



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 29, 2019 – 12:56 PM EDT

PDB ID : 6A05  
Title : Structure of pSTING complex  
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Deposited on : 2018-06-05  
Resolution : 2.20 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

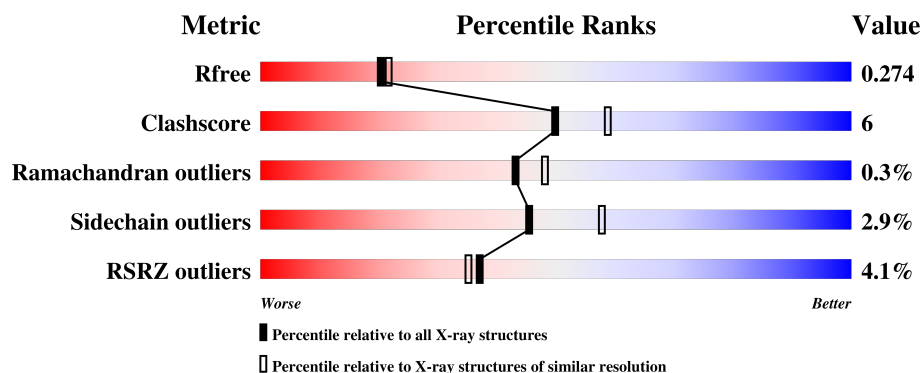
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	201	<div> <div>4%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
1	B	201	<div> <div>3%</div> <div>68%</div> <div>19%</div> <div>• 12%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3018 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.

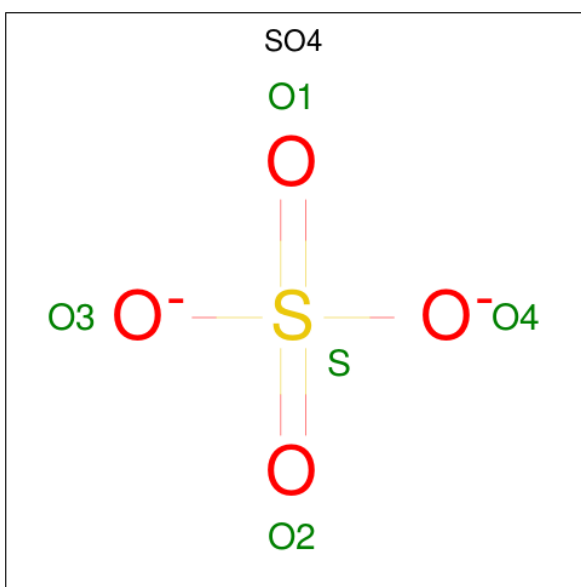
- Molecule 1 is a protein called Stimulator of interferon genes protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	2	0
			1501	944	276	275	6			
1	B	177	Total	C	N	O	S	0	1	0
			1420	898	255	261	6			

There are 22 discrepancies between the modelled and reference sequences:

