



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:40 PM UTC

PDB ID : 9NTB / pdb_00009ntb
Title : Crystal structure of human HDAC2 in complex with TNG260
Authors : McMillan, B.J.; Whittington, D.A.
Deposited on : 2025-03-18
Resolution : 1.80 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

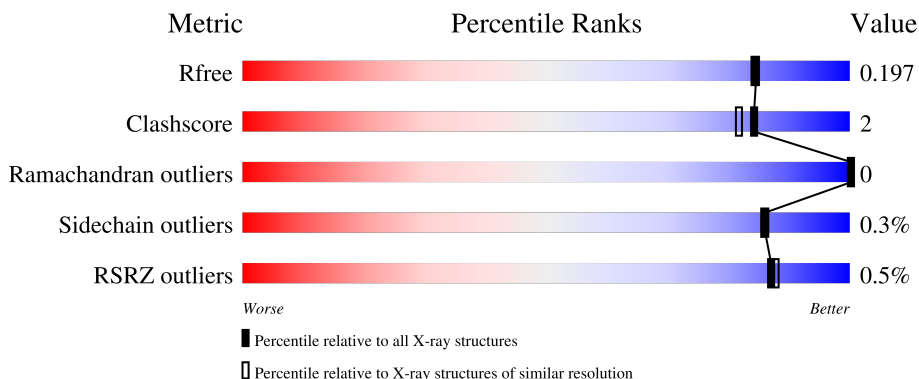
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	404	% 85% 6% 9%
1	B	404	87% 9%
1	C	404	% 86% 5% 9%

2 Entry composition [i](#)

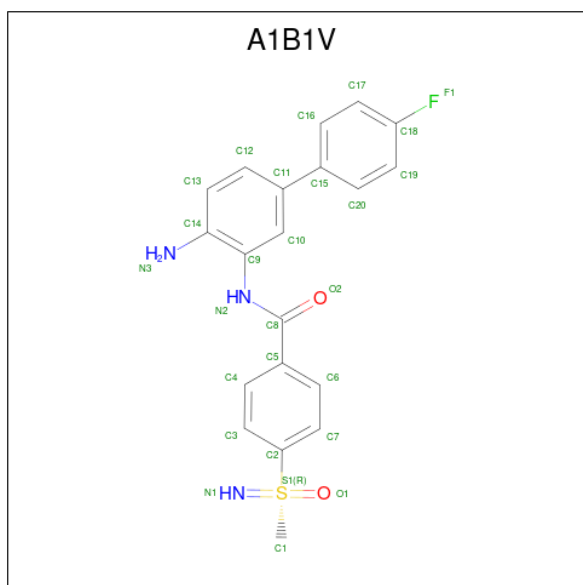
There are 10 unique types of molecules in this entry. The entry contains 10178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Histone deacetylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	9	0
			2990	1909	507	550	24			
1	B	367	Total	C	N	O	S	0	9	0
			2982	1905	501	551	25			
1	C	366	Total	C	N	O	S	0	6	0
			2970	1898	501	546	25			

- Molecule 2 is (R)-N-(4-amino-4'-fluoro-[1,1'-biphenyl]-3-yl)-4-(S-methylsulfonimidoyl)benzamide (CCD ID: A1B1V) (formula: C₂₀H₁₈FN₃O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0
			27	20	1	3	2	1	
2	B	1	Total	C	F	N	O	S	0
			27	20	1	3	2	1	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	S	
			27	20	1	3	2	1	0

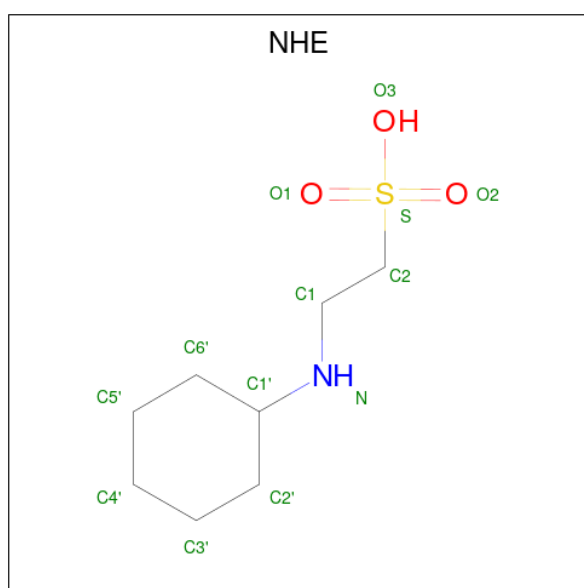
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

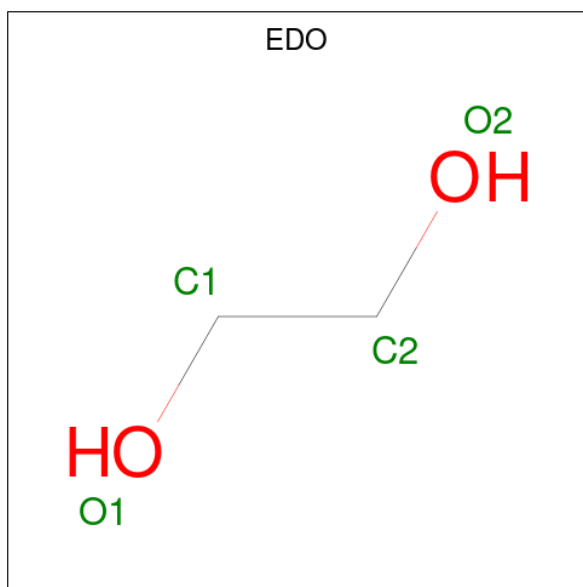
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		

- Molecule 5 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
5	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



