



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 08:06 am BST

PDB ID : 6HOY
Title : Human Sirt6 in complex with ADP-ribose and the inhibitor trichostatin A
Authors : You, W.; Steegborn, C.
Deposited on : 2018-09-18
Resolution : 1.70 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 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 : 2.11
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) : 2.11

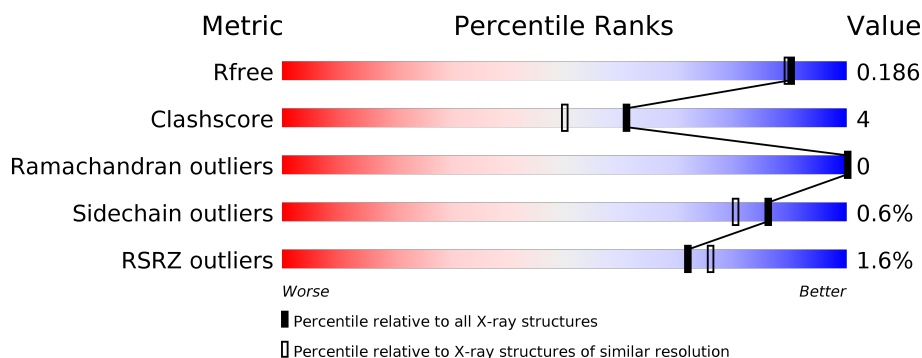
1 Overall quality at a glance

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 on 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	302	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 1%; height: 10px; background-color: red;"></div> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 12%; height: 10px; background-color: yellow;"></div> <div style="width: 7%; height: 10px; background-color: orange;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> </div> </div>
1	B	302	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 81%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 9%; height: 10px; background-color: grey;"></div> </div> </div> </div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 4902 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.

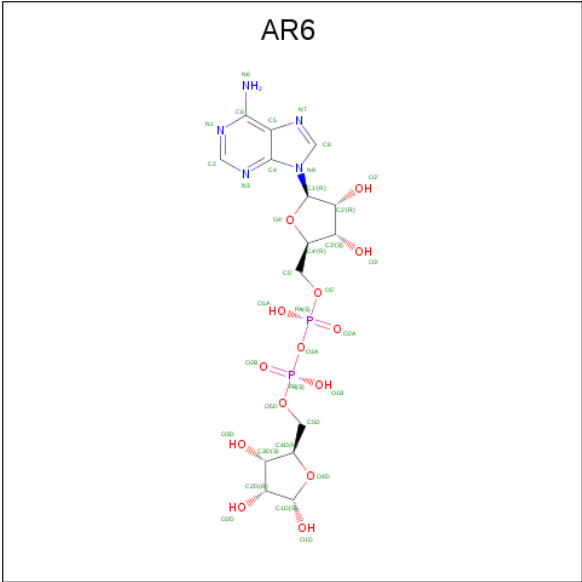
- Molecule 1 is a protein called NAD-dependent protein deacetylase sirtuin-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	4	0
			2210	1393	403	402	12			
1	B	276	Total	C	N	O	S	0	2	0
			2168	1364	400	392	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	GLY	-	expression tag	UNP Q8N6T7
A	8	ILE	-	expression tag	UNP Q8N6T7
A	9	ASP	-	expression tag	UNP Q8N6T7
A	10	PRO	-	expression tag	UNP Q8N6T7
A	11	PHE	-	expression tag	UNP Q8N6T7
A	12	THR	-	expression tag	UNP Q8N6T7
B	7	GLY	-	expression tag	UNP Q8N6T7
B	8	ILE	-	expression tag	UNP Q8N6T7
B	9	ASP	-	expression tag	UNP Q8N6T7
B	10	PRO	-	expression tag	UNP Q8N6T7
B	11	PHE	-	expression tag	UNP Q8N6T7
B	12	THR	-	expression tag	UNP Q8N6T7

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHYDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (three-letter code: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	5	14	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	5	14	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

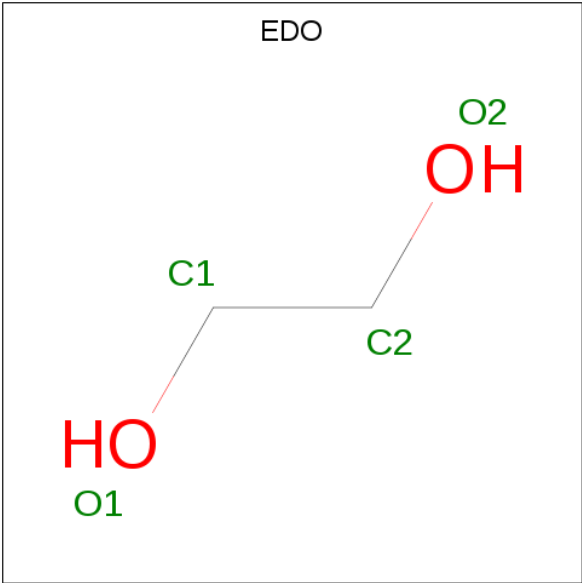
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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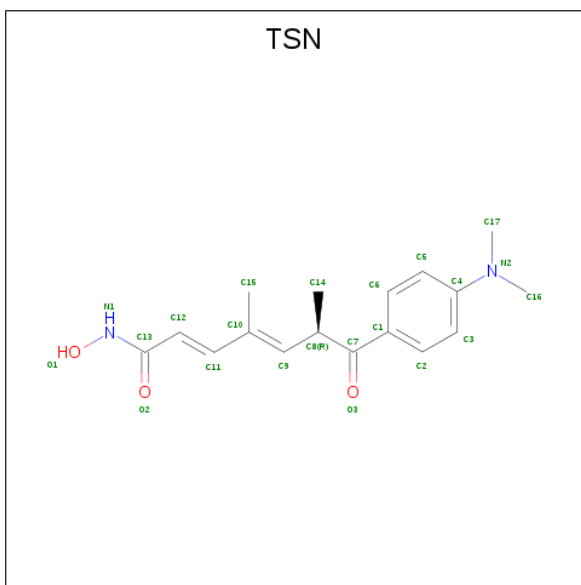
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 7 is TRICHOSTATIN A (three-letter code: TSN) (formula: C₁₇H₂₂N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			22	17	2	3		
7	B	1	Total	C	N	O	0	0
			22	17	2	3		

