



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2026 – 10:11 pm BST

PDB ID : 9S19 / pdb_00009s19
Title : WRN helicase in complex with ATPgS and ssDNA
Authors : Fletcher, C.T.; Rucktoo, P.
Deposited on : 2025-07-18
Resolution : 2.30 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 : 1.8.4, CSD as541be (2020)
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

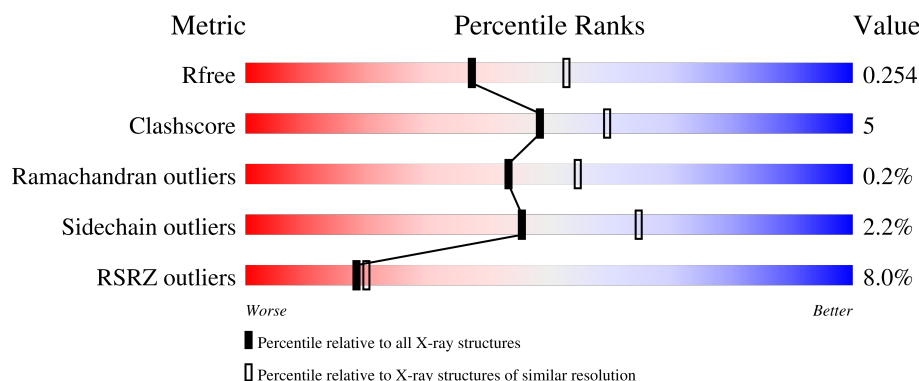
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	427	<div> <div>10%</div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	B	427	<div> <div>5%</div> <div>81%</div> <div>14%</div> <div>.</div> </div>
2	C	15	<div> <div>27%</div> <div>7%</div> <div>67%</div> </div>
2	D	15	<div> <div>13%</div> <div>20%</div> <div>33%</div> <div>47%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	B	1007	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7010 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 Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	1	0
			3184	2014	562	579	29			
1	B	409	Total	C	N	O	S	0	1	0
			3271	2072	579	591	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	515	GLY	-	expression tag	UNP Q14191
A	516	MET	-	expression tag	UNP Q14191
B	515	GLY	-	expression tag	UNP Q14191
B	516	MET	-	expression tag	UNP Q14191

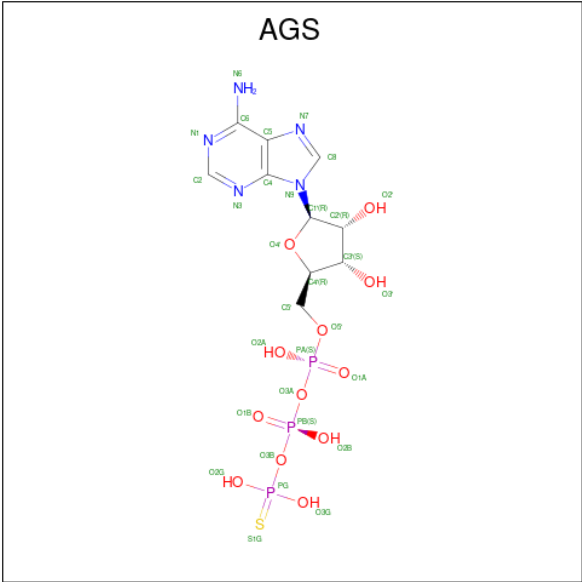
- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	P	0	0	0
			98	47	16	30	5			
2	D	8	Total	C	N	O	P	0	0	0
			163	77	31	47	8			

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

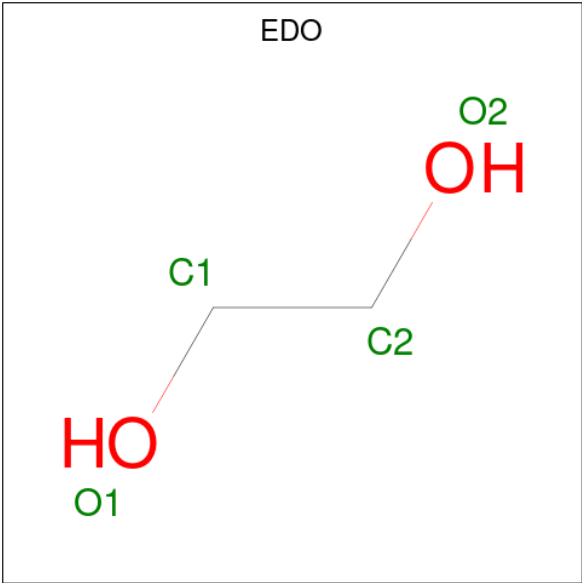
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