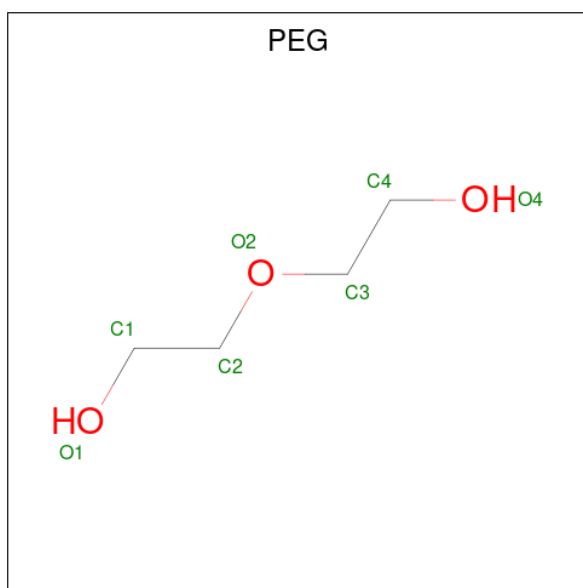
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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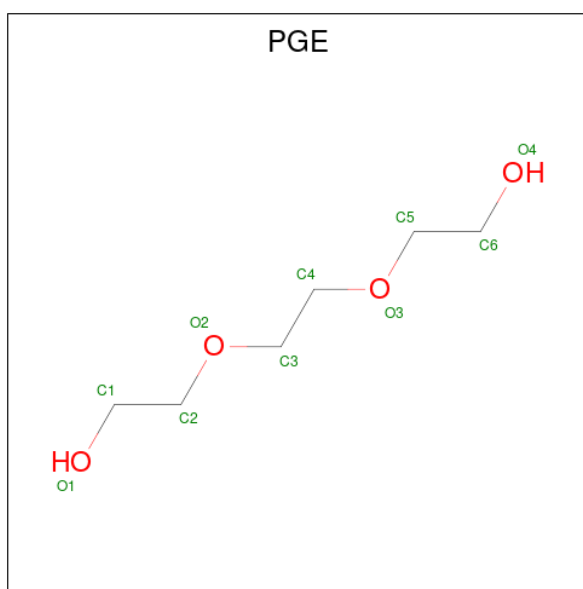
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total	C	O	0	0
			4	2	2		
6	C	1	Total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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



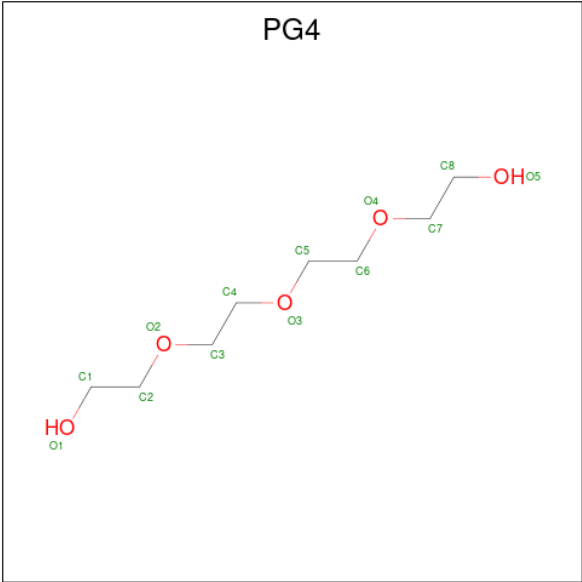
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	A	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0
7	B	1	Total C O 7 4 3	0	0

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 10 6 4	0	0
8	C	1	Total C O 10 6 4	0	0

- Molecule 9 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

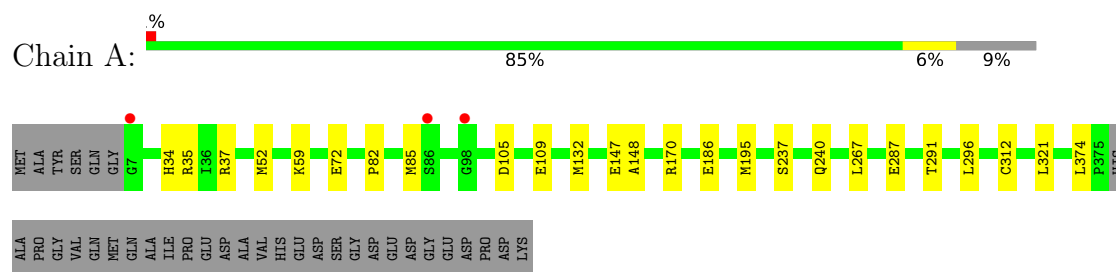
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	313	Total	O	0	0
			313	313		
10	B	351	Total	O	0	0
			351	351		
10	C	259	Total	O	0	0
			259	259		

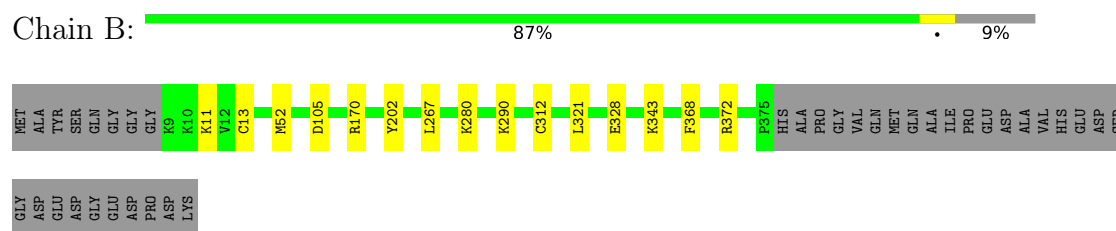
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

