



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:33 PM UTC

PDB ID : 6HOY / pdb_00006hoy
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 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

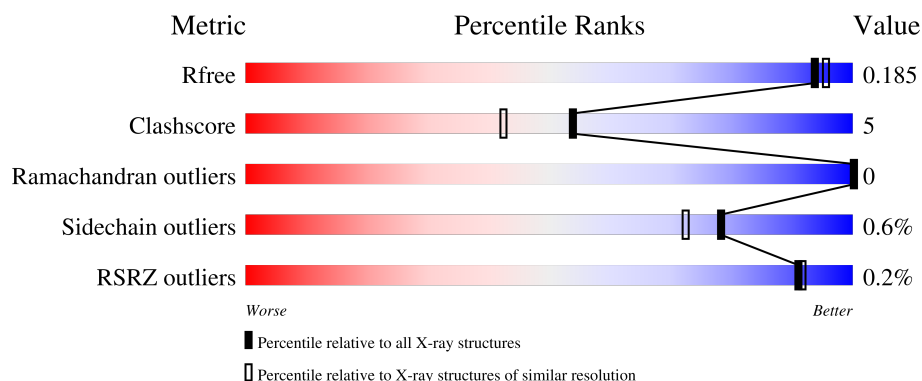
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 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	302	 72% 19% • 7%
1	B	302	 76% 14% • 9%

2 Entry composition

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.

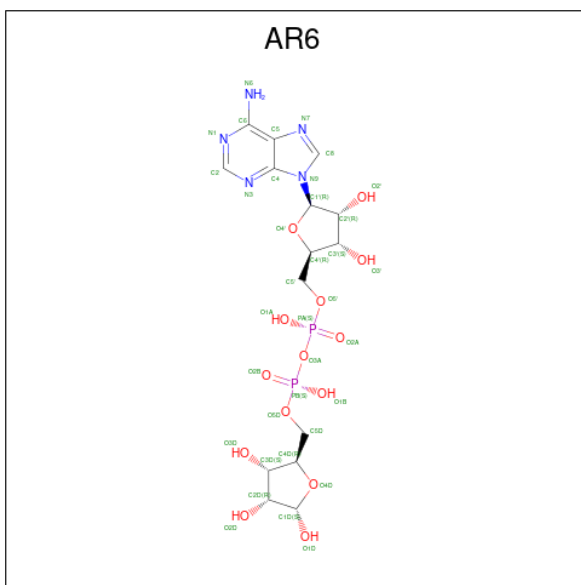
- Molecule 1 is a protein called NAD-dependent protein deacetylase sirtuin-6.

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 (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂).

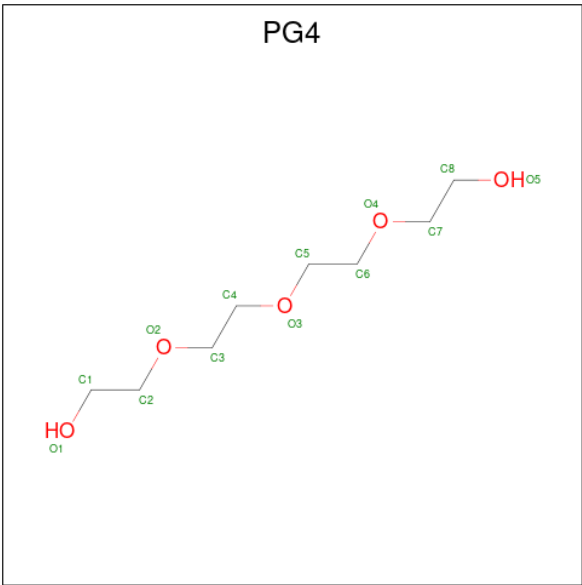


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 15	N 5	O 14	P 2	0	0
2	B	1	Total 36	C 15	N 5	O 14	P 2	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

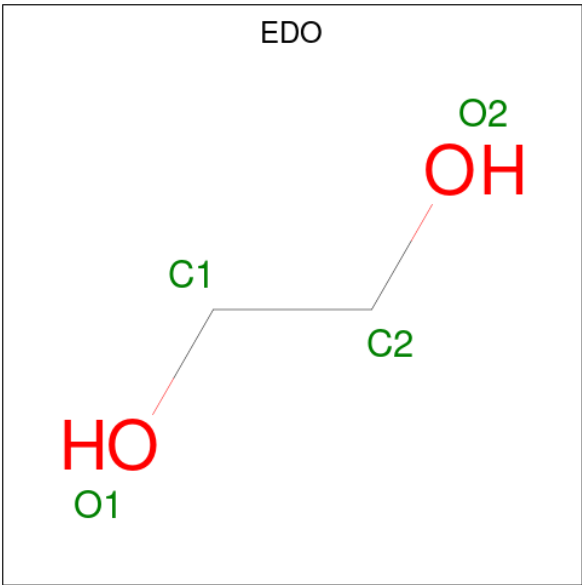
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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 (CCD ID: EDO) (formula: C₂H₆O₂).



