DEQ	C9-N2	-3.11	1.35	1.38
4	A	301	A1DEQ	C9-N4	2.63	1.46	1.37
9	B	503	EPE	O3S-S	2.30	1.55	1.47
4	A	301	A1DEQ	C7-C6	2.22	1.40	1.35
4	A	301	A1DEQ	C17-N5	-2.13	1.31	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	A1DEQ	C2-C4-C1	13.41	96.75	87.57
4	A	301	A1DEQ	C3-C4-C2	-10.33	80.50	87.57
4	A	301	A1DEQ	C17-N5-N6	7.63	109.26	103.71
4	A	301	A1DEQ	O3-C11-N3	7.30	118.11	109.50
4	A	301	A1DEQ	N4-C9-N2	7.13	121.05	114.75
4	A	301	A1DEQ	C3-C4-C1	-7.00	82.78	87.57
4	A	301	A1DEQ	C16-C17-N5	-5.48	108.22	112.14
4	A	301	A1DEQ	N2-C9-N1	-4.27	122.01	124.47
4	A	301	A1DEQ	C7-C6-N1	-3.96	119.65	125.01
4	A	301	A1DEQ	N4-C17-N5	3.89	124.02	117.50
4	A	301	A1DEQ	C7-C8-N2	3.83	120.08	115.04
4	A	301	A1DEQ	C15-C18-C12	3.57	105.65	100.75
9	B	503	EPE	O3S-S-C10	-2.95	100.23	106.00
4	A	301	A1DEQ	O3-C11-O2	-2.83	120.38	124.55
4	A	301	A1DEQ	C10-N3-C11	-2.81	119.43	126.45

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	301	A1DEQ	O2-C11-N3	-2.19	121.51	124.91

There are no chirality outliers.

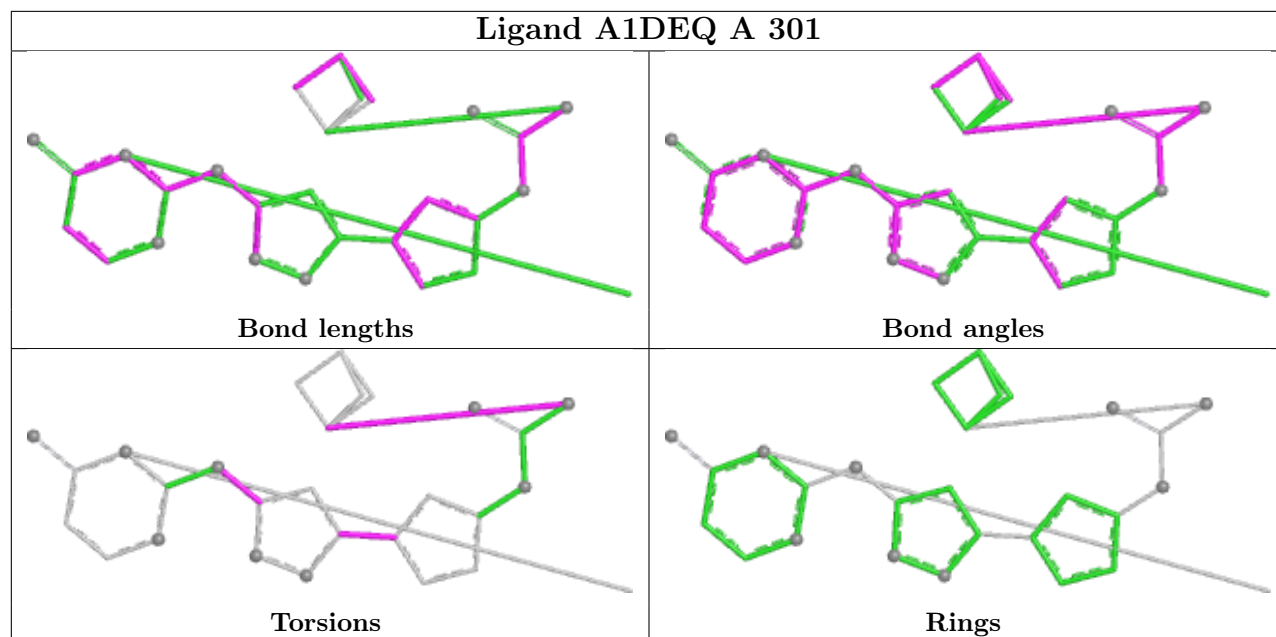
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	A1DEQ	C1-C10-N3-C11
4	A	301	A1DEQ	N5-C17-N4-C9
4	A	301	A1DEQ	C15-C18-C19-C16
4	A	301	A1DEQ	C12-C18-C19-N6
5	A	302	A1DJL	O5-C13-C14-O6
5	A	302	A1DJL	C15-C13-C14-O6
9	B	503	EPE	S-C10-C9-N1
4	A	301	A1DEQ	C16-C17-N4-C9
4	A	301	A1DEQ	C2-C10-N3-C11
4	A	301	A1DEQ	C3-C10-N3-C11
5	A	302	A1DJL	C7-C8-O4-C11
5	A	302	A1DJL	O5-C10-C11-O4
6	A	303	GOL	O1-C1-C2-O2
9	B	503	EPE	N4-C7-C8-O8