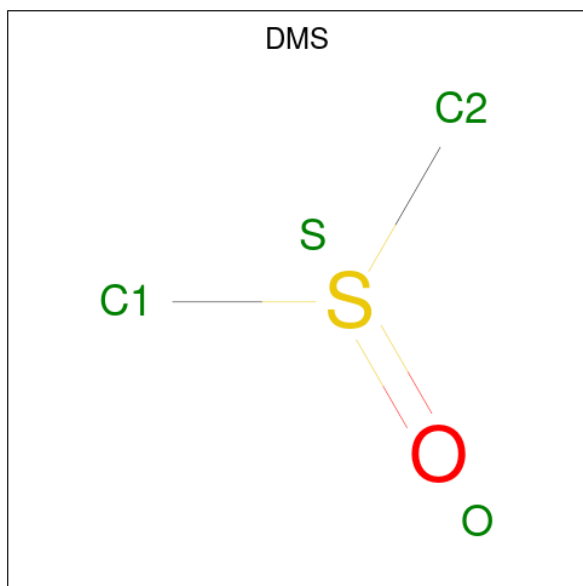
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

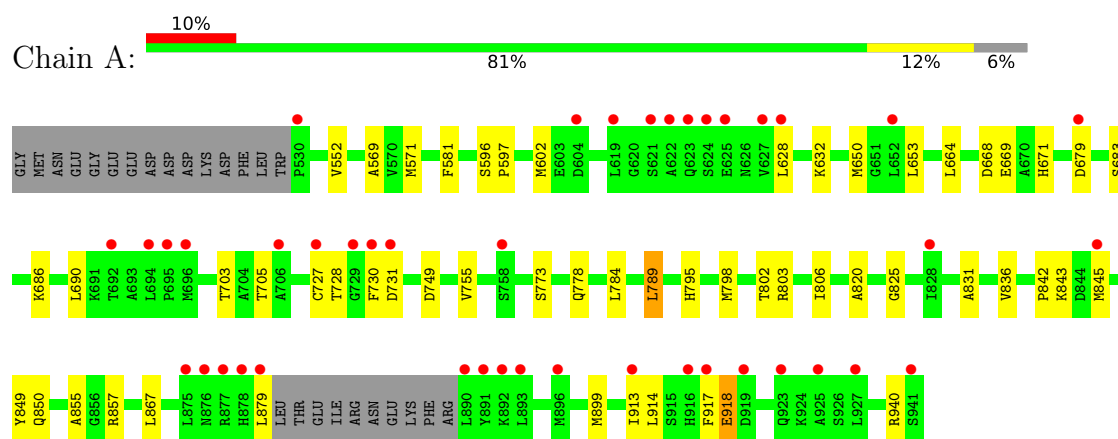
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	71	Total 71	O 71	0	0
7	B	96	Total 96	O 96	0	0
7	C	3	Total 3	O 3	0	0
7	D	8	Total 8	O 8	0	0

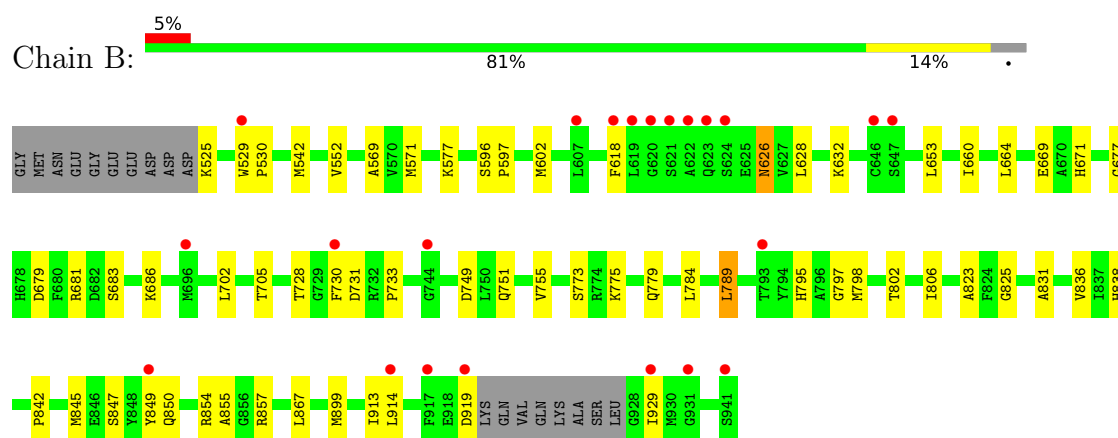
3 Residue-property plots [i](#)

