



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2025 – 01:23 pm BST

PDB ID : 9RUR / pdb_00009rur
Title : Structure of WRN in complex with ATPgS and covalent ligand Compound 4d
Authors : Fletcher, C.T.; Rucktooa, P.
Deposited on : 2025-07-04
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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

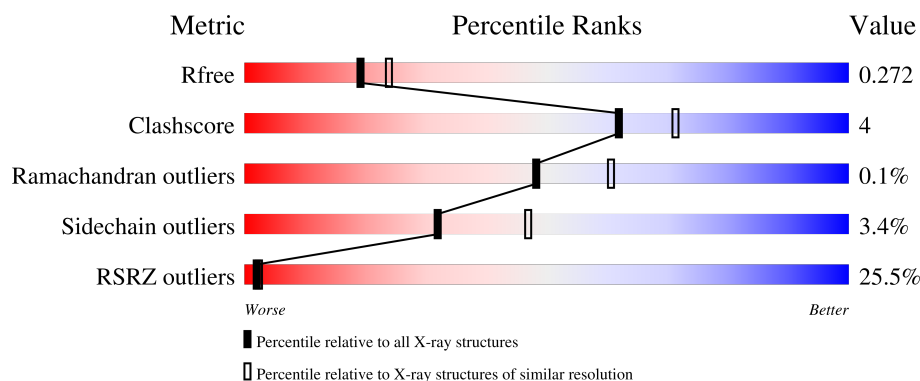
1 Overall quality at a glance

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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (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>16%</div> <div>83%</div> <div>11%</div> <div>• 5%</div> </div>
1	B	427	<div> <div>31%</div> <div>81%</div> <div>10%</div> <div>9%</div> </div>

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6715 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.

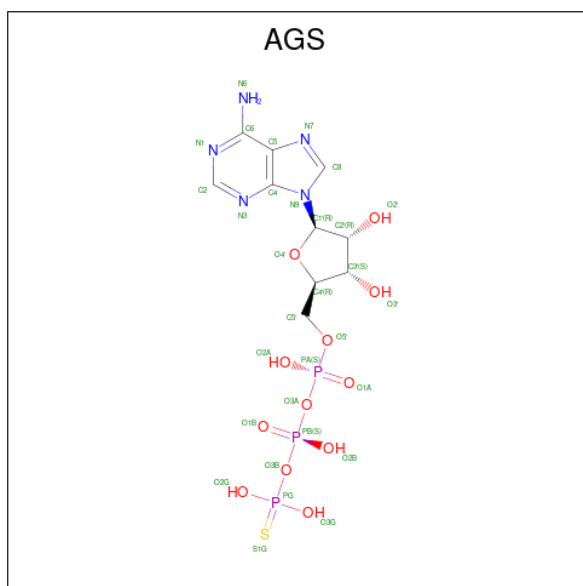
- Molecule 1 is a protein called Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	4	0
			3258	2060	579	589	30			
1	B	390	Total	C	N	O	S	0	2	0
			3110	1971	548	562	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 PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



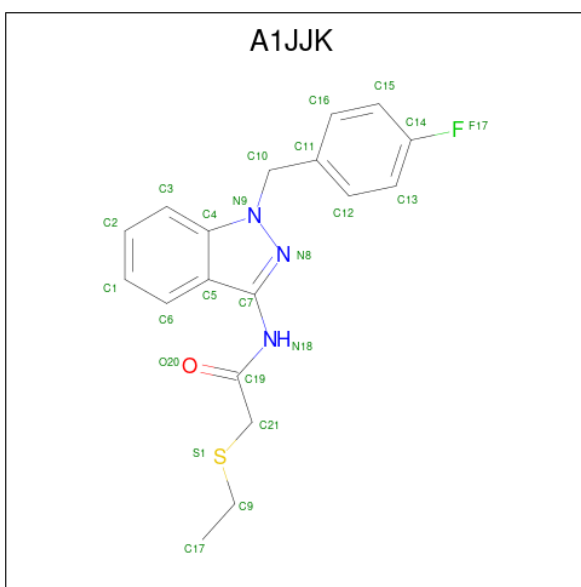
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