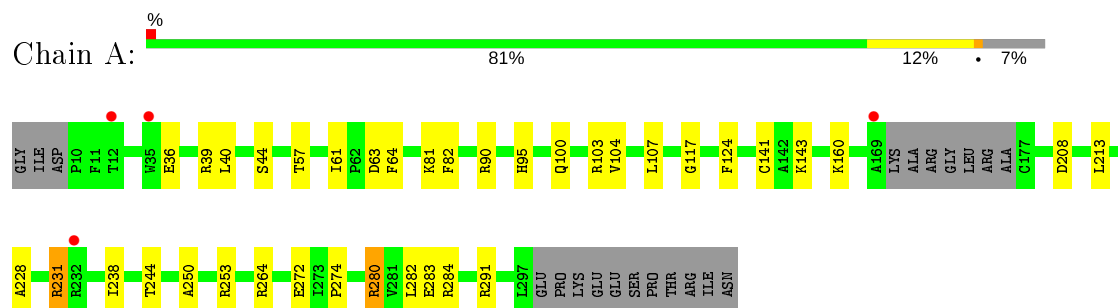
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	180	Total	O	0	0
			180	180		
8	B	153	Total	O	0	0
			153	153		

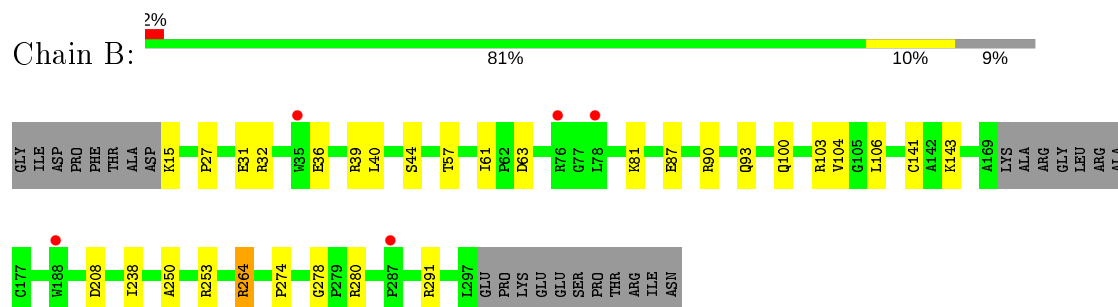
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: NAD-dependent protein deacetylase sirtuin-6



- Molecule 1: NAD-dependent protein deacetylase sirtuin-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	91.29 Å 91.29 Å 143.68 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.65 – 1.70 45.65 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.65-1.70) 99.9 (45.65-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.154 , 0.185 0.161 , 0.186	Depositor DCC
R_{free} test set	2100 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.310 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.684 for H, K, L 0.316 for -K, -H, -L	Depositor
Outliers	0 of 74415 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4902	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: TSN, ZN, AR6, EDO, PG4, 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	1.04	7/2271 (0.3%)	1.38	16/3079 (0.5%)
1	B	0.86	1/2215 (0.0%)	1.35	12/3003 (0.4%)
All	All	0.96	8/4486 (0.2%)	1.36	28/6082 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	GLU	CD-OE2	-8.09	1.16	1.25
1	A	244	THR	C-O	6.68	1.36	1.23
1	A	64	PHE	C-O	6.19	1.35	1.23
1	A	213	LEU	C-O	6.19	1.35	1.23
1	A	95	HIS	CE1-NE2	6.05	1.46	1.32
1	A	282	LEU	C-O	5.83	1.34	1.23
1	B	87	GLU	CD-OE1	5.70	1.31	1.25
1	A	117	GLY	C-O	5.12	1.31	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	NE-CZ-NH2	-20.89	109.86	120.30
1	B	264	ARG	NE-CZ-NH2	18.12	129.36	120.30
1	A	280	ARG	NE-CZ-NH2	-17.75	111.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	NE-CZ-NH1	17.55	129.07	120.30
1	B	253	ARG	NE-CZ-NH1	17.29	128.95	120.30
1	B	264	ARG	NE-CZ-NH1	-17.17	111.71	120.30
1	A	264	ARG	NE-CZ-NH2	-17.12	111.74	120.30
1	A	264	ARG	NE-CZ-NH1	15.89	128.25	120.30
1	A	103	ARG	NE-CZ-NH2	15.50	128.05	120.30
1	A	253	ARG	NE-CZ-NH1	-14.45	113.08	120.30
1	B	280	ARG	NE-CZ-NH1	-14.18	113.21	120.30
1	B	280	ARG	NE-CZ-NH2	14.14	127.37	120.30
1	B	103	ARG	NE-CZ-NH1	14.12	127.36	120.30
1	A	253	ARG	NE-CZ-NH2	13.60	127.10	120.30
1	B	253	ARG	CD-NE-CZ	13.31	142.23	123.60
1	A	280	ARG	CD-NE-CZ	11.08	139.11	123.60
1	B	253	ARG	CG-CD-NE	-10.92	88.87	111.80
1	A	264	ARG	CD-NE-CZ	10.80	138.72	123.60
1	B	264	ARG	CD-NE-CZ	10.52	138.33	123.60
1	B	280	ARG	CD-NE-CZ	9.15	136.41	123.60
1	A	253	ARG	CD-NE-CZ	8.53	135.54	123.60
1	A	264	ARG	CG-CD-NE	-8.07	94.85	111.80
1	A	103	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	B	103	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	A	280	ARG	CG-CD-NE	-5.63	99.98	111.80
1	A	124	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	A	103	ARG	CD-NE-CZ	5.21	130.89	123.60
1	A	244	THR	O-C-N	5.03	130.75	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	82	PHE	Mainchain