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: Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN



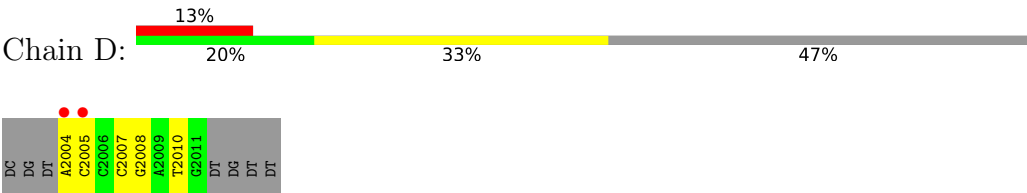
- Molecule 1: Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN



- Molecule 2: DNA (5'-D(P*TP*AP*CP*CP*C)-3')



- Molecule 2: DNA (5'-D(P*TP*AP*CP*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.42Å 70.55Å 123.47Å 90.00° 94.90° 90.00°	Depositor
Resolution (Å)	123.02 – 2.30 123.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.5 (123.02-2.30) 87.5 (123.02-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.228 , 0.257 0.222 , 0.254	Depositor DCC
R_{free} test set	2026 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7010	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: ZN, EDO, AGS, DMS

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	0.67	0/3251	1.05	7/4386 (0.2%)
1	B	0.70	3/3339 (0.1%)	1.04	1/4505 (0.0%)
2	C	0.50	0/108	0.61	0/163
2	D	0.53	0/182	0.75	0/278
All	All	0.68	3/6880 (0.0%)	1.03	8/9332 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	542	MET	SD-CE	5.44	1.93	1.79
1	B	679	ASP	CA-C	5.17	1.55	1.52
1	B	660	ILE	CG1-CD1	-5.03	1.32	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	626	ASN	CA-CB-CG	8.28	120.88	112.60
1	A	679	ASP	CA-C-N	7.05	129.95	120.65
1	A	679	ASP	C-N-CA	7.05	129.95	120.65
1	A	820	ALA	N-CA-C	5.73	117.90	109.24
1	A	918	GLU	N-CA-C	5.37	118.80	111.39
1	A	917	PHE	CA-C-N	5.22	129.78	122.36
1	A	917	PHE	C-N-CA	5.22	129.78	122.36
1	A	581	PHE	CA-CB-CG	5.12	118.92	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3184	0	3213	32	0
1	B	3271	0	3289	38	0
2	C	98	0	57	2	0
2	D	163	0	90	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	1	0
5	A	24	0	36	1	0
5	B	20	0	30	5	0
6	A	4	0	6	0	0
6	B	4	0	6	0	0
7	A	71	0	0	1	0
7	B	96	0	0	0	0
7	C	3	0	0	0	0
7	D	8	0	0	0	0
All	All	7010	0	6751	74	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 (74) 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:823:ALA:HB2	2:D:2008:DG:H5''	1.54	0.89
1:A:798:MET:HE3	1:A:802:THR:HG22	1.58	0.85
1:B:798:MET:HE3	1:B:802:THR:HG22	1.62	0.81
1:B:705:THR:HG22	1:B:849:TYR:HD2	1.50	0.76
1:B:730:PHE:HD2	1:B:919:ASP:HB2	1.50	0.74
1:A:705:THR:HG22	1:A:849:TYR:HD2	1.56	0.70
1:A:731:ASP:HB2	1:A:914:LEU:HD21	1.75	0.67
1:B:845:MET:HE1	1:B:913:ILE:HG12	1.76	0.67
1:B:705:THR:HG22	1:B:849:TYR:CD2	2.30	0.67
1:B:775:LYS:HG2	1:B:779:GLN:HE21	1.60	0.66
1:A:940:ARG:NH1	5:A:1006:EDO:O1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:THR:HG22	1:A:849:TYR:CD2	2.33	0.64
1:B:705:THR:CG2	1:B:849:TYR:HD2	2.10	0.64
1:A:845:MET:HE1	1:A:913:ILE:HG12	1.79	0.64
1:A:705:THR:HG21	1:A:850:GLN:HG2	1.81	0.63
1:B:730:PHE:CD2	1:B:919:ASP:HB2	2.32	0.63
1:A:596:SER:HB3	1:A:602:MET:HE2	1.81	0.62
