



wwPDB EM Validation Summary Report ⓘ

Apr 2, 2025 – 02:46 am BST

PDB ID : 6QPW / pdb_00006qpw
EMDB ID : EMD-4616
Title : Structural basis of cohesin ring opening
Authors : Panne, D.; Muir, K.W.; Li, Y.; Weis, F.
Deposited on : 2019-02-15
Resolution : 3.30 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

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:

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

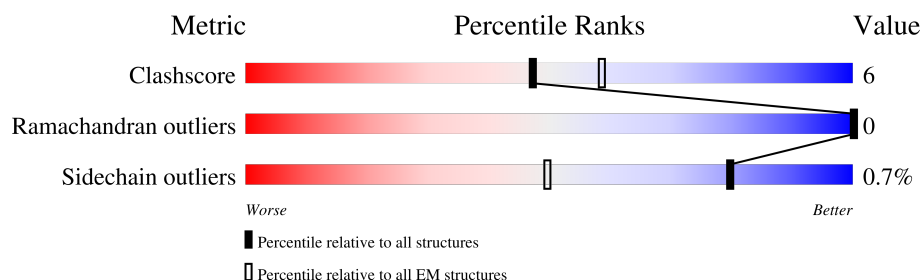
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	242	67% 9% 24%
2	B	85	89% 5% • 5%
3	C	535	57% 12% • 30%
4	E	372	47% 6% 47%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6784 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Structural maintenance of chromosomes protein, Structural maintenance of chromosomes protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	183	Total	C	N	O	S	0	0
			1486	931	267	286	2		

- Molecule 2 is a protein called Sister chromatid cohesion protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	81	Total	C	N	O	S	0	0
			637	405	107	123	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	480	MET	-	initiating methionine	UNP Q12158

- Molecule 3 is a protein called Structural maintenance of chromosomes protein 3, Structural maintenance of chromosomes protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	377	Total	C	N	O	S	0	0
			2987	1882	519	574	12		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P47037
C	1	ALA	-	expression tag	UNP P47037
C	958	SER	-	linker	UNP P47037
C	959	SER	-	linker	UNP P47037
C	960	LYS	-	linker	UNP P47037
C	961	HIS	-	linker	UNP P47037
C	962	PRO	-	linker	UNP P47037
C	963	THR	-	linker	UNP P47037

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Chain	Residue	Modelled	Actual	Comment	Reference
C	964	SER	-	linker	UNP P47037
C	965	LEU	-	linker	UNP P47037
C	966	VAL	-	linker	UNP P47037
C	967	PRO	-	linker	UNP P47037
C	968	ARG	-	linker	UNP P47037
C	969	GLY	-	linker	UNP P47037
C	1159	CYS	ALA	engineered mutation	UNP P47037
C	1204	CYS	ASN	engineered mutation	UNP P47037

- Molecule 4 is a protein called Sister chromatid cohesion protein 1, Structural maintenance of chromosomes protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	198	Total	C	N	O	S	0	0
			1610	1022	284	298	6		

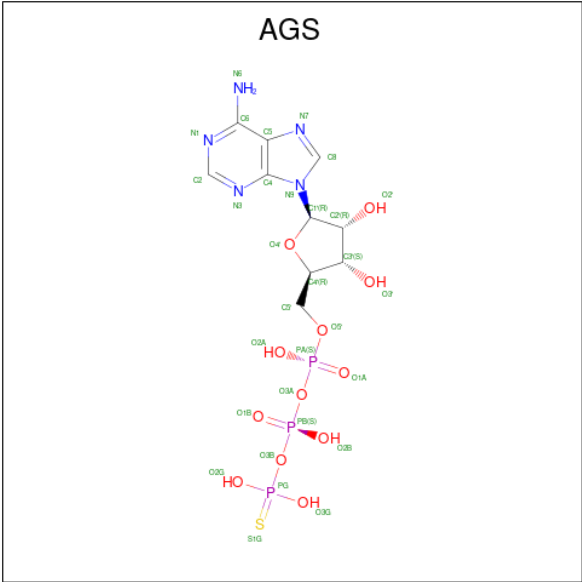
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	954	SER	CYS	engineered mutation	UNP Q12158
E	1160	CYS	LEU	engineered mutation	UNP G0SGH3
E	1201	CYS	ALA	engineered mutation	UNP G0SGH3
E	1265	HIS	-	expression tag	UNP G0SGH3
E	1266	HIS	-	expression tag	UNP G0SGH3
E	1267	HIS	-	expression tag	UNP G0SGH3
E	1268	HIS	-	expression tag	UNP G0SGH3
E	1269	HIS	-	expression tag	UNP G0SGH3
E	1270	HIS	-	expression tag	UNP G0SGH3