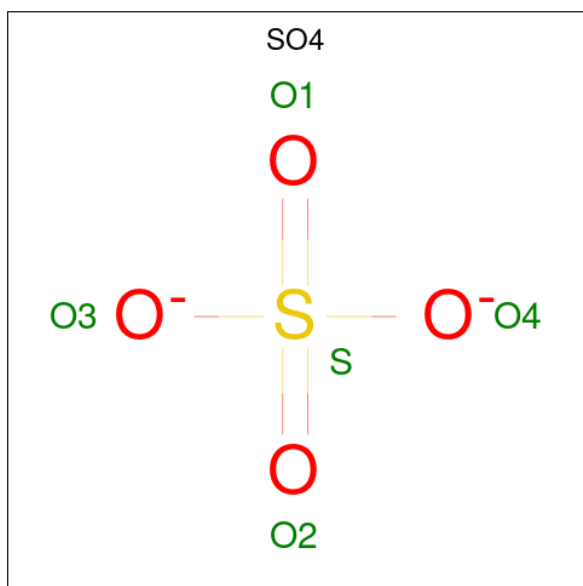
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

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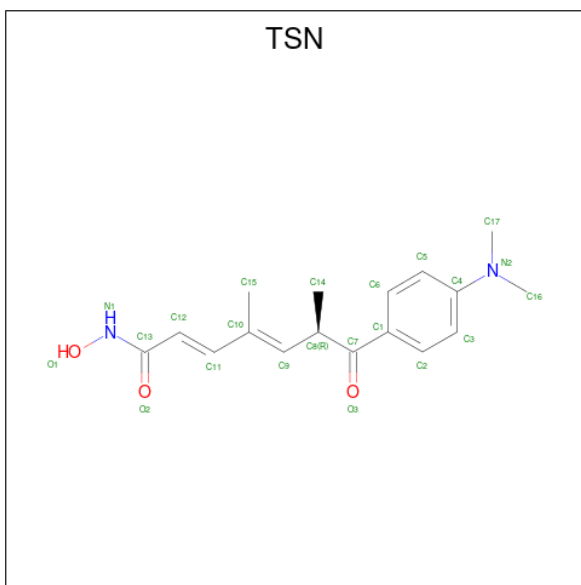
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is SULFATE ION (CCD ID: 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 (CCD ID: 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		

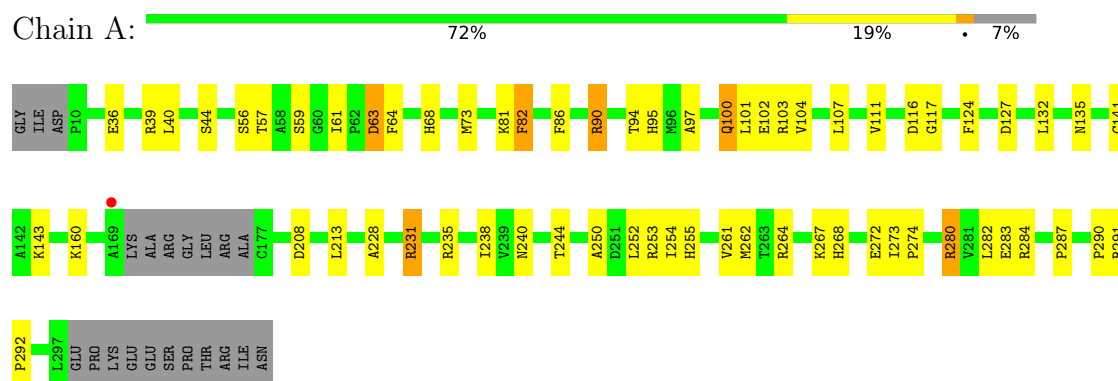
- Molecule 8 is water.

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

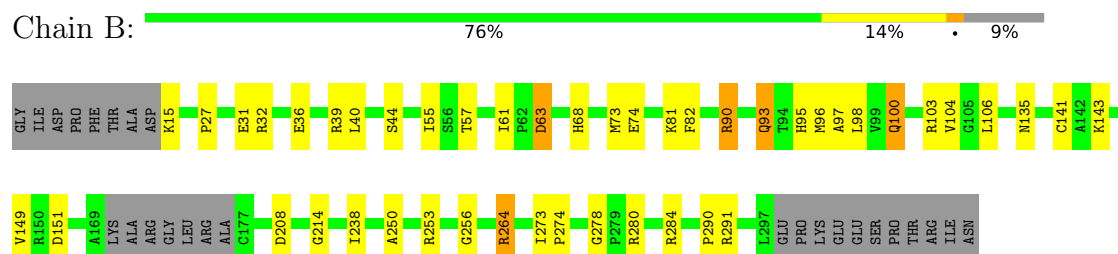
3 Residue-property plots

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 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	91.29Å 91.29Å 143.68Å 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) 100.0 (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 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.154 , 0.185 0.159 , 0.185	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)	0.35 , 29.4	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	0.98	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PG4, AR6, EDO, SO4, TSN

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	1.49	20/2271 (0.9%)	1.67	29/3079 (0.9%)
1	B	1.25	8/2215 (0.4%)	1.61	26/3003 (0.9%)
All	All	1.38	28/4486 (0.6%)	1.64	55/6082 (0.9%)