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	2210	0	2235	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2168	0	2185	21	0
2	A	36	0	21	1	0
2	B	36	0	21	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	13	0	18	0	0
4	B	13	0	18	0	0
5	A	4	0	6	0	0
5	B	8	0	12	0	0
6	A	20	0	0	1	0
6	B	15	0	0	0	0
7	A	22	0	22	1	0
7	B	22	0	22	1	0
8	A	180	0	0	6	0
8	B	153	0	0	6	0
All	All	4902	0	4560	41	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 4.

All (41) 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:31:GLU:CD	1:B:264:ARG:HH11	1.61	1.04
1:B:31:GLU:OE1	1:B:264:ARG:NH1	1.96	0.97
1:B:31:GLU:CD	1:B:264:ARG:NH1	2.29	0.85
1:A:272[B]:GLU:HG2	8:A:633:HOH:O	1.77	0.84
1:B:31:GLU:OE2	1:B:264:ARG:NH1	2.25	0.67
1:A:280:ARG:HB2	8:A:655:HOH:O	2.00	0.61
1:A:36:GLU:OE2	1:A:39:ARG:NH1	2.34	0.61
1:A:284:ARG:NH2	8:A:502:HOH:O	2.34	0.59
1:B:36:GLU:OE2	1:B:39[A]:ARG:NH1	2.36	0.58
1:A:160:LYS:HE2	8:A:675:HOH:O	2.04	0.58
1:B:44:SER:HB3	1:B:208:ASP:OD1	2.04	0.58
1:B:32:ARG:HD3	8:B:899:HOH:O	2.04	0.57
1:A:280:ARG:NH2	8:A:503:HOH:O	2.38	0.56
1:A:44:SER:HB3	1:A:208:ASP:OD1	2.09	0.53
1:B:90:ARG:NH2	8:B:803:HOH:O	2.40	0.52
1:B:15:LYS:NZ	8:B:804:HOH:O	2.40	0.51
1:A:90:ARG:NH2	8:A:509:HOH:O	2.44	0.50
1:A:57:THR:HA	1:A:61:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASP:OD2	2:A:401:AR6:H8	2.12	0.50
1:A:104:VAL:HB	1:A:291:ARG:HB3	1.94	0.49
7:A:409:TSN:H121	7:A:409:TSN:H151	1.68	0.48
1:B:27:PRO:O	1:B:31:GLU:HG2	2.13	0.48
1:A:40:LEU:O	1:A:44:SER:OG	2.30	0.47
1:B:104:VAL:HB	1:B:291:ARG:HB3	1.95	0.47
1:A:100:GLN:HB2	1:A:274:PRO:HD3	1.97	0.46
1:B:141:CYS:SG	1:B:143:LYS:HB2	2.56	0.46
1:B:57:THR:HA	1:B:61:ILE:O	2.16	0.46
1:A:141:CYS:SG	1:A:143:LYS:HB2	2.56	0.45
1:A:231:ARG:NE	6:A:406:SO4:O4	2.48	0.44
1:B:100:GLN:HB2	1:B:274:PRO:HD3	2.00	0.44
1:B:40:LEU:O	1:B:44:SER:OG	2.28	0.43
1:A:238:ILE:HD12	1:A:250:ALA:HB2	2.00	0.43
1:A:107:LEU:C	1:A:107:LEU:HD23	2.40	0.42
1:B:15:LYS:N	8:B:815:HOH:O	2.52	0.42
1:B:238:ILE:HD12	1:B:250:ALA:HB2	2.02	0.41
1:B:63:ASP:OD2	2:B:702:AR6:H8	2.19	0.41
1:B:93:GLN:NE2	8:B:806:HOH:O	2.54	0.41
1:B:278:GLY:N	8:B:802:HOH:O	2.53	0.41
1:A:228:ALA:O	1:A:231:ARG:HD2	2.21	0.41
7:B:709:TSN:H121	7:B:709:TSN:H151	1.92	0.40
1:B:106:LEU:HA	1:B:106:LEU:HD23	1.86	0.40

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	281/302 (93%)	278 (99%)	3 (1%)	0	100	100
1	B	274/302 (91%)	269 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	555/604 (92%)	547 (99%)	8 (1%)	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	242/256 (94%)	240 (99%)	2 (1%)	81	74
1	B	235/256 (92%)	234 (100%)	1 (0%)	91	87
All	All	477/512 (93%)	474 (99%)	3 (1%)	86	80