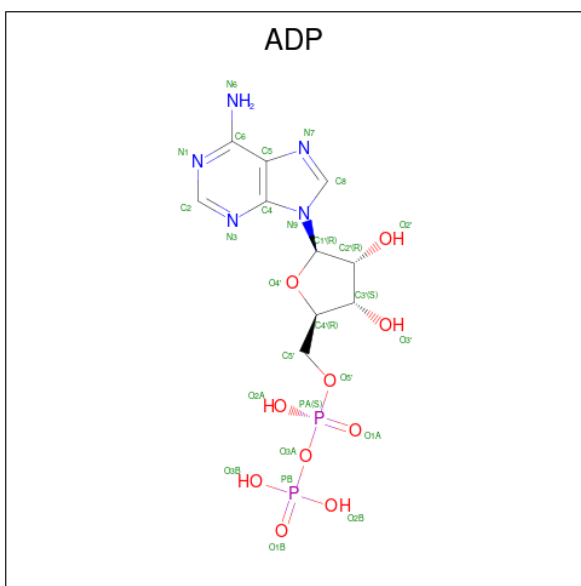
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-ethylsulfanyl- {N}-[1-[(4-fluorophenyl)methyl]indazol-3-yl]ethanamide (CCD ID: A1JJK) (formula: C₁₈H₁₈FN₃OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	1
			21	16	1	3	1		

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	1
			27	10	5	10	2		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Mg 1	0	0

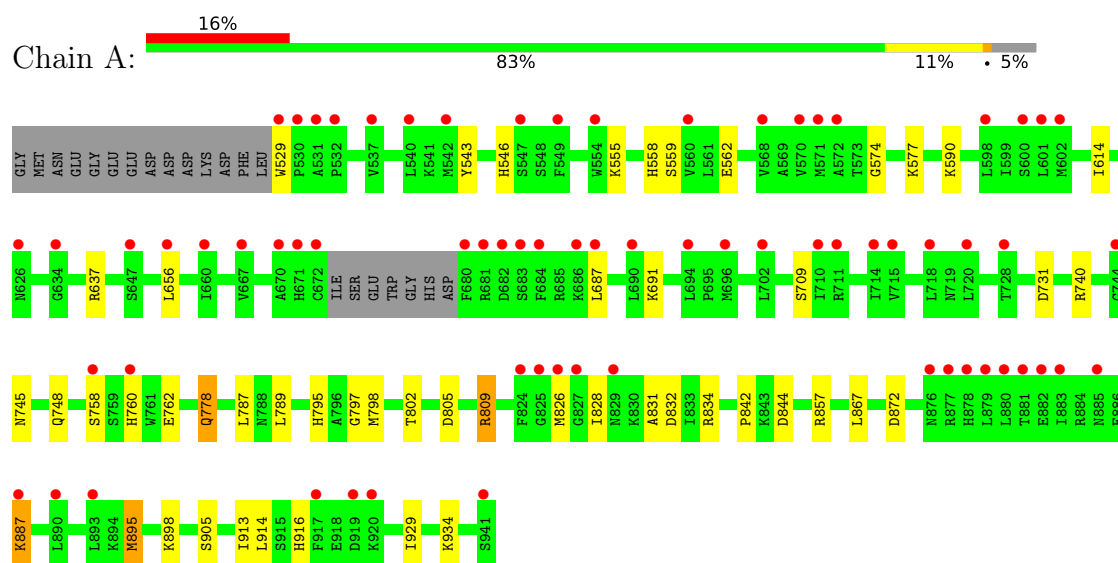
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	106	Total 106	O 106	0	0
9	B	76	Total 76	O 76	0	0