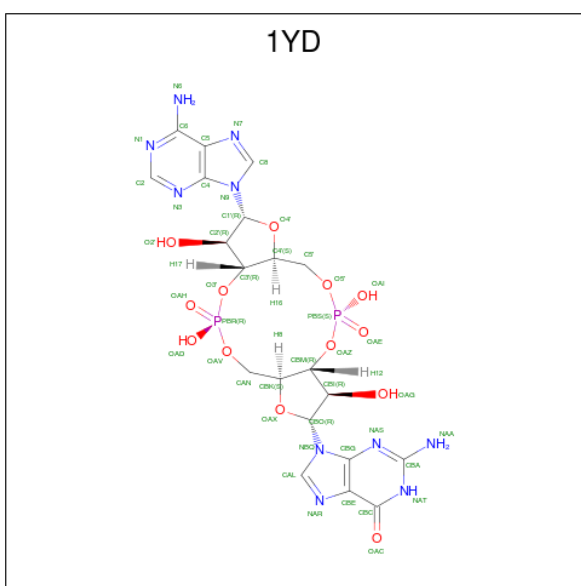
Chain	Residue	Modelled	Actual	Comment	Reference
A	150	ALA	-	expression tag	UNP B8XX90
A	151	ALA	-	expression tag	UNP B8XX90
A	260	GLU	GLY	conflict	UNP B8XX90
A	343	LEU	-	expression tag	UNP B8XX90
A	344	GLU	-	expression tag	UNP B8XX90
A	345	HIS	-	expression tag	UNP B8XX90
A	346	HIS	-	expression tag	UNP B8XX90
A	347	HIS	-	expression tag	UNP B8XX90
A	348	HIS	-	expression tag	UNP B8XX90
A	349	HIS	-	expression tag	UNP B8XX90
A	350	HIS	-	expression tag	UNP B8XX90
B	150	ALA	-	expression tag	UNP B8XX90
B	151	ALA	-	expression tag	UNP B8XX90
B	260	GLU	GLY	conflict	UNP B8XX90
B	343	LEU	-	expression tag	UNP B8XX90
B	344	GLU	-	expression tag	UNP B8XX90
B	345	HIS	-	expression tag	UNP B8XX90
B	346	HIS	-	expression tag	UNP B8XX90
B	347	HIS	-	expression tag	UNP B8XX90
B	348	HIS	-	expression tag	UNP B8XX90
B	349	HIS	-	expression tag	UNP B8XX90
B	350	HIS	-	expression tag	UNP B8XX90

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



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

- Molecule 3 is 2-amino-9-[(2R,3R,3aR,5S,7aS,9R,10R,10aR,12R,14aS)-9-(6-amino-9H-purin-9-yl)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecin-2-yl]-1,9-dihydro-6H-purin-6-one (three-letter code: 1YD) (formula: C<sub>20</sub>H<sub>24</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 45	C 20	N 10	O 13	P 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	16	Total 16	O 16	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.41Å 64.74Å 100.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.38 – 2.20 44.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.38-2.20) 91.1 (44.38-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.20Å)	Xtriage
Refinement program	PHENIX (dev_3092: ???)	Depositor
R, $R_{free}$	0.215 , 0.274 0.215 , 0.274	Depositor DCC
$R_{free}$ test set	1702 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.731	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7511e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: 1YD, SO4

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	0.41	0/1538	0.59	0/2082
1	B	0.41	0/1451	0.59	0/1964
All	All	0.41	0/2989	0.59	0/4046

There are no bond length outliers.

There are no bond angle outliers.

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	1501	0	1481	11	0
1	B	1420	0	1391	27	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	45	0	22	3	0
4	A	21	0	0	1	0
4	B	16	0	0	1	0
All	All	3018	0	2894	37	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.



