



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 10, 2025 – 10:09 am BST

PDB ID : 8R66 / pdb_00008r66
Title : Crystal structure of ThsA Macro domain in complex with signaling molecule
Authors : Tamulaitiene, G.; Sabonis, D.
Deposited on : 2023-11-21
Resolution : 2.23 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

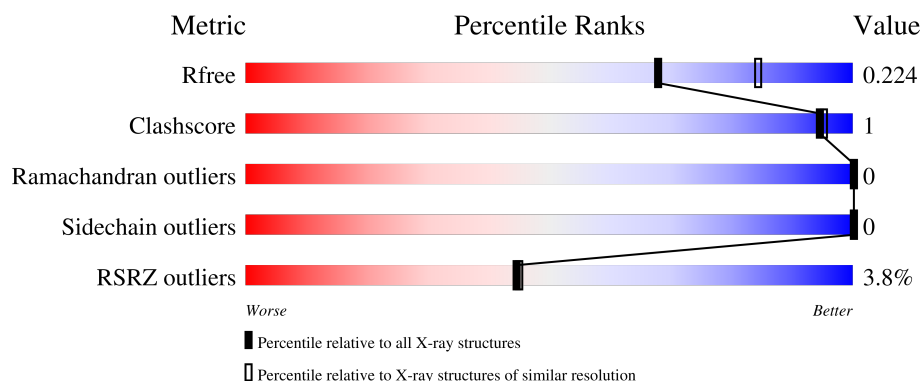
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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}	164625	3139 (2.26-2.22)
Clashscore	180529	3381 (2.26-2.22)
Ramachandran outliers	177936	3334 (2.26-2.22)
Sidechain outliers	177891	3335 (2.26-2.22)
RSRZ outliers	164620	3138 (2.26-2.22)

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	253	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>•</div> <div>17%</div> </div> </div>
1	B	253	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>•</div> <div>18%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3614 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 Thoeris protein ThsA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	4	0
			1757	1130	296	327	4			
1	B	207	Total	C	N	O	S	0	3	0
			1678	1075	288	311	4			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	-	initiating methionine	UNP I2C645
A	82	GLY	-	expression tag	UNP I2C645
A	298	VAL	-	expression tag	UNP I2C645
A	299	ASP	-	expression tag	UNP I2C645
A	300	THR	-	expression tag	UNP I2C645
A	301	GLY	-	expression tag	UNP I2C645
A	302	ASN	-	expression tag	UNP I2C645
A	303	GLY	-	expression tag	UNP I2C645
A	304	SER	-	expression tag	UNP I2C645
A	305	ALA	-	expression tag	UNP I2C645
A	306	TRP	-	expression tag	UNP I2C645
A	307	SER	-	expression tag	UNP I2C645
A	308	HIS	-	expression tag	UNP I2C645
A	309	PRO	-	expression tag	UNP I2C645
A	310	GLN	-	expression tag	UNP I2C645
A	311	PHE	-	expression tag	UNP I2C645
A	312	GLU	-	expression tag	UNP I2C645
A	313	LYS	-	expression tag	UNP I2C645
A	314	GLY	-	expression tag	UNP I2C645
A	315	GLY	-	expression tag	UNP I2C645
A	316	GLY	-	expression tag	UNP I2C645
A	317	SER	-	expression tag	UNP I2C645
A	318	GLY	-	expression tag	UNP I2C645
A	319	GLY	-	expression tag	UNP I2C645
A	320	GLY	-	expression tag	UNP I2C645