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 (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	HIS	CE1-NE2	14.02	1.46	1.32
1	A	213	LEU	C-O	9.93	1.35	1.24
1	A	244	THR	C-O	9.70	1.36	1.23
1	A	282	LEU	C-O	9.11	1.34	1.24
1	A	64	PHE	C-O	8.00	1.35	1.23
1	B	95	HIS	CE1-NE2	7.89	1.40	1.32
1	A	111	VAL	C-O	-6.96	1.16	1.24
1	A	240	ASN	C-O	6.60	1.32	1.23
1	A	254	ILE	C-O	6.31	1.31	1.24
1	A	255	HIS	C-O	6.01	1.31	1.23
1	B	149	VAL	C-O	5.98	1.30	1.24
1	A	268	HIS	C-O	5.82	1.30	1.24
1	A	132	LEU	C-O	5.77	1.31	1.24
1	A	94	THR	C-O	5.63	1.30	1.24
1	A	117	GLY	C-O	5.61	1.31	1.24
1	A	283	GLU	C-O	5.60	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	GLY	C-O	-5.46	1.18	1.24
1	B	280	ARG	C-O	5.30	1.30	1.23
1	A	290	PRO	C-O	5.26	1.29	1.23
1	A	235	ARG	C-O	5.24	1.29	1.23
1	B	256	GLY	C-O	5.21	1.29	1.23
1	B	98	LEU	N-CA	5.18	1.52	1.46
1	A	262	MET	C-O	-5.16	1.17	1.24
1	B	284	ARG	C-O	5.11	1.29	1.24
1	A	102	GLU	N-CA	5.08	1.52	1.46
1	A	261	VAL	C-O	-5.08	1.18	1.24
1	B	290	PRO	C-O	5.08	1.29	1.23
1	A	252	LEU	C-O	5.07	1.30	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ARG	CD-NE-CZ	12.74	142.23	124.40
1	B	264	ARG	NE-CZ-NH2	11.29	129.36	119.20
1	B	253	ARG	CG-CD-NE	-10.52	88.87	112.00
1	A	280	ARG	CD-NE-CZ	10.51	139.11	124.40
1	B	253	ARG	NE-CZ-NH2	-10.38	109.86	119.20
1	A	264	ARG	CD-NE-CZ	10.23	138.72	124.40
1	B	264	ARG	CD-NE-CZ	9.95	138.33	124.40
1	A	103	ARG	NE-CZ-NH2	9.84	128.05	119.20
1	B	264	ARG	NE-CZ-NH1	-9.79	111.71	121.50
1	B	280	ARG	NE-CZ-NH2	9.08	127.37	119.20
1	A	253	ARG	NE-CZ-NH2	8.78	127.10	119.20
1	A	280	ARG	NE-CZ-NH2	-8.64	111.43	119.20
1	B	280	ARG	CD-NE-CZ	8.58	136.41	124.40
1	A	253	ARG	NE-CZ-NH1	-8.42	113.08	121.50
1	A	264	ARG	NE-CZ-NH2	-8.29	111.74	119.20
1	B	280	ARG	NE-CZ-NH1	-8.29	113.21	121.50
1	A	253	ARG	CD-NE-CZ	7.96	135.54	124.40
1	A	264	ARG	CG-CD-NE	-7.79	94.85	112.00
1	A	90	ARG	CB-CA-C	7.67	119.27	108.76
1	A	280	ARG	NE-CZ-NH1	7.58	129.07	121.50
1	B	253	ARG	NE-CZ-NH1	7.45	128.95	121.50
1	B	273	ILE	CA-C-O	6.96	123.25	119.15
1	A	264	ARG	NE-CZ-NH1	6.75	128.25	121.50
1	B	97	ALA	N-CA-C	-6.71	103.97	111.28
1	A	127	ASP	CA-CB-CG	6.70	119.30	112.60
1	B	100	GLN	CA-C-O	-6.63	113.40	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	82	PHE	CA-C-O	-6.43	113.67	120.80
1	A	86	PHE	CA-C-O	-6.41	113.62	120.42
1	B	264	ARG	CA-C-O	-6.33	114.17	120.82
1	A	101	LEU	N-CA-C	-6.12	104.72	111.82
1	B	90	ARG	CB-CA-C	6.06	117.89	108.61
1	A	292	PRO	CB-CA-C	6.03	117.06	111.39
1	B	135	ASN	CB-CA-C	6.02	120.18	109.65
1	A	244	THR	CA-C-O	-5.95	114.48	121.44
1	A	63	ASP	CA-CB-CG	5.89	118.49	112.60
1	B	103	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	A	244	THR	O-C-N	5.84	130.75	123.15
1	B	55	ILE	CA-C-N	5.73	131.36	122.26
1	B	55	ILE	C-N-CA	5.73	131.36	122.26
1	A	135	ASN	CB-CA-C	5.70	119.63	109.65
1	B	63	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	267	LYS	CA-C-O	-5.53	115.02	120.82
1	A	280	ARG	CG-CD-NE	-5.46	99.98	112.00
1	A	100	GLN	CA-C-O	-5.46	114.76	120.55
1	A	97	ALA	CA-C-O	-5.42	115.12	120.82
1	B	96	MET	CA-C-O	-5.41	113.75	119.97
1	A	273	ILE	CA-C-O	5.36	122.31	119.15
1	A	82	PHE	CA-C-O	-5.27	114.95	120.80
1	B	74	GLU	CA-C-N	5.26	127.58	120.38
1	B	74	GLU	C-N-CA	5.26	127.58	120.38
1	B	93	GLN	OE1-CD-NE2	-5.17	117.43	122.60
1	A	124	PHE	CA-C-O	-5.16	114.67	120.25
1	A	287	PRO	CA-C-N	5.04	124.95	119.76
1	A	287	PRO	C-N-CA	5.04	124.95	119.76

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	22	0
1	B	2168	0	2185	23	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	2	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	45	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 5.