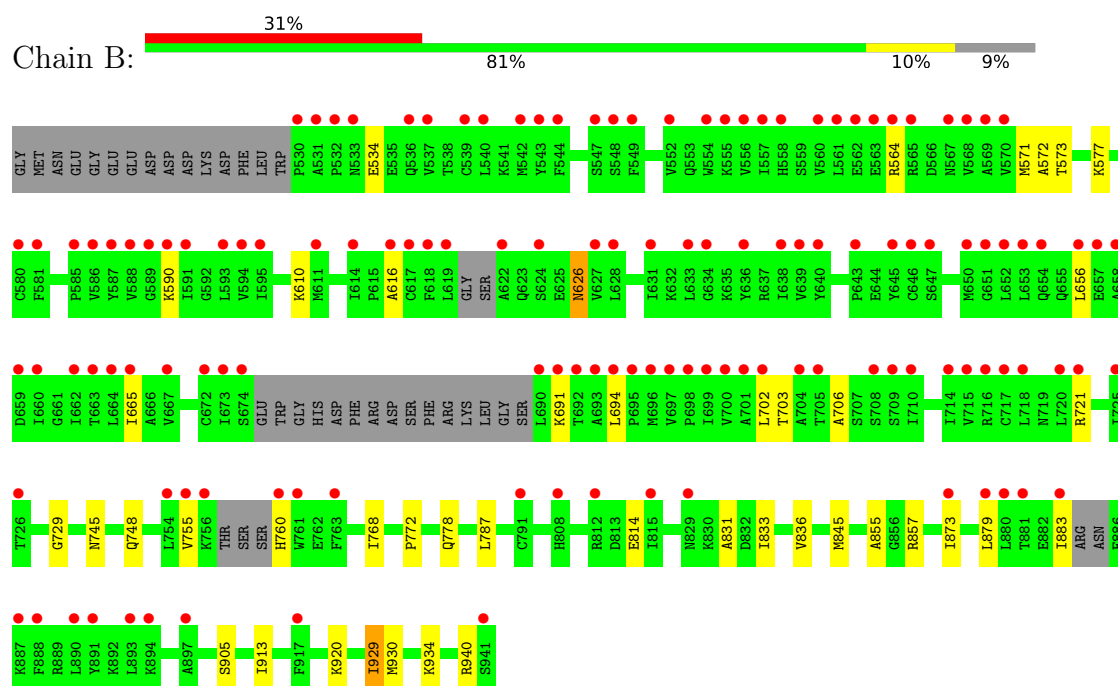
3 Residue-property plots

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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.98Å 89.98Å 241.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.31 – 2.30 84.31 – 2.30	Depositor EDS
% Data completeness (in resolution range)	72.0 (84.31-2.30) 72.0 (84.31-2.30)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.250 , 0.281 0.239 , 0.272	Depositor DCC
R_{free} test set	1599 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6715	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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, ADP, MG, AGS, EDO, A1JJK, 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	0/3322	1.06	2/4480 (0.0%)
1	B	0.69	3/3168 (0.1%)	1.09	4/4270 (0.1%)
All	All	0.68	3/6490 (0.0%)	1.07	6/8750 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	571	MET	SD-CE	-6.63	1.62	1.79
1	B	929	ILE	CG1-CD1	-5.57	1.30	1.51
1	B	930	MET	SD-CE	-5.10	1.66	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	872	ASP	CA-CB-CG	10.21	122.81	112.60
1	B	626	ASN	CA-CB-CG	5.90	118.50	112.60
1	B	814	GLU	CA-C-N	5.84	130.43	123.19
1	B	814	GLU	C-N-CA	5.84	130.43	123.19
1	A	905	SER	N-CA-C	5.53	117.86	110.35
1	B	905	SER	N-CA-C	5.05	117.22	110.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3258	0	3291	37	0
1	B	3110	0	3151	18	0
2	A	31	0	12	0	0
2	B	31	0	12	1	0
3	A	12	0	18	4	0
3	B	8	0	12	1	0
4	A	16	0	24	2	0
4	B	16	0	24	0	0
5	A	21	0	0	1	0
6	A	27	0	12	6	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	1	0	0	0	0
9	A	106	0	0	0	0
9	B	76	0	0	0	0
All	All	6715	0	6556	52	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 (52) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:HIS:HD1	1:A:797:GLY:H	1.36	0.73
1:A:760:HIS:CE1	1:B:873:ILE:HD12	2.23	0.73
1:A:798:MET:HE3	1:A:802:THR:HG22	1.74	0.70
1:A:832:ASP:OD2	1:B:778:GLN:NE2	2.27	0.67
1:A:546:HIS:CE1	6:A:1007[B]:ADP:C4	2.86	0.63
1:A:898:LYS:HD3	1:A:916:HIS:HE1	1.64	0.61
1:A:709:SER:HB2	1:A:887:LYS:NZ	2.18	0.59
1:A:898:LYS:HD3	1:A:916:HIS:CE1	2.38	0.58
1:A:709:SER:HB2	1:A:887:LYS:HZ3	1.68	0.58