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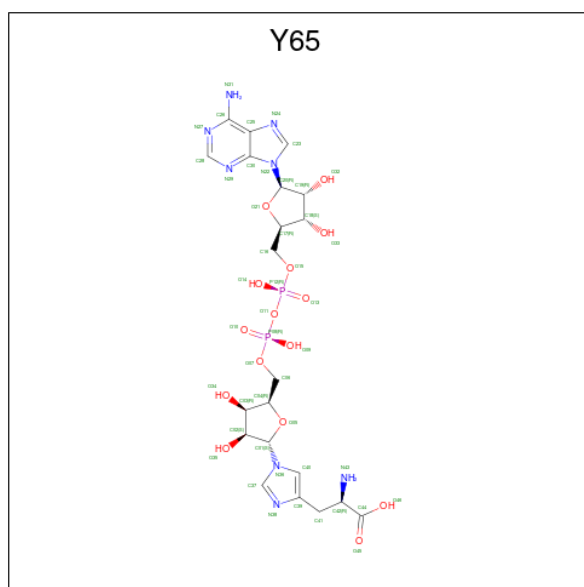
Chain	Residue	Modelled	Actual	Comment	Reference
A	321	SER	-	expression tag	UNP I2C645
A	322	GLY	-	expression tag	UNP I2C645
A	323	GLY	-	expression tag	UNP I2C645
A	324	SER	-	expression tag	UNP I2C645
A	325	ALA	-	expression tag	UNP I2C645
A	326	TRP	-	expression tag	UNP I2C645
A	327	SER	-	expression tag	UNP I2C645
A	328	HIS	-	expression tag	UNP I2C645
A	329	PRO	-	expression tag	UNP I2C645
A	330	GLN	-	expression tag	UNP I2C645
A	331	PHE	-	expression tag	UNP I2C645
A	332	GLU	-	expression tag	UNP I2C645
A	333	LYS	-	expression tag	UNP I2C645
B	81	MET	-	initiating methionine	UNP I2C645
B	82	GLY	-	expression tag	UNP I2C645
B	298	VAL	-	expression tag	UNP I2C645
B	299	ASP	-	expression tag	UNP I2C645
B	300	THR	-	expression tag	UNP I2C645
B	301	GLY	-	expression tag	UNP I2C645
B	302	ASN	-	expression tag	UNP I2C645
B	303	GLY	-	expression tag	UNP I2C645
B	304	SER	-	expression tag	UNP I2C645
B	305	ALA	-	expression tag	UNP I2C645
B	306	TRP	-	expression tag	UNP I2C645
B	307	SER	-	expression tag	UNP I2C645
B	308	HIS	-	expression tag	UNP I2C645
B	309	PRO	-	expression tag	UNP I2C645
B	310	GLN	-	expression tag	UNP I2C645
B	311	PHE	-	expression tag	UNP I2C645
B	312	GLU	-	expression tag	UNP I2C645
B	313	LYS	-	expression tag	UNP I2C645
B	314	GLY	-	expression tag	UNP I2C645
B	315	GLY	-	expression tag	UNP I2C645
B	316	GLY	-	expression tag	UNP I2C645
B	317	SER	-	expression tag	UNP I2C645
B	318	GLY	-	expression tag	UNP I2C645
B	319	GLY	-	expression tag	UNP I2C645
B	320	GLY	-	expression tag	UNP I2C645
B	321	SER	-	expression tag	UNP I2C645
B	322	GLY	-	expression tag	UNP I2C645
B	323	GLY	-	expression tag	UNP I2C645
B	324	SER	-	expression tag	UNP I2C645

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Chain	Residue	Modelled	Actual	Comment	Reference
B	325	ALA	-	expression tag	UNP I2C645
B	326	TRP	-	expression tag	UNP I2C645
B	327	SER	-	expression tag	UNP I2C645
B	328	HIS	-	expression tag	UNP I2C645
B	329	PRO	-	expression tag	UNP I2C645
B	330	GLN	-	expression tag	UNP I2C645
B	331	PHE	-	expression tag	UNP I2C645
B	332	GLU	-	expression tag	UNP I2C645
B	333	LYS	-	expression tag	UNP I2C645