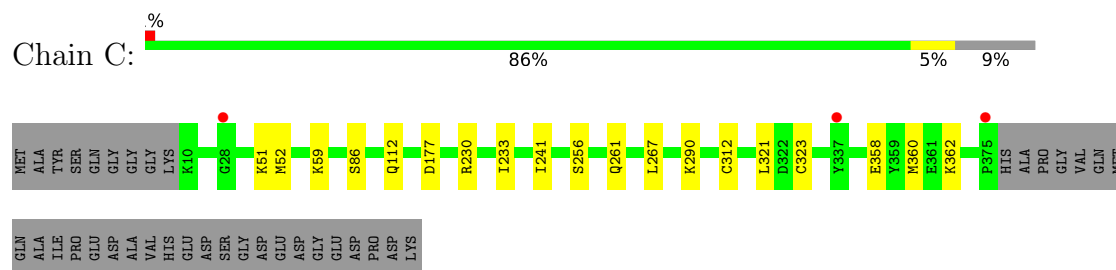
• Molecule 1: Histone deacetylase 2



• Molecule 1: Histone deacetylase 2



• Molecule 1: Histone deacetylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.23Å 97.31Å 139.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.66 – 1.80 48.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.66-1.80) 98.7 (48.66-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.160 , 0.197 0.162 , 0.197	Depositor DCC
R_{free} test set	1990 reflections (1.71%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10178	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: PG4, CA, EDO, PEG, NHE, A1B1V, PGE, ZN

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	0.28	0/3079	0.48	0/4156
1	B	0.29	0/3079	0.48	0/4157
1	C	0.24	0/3060	0.43	0/4132
All	All	0.27	0/9218	0.47	0/12445

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	ARG	Sidechain

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	2990	0	2890	16	0
1	B	2982	0	2886	11	0
1	C	2970	0	2876	11	0
2	A	27	0	0	0	0
2	B	27	0	0	0	0
2	C	27	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	A	13	0	17	3	0
5	B	13	0	17	0	0
6	A	44	0	66	1	0
6	B	24	0	36	1	0
6	C	20	0	30	0	0
7	A	28	0	40	0	0
7	B	35	0	50	1	0
8	A	10	0	14	1	0
8	C	10	0	14	0	0
9	B	26	0	36	2	0
10	A	313	0	0	2	0
10	B	351	0	0	3	0
10	C	259	0	0	2	0
All	All	10178	0	8972	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 2.

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:C:51:LYS:NZ	1:C:323[B]:CYS:SG	2.47	0.87
1:B:11:LYS:NZ	1:B:13[A]:CYS:SG	2.57	0.78
1:A:85:MET:SD	6:A:506:EDO:H11	2.33	0.69
1:C:230:ARG:NH1	10:C:601:HOH:O	2.25	0.69
1:A:105:ASP:HB3	5:A:505:NHE:H4'1	1.80	0.62
1:A:132:MET:HE3	1:A:296:LEU:HD23	1.80	0.62
1:A:186:GLU:OE1	10:A:601:HOH:O	2.16	0.61
1:A:195:MET:HE1	1:A:374:LEU:HD21	1.84	0.57
6:B:508:EDO:O1	10:B:601:HOH:O	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:MET:HB3	1:B:321:LEU:HD21	1.91	0.53
1:B:105:ASP:HB3	9:B:518:PG4:H11	1.90	0.53
1:A:287:GLU:O	1:A:291:THR:HG23	2.09	0.52
1:A:34:HIS:CD2	1:A:37:ARG:HH21	2.27	0.51
1:C:358:GLU:HG2	1:C:362:LYS:HE2	1.93	0.51
1:A:52:MET:HB3	1:A:321:LEU:HD21	1.91	0.50
1:C:241:ILE:HG21	1:C:360:MET:HE3	1.92	0.49
1:A:72:GLU:H	1:A:72:GLU:CD	2.22	0.48
1:C:290:LYS:HB3	1:C:290:LYS:HE2	1.71	0.46
1:A:170:ARG:HH11	8:A:521:PGE:H6	1.81	0.45
1:B:11:LYS:HG3	10:B:811:HOH:O	2.16	0.45
1:C:59:LYS:HB3	1:C:112:GLN:HB3	1.98	0.45
5:A:505:NHE:HC22	5:A:505:NHE:HC'1	1.61	0.45
1:C:52:MET:HB3	1:C:321:LEU:HD21	1.99	0.44
1:C:362:LYS:NZ	10:C:606:HOH:O	2.50	0.44
1:A:237:SER:O	1:A:240[A]:GLN:HB2	2.17	0.44
1:B:368:PHE:O	1:B:372:ARG:HG3	2.16	0.44
1:B:280:LYS:HE2	9:B:517:PG4:H72	2.00	0.44
1:A:82:PRO:HA	1:A:85:MET:HG3	2.00	0.43
1:A:147:GLU:HG2	1:A:148:ALA:O	2.18	0.43
5:A:505:NHE:H3'1	10:A:885:HOH:O	2.18	0.43
1:C:51:LYS:HE2	1:C:51:LYS:HB3	1.78	0.43
1:C:267:LEU:HD11	1:C:312:CYS:HB2	1.99	0.43
1:A:59:LYS:NZ	1:A:109:GLU:OE1	2.43	0.42
1:B:170:ARG:HD3	7:B:516:PEG:H32	2.01	0.42
1:B:267:LEU:HD11	1:B:312:CYS:HB2	2.02	0.42
1:B:290:LYS:HE2	1:B:290:LYS:HB3	1.83	0.42
1:C:177:ASP:HB2	1:C:261:GLN:OE1	2.20	0.41
1:B:202:TYR:O	10:B:602:HOH:O	2.22	0.41
1:B:328:GLU:OE1	1:B:343:LYS:NZ	2.53	0.41
1:A:34:HIS:HD2	1:A:37:ARG:HH21	1.69	0.41
1:A:267:LEU:HD11	1:A:312:CYS:HB2	2.01	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	371/404 (92%)	363 (98%)	8 (2%)	0	100	100
1	B	371/404 (92%)	363 (98%)	8 (2%)	0	100	100
1	C	368/404 (91%)	362 (98%)	6 (2%)	0	100	100
All	All	1110/1212 (92%)	1088 (98%)	22 (2%)	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	321/344 (93%)	321 (100%)	0	100	100
1	B	323/344 (94%)	323 (100%)	0	100	100
1	C	320/344 (93%)	317 (99%)	3 (1%)	70	67
All	All	964/1032 (93%)	961 (100%)	3 (0%)	86	86