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	A	231	ARG
1	B	81	LYS

Some 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 carbohydrates in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	TSN	A	409	-	22,22,22	2.36	7 (31%)	27,29,29	5.31	6 (22%)
6	SO4	A	405	-	4,4,4	0.44	0	6,6,6	0.20	0
6	SO4	B	708	-	4,4,4	0.34	0	6,6,6	0.07	0
2	AR6	B	702	-	34,39,39	0.84	1 (2%)	40,60,60	0.97	2 (5%)
4	PG4	B	704	-	12,12,12	0.28	0	11,11,11	0.12	0
6	SO4	A	406	-	4,4,4	0.37	0	6,6,6	0.08	0
6	SO4	B	707	-	4,4,4	0.48	0	6,6,6	0.17	0
7	TSN	B	709	-	22,22,22	2.54	8 (36%)	27,29,29	2.53	5 (18%)
6	SO4	A	408	-	4,4,4	0.35	0	6,6,6	0.31	0
6	SO4	B	706	-	4,4,4	0.51	0	6,6,6	0.35	0
5	EDO	B	705	-	3,3,3	0.21	0	2,2,2	0.53	0
2	AR6	A	401	-	34,39,39	0.99	1 (2%)	40,60,60	1.14	3 (7%)
6	SO4	A	407	-	4,4,4	0.37	0	6,6,6	0.26	0
4	PG4	A	403	-	12,12,12	0.26	0	11,11,11	0.11	0
5	EDO	B	701	-	3,3,3	0.10	0	2,2,2	0.25	0
5	EDO	A	404	-	3,3,3	0.40	0	2,2,2	0.65	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
7	TSN	A	409	-	-	3/23/23/23	0/1/1/1
2	AR6	B	702	-	-	2/18/54/54	0/4/4/4
4	PG4	B	704	-	-	7/10/10/10	-
7	TSN	B	709	-	-	5/23/23/23	0/1/1/1
5	EDO	B	705	-	-	1/1/1/1	-
2	AR6	A	401	-	-	2/18/54/54	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	A	403	-	-	4/10/10/10	-
5	EDO	B	701	-	-	1/1/1/1	-
5	EDO	A	404	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	709	TSN	C13-N1	5.46	1.42	1.33
7	A	409	TSN	C8-C9	5.22	1.59	1.51
7	A	409	TSN	O3-C7	-5.04	1.15	1.22
7	A	409	TSN	C4-N2	4.97	1.49	1.37
7	B	709	TSN	C11-C10	4.22	1.55	1.45
7	B	709	TSN	C1-C7	4.05	1.55	1.49
7	B	709	TSN	C4-N2	4.02	1.46	1.37
7	B	709	TSN	O1-N1	-4.00	1.29	1.40
7	B	709	TSN	C8-C9	3.70	1.56	1.51
7	A	409	TSN	C1-C7	3.33	1.54	1.49
7	B	709	TSN	C12-C13	3.30	1.55	1.48
2	B	702	AR6	O4D-C1D	-2.99	1.39	1.43
7	B	709	TSN	O3-C7	-2.84	1.18	1.22
7	A	409	TSN	C11-C10	2.49	1.51	1.45
7	A	409	TSN	C14-C8	2.48	1.57	1.54
2	A	401	AR6	C2-N3	2.13	1.35	1.32
7	A	409	TSN	O1-N1	-2.01	1.35	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	409	TSN	C1-C7-C8	21.21	138.90	119.29
7	A	409	TSN	O3-C7-C1	-11.05	106.38	120.66
7	A	409	TSN	C14-C8-C9	-8.33	102.95	110.75
7	A	409	TSN	O3-C7-C8	-7.89	112.51	119.81
7	B	709	TSN	C1-C7-C8	7.59	126.31	119.29
7	A	409	TSN	C15-C10-C11	-6.22	108.27	118.08
7	B	709	TSN	O3-C7-C8	-5.99	114.26	119.81
7	B	709	TSN	O1-N1-C13	5.51	132.93	119.62
7	B	709	TSN	C14-C8-C9	-4.80	106.25	110.75
7	B	709	TSN	C15-C10-C11	-2.95	113.43	118.08
2	B	702	AR6	C2D-C3D-C4D	-2.35	98.08	102.64
2	B	702	AR6	O5D-PB-O2B	2.28	117.99	109.07
2	A	401	AR6	O2D-C2D-C1D	2.23	117.97	111.82
2	A	401	AR6	O3'-C3'-C2'	-2.14	104.91	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	AR6	O1D-C1D-O4D	2.08	113.79	111.13
7	A	409	TSN	C11-C12-C13	-2.06	117.33	125.72

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	TSN	C1-C7-C8-C9
7	A	409	TSN	C1-C7-C8-C14
7	B	709	TSN	C5-C4-N2-C16
7	B	709	TSN	C3-C4-N2-C17
7	B	709	TSN	C3-C4-N2-C16
7	B	709	TSN	C5-C4-N2-C17
4	A	403	PG4	O3-C5-C6-O4
4	B	704	PG4	O2-C3-C4-O3
4	B	704	PG4	O4-C7-C8-O5
5	A	404	EDO	O1-C1-C2-O2
4	B	704	PG4	O3-C5-C6-O4
4	A	403	PG4	C8-C7-O4-C6
5	B	701	EDO	O1-C1-C2-O2
7	B	709	TSN	C7-C8-C9-C10
4	B	704	PG4	O1-C1-C2-O2
4	B	704	PG4	C6-C5-O3-C4
4	B	704	PG4	C3-C4-O3-C5
2	B	702	AR6	O4'-C4'-C5'-O5'
4	A	403	PG4	O2-C3-C4-O3
4	A	403	PG4	C4-C3-O2-C2
5	B	705	EDO	O1-C1-C2-O2
4	B	704	PG4	C4-C3-O2-C2
2	A	401	AR6	O4'-C4'-C5'-O5'
2	B	702	AR6	C5D-O5D-PB-O2B
2	A	401	AR6	C5D-O5D-PB-O2B
7	A	409	TSN	O3-C7-C8-C9

There are no ring outliers.