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	E	1	Total	Mg	0
			1	1	

- Molecule 6 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

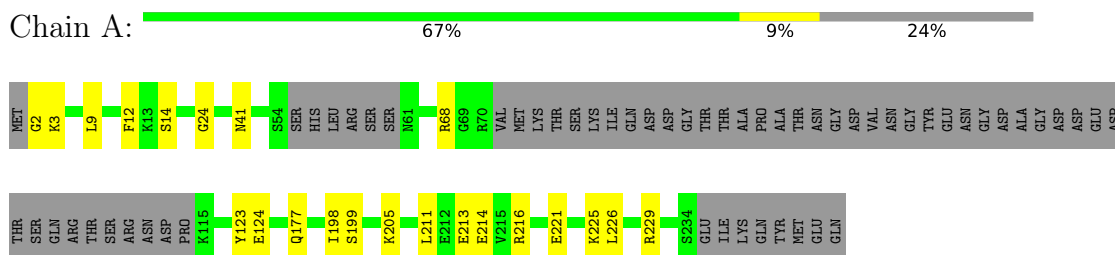


Mol	Chain	Residues	Atoms						AltConf
6	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
6	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

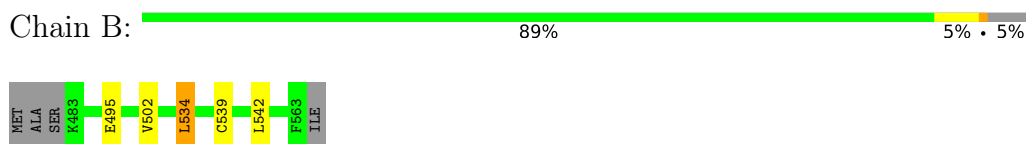
3 Residue-property plots [i](#)

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. 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. 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.

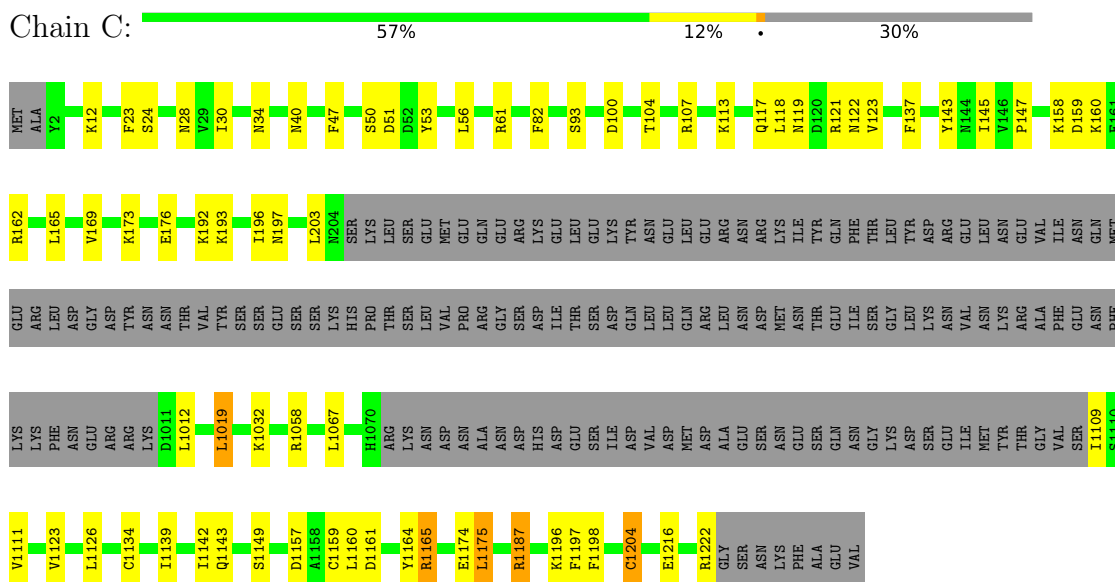
- Molecule 1: Structural maintenance of chromosomes protein, Structural maintenance of chromosomes protein