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

Mol	Chain	Res	Type
1	C	86	SER
1	C	233	ILE
1	C	256	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	B	91	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 9 are monoatomic - leaving 40 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	$\# Z > 2$
2	A1B1V	C	501	3	29,29,29	0.47	1 (3%)	40,42,42	1.35	2 (5%)
6	EDO	B	508	-	3,3,3	0.40	0	2,2,2	0.60	0
7	PEG	B	511	-	6,6,6	0.14	0	5,5,5	0.09	0
7	PEG	B	516	-	6,6,6	0.18	0	5,5,5	0.07	0
7	PEG	A	516	-	6,6,6	0.09	0	5,5,5	0.17	0
6	EDO	A	509	-	3,3,3	0.45	0	2,2,2	0.33	0
6	EDO	B	513	-	3,3,3	0.48	0	2,2,2	0.21	0
6	EDO	A	513	-	3,3,3	0.45	0	2,2,2	0.38	0
7	PEG	B	515	-	6,6,6	0.18	0	5,5,5	0.07	0
7	PEG	A	517	-	6,6,6	0.15	0	5,5,5	0.08	0
2	A1B1V	B	501	3	29,29,29	0.52	1 (3%)	40,42,42	1.21	3 (7%)
5	NHE	B	505	-	13,13,13	0.22	0	16,17,17	0.57	0
6	EDO	B	512	-	3,3,3	0.53	0	2,2,2	0.09	0
6	EDO	C	507	-	3,3,3	0.46	0	2,2,2	0.20	0
7	PEG	A	519	-	6,6,6	0.11	0	5,5,5	0.14	0
8	PGE	C	510	-	9,9,9	0.29	0	8,8,8	0.42	0
6	EDO	A	510	-	3,3,3	0.41	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	A	515	-	3,3,3	0.49	0	2,2,2	0.25	0
6	EDO	A	512	-	3,3,3	0.45	0	2,2,2	0.46	0
6	EDO	B	510	-	3,3,3	0.42	0	2,2,2	0.41	0
5	NHE	A	505	-	13,13,13	0.24	0	16,17,17	0.31	0
8	PGE	A	521	-	9,9,9	0.32	0	8,8,8	0.38	0
6	EDO	C	505	-	3,3,3	0.47	0	2,2,2	0.22	0
2	A1B1V	A	501	3	29,29,29	0.51	0	40,42,42	1.20	2 (5%)
6	EDO	A	511	-	3,3,3	0.45	0	2,2,2	0.31	0
7	PEG	B	506	-	6,6,6	0.11	0	5,5,5	0.17	0
6	EDO	A	506	-	3,3,3	0.36	0	2,2,2	0.43	0
6	EDO	B	509	-	3,3,3	0.44	0	2,2,2	0.51	0
6	EDO	B	507	-	3,3,3	0.44	0	2,2,2	0.68	0
9	PG4	B	518	-	12,12,12	0.13	0	11,11,11	0.64	0
6	EDO	A	508	-	3,3,3	0.43	0	2,2,2	0.37	0
7	PEG	B	514	-	6,6,6	0.15	0	5,5,5	0.08	0
6	EDO	C	509	-	3,3,3	0.43	0	2,2,2	0.40	0
9	PG4	B	517	-	12,12,12	0.15	0	11,11,11	0.57	0
6	EDO	A	514	-	3,3,3	0.32	0	2,2,2	0.27	0
6	EDO	C	506	-	3,3,3	0.45	0	2,2,2	0.27	0
6	EDO	C	508	-	3,3,3	0.43	0	2,2,2	0.38	0
6	EDO	A	520	-	3,3,3	0.44	0	2,2,2	0.32	0
6	EDO	A	507	-	3,3,3	0.33	0	2,2,2	0.69	0
7	PEG	A	518	-	6,6,6	0.11	0	5,5,5	0.17	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	A1B1V	C	501	3	-	0/18/18/18	0/3/3/3
6	EDO	B	508	-	-	0/1/1/1	-
7	PEG	B	511	-	-	1/4/4/4	-
7	PEG	B	516	-	-	2/4/4/4	-
7	PEG	A	516	-	-	2/4/4/4	-
6	EDO	A	509	-	-	0/1/1/1	-
6	EDO	B	513	-	-	0/1/1/1	-
6	EDO	A	513	-	-	1/1/1/1	-
7	PEG	B	515	-	-	2/4/4/4	-
7	PEG	A	517	-	-	1/4/4/4	-
2	A1B1V	B	501	3	-	2/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NHE	B	505	-	-	0/7/15/15	0/1/1/1
6	EDO	B	512	-	-	1/1/1/1	-
6	EDO	C	507	-	-	0/1/1/1	-
7	PEG	A	519	-	-	2/4/4/4	-
8	PGE	C	510	-	-	1/7/7/7	-
6	EDO	A	510	-	-	1/1/1/1	-
6	EDO	A	515	-	-	1/1/1/1	-
6	EDO	A	512	-	-	0/1/1/1	-
6	EDO	B	510	-	-	0/1/1/1	-
5	NHE	A	505	-	-	4/7/15/15	0/1/1/1
8	PGE	A	521	-	-	2/7/7/7	-
6	EDO	C	505	-	-	0/1/1/1	-
2	A1B1V	A	501	3	-	0/18/18/18	0/3/3/3
6	EDO	A	511	-	-	0/1/1/1	-
7	PEG	B	506	-	-	4/4/4/4	-
6	EDO	A	506	-	-	1/1/1/1	-
6	EDO	B	509	-	-	0/1/1/1	-
6	EDO	B	507	-	-	1/1/1/1	-
9	PG4	B	518	-	-	3/10/10/10	-
6	EDO	A	508	-	-	1/1/1/1	-
7	PEG	B	514	-	-	2/4/4/4	-
6	EDO	C	509	-	-	0/1/1/1	-
9	PG4	B	517	-	-	2/10/10/10	-
6	EDO	A	514	-	-	0/1/1/1	-
6	EDO	C	506	-	-	1/1/1/1	-
6	EDO	C	508	-	-	1/1/1/1	-
6	EDO	A	520	-	-	0/1/1/1	-
6	EDO	A	507	-	-	1/1/1/1	-
7	PEG	A	518	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1B1V	S1-N1	2.25	1.55	1.51
2	C	501	A1B1V	S1-N1	2.01	1.54	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	A1B1V	O1-S1-N1	-7.31	112.99	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	A1B1V	O1-S1-N1	-6.41	114.20	122.87
2	A	501	A1B1V	O1-S1-N1	-6.04	114.71	122.87
2	A	501	A1B1V	C1-S1-C2	2.82	108.39	104.83
2	C	501	A1B1V	C1-S1-C2	2.45	107.92	104.83
2	B	501	A1B1V	O1-S1-C1	-2.18	106.01	109.02
2	B	501	A1B1V	C1-S1-C2	2.11	107.50	104.83