5 monomers are involved in 5 short contacts:

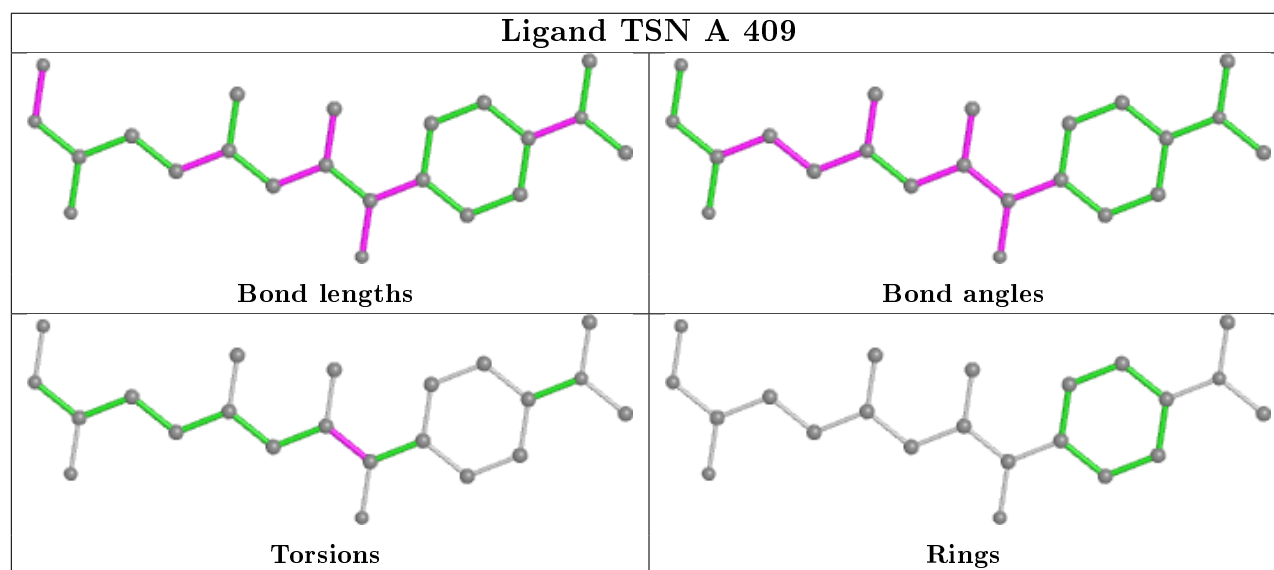
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	409	TSN	1	0
2	B	702	AR6	1	0
6	A	406	SO4	1	0

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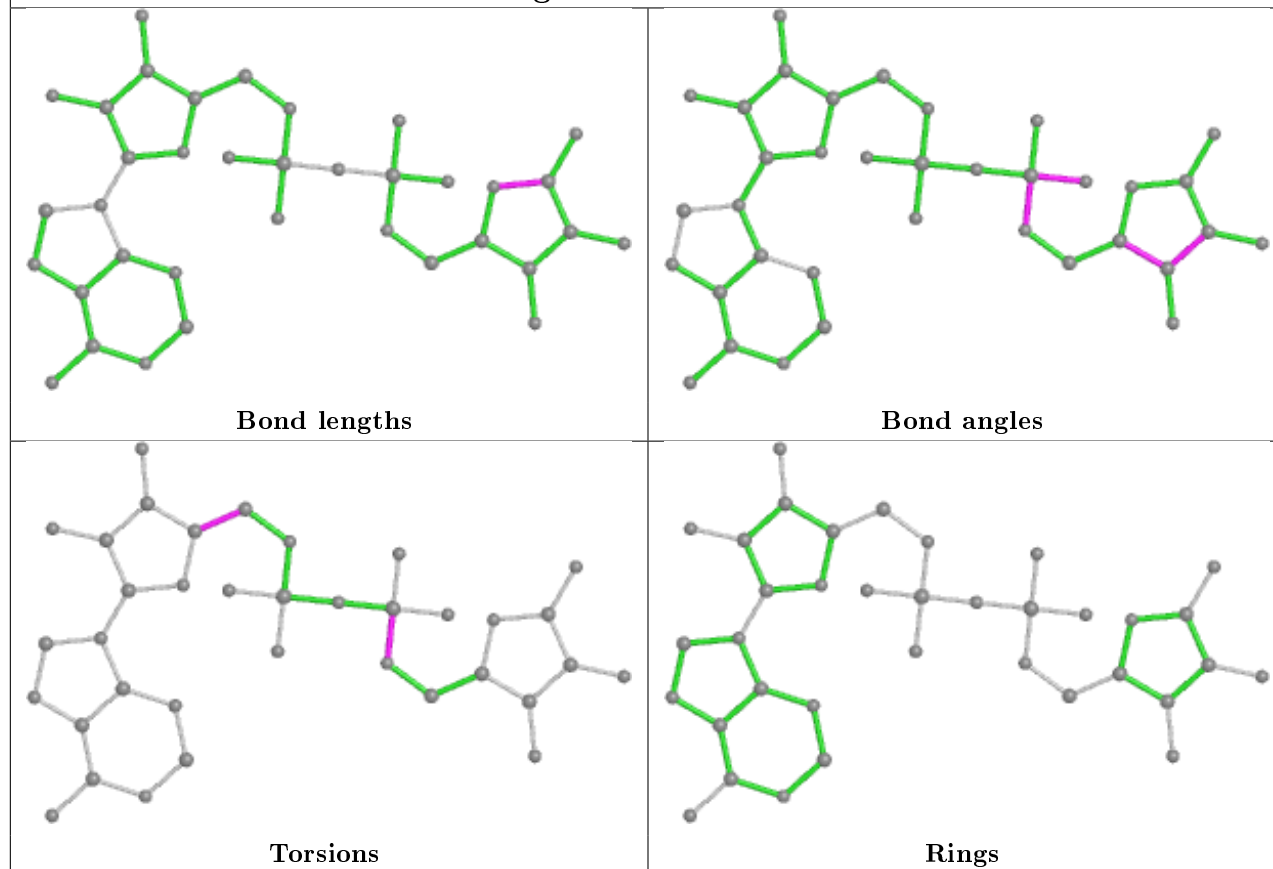
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	709	TSN	1	0
2	A	401	AR6	1	0