- Molecule 2 is (2 {S})-3-[1-[(2 {R},3 {R},4 {S},5 {R})-5-[[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxymethyl]-3,4-bis(oxidanyl)oxolan-2-yl]imidazol-4-yl]-2-azanyl-propanoic acid (CCD ID: Y65) (formula: C₂₁H₃₀N₈O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			46	21	8	15	2	
2	B	1	Total	C	N	O	P	0
			46	21	8	15	2	

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

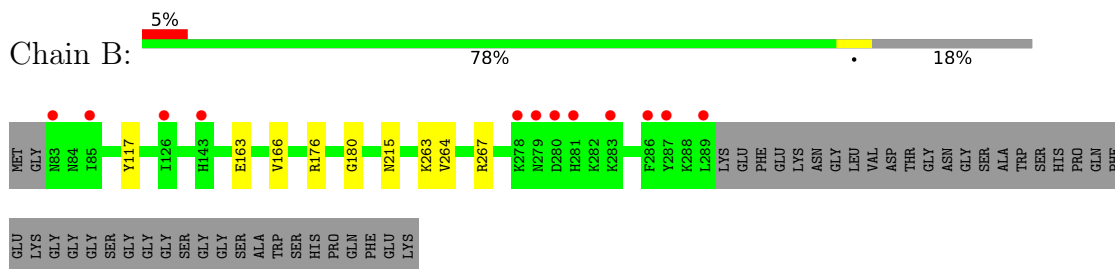


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	39	Total	O	0	0
			39	39		

- Molecule 1: Thoeris protein ThsA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.30Å 71.06Å 51.96Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	69.66 – 2.23 69.66 – 2.23	Depositor EDS
% Data completeness (in resolution range)	95.7 (69.66-2.23) 97.6 (69.66-2.23)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.185 , 0.226 0.185 , 0.224	Depositor DCC
R_{free} test set	2438 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.903	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3614	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.81% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, Y65

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	0.26	0/1792	0.48	0/2418
1	B	0.26	0/1710	0.48	0/2313
All	All	0.26	0/3502	0.48	0/4731

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	1757	0	1729	4	0
1	B	1678	0	1633	6	0
2	A	46	0	0	0	0
2	B	46	0	0	0	0
3	A	5	0	0	0	0
4	A	43	0	0	0	0
4	B	39	0	0	0	0
All	All	3614	0	3362	8	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 1.

All (8) 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:163:GLU:OE1	1:A:176:ARG:NH1	2.39	0.55
1:A:182:VAL:HG22	1:A:191:VAL:HG22	1.89	0.54
1:A:250:GLU:OE2	1:B:267:ARG:NH1	2.43	0.50
1:B:263:LYS:HE2	1:B:263:LYS:HB3	1.67	0.48
1:B:163:GLU:OE1	1:B:176:ARG:NH1	2.50	0.45
1:B:117:TYR:CE1	1:B:166:VAL:HG21	2.52	0.44
1:A:206:LEU:HD21	1:B:264:VAL:HB	2.03	0.41
1:B:180:GLY:HA3	1:B:215[A]:ASN:HB3	2.03	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	213/253 (84%)	207 (97%)	6 (3%)	0	100	100
1	B	208/253 (82%)	199 (96%)	9 (4%)	0	100	100
All	All	421/506 (83%)	406 (96%)	15 (4%)	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 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	192/223 (86%)	192 (100%)	0	100	100
1	B	179/223 (80%)	179 (100%)	0	100	100
All	All	371/446 (83%)	371 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