1:B:847:SER:HA	5:B:1007:EDO:H12	1.81	0.62
1:B:705:THR:HG21	1:B:850:GLN:HG2	1.82	0.62
1:A:705:THR:CG2	1:A:849:TYR:HD2	2.12	0.61
1:B:823:ALA:HB2	2:D:2008:DG:C5'	2.28	0.59
1:B:677:GLY:HA2	1:B:681:ARG:O	2.05	0.56
1:B:847:SER:HA	5:B:1007:EDO:C1	2.36	0.54
1:A:773:SER:HA	2:C:2007:DT:H5''	1.89	0.54
7:A:1129:HOH:O	2:D:2010:DT:H73	2.10	0.52
1:B:731:ASP:HB2	1:B:914:LEU:HD21	1.92	0.52
1:B:795:HIS:HD2	1:B:797:GLY:H	1.56	0.52
1:A:798:MET:HE3	1:A:802:THR:CG2	2.36	0.51
1:A:650:MET:HE1	1:A:690:LEU:HA	1.91	0.51
1:B:671:HIS:CD2	5:B:1007:EDO:H21	2.47	0.50
1:B:798:MET:HE3	1:B:802:THR:CG2	2.40	0.50
1:B:552:VAL:HG21	1:B:728:THR:HG22	1.94	0.48
1:A:795:HIS:O	1:A:803:ARG:HD3	2.13	0.47
1:B:831:ALA:HA	1:B:857:ARG:HB2	1.95	0.47
1:A:831:ALA:HA	1:A:857:ARG:HB2	1.96	0.47
1:B:784:LEU:HD22	1:B:789:LEU:HD13	1.96	0.47
1:A:784:LEU:HD22	1:A:789:LEU:HD13	1.97	0.47
1:A:798:MET:HE2	1:A:803:ARG:HG2	1.96	0.47
1:A:552:VAL:HG21	1:A:728:THR:HG22	1.97	0.46
1:B:602:MET:SD	1:B:618:PHE:CD1	3.08	0.46
2:D:2004:DA:H4'	2:D:2005:DC:OP1	2.16	0.46
2:D:2005:DC:O2	2:D:2005:DC:H2'	2.16	0.46
1:B:705:THR:CG2	1:B:850:GLN:HG2	2.45	0.46
1:A:842:PRO:HD2	1:A:899:MET:HE2	1.97	0.46
1:B:836:VAL:HG23	1:B:855:ALA:HB2	1.99	0.45
1:B:596:SER:HB3	1:B:602:MET:HE2	1.99	0.45
1:A:668:ASP:OD2	4:A:1002:AGS:S1G	2.75	0.45
1:A:569:ALA:HB1	1:A:571:MET:HE3	1.99	0.45
1:A:705:THR:CG2	1:A:850:GLN:HG2	2.46	0.44
1:A:597:PRO:HG3	1:A:669:GLU:HB2	2.00	0.44
1:B:842:PRO:HD2	1:B:899:MET:HE2	1.99	0.44
1:A:628:LEU:HG	1:A:632:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:VAL:HG23	1:A:855:ALA:HB2	2.01	0.43
1:B:733:PRO:HB3	1:B:929:ILE:HG13	1.99	0.43
1:B:577:LYS:HE2	4:B:1006:AGS:S1G	2.58	0.43
1:A:778:GLN:HG2	2:D:2005:DC:OP1	2.18	0.43
1:B:552:VAL:HG12	1:B:571:MET:HE2	2.01	0.43
1:A:552:VAL:HG12	1:A:571:MET:HE2	2.01	0.42
1:B:569:ALA:HB1	1:B:571:MET:HE3	2.01	0.42
1:A:727:CYS:SG	1:A:730:PHE:CE2	3.13	0.42
1:B:749:ASP:HB3	1:B:867:LEU:HD13	2.02	0.41
1:A:749:ASP:HB3	1:A:867:LEU:HD13	2.02	0.41
1:B:683:SER:HA	1:B:686:LYS:HD2	2.02	0.41
1:A:843:LYS:HE3	1:A:879:LEU:CD1	2.50	0.41
1:B:773:SER:HA	2:D:2007:DC:C5'	2.50	0.41
1:B:597:PRO:HG3	1:B:669:GLU:HB2	2.03	0.41
1:B:838:HIS:HD2	5:B:1008:EDO:H21	1.85	0.41
1:A:683:SER:HA	1:A:686:LYS:HD2	2.03	0.41
2:D:2005:DC:O2	2:D:2005:DC:C2'	2.68	0.41
1:A:671:HIS:ND1	1:A:703:THR:OG1	2.51	0.41
1:B:671:HIS:HD2	5:B:1007:EDO:H21	1.85	0.41
1:B:628:LEU:HG	1:B:632:LYS:HE3	2.02	0.40
1:A:773:SER:HA	2:C:2007:DT:C5'	2.52	0.40
1:B:529:TRP:HA	1:B:530:PRO:HA	1.89	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	399/427 (93%)	385 (96%)	13 (3%)	1 (0%)	36	46
1	B	406/427 (95%)	391 (96%)	14 (3%)	1 (0%)	43	55
All	All	805/854 (94%)	776 (96%)	27 (3%)	2 (0%)	43	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	825	GLY
1	B	825	GLY