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	NHE	C2-C1-N-C1'
7	A	517	PEG	O2-C3-C4-O4
7	A	518	PEG	O1-C1-C2-O2
7	B	511	PEG	O2-C3-C4-O4
7	B	516	PEG	O1-C1-C2-O2
7	B	516	PEG	O2-C3-C4-O4
6	A	508	EDO	O1-C1-C2-O2
6	B	512	EDO	O1-C1-C2-O2
6	C	506	EDO	O1-C1-C2-O2
6	C	508	EDO	O1-C1-C2-O2
7	B	506	PEG	O2-C3-C4-O4
7	A	516	PEG	O2-C3-C4-O4
5	A	505	NHE	C6'-C1'-N-C1
6	A	510	EDO	O1-C1-C2-O2
6	A	513	EDO	O1-C1-C2-O2
7	B	515	PEG	O2-C3-C4-O4
9	B	518	PG4	O2-C3-C4-O3
6	A	515	EDO	O1-C1-C2-O2
8	A	521	PGE	O2-C3-C4-O3
7	A	519	PEG	O2-C3-C4-O4
8	A	521	PGE	C3-C4-O3-C5
7	B	506	PEG	C1-C2-O2-C3
9	B	518	PG4	O4-C7-C8-O5
7	A	519	PEG	C4-C3-O2-C2
7	A	518	PEG	O2-C3-C4-O4
2	B	501	A1B1V	C7-C2-S1-N1
2	B	501	A1B1V	C3-C2-S1-N1
7	A	516	PEG	O1-C1-C2-O2
7	A	518	PEG	C1-C2-O2-C3
7	B	514	PEG	O2-C3-C4-O4
6	A	506	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	B	507	EDO	O1-C1-C2-O2
7	B	515	PEG	O1-C1-C2-O2
7	B	506	PEG	C4-C3-O2-C2
7	B	514	PEG	C1-C2-O2-C3
9	B	518	PG4	C5-C6-O4-C7
5	A	505	NHE	C2'-C1'-N-C1
7	B	506	PEG	O1-C1-C2-O2
9	B	517	PG4	O2-C3-C4-O3
6	A	507	EDO	O1-C1-C2-O2
8	C	510	PGE	O3-C5-C6-O4
9	B	517	PG4	O1-C1-C2-O2
5	A	505	NHE	N-C1-C2-S

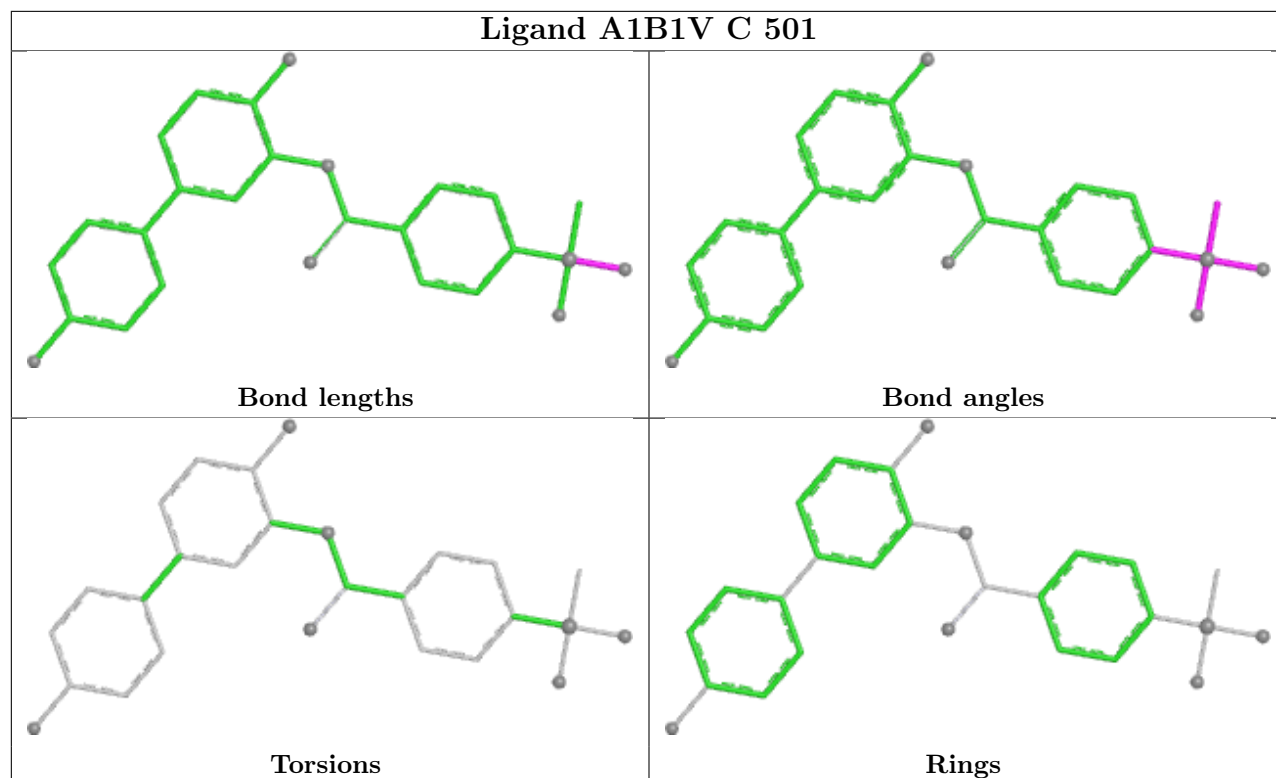
There are no ring outliers.