All (37) 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:B:284:ARG:HH11	1:B:284:ARG:HG2	1.53	0.73
1:B:171:ILE:HD12	1:B:172:LEU:N	2.15	0.61
1:A:155:VAL:HG22	1:B:158:GLY:HA2	1.85	0.57
1:B:169:ARG:HH21	1:B:170:LEU:HD21	1.69	0.57
1:B:167:TYR:O	1:B:171:ILE:HG13	2.05	0.57
3:A:403:1YD:NAT	4:A:502:HOH:O	2.32	0.57
1:B:168:LEU:HA	1:B:171:ILE:HD11	1.86	0.57
1:B:171:ILE:HD12	1:B:172:LEU:H	1.70	0.55
1:A:158:GLY:HA2	1:B:155:VAL:HG22	1.90	0.53
1:A:158:GLY:HA2	1:B:155:VAL:CG2	2.39	0.53
1:B:185:ARG:NH2	4:B:501:HOH:O	2.42	0.51
1:B:284:ARG:NH1	1:B:284:ARG:HG2	2.23	0.51
1:B:186:HIS:HB3	1:B:190:LEU:HB3	1.92	0.50
1:B:226:PRO:O	1:B:227:GLN:HB2	2.12	0.49
1:B:202:PHE:HB3	1:B:313:VAL:HG12	1.96	0.48
1:A:202:PHE:CE1	1:A:311:LEU:HG	2.48	0.48
1:A:332:HIS:O	1:A:336:GLU:HG3	2.14	0.47
1:A:208:VAL:HG21	1:A:266:GLN:HG2	1.95	0.47
1:A:186:HIS:HB3	1:A:190:LEU:HB2	1.98	0.46
1:A:320:GLY:C	1:A:322:SER:H	2.18	0.46
1:B:220:ARG:NH2	1:B:248:LEU:HD21	2.30	0.46
1:B:303:PRO:HD2	1:B:304:GLU:OE1	2.17	0.45
1:B:304:GLU:HG2	1:B:305:ALA:H	1.82	0.45
1:A:249:GLU:HG3	1:A:327:GLN:OE1	2.17	0.44
1:B:208:VAL:HG13	1:B:261:TYR:CG	2.52	0.44
1:B:314:TYR:HE2	1:B:318:THR:HG22	1.82	0.44
1:B:183:ASN:HB3	1:B:187:LYS:NZ	2.33	0.43
1:A:175:LEU:HD22	1:A:198:LEU:HB2	2.01	0.43
1:B:201:LEU:HD21	1:B:259:LEU:HD11	2.01	0.43
1:B:332:HIS:O	1:B:336:GLU:HG3	2.19	0.42
1:A:165:ILE:HG21	1:B:267:THR:HA	2.00	0.42
1:B:331:ARG:HH11	1:B:331:ARG:HG2	1.85	0.42
1:B:336:GLU:O	1:B:340:VAL:HG23	2.20	0.41
3:A:403:1YD:H6	3:A:403:1YD:OAI	2.19	0.41
3:A:403:1YD:C8	3:A:403:1YD:H16	2.51	0.41
1:B:204:LEU:HD11	1:B:292[B]:CYS:SG	2.60	0.41
1:B:282:GLU:OE2	1:B:282:GLU:N	2.53	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/201 (93%)	172 (92%)	14 (8%)	1 (0%)	31	33
1	B	170/201 (85%)	163 (96%)	7 (4%)	0	100	100
All	All	357/402 (89%)	335 (94%)	21 (6%)	1 (0%)	43	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	GLU

### 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 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	159/169 (94%)	156 (98%)	3 (2%)	60	74
1	B	152/169 (90%)	146 (96%)	6 (4%)	35	44
All	All	311/338 (92%)	302 (97%)	9 (3%)	45	58

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	LEU
1	A	222	LEU
1	A	229	SER
1	B	187	LYS
1	B	202	PHE

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Mol	Chain	Res	Type
1	B	238	ARG
1	B	281	ARG
1	B	286	GLU
1	B	301	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	$\# Z  > 2$
2	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.30	0
2	SO4	A	402	-	4,4,4	0.17	0	6,6,6	0.08	0
3	1YD	A	403	-	42,51,51	0.91	2 (4%)	50,80,80	2.66	18 (36%)
2	SO4	B	401	-	4,4,4	0.19	0	6,6,6	0.21	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
3	1YD	A	403	-	-	12/22/62/62	0/6/7/7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	1YD	C8-N7	-2.76	1.29	1.34
3	A	403	1YD	CAL-NAR	-2.51	1.30	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	1YD	C4'-O4'-C1'	-9.95	99.45	109.83
3	A	403	1YD	CBK-OAX-CBO	-4.98	104.63	109.83
3	A	403	1YD	CBA-NAS-CBG	4.77	120.80	115.36
3	A	403	1YD	C2'-C3'-C4'	-4.70	94.88	103.22
3	A	403	1YD	CBE-CBC-NAT	-4.10	117.76	123.47
3	A	403	1YD	PBR-O3'-C3'	4.05	134.15	119.41
3	A	403	1YD	N3-C2-N1	-3.96	122.30	128.68
3	A	403	1YD	PBS-OAZ-CBM	3.72	132.94	119.41
3	A	403	1YD	NAS-CBA-NAT	-3.49	122.53	127.25
3	A	403	1YD	CBI-CBM-CBK	-3.37	97.24	103.22
3	A	403	1YD	CBC-NAT-CBA	2.97	120.29	116.06
3	A	403	1YD	CBG-CBE-NAR	-2.80	106.48	109.40
3	A	403	1YD	OAV-CAN-CBK	-2.77	99.45	108.99
3	A	403	1YD	O5'-C5'-C4'	-2.73	99.56	108.99
3	A	403	1YD	C3'-C2'-C1'	2.61	105.68	99.89
3	A	403	1YD	CBM-CBI-CBO	2.53	105.50	99.89
3	A	403	1YD	OAI-PBS-OAZ	2.41	116.31	106.78
3	A	403	1YD	OAG-CBI-CBM	-2.33	104.55	111.15