All (45) 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	1.08
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	0.89
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:68:HIS:CE1	1:B:73:MET:HE2	2.42	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	0.48
1:A:73:MET:HE2	1:B:68:HIS:CE1	2.49	0.48
1:B:104:VAL:HB	1:B:291:ARG:HB3	1.95	0.47
1:A:107:LEU:C	1:A:107:LEU:HD23	2.40	0.47
1:A:116:ASP:OD2	7:A:409:TSN:O1	2.28	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:B:15:LYS:N	8:B:815:HOH:O	2.52	0.42
1:B:63:ASP:OD2	2:B:702:AR6:H8	2.19	0.41
1:B:238:ILE:HD12	1:B:250:ALA:HB2	2.02	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:A:56:SER:O	1:A:59[A]:SER:OG	2.35	0.40
1:B:106:LEU:HD23	1:B:106:LEU:HA	1.86	0.40

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	281/302 (93%)	278 (99%)	3 (1%)	0	100	100
1	B	274/302 (91%)	269 (98%)	5 (2%)	0	100	100
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%)	73	65
1	B	235/256 (92%)	234 (100%)	1 (0%)	84	80
All	All	477/512 (93%)	474 (99%)	3 (1%)	78	72

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	255	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
6	SO4	B	706	-	4,4,4	0.51	0	6,6,6	0.35	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	0.18	0
6	SO4	A	408	-	4,4,4	0.34	0	6,6,6	0.31	0
6	SO4	A	406	-	4,4,4	0.35	0	6,6,6	0.10	0
6	SO4	B	708	-	4,4,4	0.33	0	6,6,6	0.11	0
6	SO4	A	407	-	4,4,4	0.32	0	6,6,6	0.27	0
7	TSN	B	709	-	21,22,22	2.38	7 (33%)	27,29,29	2.57	5 (18%)
5	EDO	A	404	-	3,3,3	0.40	0	2,2,2	0.67	0
6	SO4	A	405	-	4,4,4	0.39	0	6,6,6	0.23	0
6	SO4	B	707	-	4,4,4	0.39	0	6,6,6	0.19	0
7	TSN	A	409	-	21,22,22	2.52	7 (33%)	27,29,29	5.44	7 (25%)
4	PG4	B	704	-	12,12,12	0.27	0	11,11,11	0.12	0
2	AR6	A	401	-	39,39,39	1.43	2 (5%)	56,60,60	1.14	5 (8%)
5	EDO	B	705	-	3,3,3	0.21	0	2,2,2	0.56	0
2	AR6	B	702	-	39,39,39	0.87	2 (5%)	56,60,60	1.10	6 (10%)

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
4	PG4	A	403	-	-	4/10/10/10	-
5	EDO	B	701	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TSN	B	709	-	-	4/23/23/23	0/1/1/1
5	EDO	A	404	-	-	1/1/1/1	-
7	TSN	A	409	-	-	3/23/23/23	0/1/1/1
4	PG4	B	704	-	-	7/10/10/10	-
2	AR6	A	401	-	-	1/22/54/54	0/4/4/4
5	EDO	B	705	-	-	1/1/1/1	-
2	AR6	B	702	-	-	2/22/54/54	0/4/4/4

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	AR6	PA-O3A	6.07	1.66	1.59
7	A	409	TSN	C8-C9	5.52	1.59	1.50
7	A	409	TSN	O3-C7	-5.34	1.15	1.22
7	A	409	TSN	C4-N2	5.00	1.49	1.37
2	A	401	AR6	PB-O3A	4.24	1.64	1.59
7	B	709	TSN	C11-C10	4.23	1.55	1.46
7	B	709	TSN	O1-N1	-4.19	1.29	1.40
7	B	709	TSN	C1-C7	4.17	1.55	1.49
7	B	709	TSN	C4-N2	4.03	1.46	1.37
7	B	709	TSN	C8-C9	3.93	1.56	1.50
7	A	409	TSN	C1-C7	3.43	1.54	1.49
7	B	709	TSN	C12-C13	3.26	1.55	1.48
7	B	709	TSN	O3-C7	-3.00	1.18	1.22
2	B	702	AR6	O4D-C1D	-2.85	1.39	1.43
7	A	409	TSN	C14-C8	2.71	1.57	1.54
7	A	409	TSN	C11-C10	2.50	1.51	1.46
2	B	702	AR6	PB-O3A	2.37	1.62	1.59
7	A	409	TSN	O1-N1	-2.09	1.35	1.40