1:A:934:LYS:HD3	3:A:1003:DMS:H13	1.87	0.57
1:A:913:ILE:HG23	5:A:1006[B]:A1JJK:F17	1.94	0.57
1:B:577:LYS:HB3	1:B:702:LEU:HD13	1.86	0.57
1:A:762:GLU:HA	1:A:789:LEU:HD21	1.91	0.51
1:B:836:VAL:HG23	1:B:855:ALA:HB2	1.94	0.50
1:A:844:ASP:HB2	1:A:895:MET:HB3	1.95	0.49
1:A:577:LYS:HE3	6:A:1007[B]:ADP:O1B	2.13	0.49
1:B:665:ILE:HD11	1:B:694:LEU:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:GLU:HA	1:A:789:LEU:CD2	2.42	0.49
1:B:703:THR:HG21	1:B:706:ALA:HB3	1.95	0.48
1:B:929:ILE:HG12	1:B:934:LYS:HD3	1.96	0.48
1:A:934:LYS:CD	3:A:1003:DMS:H13	2.43	0.47
1:A:546:HIS:CE1	6:A:1007[B]:ADP:N9	2.83	0.47
1:A:574:GLY:N	6:A:1007[B]:ADP:O2B	2.27	0.47
1:B:940:ARG:HH12	3:B:1003:DMS:H12	1.80	0.46
1:A:529:TRP:NE1	1:A:555:LYS:HE3	2.31	0.46
1:A:778:GLN:NE2	1:A:795:HIS:NE2	2.65	0.45
1:B:772:PRO:HB2	1:B:873:ILE:HD11	1.97	0.45
1:B:768:ILE:HD11	1:B:833:ILE:HD13	1.99	0.45
1:A:691:LYS:HA	1:A:691:LYS:HD2	1.83	0.45
1:A:828:ILE:HG12	3:A:1008:DMS:H22	1.98	0.45
1:A:798:MET:HE3	1:A:802:THR:CG2	2.45	0.45
1:B:572:ALA:HB2	1:B:729:GLY:O	2.17	0.45
1:A:831:ALA:HA	1:A:857:ARG:HB2	1.98	0.44
1:B:703:THR:HG21	1:B:706:ALA:CB	2.47	0.44
1:A:826:MET:O	3:A:1008:DMS:S	2.75	0.44
1:B:745:ASN:HB3	1:B:748:GLN:HB3	1.99	0.44
1:A:543:TYR:HB3	1:A:614:ILE:HD11	2.00	0.44
1:A:805:ASP:O	1:A:809:ARG:HG3	2.18	0.44
1:A:577:LYS:HG2	6:A:1007[B]:ADP:O3B	2.18	0.43
1:A:745:ASN:HB3	1:A:748:GLN:HB3	2.00	0.43
1:B:610:LYS:HE2	1:B:616:ALA:O	2.19	0.43
1:A:558:HIS:CE1	1:A:562:GLU:HG3	2.53	0.43
1:B:573:THR:HA	2:B:1001:AGS:S1G	2.59	0.42
1:A:913:ILE:O	1:A:916:HIS:HD2	2.03	0.42
1:A:842:PRO:HA	4:A:1009:EDO:H22	2.02	0.42
1:A:546:HIS:CE1	6:A:1007[B]:ADP:C8	3.08	0.42
1:A:731:ASP:HB2	1:A:914:LEU:HD21	2.03	0.41
1:A:834:ARG:O	4:A:1004:EDO:H11	2.21	0.41
1:B:831:ALA:HA	1:B:857:ARG:HB2	2.02	0.41
1:A:760:HIS:CE1	1:B:873:ILE:CD1	3.00	0.40
1:A:740:ARG:HG3	1:A:867:LEU:HD23	2.03	0.40
1:B:845:MET:HE1	1:B:913:ILE:HG12	2.04	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	406/427 (95%)	399 (98%)	6 (2%)	1 (0%)	44	55
1	B	382/427 (90%)	371 (97%)	11 (3%)	0	100	100
All	All	788/854 (92%)	770 (98%)	17 (2%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	758	SER