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/316 (91%)	0.04	12 (4%) 40 36	30, 59, 100, 143	1 (0%)
2	B	270/273 (98%)	-0.05	7 (2%) 57 53	36, 61, 117, 155	1 (0%)
3	C	76/80 (95%)	0.10	2 (2%) 57 53	52, 69, 105, 113	0
All	All	634/669 (94%)	0.01	21 (3%) 49 45	30, 61, 107, 155	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ILE	5.7
3	C	1	SER	3.8
2	B	357	ASN	3.2
1	A	71	MET	3.0
2	B	163	MET	2.9
1	A	1	MET	2.8
1	A	15	TYR	2.8
1	A	36	ARG	2.8
2	B	360	TRP	2.7
3	C	3	HIS	2.6
1	A	248	SER	2.5
2	B	165	LEU	2.5
1	A	72	GLN	2.5
1	A	292	ASN	2.5
1	A	14	THR	2.4
2	B	162	HIS	2.3
2	B	367	TYR	2.3
1	A	35	ILE	2.2
1	A	70	LEU	2.1
2	B	312	GLY	2.1
1	A	73	ASP	2.1

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	A	161	11/12	0.98	0.06	47,50,50,52	0

6.3 Carbohydrates [i](#)

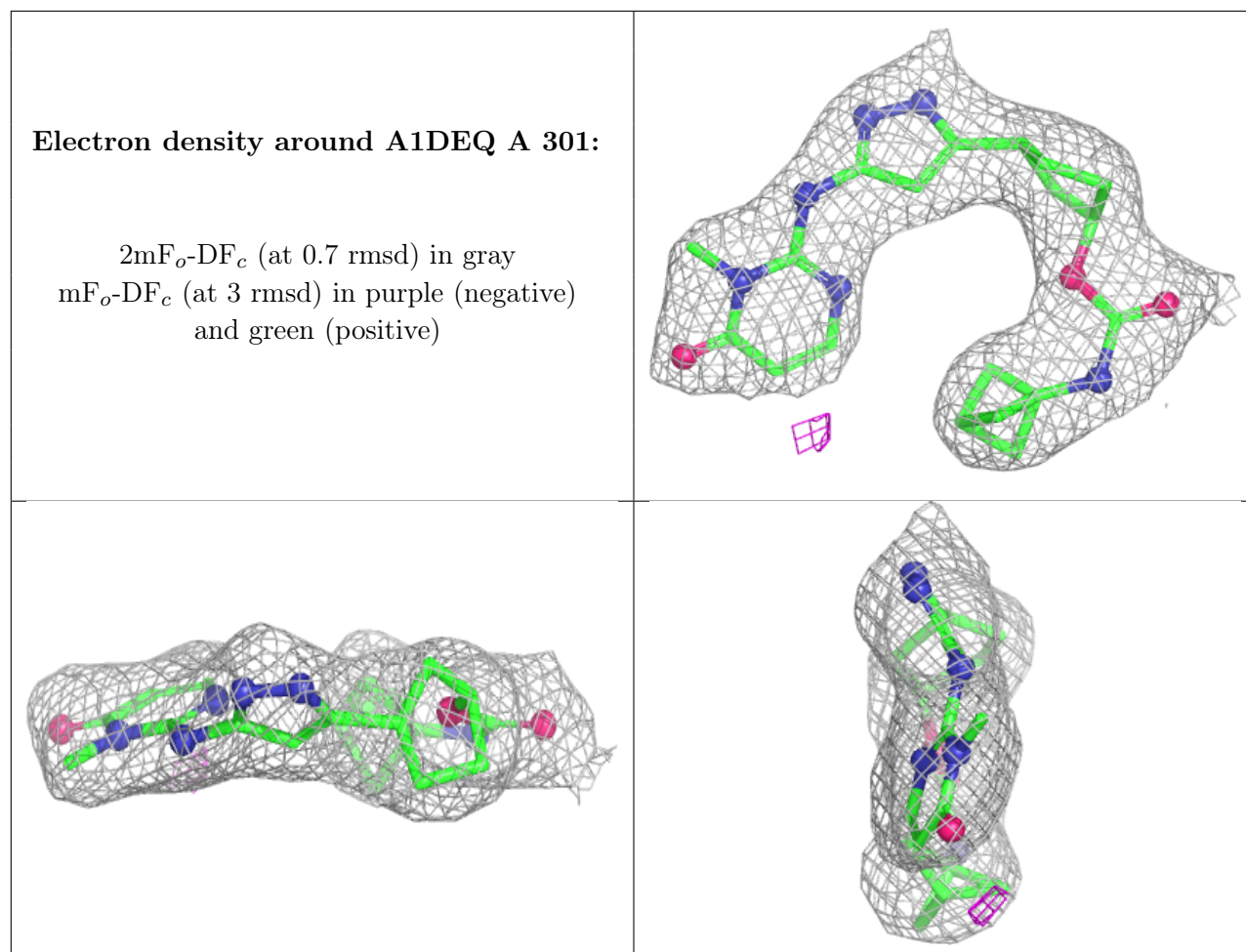
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	DMS	B	502	4/4	0.76	0.27	112,113,118,122	0
9	EPE	B	503	15/15	0.76	0.19	91,100,124,126	0
7	SO4	A	304	5/5	0.79	0.12	115,115,124,125	0
7	SO4	B	505	5/5	0.82	0.12	109,116,118,119	0
7	SO4	B	506	5/5	0.83	0.15	83,87,105,110	0
7	SO4	A	305	5/5	0.83	0.11	106,114,119,122	0
5	A1DJL	A	302	17/17	0.83	0.21	94,109,118,121	0
6	GOL	A	303	6/6	0.86	0.11	67,72,74,76	0
7	SO4	C	101	5/5	0.89	0.10	76,80,84,86	0
6	GOL	B	501	6/6	0.92	0.13	62,67,72,75	0
4	A1DEQ	A	301	28/28	0.96	0.08	49,56,65,68	0
7	SO4	B	504	5/5	0.98	0.07	69,70,72,72	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.