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	409	TSN	C1-C7-C8	21.77	138.90	119.27
7	A	409	TSN	O3-C7-C1	-11.52	106.38	120.70
7	A	409	TSN	C14-C8-C9	-8.11	102.95	110.73
7	A	409	TSN	O3-C7-C8	-7.89	112.51	119.81
7	B	709	TSN	C1-C7-C8	7.80	126.31	119.27
7	A	409	TSN	C15-C10-C11	-6.43	108.27	118.09
7	B	709	TSN	O3-C7-C8	-5.99	114.26	119.81
7	B	709	TSN	O1-N1-C13	5.56	132.93	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	709	TSN	C14-C8-C9	-4.67	106.25	110.73
2	B	702	AR6	O3A-PA-O2A	-3.33	100.67	110.70
7	B	709	TSN	C15-C10-C11	-3.05	113.43	118.09
2	B	702	AR6	C2'-C1'-N9	2.74	120.11	113.30
2	B	702	AR6	O1A-PA-O3A	2.57	114.23	107.27
2	B	702	AR6	C2D-C3D-C4D	-2.34	98.08	102.61
7	A	409	TSN	C11-C10-C9	2.31	125.00	118.82
2	B	702	AR6	O5D-PB-O2B	2.28	117.99	108.94
2	A	401	AR6	O2D-C2D-C1D	2.20	117.97	111.85
2	A	401	AR6	O3'-C3'-C2'	-2.16	104.91	111.82
2	A	401	AR6	C4-N9-C8	2.11	107.95	105.74
2	A	401	AR6	O1D-C1D-O4D	2.10	113.79	111.12
2	B	702	AR6	O3A-PB-O2B	-2.07	104.49	110.70
2	A	401	AR6	C2'-C3'-C4'	2.02	106.51	102.61
7	A	409	TSN	C11-C12-C13	-2.01	117.33	125.43

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

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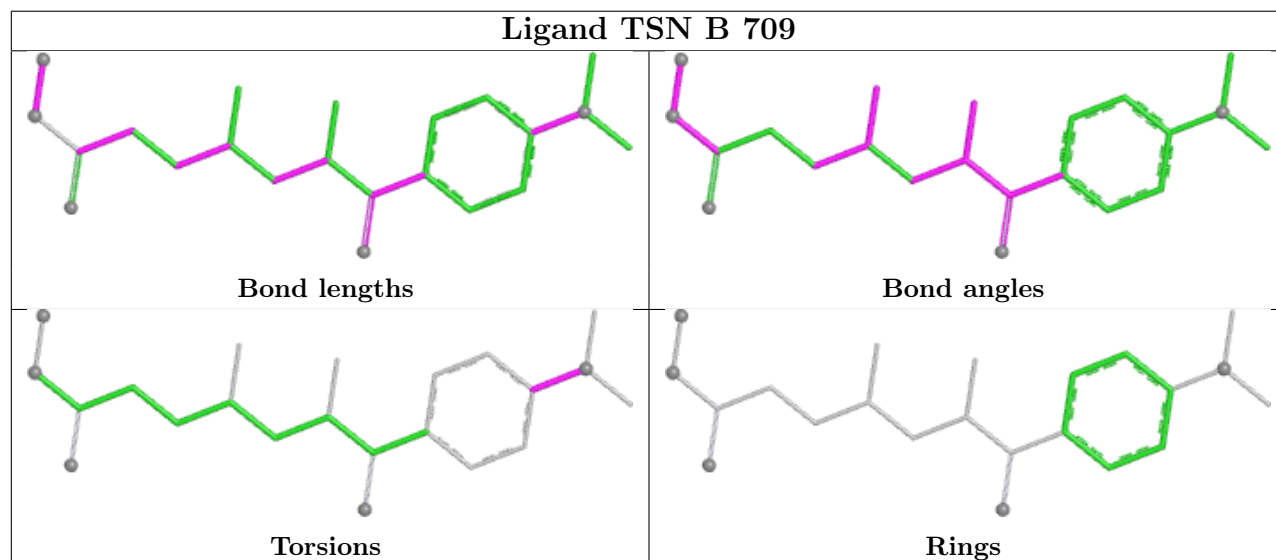
Mol	Chain	Res	Type	Atoms
5	B	705	EDO	O1-C1-C2-O2
2	B	702	AR6	O4'-C4'-C5'-O5'