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	363/377 (96%)	352 (97%)	11 (3%)	36	52
1	B	347/377 (92%)	334 (96%)	13 (4%)	29	43
All	All	710/754 (94%)	686 (97%)	24 (3%)	32	47

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	559	SER
1	A	590	LYS
1	A	637	ARG
1	A	656	LEU
1	A	687	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	778	GLN
1	A	787	LEU
1	A	809	ARG
1	A	887	LYS
1	A	895	MET
1	A	929	ILE
1	B	534	GLU
1	B	564	ARG
1	B	590	LYS
1	B	626	ASN
1	B	656	LEU
1	B	691	LYS
1	B	721	ARG
1	B	755	VAL
1	B	760	HIS
1	B	787	LEU
1	B	879	LEU
1	B	883	ILE
1	B	920	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	719	ASN
1	A	760	HIS
1	A	778	GLN
1	A	916	HIS
1	A	923	GLN
1	B	623	GLN
1	B	626	ASN
1	B	671	HIS
1	B	724	GLN
1	B	779	GLN
1	B	807	HIS
1	B	835	GLN
1	B	876	ASN

5.3.3 RNA ⓘ

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 20 ligands modelled in this entry, 3 are monoatomic - leaving 17 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	$\# Z > 2$
4	EDO	A	1005	-	3,3,3	0.15	0	2,2,2	0.27	0
4	EDO	B	1006	-	3,3,3	0.25	0	2,2,2	0.31	0
3	DMS	B	1004	-	3,3,3	0.58	0	3,3,3	0.41	0
3	DMS	B	1003	-	3,3,3	0.43	0	3,3,3	0.50	0
4	EDO	A	1004	-	3,3,3	0.20	0	2,2,2	0.46	0
4	EDO	A	1009	-	3,3,3	0.16	0	2,2,2	0.42	0
4	EDO	A	1010	-	3,3,3	0.20	0	2,2,2	0.35	0
4	EDO	B	1002	-	3,3,3	0.13	0	2,2,2	0.37	0
4	EDO	B	1005	-	3,3,3	0.29	0	2,2,2	0.17	0
2	AGS	A	1001[A]	-	26,33,33	0.87	1 (3%)	26,52,52	0.94	2 (7%)
3	DMS	A	1002	-	3,3,3	0.39	0	3,3,3	0.63	0
6	ADP	A	1007[B]	-	24,29,29	0.67	0	29,45,45	0.87	2 (6%)
5	A1JJK	A	1006[B]	1	20,23,26	0.90	1 (5%)	21,32,35	0.59	0
3	DMS	A	1003	-	3,3,3	0.54	0	3,3,3	0.40	0
3	DMS	A	1008	-	3,3,3	0.46	0	3,3,3	0.90	0
4	EDO	B	1007	-	3,3,3	0.51	0	2,2,2	0.05	0
2	AGS	B	1001	8	26,33,33	0.77	1 (3%)	26,52,52	0.88	1 (3%)