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 ⓘ

3 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	Y65	A	401	-	41,50,50	1.08	5 (12%)	46,76,76	1.10	2 (4%)
2	Y65	B	401	-	41,50,50	1.07	5 (12%)	46,76,76	1.10	2 (4%)
3	SO4	A	402	-	4,4,4	0.29	0	6,6,6	0.06	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
2	Y65	A	401	-	-	7/26/66/66	0/5/5/5
2	Y65	B	401	-	-	6/26/66/66	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	Y65	O21-C20	2.65	1.44	1.41
2	B	401	Y65	O21-C20	2.64	1.44	1.41
2	A	401	Y65	O05-C01	2.60	1.44	1.41
2	A	401	Y65	C25-N24	-2.60	1.30	1.39
2	A	401	Y65	C23-N24	-2.60	1.30	1.34
2	B	401	Y65	C25-N24	-2.58	1.30	1.39
2	B	401	Y65	C23-N24	-2.57	1.30	1.34
2	B	401	Y65	O05-C01	2.55	1.44	1.41
2	A	401	Y65	C26-N31	2.29	1.42	1.34
2	B	401	Y65	C26-N31	2.29	1.42	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	Y65	N29-C28-N27	-5.00	120.87	128.68
2	B	401	Y65	N29-C28-N27	-4.98	120.90	128.68
2	B	401	Y65	P12-O11-P08	-2.40	124.59	132.83
2	A	401	Y65	P12-O11-P08	-2.15	125.43	132.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	Y65	C39-C41-C42-C44
2	A	401	Y65	C39-C41-C42-N43
2	B	401	Y65	C39-C41-C42-C44
2	B	401	Y65	C39-C41-C42-N43
2	A	401	Y65	N38-C39-C41-C42
2	B	401	Y65	N38-C39-C41-C42
2	B	401	Y65	O05-C04-C06-O07
2	A	401	Y65	P08-O11-P12-O14
2	A	401	Y65	C16-O15-P12-O13