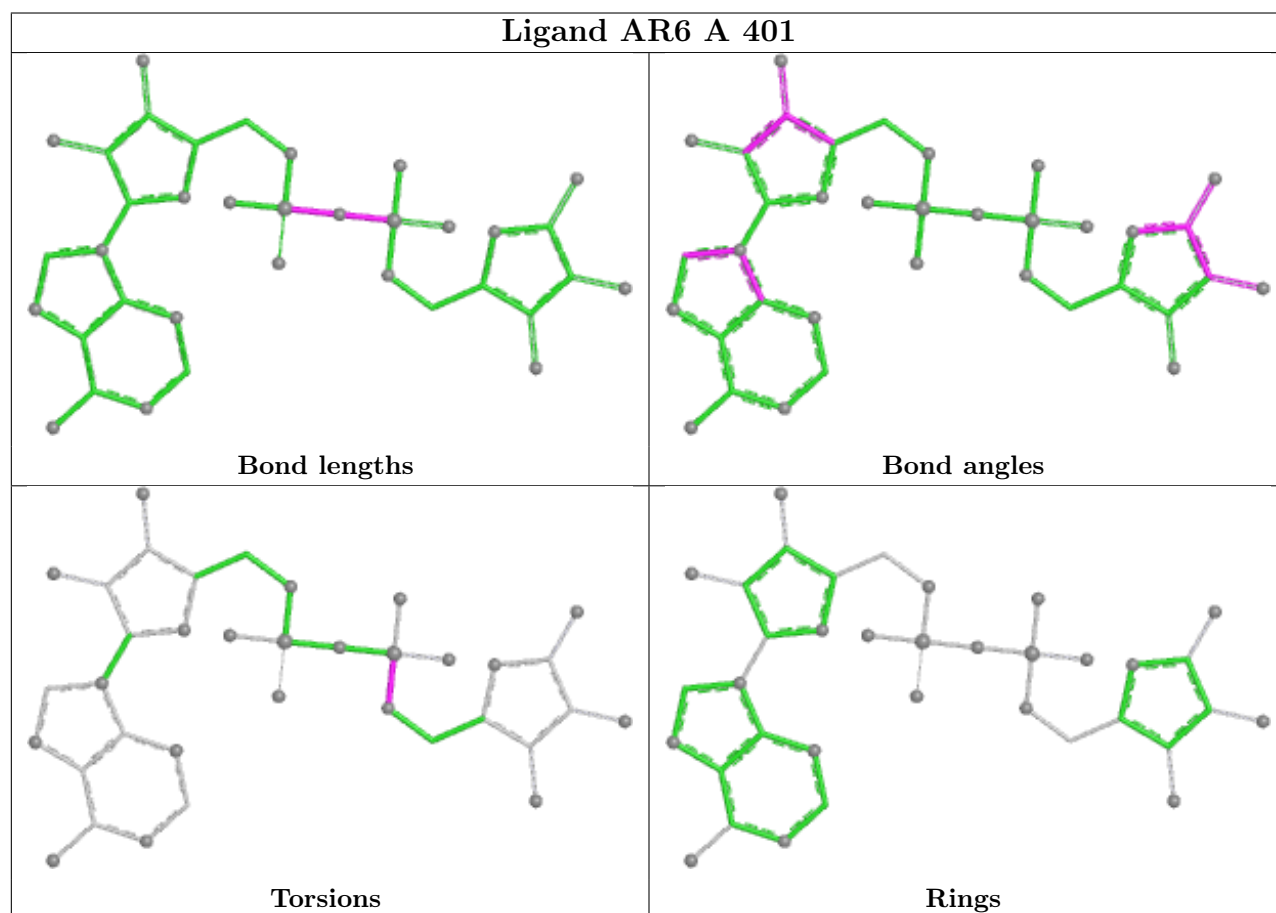
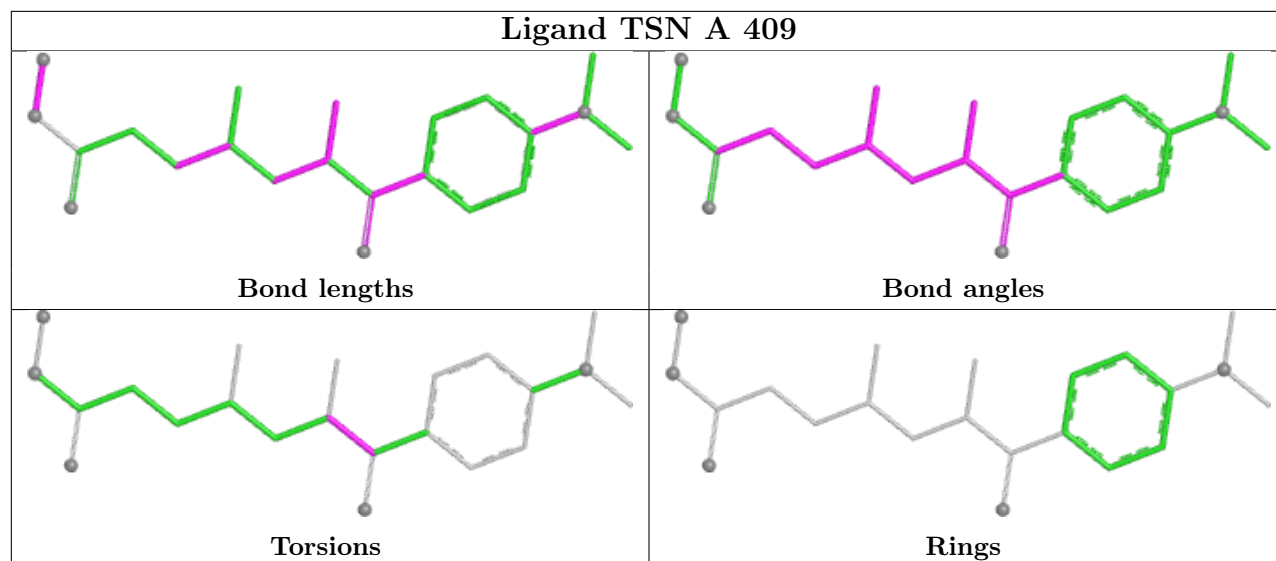
There are no ring outliers.