- Molecule 2: Sister chromatid cohesion protein 1



- Molecule 3: Structural maintenance of chromosomes protein 3, Structural maintenance of chromosomes protein 3



- [illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	178162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.08	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: MG, AGS

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	0.31	0/1508	0.53	0/2024
2	B	0.33	0/644	0.60	1/862 (0.1%)
3	C	0.32	0/3024	0.60	4/4061 (0.1%)
4	E	0.31	0/1645	0.56	1/2215 (0.0%)
All	All	0.32	0/6821	0.57	6/9162 (0.1%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1160	CYS	CA-CB-SG	7.32	127.18	114.00
3	C	1175	LEU	CB-CG-CD2	-6.01	100.78	111.00
3	C	165	LEU	CA-CB-CG	5.41	127.74	115.30
3	C	1204	CYS	CA-CB-SG	5.31	123.56	114.00
3	C	1019	LEU	CA-CB-CG	5.20	127.27	115.30

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	1486	0	1463	13	0
2	B	637	0	655	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2987	0	3036	51	0
4	E	1610	0	1594	15	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	A	31	0	12	1	0
6	E	31	0	12	3	0
All	All	6784	0	6772	78	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 6.

The worst 5 of 78 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)
3:C:61:ARG:HH22	3:C:113:LYS:HA	1.60	0.65
2:B:495:GLU:HB3	2:B:502:VAL:HG21	1.78	0.65
1:A:221:GLU:O	1:A:225:LYS:HB2	1.97	0.64
3:C:193:LYS:HA	3:C:196:ILE:HB	1.81	0.63
3:C:117:GLN:HA	3:C:122:ASN:HA	1.80	0.63

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 PDB entries followed by that with respect to all EM entries.

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	177/242 (73%)	172 (97%)	5 (3%)	0	100	100
2	B	79/85 (93%)	79 (100%)	0	0	100	100
3	C	371/535 (69%)	340 (92%)	31 (8%)	0	100	100
4	E	196/372 (53%)	191 (97%)	5 (3%)	0	100	100
All	All	823/1234 (67%)	782 (95%)	41 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	157/208 (76%)	156 (99%)	1 (1%)	84	90
2	B	69/72 (96%)	69 (100%)	0	100	100
3	C	334/481 (69%)	331 (99%)	3 (1%)	75	85
4	E	172/327 (53%)	171 (99%)	1 (1%)	84	90
All	All	732/1088 (67%)	727 (99%)	5 (1%)	80	88

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

Mol	Chain	Res	Type
1	A	68	ARG
3	C	1134	CYS
3	C	1165	ARG
3	C	1187	ARG
4	E	1087	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	1248	GLN
4	E	1076	GLN
3	C	1036	GLN
3	C	197	ASN
3	C	1125	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
6	AGS	E	1302	5,4	26,33,33	0.82	1 (3%)	26,52,52	1.28	2 (7%)
6	AGS	A	302	1,5	26,33,33	0.69	0	26,52,52	1.09	2 (7%)

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	AGS	E	1302	5,4	-	4/17/38/38	0/3/3/3
6	AGS	A	302	1,5	-	3/17/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1302	AGS	PG-S1G	2.59	1.96	1.90

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	1302	AGS	PA-O3A-PB	-5.30	114.64	132.83
6	A	302	AGS	PA-O3A-PB	-3.61	120.43	132.83
6	A	302	AGS	C5-C6-N6	2.41	124.01	120.35
6	E	1302	AGS	C5-C6-N6	2.33	123.89	120.35