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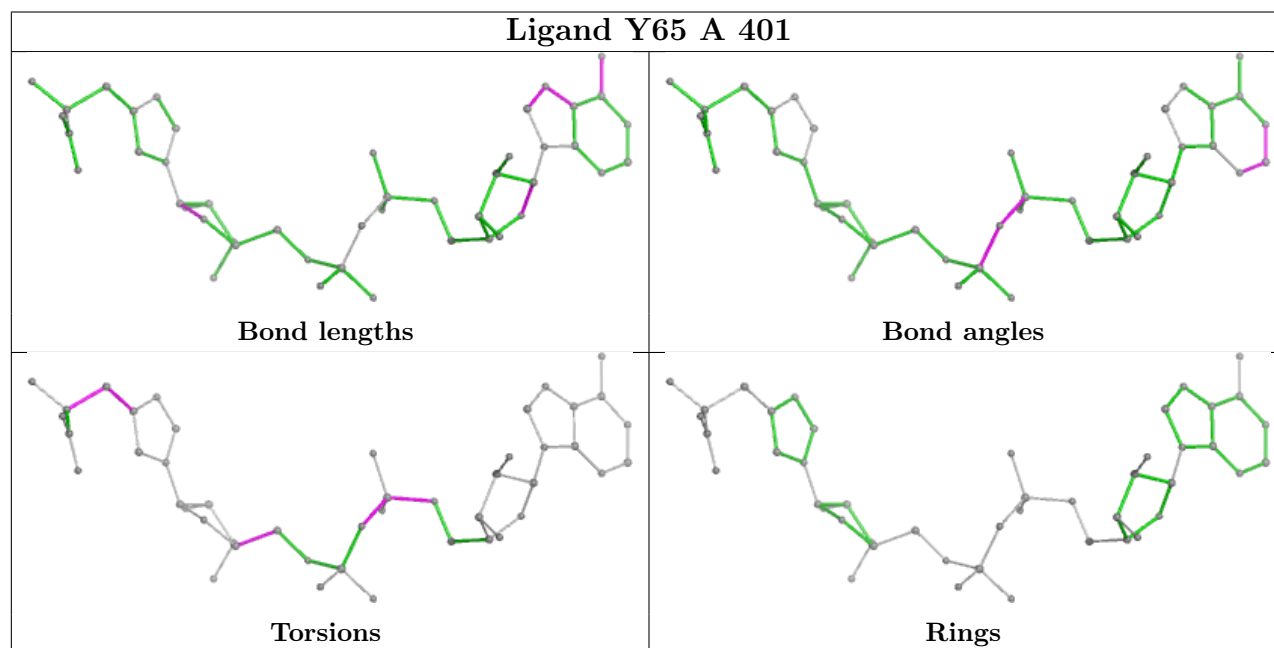
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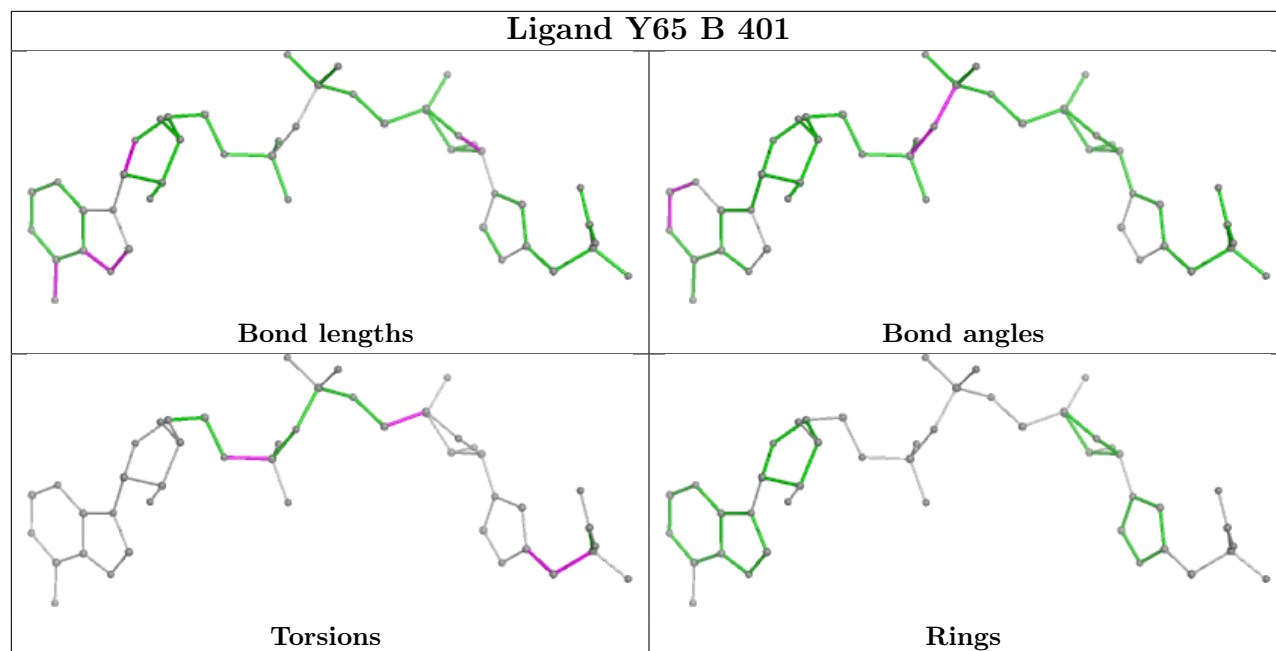
Mol	Chain	Res	Type	Atoms
2	B	401	Y65	C16-O15-P12-O13
2	A	401	Y65	O05-C04-C06-O07
2	A	401	Y65	C40-C39-C41-C42
2	B	401	Y65	C40-C39-C41-C42

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 [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, 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	211/253 (83%)	0.24	4 (1%) 66 66	23, 51, 79, 93	4 (1%)
1	B	207/253 (81%)	0.29	12 (5%) 30 30	23, 51, 93, 108	3 (1%)
All	All	418/506 (82%)	0.27	16 (3%) 44 45	23, 51, 89, 108	7 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	HIS	4.8
1	A	83	ASN	4.5
1	B	279	ASN	3.4
1	B	83	ASN	3.4
1	B	280	ASP	3.4
1	B	289	LEU	3.1
1	A	165[A]	ASN	2.9
1	B	278	LYS	2.8
1	B	286	PHE	2.8
1	B	283	LYS	2.6
1	A	85	ILE	2.5
1	A	280	ASP	2.4
1	B	85	ILE	2.4
1	B	287	TYR	2.4
1	B	143[A]	HIS	2.2
1	B	126	ILE	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 monosaccharides in this entry.