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	355/377 (94%)	349 (98%)	6 (2%)	53	72
1	B	363/377 (96%)	353 (97%)	10 (3%)	38	56
All	All	718/754 (95%)	702 (98%)	16 (2%)	45	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	653	LEU
1	A	664	LEU
1	A	755	VAL
1	A	789	LEU
1	A	806	ILE
1	A	918	GLU
1	B	525	LYS
1	B	626	ASN
1	B	653	LEU
1	B	664	LEU
1	B	702	LEU
1	B	751	GLN
1	B	755	VAL
1	B	789	LEU
1	B	806	ILE
1	B	854	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	546	HIS
1	A	745	ASN
1	A	748	GLN
1	A	916	HIS
1	B	546	HIS
1	B	558	HIS
1	B	605	GLN
1	B	779	GLN
1	B	795	HIS
1	B	916	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\# Z > 2$
5	EDO	A	1009	-	3,3,3	0.34	0	2,2,2	0.13	0
5	EDO	B	1008	-	3,3,3	0.38	0	2,2,2	0.17	0
5	EDO	A	1005	-	3,3,3	0.18	0	2,2,2	0.43	0
5	EDO	B	1005	-	3,3,3	0.20	0	2,2,2	0.37	0
6	DMS	A	1008	-	3,3,3	0.59	0	3,3,3	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	1007	-	3,3,3	0.26	0	2,2,2	0.09	0
5	EDO	A	1004	-	3,3,3	0.13	0	2,2,2	0.55	0
5	EDO	B	1003	-	3,3,3	0.20	0	2,2,2	0.37	0
6	DMS	B	1002	-	3,3,3	0.71	0	3,3,3	0.78	0
5	EDO	A	1006	-	3,3,3	0.19	0	2,2,2	0.42	0
5	EDO	B	1004	-	3,3,3	0.22	0	2,2,2	0.20	0
5	EDO	A	1003	-	3,3,3	0.29	0	2,2,2	0.28	0
4	AGS	A	1002	-	29,33,33	0.65	1 (3%)	39,52,52	0.53	0
5	EDO	A	1007	-	3,3,3	0.27	0	2,2,2	0.23	0
4	AGS	B	1006	-	29,33,33	0.75	1 (3%)	39,52,52	0.68	1 (2%)