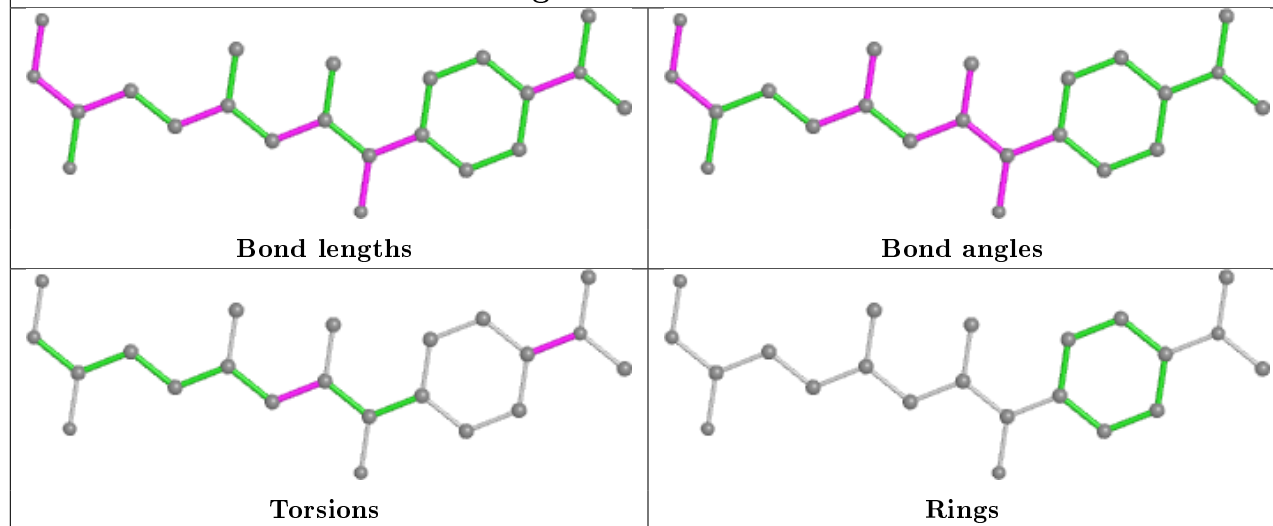
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