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

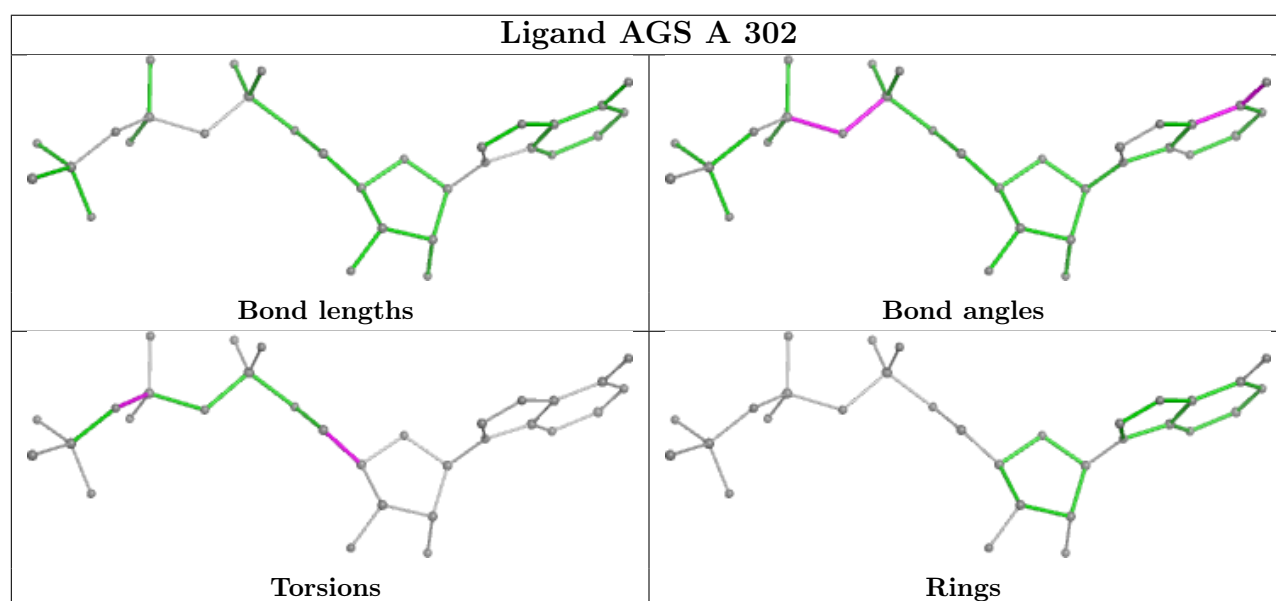
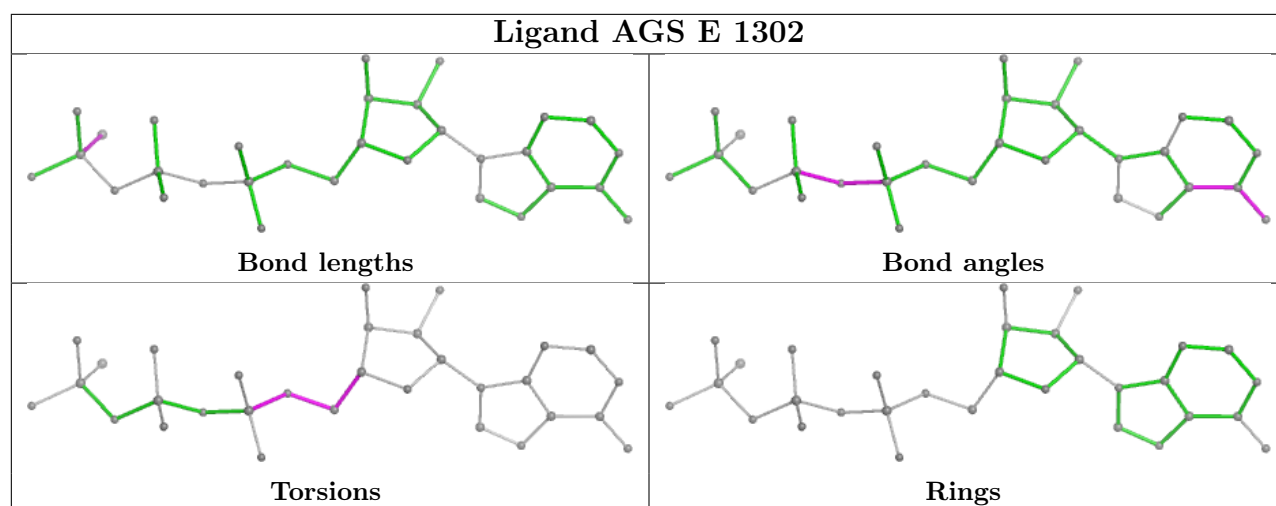
Mol	Chain	Res	Type	Atoms
6	E	1302	AGS	C5'-O5'-PA-O2A
6	E	1302	AGS	C5'-O5'-PA-O3A
6	A	302	AGS	PG-O3B-PB-O1B
6	E	1302	AGS	C4'-C5'-O5'-PA
6	A	302	AGS	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1302	AGS	3	0
6	A	302	AGS	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 Map visualisation

This section contains visualisations of the EMDB entry EMD-4616. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.