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
5	EDO	A	1009	-	-	1/1/1/1	-
5	EDO	B	1008	-	-	1/1/1/1	-
5	EDO	A	1005	-	-	1/1/1/1	-
5	EDO	B	1005	-	-	0/1/1/1	-
5	EDO	B	1007	-	-	1/1/1/1	-
5	EDO	A	1004	-	-	1/1/1/1	-
5	EDO	B	1003	-	-	0/1/1/1	-
5	EDO	A	1006	-	-	1/1/1/1	-
5	EDO	B	1004	-	-	0/1/1/1	-
5	EDO	A	1003	-	-	1/1/1/1	-
4	AGS	A	1002	-	-	0/21/38/38	0/3/3/3
5	EDO	A	1007	-	-	0/1/1/1	-
4	AGS	B	1006	-	-	3/21/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1006	AGS	PG-S1G	3.16	1.97	1.90
4	A	1002	AGS	PG-S1G	2.47	1.96	1.90

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1006	AGS	O2'-C2'-C1'	2.08	116.96	110.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

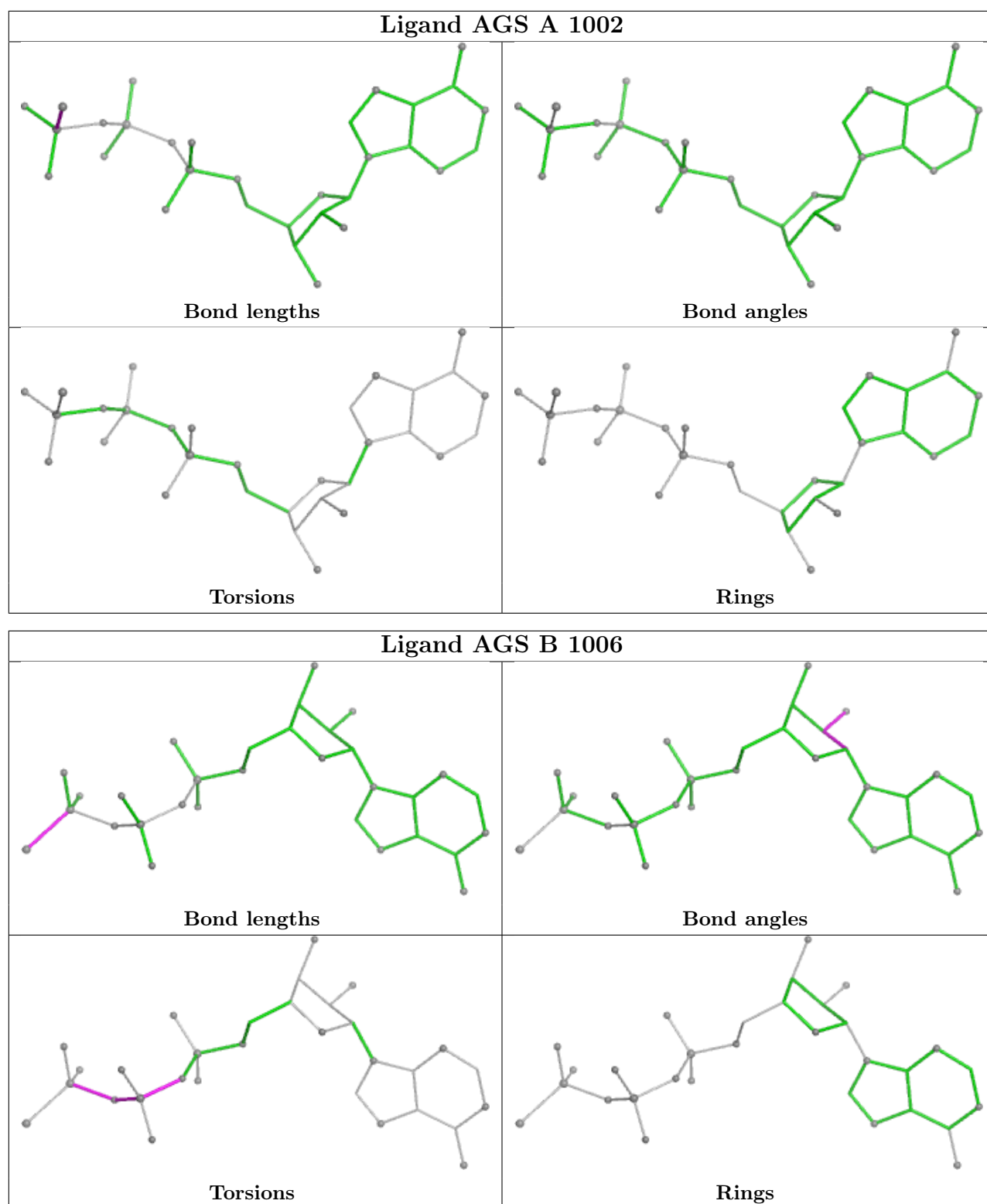
Mol	Chain	Res	Type	Atoms
5	B	1007	EDO	O1-C1-C2-O2
5	A	1005	EDO	O1-C1-C2-O2
5	A	1006	EDO	O1-C1-C2-O2
5	B	1008	EDO	O1-C1-C2-O2
4	B	1006	AGS	PB-O3B-PG-O3G
5	A	1003	EDO	O1-C1-C2-O2
4	B	1006	AGS	PG-O3B-PB-O2B
4	B	1006	AGS	PA-O3A-PB-O2B
5	A	1004	EDO	O1-C1-C2-O2
5	A	1009	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1008	EDO	1	0
5	B	1007	EDO	4	0
5	A	1006	EDO	1	0
4	A	1002	AGS	1	0
4	B	1006	AGS	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	402/427 (94%)	0.70	42 (10%) 11 13	27, 56, 89, 116	1 (0%)
1	B	409/427 (95%)	0.58	22 (5%) 31 33	21, 52, 83, 102	1 (0%)
2	C	5/15 (33%)	0.65	0 100 100	63, 65, 69, 75	0