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	1YD	CBI-CBM-OAZ-PBS
3	A	403	1YD	CBM-OAZ-PBS-OAI
3	A	403	1YD	CBM-OAZ-PBS-OAE
3	A	403	1YD	C5'-O5'-PBS-OAE

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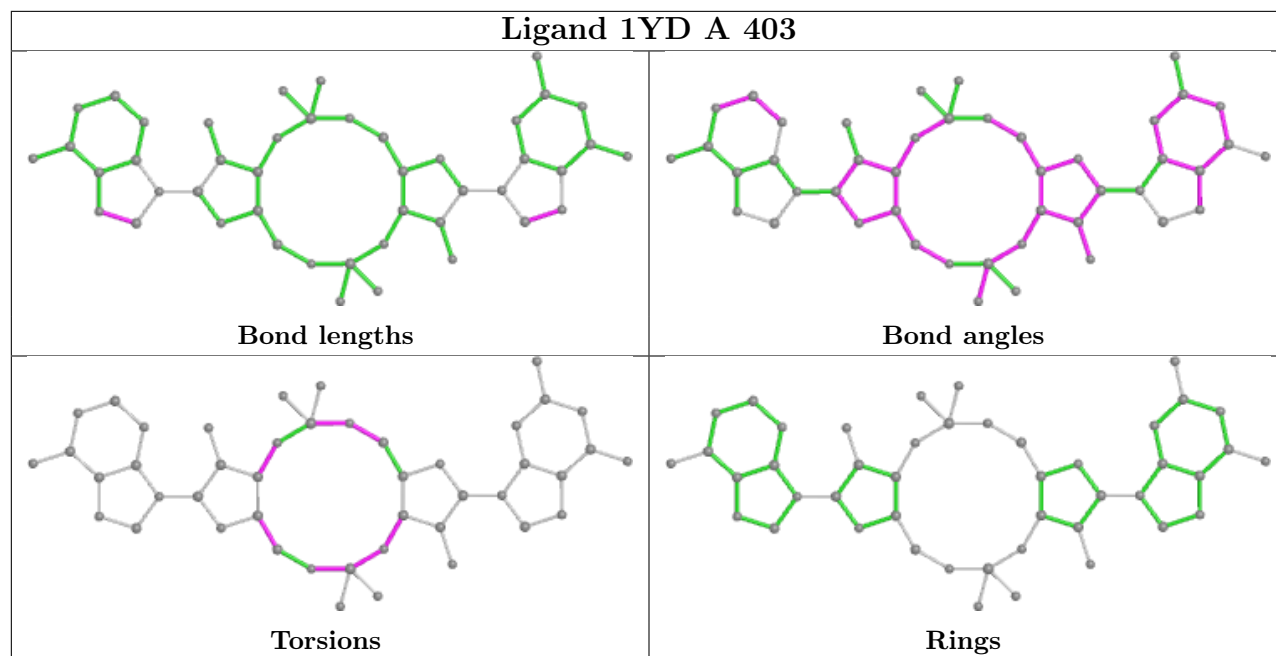
Mol	Chain	Res	Type	Atoms
3	A	403	1YD	C3'-C4'-C5'-O5'
3	A	403	1YD	C2'-C3'-O3'-PBR
3	A	403	1YD	CAN-OAV-PBR-O3'
3	A	403	1YD	C5'-O5'-PBS-OAZ
3	A	403	1YD	CBM-OAZ-PBS-O5'
3	A	403	1YD	CAN-OAV-PBR-OAD
3	A	403	1YD	CBK-CAN-OAV-PBR
3	A	403	1YD	CAN-OAV-PBR-OAH