7 monomers are involved in 9 short contacts:

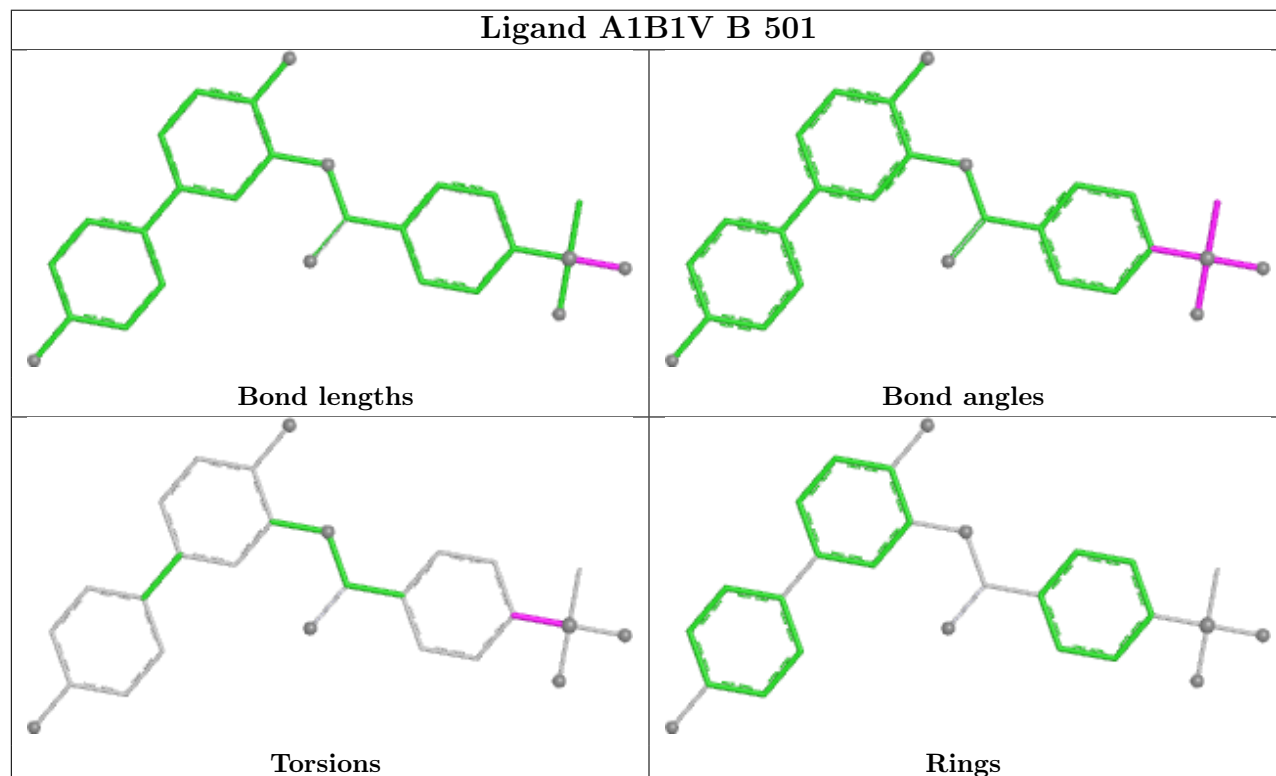
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	508	EDO	1	0
7	B	516	PEG	1	0
5	A	505	NHE	3	0
8	A	521	PGE	1	0
6	A	506	EDO	1	0
9	B	518	PG4	1	0
9	B	517	PG4	1	0