2	D	8/15 (53%)	0.97	2 (25%) 2 2	53, 64, 97, 110	0
All	All	824/884 (93%)	0.64	66 (8%) 18 20	21, 54, 86, 116	2 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	879	LEU	6.5
1	A	730	PHE	6.1
1	A	875	LEU	5.9
1	A	890	LEU	5.7
1	A	622	ALA	5.5
1	A	917	PHE	5.0
1	B	622	ALA	4.6
1	A	621	SER	4.2
1	B	620	GLY	3.9
1	B	941	SER	3.6
1	A	878	HIS	3.6
1	A	758	SER	3.5
1	B	646	CYS	3.4
1	A	624	SER	3.3
1	B	919	ASP	3.2
1	A	876	ASN	3.1
1	A	893	LEU	3.0
1	B	696	MET	2.9
1	B	744	GLY	2.9
1	B	929	ILE	2.9
1	A	694	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	729	GLY	2.8
1	A	916	HIS	2.8
1	A	923	GLN	2.7
1	B	647	SER	2.7
1	A	706	ALA	2.7
1	A	731	ASP	2.7
1	B	917	PHE	2.7
1	B	849	TYR	2.7
1	A	696	MET	2.6
1	B	621	SER	2.6
1	A	727	CYS	2.5
1	A	927	LEU	2.5
1	B	931	GLY	2.5
1	A	891	TYR	2.5
1	A	652	LEU	2.5
1	B	607	LEU	2.5
1	A	941	SER	2.4
1	B	730	PHE	2.4
1	B	624	SER	2.4
1	A	913	ILE	2.4
1	B	623	GLN	2.4
1	B	793	THR	2.4
1	A	877	ARG	2.4
2	D	2005	DC	2.4
1	A	919	ASP	2.3
1	B	618	PHE	2.3
2	D	2004	DA	2.3
1	A	845	MET	2.3
1	A	925	ALA	2.3
1	A	828	ILE	2.3
1	A	627	VAL	2.3
1	A	628	LEU	2.3
1	A	625	GLU	2.2
1	A	695	PRO	2.2
1	A	623	GLN	2.2
1	A	619	LEU	2.2
1	A	892	LYS	2.1
1	A	604	ASP	2.1
1	A	692	THR	2.1
1	B	619	LEU	2.1
1	A	679	ASP	2.1
1	B	529	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	896	MET	2.0
1	B	914	LEU	2.0
1	A	530	PRO	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.