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	EDO	A	1005	-	-	1/1/1/1	-
4	EDO	B	1006	-	-	1/1/1/1	-
4	EDO	A	1004	-	-	1/1/1/1	-
4	EDO	A	1010	-	-	0/1/1/1	-
4	EDO	B	1002	-	-	0/1/1/1	-
4	EDO	B	1005	-	-	0/1/1/1	-
2	AGS	A	1001[A]	-	-	1/17/38/38	0/3/3/3
6	ADP	A	1007[B]	-	-	2/12/32/32	0/3/3/3
5	A1JJK	A	1006[B]	1	-	1/6/8/12	0/3/3/3
4	EDO	A	1009	-	-	0/1/1/1	-
4	EDO	B	1007	-	-	1/1/1/1	-
2	AGS	B	1001	8	-	1/17/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006[B]	A1JJK	C7-N18	2.60	1.40	1.36
2	A	1001[A]	AGS	PG-S1G	2.53	1.96	1.90
2	B	1001	AGS	PG-S1G	2.06	1.95	1.90

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1007[B]	ADP	PA-O3A-PB	2.59	141.70	132.83
2	A	1001[A]	AGS	O4'-C1'-C2'	-2.37	103.46	106.93
2	B	1001	AGS	C5-C6-N6	2.37	123.95	120.35
6	A	1007[B]	ADP	C5-C6-N6	2.32	123.88	120.35
2	A	1001[A]	AGS	C5-C6-N6	2.25	123.77	120.35

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	AGS	C5'-O5'-PA-O1A
6	A	1007[B]	ADP	O4'-C4'-C5'-O5'
6	A	1007[B]	ADP	C3'-C4'-C5'-O5'
4	A	1004	EDO	O1-C1-C2-O2
4	B	1006	EDO	O1-C1-C2-O2
4	A	1005	EDO	O1-C1-C2-O2
4	B	1007	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1001[A]	AGS	PA-O3A-PB-O2B
5	A	1006[B]	A1JJK	C11-C10-N9-N8

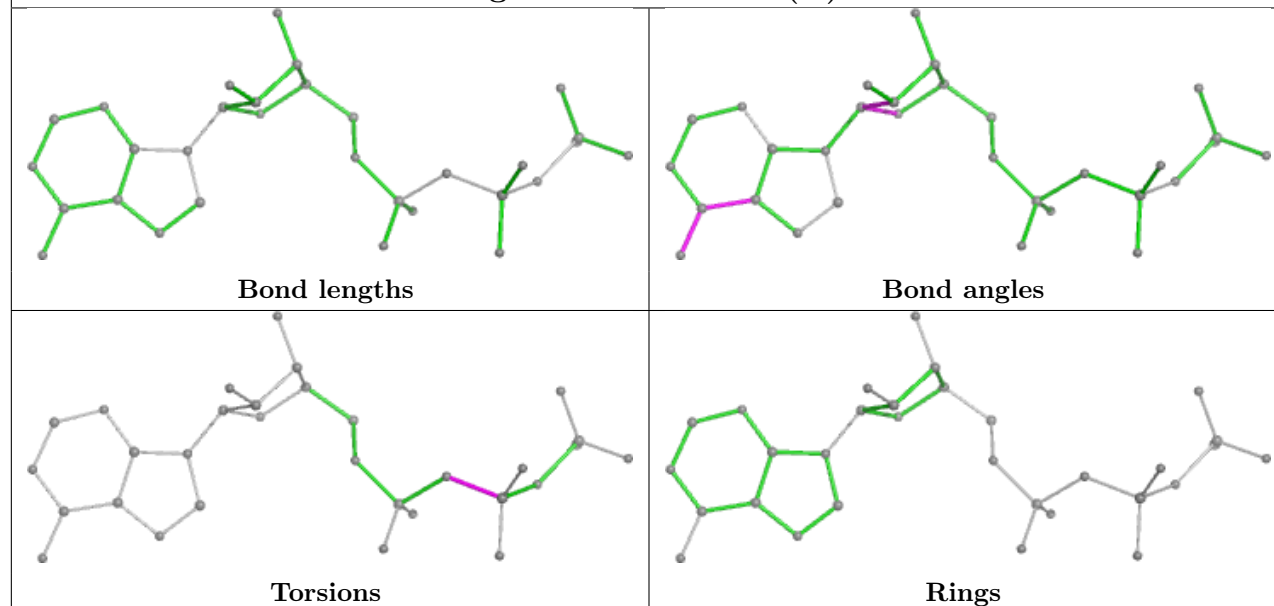
There are no ring outliers.