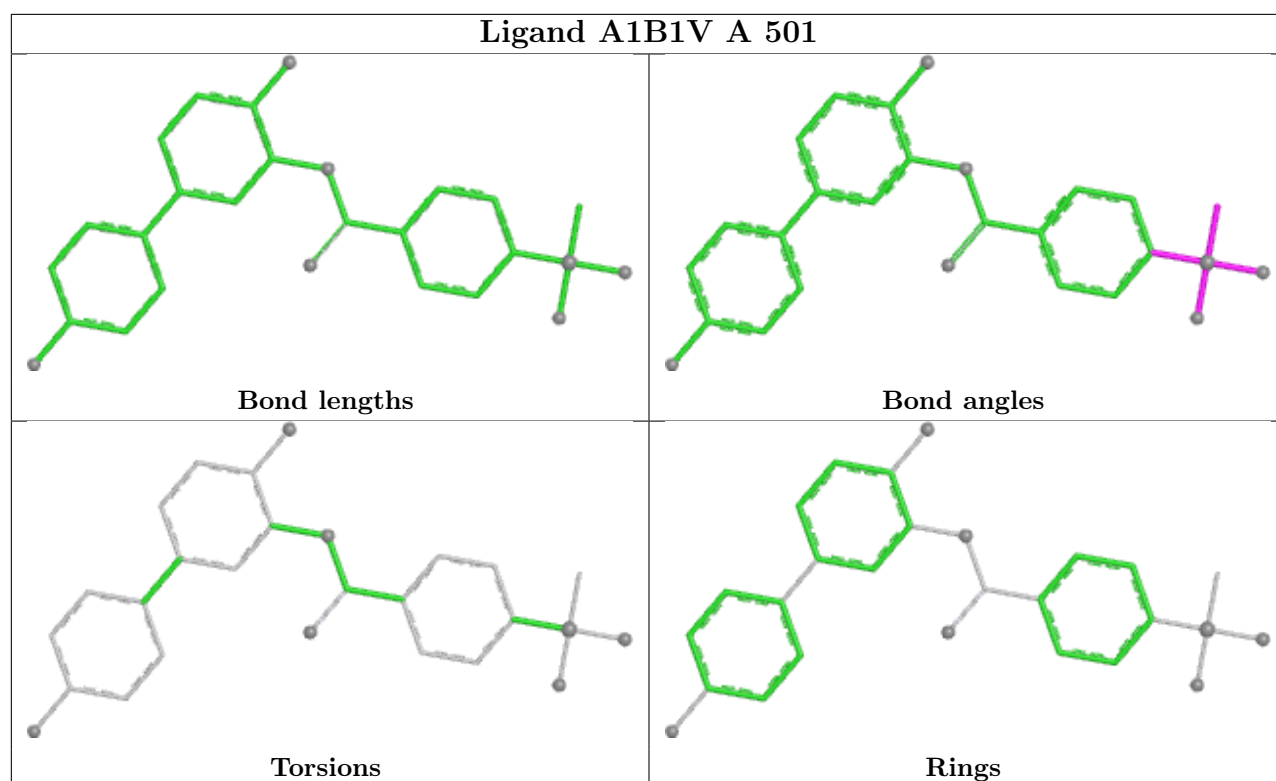
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 A1B1V C 501



Ligand A1B1V B 501





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	369/404 (91%)	-0.31	3 (0%) 82 83	17, 24, 40, 56	7 (1%)
1	B	367/404 (90%)	-0.38	0 100 100	15, 23, 40, 55	8 (2%)
1	C	366/404 (90%)	0.04	3 (0%) 82 83	17, 31, 47, 63	6 (1%)
All	All	1102/1212 (90%)	-0.22	6 (0%) 87 88	15, 26, 43, 63	21 (1%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	375	PRO	3.8
1	A	86	SER	2.9
1	A	98	GLY	2.9
1	C	28	GLY	2.3
1	A	7	GLY	2.2
1	C	337	TYR	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($\text{\AA}^2$)	Q<0.9
5	NHE	A	505	13/13	0.71	0.18	41,50,68,72	0
6	EDO	C	508	4/4	0.76	0.15	50,54,56,60	0
7	PEG	A	516	7/7	0.77	0.17	45,51,56,58	0
6	EDO	B	512	4/4	0.78	0.20	38,44,44,45	0
7	PEG	B	506	7/7	0.78	0.15	46,49,54,55	0
6	EDO	C	509	4/4	0.79	0.15	46,51,51,57	0
6	EDO	B	513	4/4	0.79	0.19	40,42,44,46	0
6	EDO	B	507	4/4	0.79	0.14	46,47,48,52	0
7	PEG	B	515	7/7	0.79	0.15	46,50,53,55	0
6	EDO	A	509	4/4	0.81	0.13	41,42,50,50	0
7	PEG	A	519	7/7	0.83	0.12	43,48,54,55	0
9	PG4	B	517	13/13	0.83	0.13	32,45,52,61	0
6	EDO	B	510	4/4	0.84	0.12	42,45,48,50	0
6	EDO	B	508	4/4	0.84	0.14	48,48,51,52	0
6	EDO	B	509	4/4	0.85	0.12	44,46,47,51	0
7	PEG	A	517	7/7	0.85	0.12	45,48,52,59	0
6	EDO	A	506	4/4	0.86	0.15	32,43,53,56	0
7	PEG	B	516	7/7	0.86	0.12	43,45,50,51	0
7	PEG	B	514	7/7	0.86	0.12	40,41,48,54	0
6	EDO	A	512	4/4	0.87	0.12	47,52,52,53	0
7	PEG	B	511	7/7	0.87	0.11	42,44,51,58	0
6	EDO	A	507	4/4	0.87	0.13	34,35,36,45	0
6	EDO	A	510	4/4	0.87	0.11	41,43,52,55	0
7	PEG	A	518	7/7	0.87	0.11	44,44,53,59	0
8	PGE	A	521	10/10	0.87	0.11	39,44,50,50	0
6	EDO	A	511	4/4	0.87	0.11	46,48,54,56	0
9	PG4	B	518	13/13	0.87	0.12	32,42,52,58	0
6	EDO	C	505	4/4	0.88	0.11	42,45,51,53	0
6	EDO	A	513	4/4	0.88	0.10	40,46,48,56	0
6	EDO	A	520	4/4	0.88	0.09	42,45,50,58	0
6	EDO	A	515	4/4	0.89	0.11	45,47,50,52	0
2	A1B1V	A	501	27/27	0.90	0.10	14,19,43,52	0
6	EDO	C	507	4/4	0.90	0.10	44,45,47,48	0
2	A1B1V	B	501	27/27	0.91	0.10	15,19,48,51	0
6	EDO	A	508	4/4	0.91	0.10	46,49,51,52	0
5	NHE	B	505	13/13	0.91	0.10	26,33,45,48	0
2	A1B1V	C	501	27/27	0.91	0.10	16,23,50,53	0
6	EDO	C	506	4/4	0.91	0.12	36,40,42,45	0
8	PGE	C	510	10/10	0.95	0.07	30,33,46,53	0
6	EDO	A	514	4/4	0.97	0.07	23,27,33,36	0
4	CA	C	504	1/1	0.98	0.17	34,34,34,34	0
4	CA	B	504	1/1	0.99	0.06	28,28,28,28	0
3	ZN	C	502	1/1	0.99	0.03	23,23,23,23	0