6.4 Ligands [i](#)

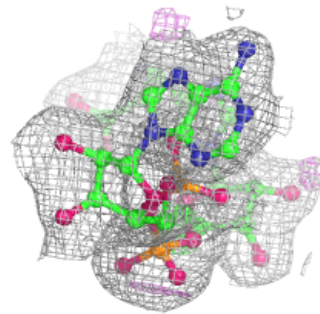
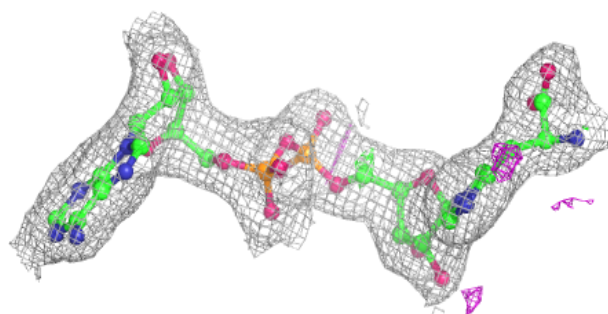
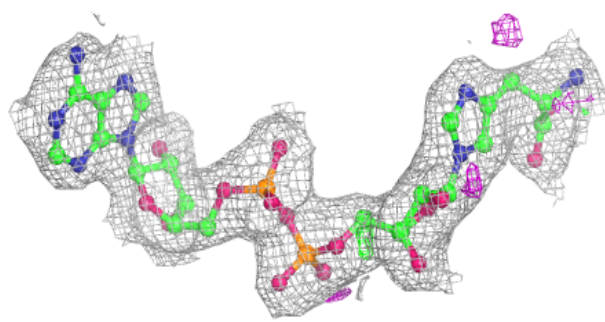
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	402	5/5	0.75	0.11	73,75,94,96	0
2	Y65	B	401	46/46	0.96	0.07	38,50,58,60	0
2	Y65	A	401	46/46	0.97	0.07	36,44,55,59	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.

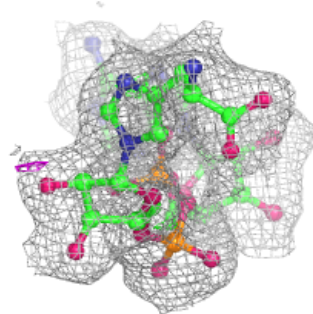
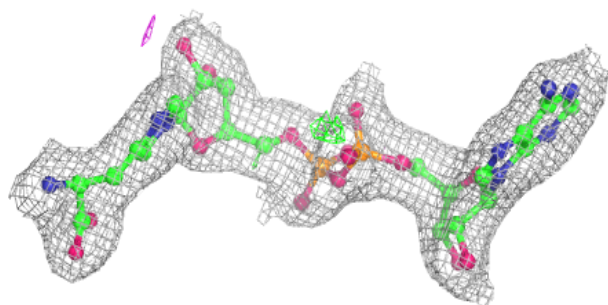
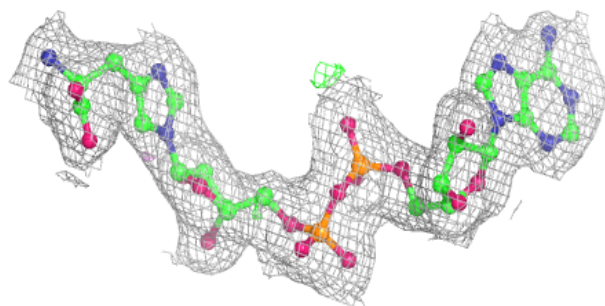
Electron density around Y65 B 401:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Y65 A 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.