8 monomers are involved in 15 short contacts:

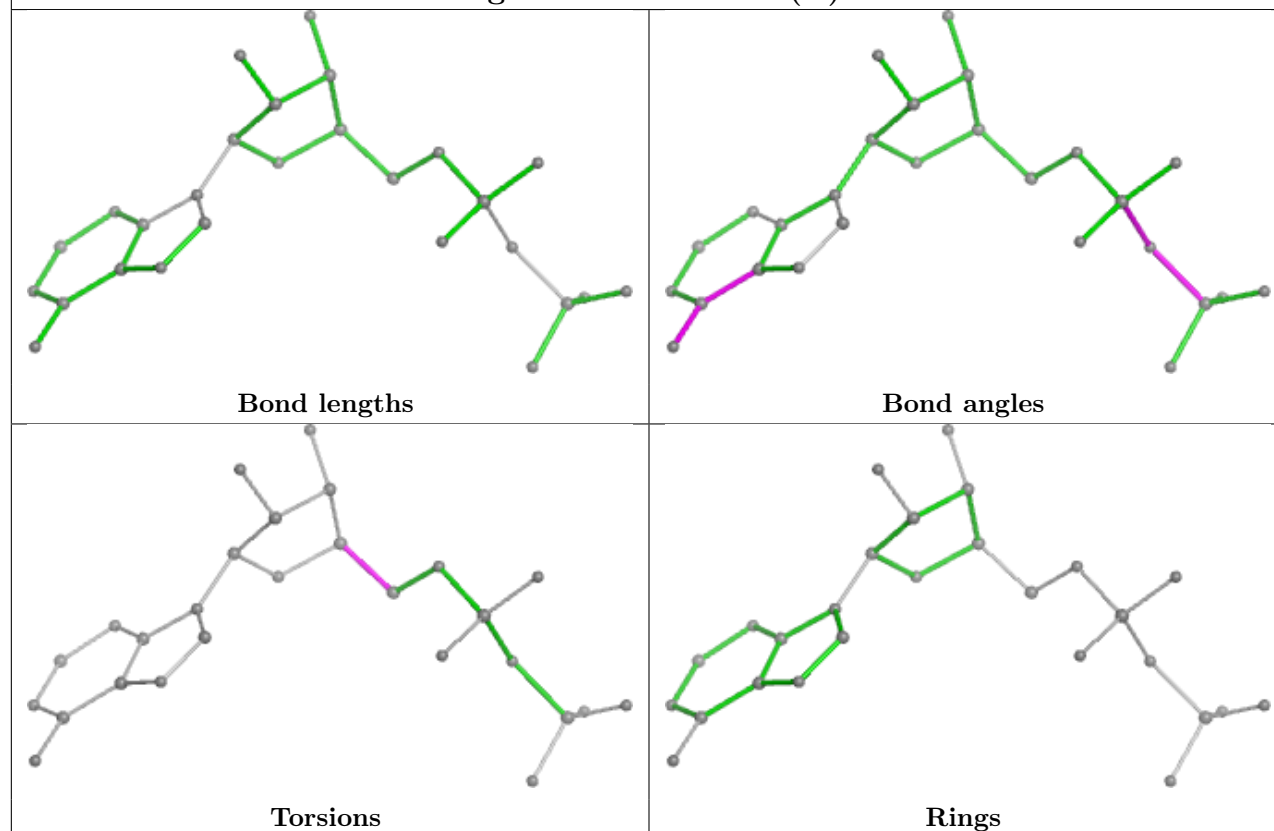
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1003	DMS	1	0
4	A	1004	EDO	1	0
4	A	1009	EDO	1	0
6	A	1007[B]	ADP	6	0
5	A	1006[B]	A1JJK	1	0
3	A	1003	DMS	2	0
3	A	1008	DMS	2	0
2	B	1001	AGS	1	0