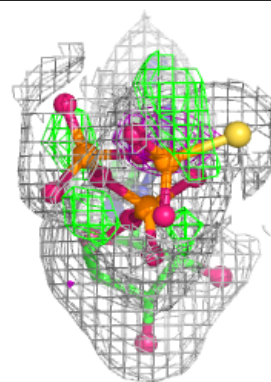
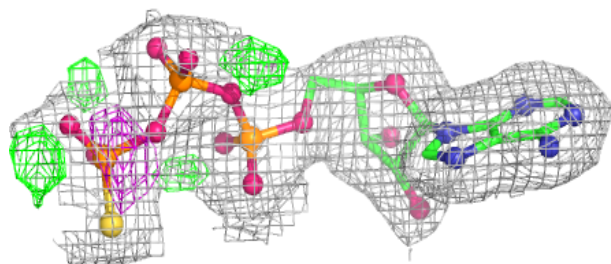
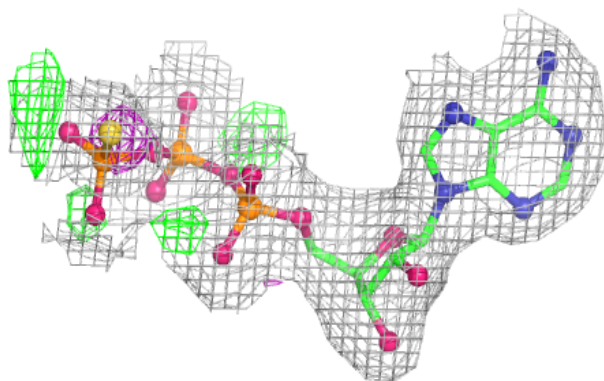
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	EDO	A	1009	4/4	0.75	0.18	63,63,63,64	0
5	EDO	A	1003	4/4	0.80	0.17	77,77,77,78	0
5	EDO	A	1006	4/4	0.82	0.18	73,73,73,73	0
5	EDO	A	1005	4/4	0.82	0.17	58,59,59,59	0
5	EDO	B	1007	4/4	0.82	0.19	69,69,69,69	0
5	EDO	B	1008	4/4	0.83	0.18	59,59,59,60	0
5	EDO	A	1007	4/4	0.84	0.17	70,70,71,71	0
5	EDO	B	1003	4/4	0.84	0.17	68,69,69,69	0
5	EDO	A	1004	4/4	0.85	0.18	55,56,56,56	0
5	EDO	B	1004	4/4	0.85	0.19	84,84,84,84	0
5	EDO	B	1005	4/4	0.86	0.26	83,83,83,83	0
4	AGS	A	1002	31/31	0.91	0.09	44,49,63,64	0
4	AGS	B	1006	31/31	0.92	0.07	37,43,54,57	0
6	DMS	A	1008	4/4	0.98	0.06	35,35,35,35	0
6	DMS	B	1002	4/4	0.98	0.06	43,44,44,44	0
3	ZN	B	1001	1/1	0.99	0.06	69,69,69,69	0
3	ZN	A	1001	1/1	0.99	0.04	65,65,65,65	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.

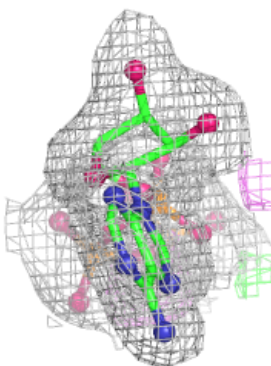
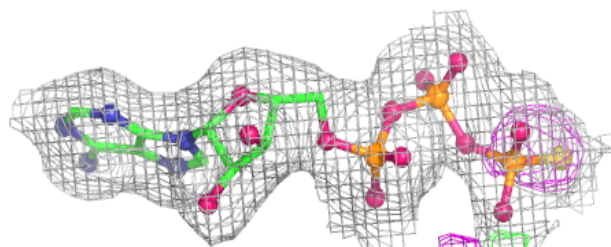
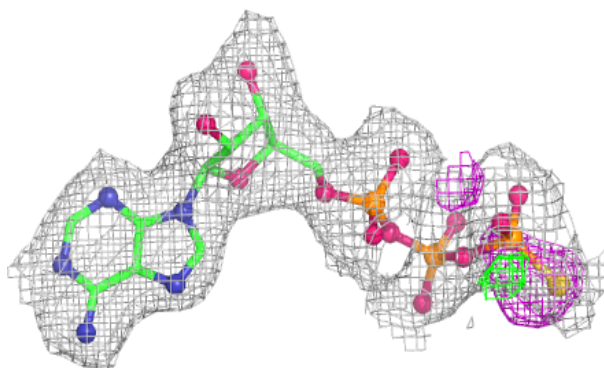
Electron density around AGS A 1002:

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



Electron density around AGS B 1006:

$2mF_o-DF_c$ (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.