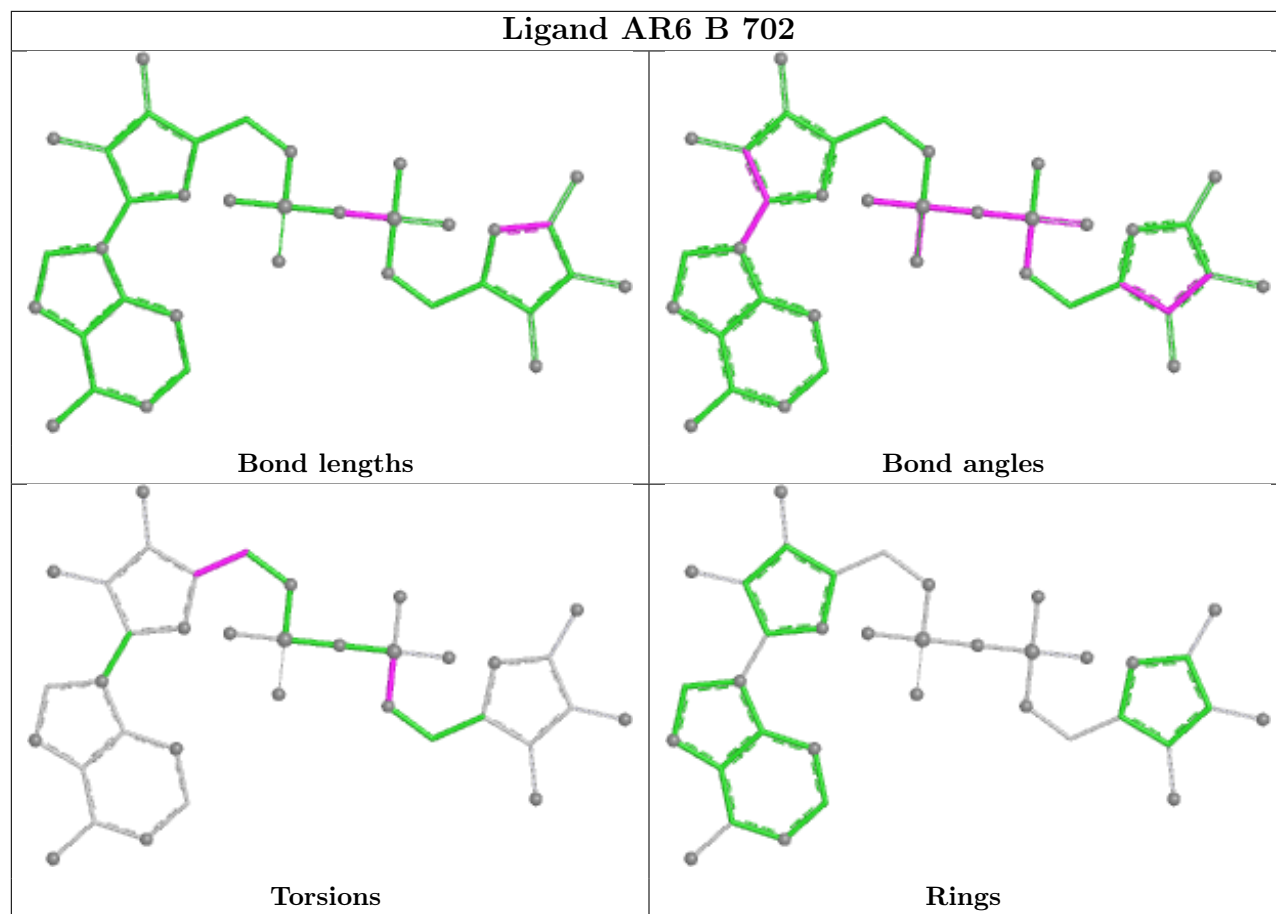
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	406	SO4	1	0
7	B	709	TSN	1	0
7	A	409	TSN	2	0
2	A	401	AR6	1	0
2	B	702	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.







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%)	-0.97	1 (0%) 88 90	15, 29, 51, 70	4 (1%)
1	B	276/302 (91%)	-0.83	0 100 100	17, 36, 60, 77	2 (0%)
All	All	557/604 (92%)	-0.90	1 (0%) 91 92	15, 33, 57, 77	6 (1%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	ALA	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 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
4	PG4	B	704	13/13	0.97	0.08	64,78,83,85	0
5	EDO	B	705	4/4	0.97	0.10	47,55,58,58	0
5	EDO	A	404	4/4	0.98	0.06	37,43,43,46	0
4	PG4	A	403	13/13	0.98	0.07	52,63,69,71	0

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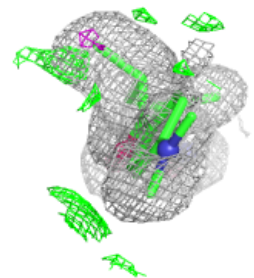
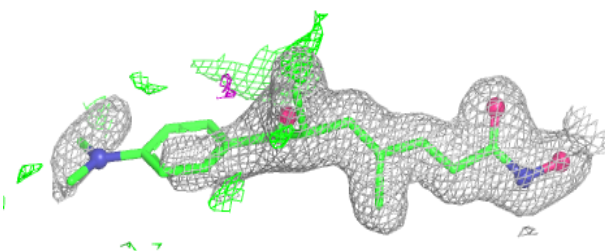
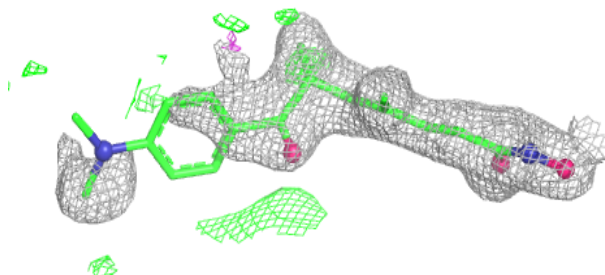
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	A	405	5/5	0.98	0.05	46,52,54,60	0
6	SO4	A	406	5/5	0.98	0.04	82,86,88,90	0
6	SO4	B	707	5/5	0.98	0.04	54,64,71,72	0
7	TSN	A	409	22/22	0.98	0.09	23,35,79,84	0
7	TSN	B	709	22/22	0.98	0.10	24,43,98,100	0
3	ZN	A	402	1/1	0.99	0.03	47,47,47,47	0
6	SO4	A	407	5/5	0.99	0.03	48,59,67,67	0
6	SO4	A	408	5/5	0.99	0.05	44,47,58,63	0
6	SO4	B	706	5/5	0.99	0.04	38,38,47,52	0
5	EDO	B	701	4/4	0.99	0.06	53,53,58,58	0
6	SO4	B	708	5/5	0.99	0.03	53,63,66,74	0
2	AR6	A	401	36/36	0.99	0.03	20,23,27,27	0
2	AR6	B	702	36/36	0.99	0.03	24,30,34,38	0
3	ZN	B	703	1/1	1.00	0.02	52,52,52,52	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.