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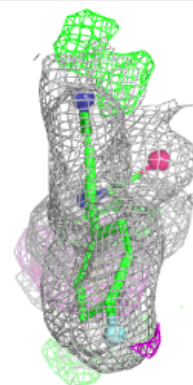
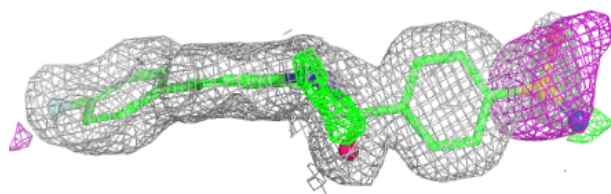
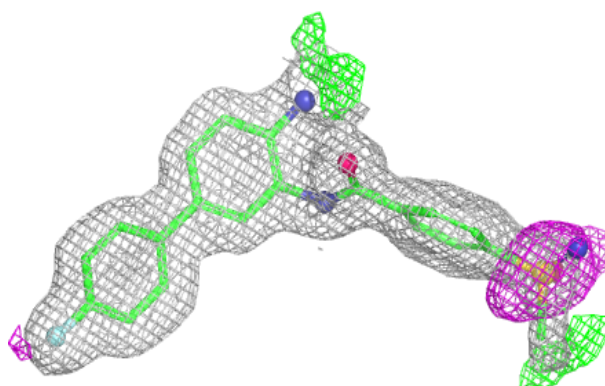
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	A	504	1/1	0.99	0.11	28,28,28,28	0
3	ZN	A	502	1/1	1.00	0.03	19,19,19,19	0
4	CA	C	503	1/1	1.00	0.09	27,27,27,27	0
4	CA	A	503	1/1	1.00	0.06	22,22,22,22	0
3	ZN	B	502	1/1	1.00	0.02	17,17,17,17	0
4	CA	B	503	1/1	1.00	0.05	21,21,21,21	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.

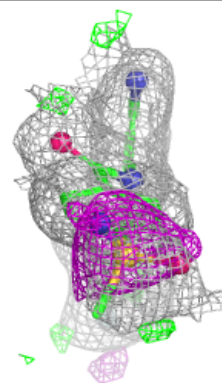
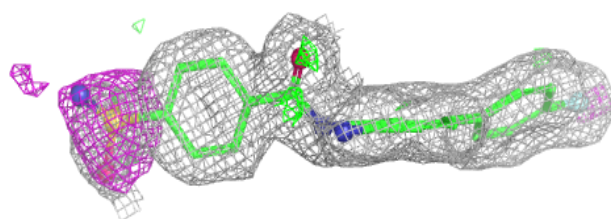
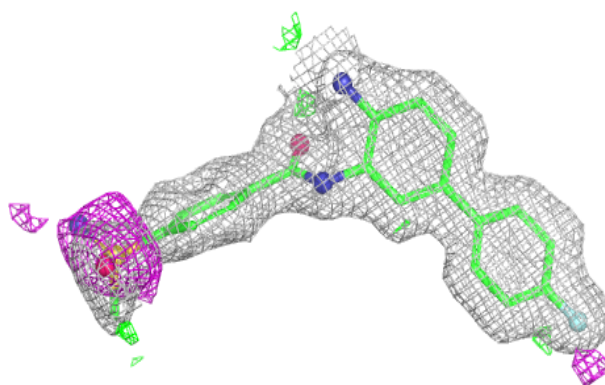
Electron density around A1B1V A 501:

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

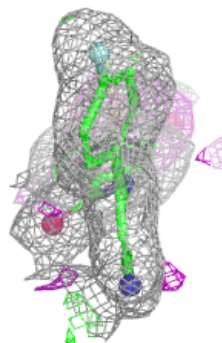
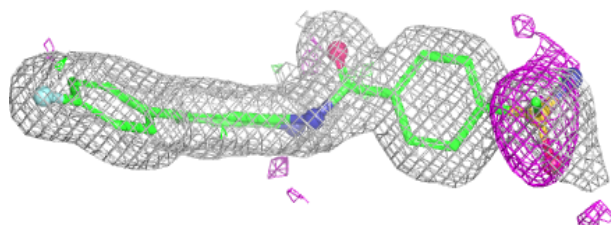
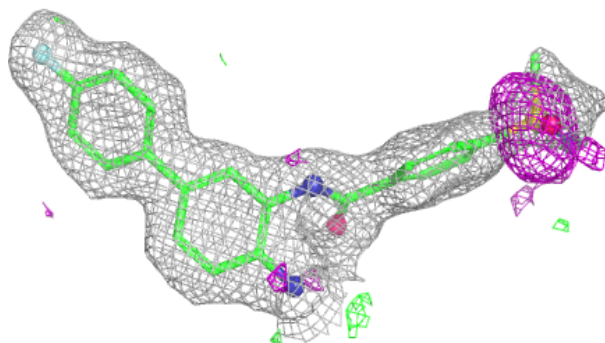


Electron density around A1B1V B 501:

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

**Electron density around A1B1V C 501:**

$2mF_o-DF_c$ (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.