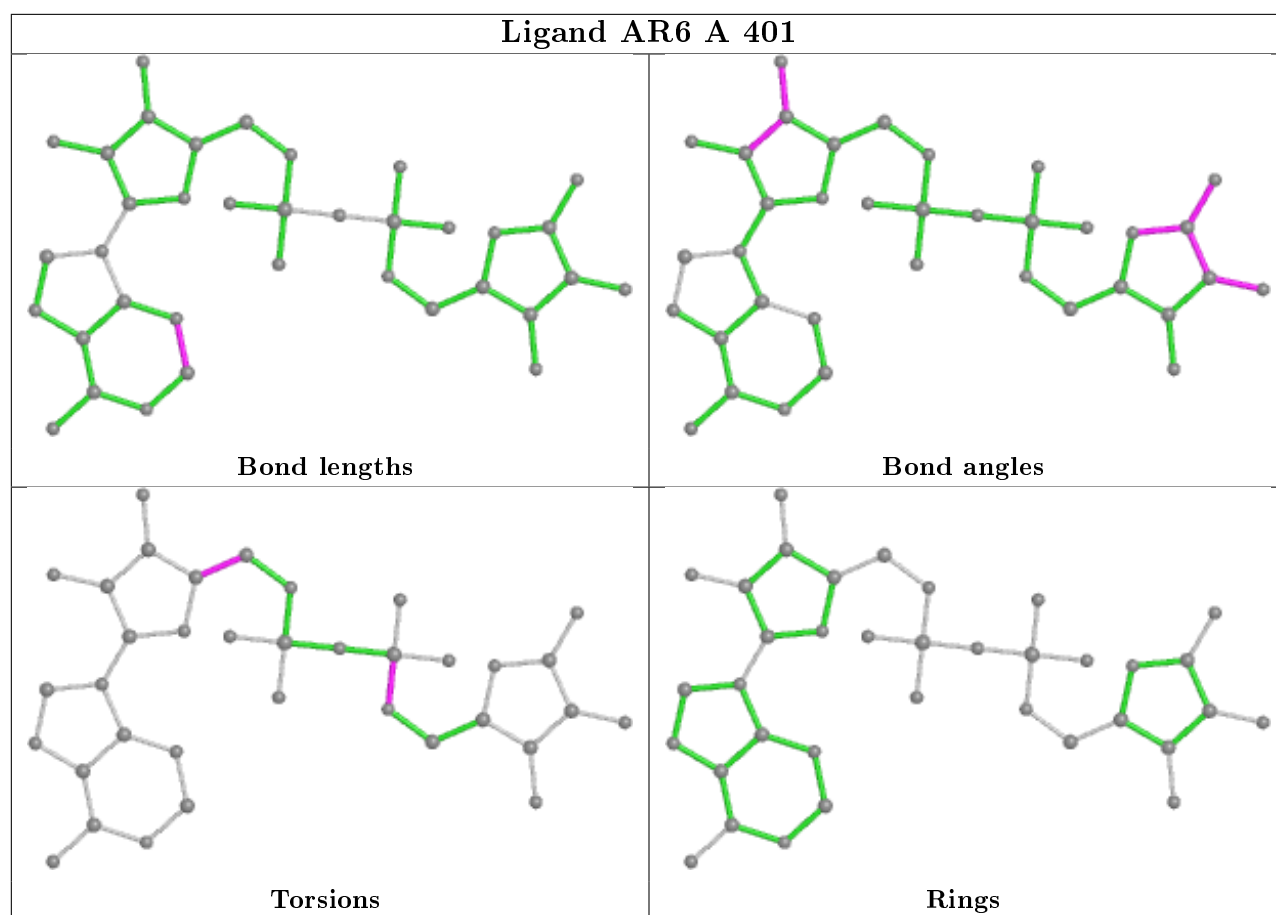


Ligand AR6 B 702



Ligand TSN B 709





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	281/302 (93%)	-0.22	4 (1%) 75 79	18, 29, 51, 70	0
1	B	276/302 (91%)	-0.13	5 (1%) 68 72	22, 36, 60, 77	0
All	All	557/604 (92%)	-0.17	9 (1%) 72 76	18, 33, 57, 77	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	35	TRP	4.2
1	B	188	TRP	3.8
1	A	169	ALA	3.6
1	A	35	TRP	2.9
1	B	78	LEU	2.9
1	A	12	THR	2.8
1	B	287	PRO	2.4
1	B	76	ARG	2.3
1	A	232	ARG	2.1

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 [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,

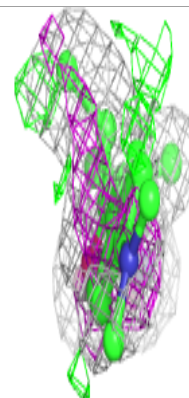
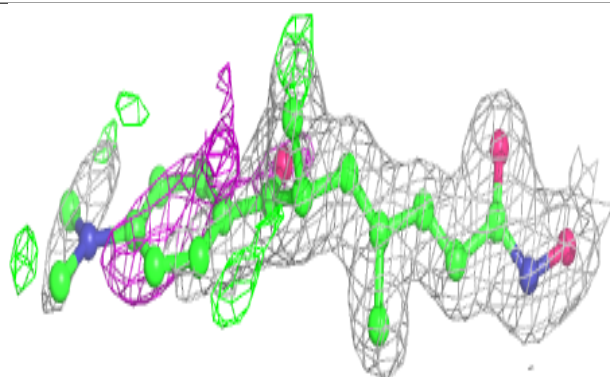
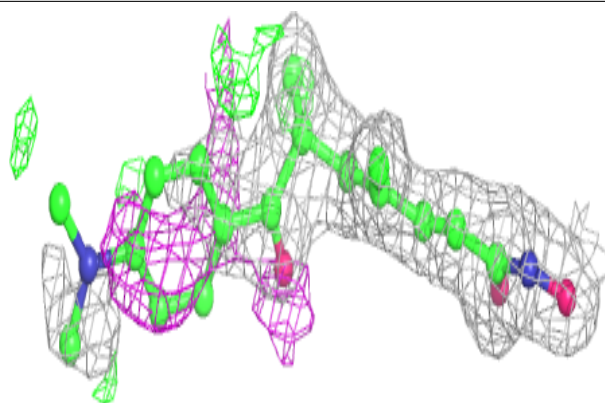
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	B	705	4/4	0.72	0.17	47,55,58,58	0
4	PG4	B	704	13/13	0.73	0.17	64,78,83,85	0
5	EDO	B	701	4/4	0.74	0.15	53,53,58,58	0
4	PG4	A	403	13/13	0.89	0.13	52,63,69,71	0
5	EDO	A	404	4/4	0.89	0.15	37,43,43,46	0
7	TSN	A	409	22/22	0.90	0.19	23,35,79,84	0
7	TSN	B	709	22/22	0.91	0.22	24,43,98,100	0
6	SO4	A	406	5/5	0.95	0.08	82,86,88,90	0
6	SO4	A	407	5/5	0.96	0.12	48,59,67,67	0
3	ZN	A	402	1/1	0.96	0.06	47,47,47,47	0
6	SO4	A	405	5/5	0.96	0.13	46,52,54,60	0
6	SO4	B	708	5/5	0.96	0.12	53,63,66,74	0
6	SO4	A	408	5/5	0.97	0.12	44,47,58,63	0
3	ZN	B	703	1/1	0.97	0.06	52,52,52,52	0
6	SO4	B	707	5/5	0.97	0.10	54,64,71,72	0
2	AR6	B	702	36/36	0.98	0.07	24,30,34,38	0
2	AR6	A	401	36/36	0.98	0.07	20,23,27,27	0
6	SO4	B	706	5/5	0.99	0.07	38,38,47,52	0