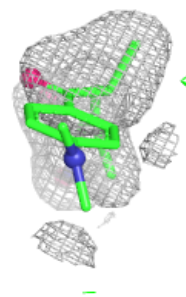
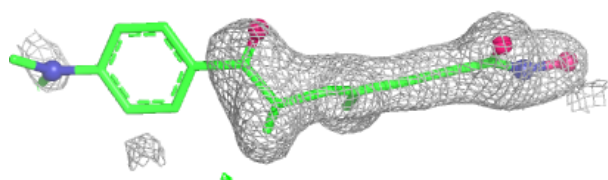
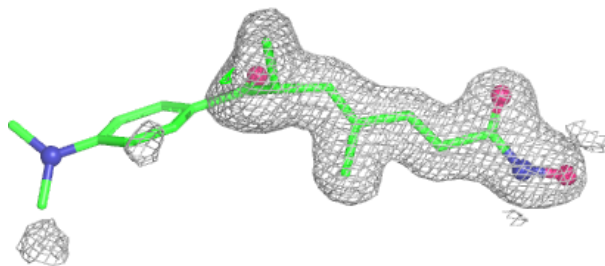
Electron density around TSN A 409:

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

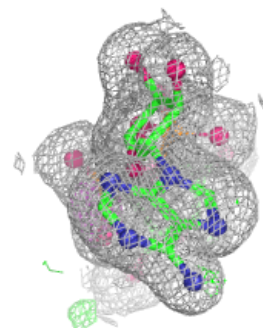
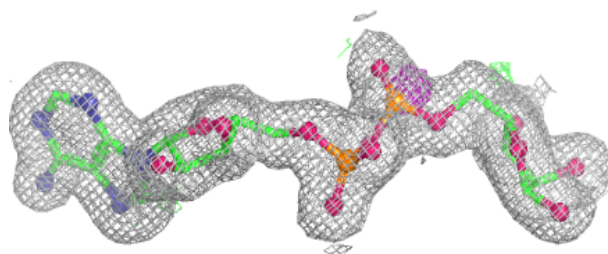
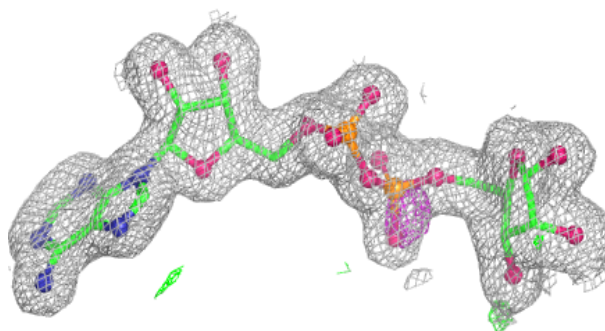


Electron density around TSN B 709:

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

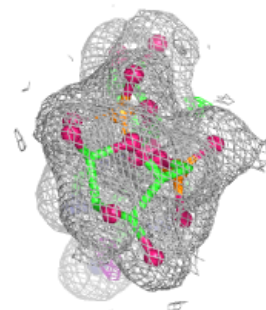
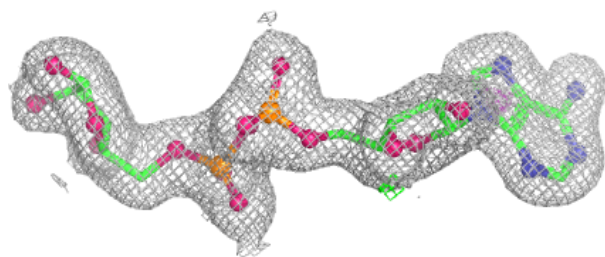
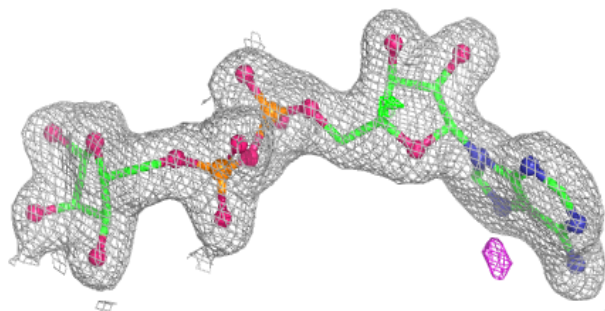
**Electron density around AR6 A 401:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.