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403	1YD	3	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	187/201 (93%)	0.06	8 (4%) 35 33	31, 44, 69, 83	0
1	B	177/201 (88%)	0.14	7 (3%) 38 36	28, 45, 71, 81	0
All	All	364/402 (90%)	0.10	15 (4%) 37 35	28, 45, 70, 83	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	THR	5.4
1	B	340	VAL	3.9
1	B	320	GLY	3.6
1	B	237	GLY	3.4
1	B	278	GLY	3.2
1	A	317	PRO	2.7
1	B	153	PHE	2.5
1	A	222	LEU	2.5
1	A	187	LYS	2.3
1	A	337	GLU	2.2
1	B	187	LYS	2.2
1	A	320	GLY	2.2
1	A	282	GLU	2.1
1	A	277	ALA	2.1
1	A	318	THR	2.0

### 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 carbohydrates in this entry.

## 6.4 Ligands

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.

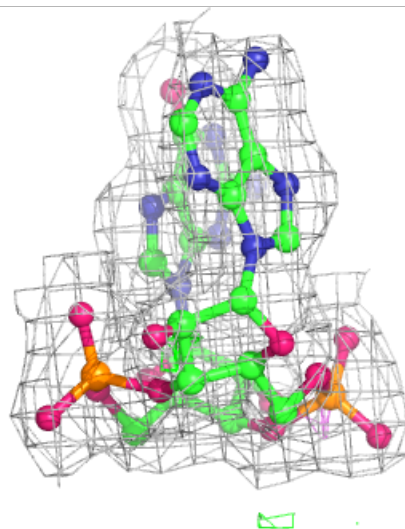
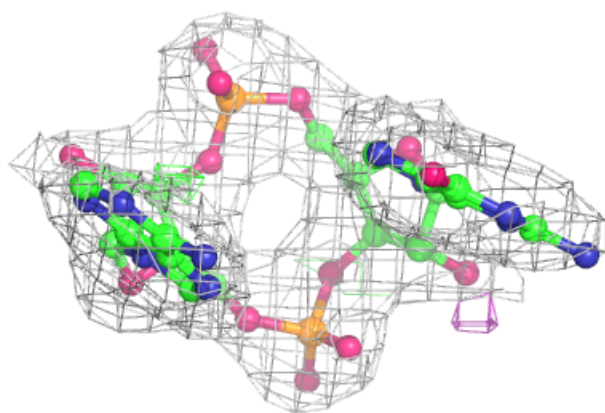
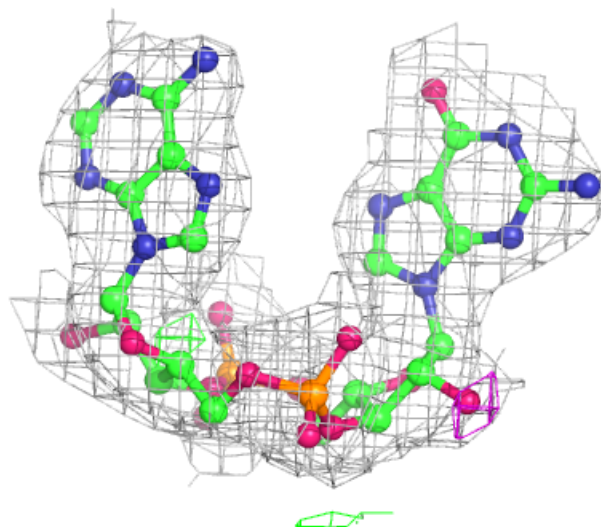
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	401	5/5	0.86	0.16	61,79,89,95	0
2	SO4	A	402	5/5	0.90	0.18	66,75,81,89	0
3	1YD	A	403	45/45	0.94	0.11	30,41,46,48	0
2	SO4	A	401	5/5	0.95	0.08	56,57,62,71	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around 1YD A 403:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.