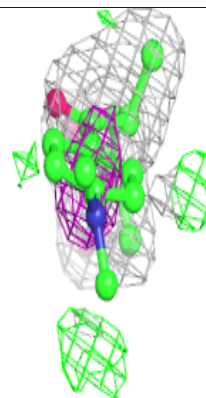
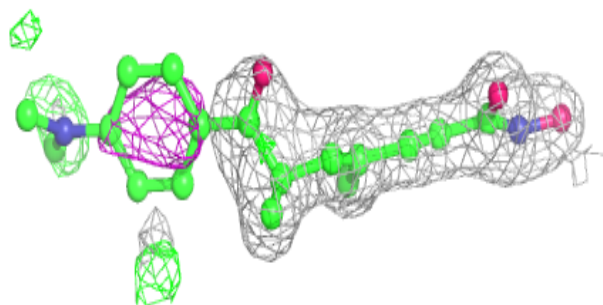
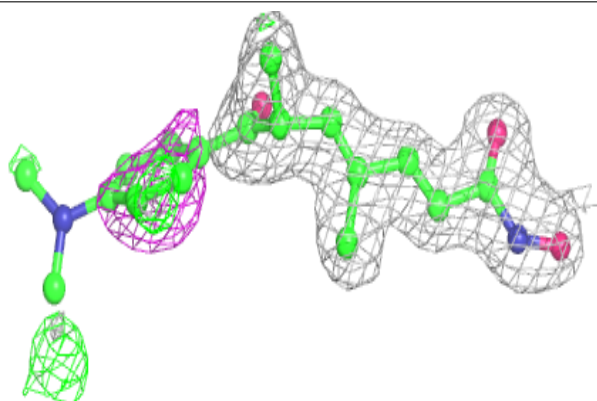
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TSN A 409:

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

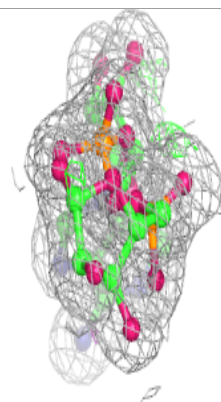
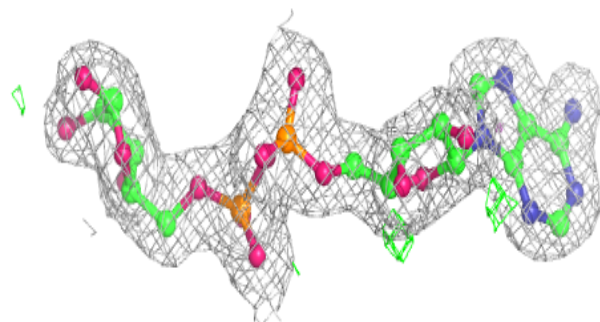
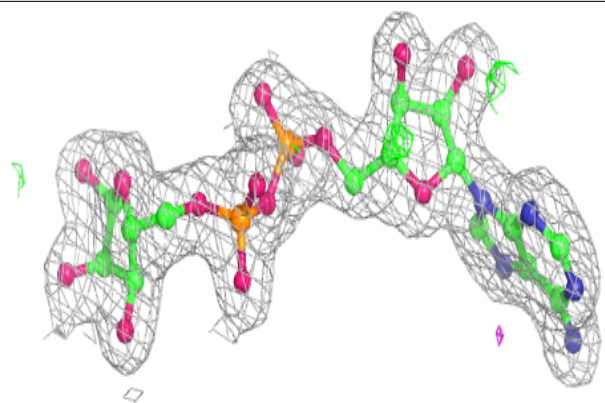
**Electron density around TSN B 709:**

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

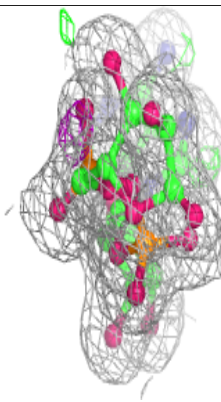
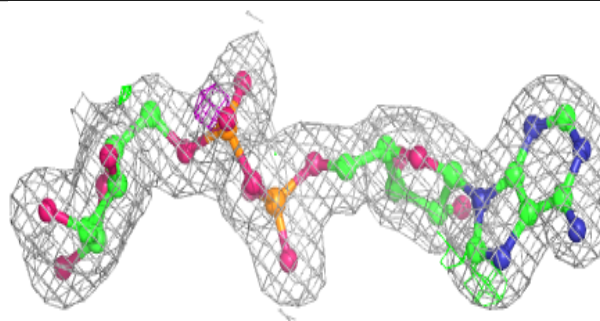
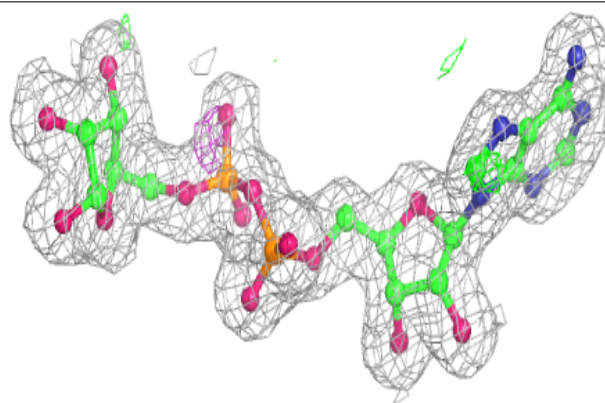


Electron density around AR6 B 702:

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

**Electron density around AR6 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.