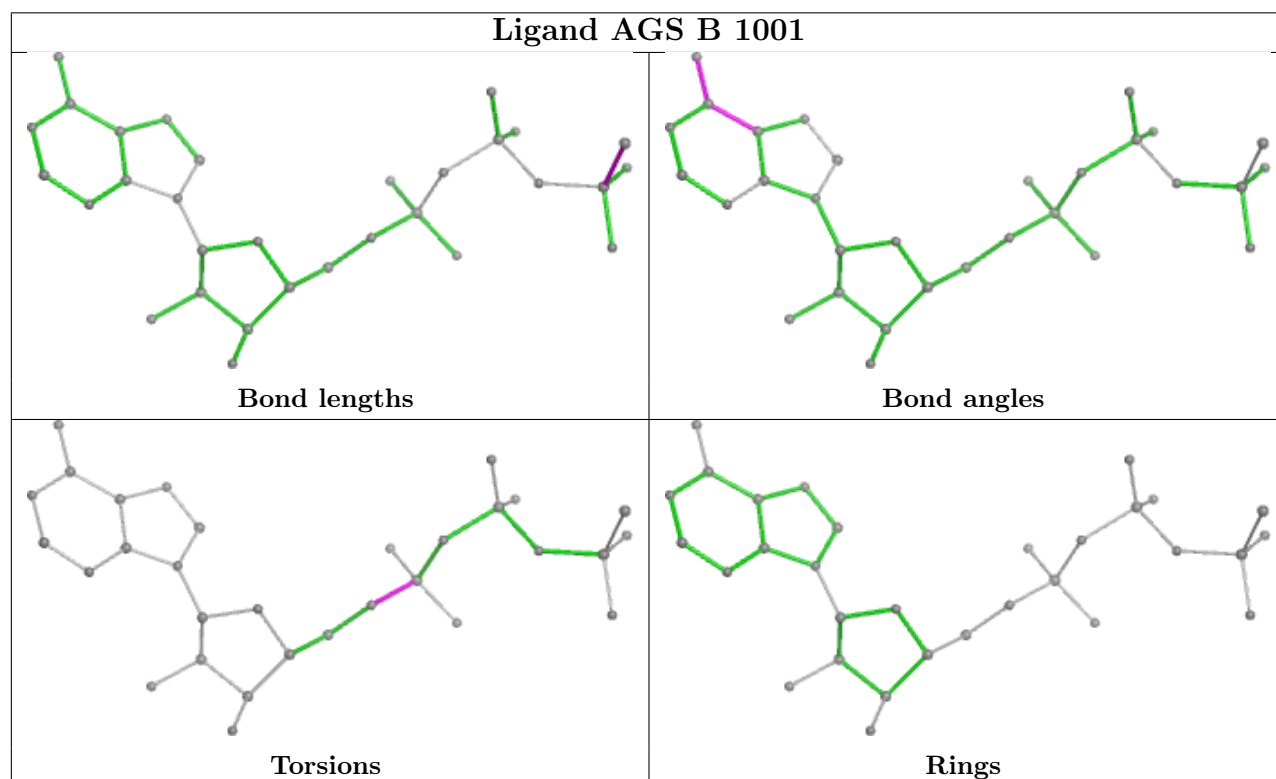
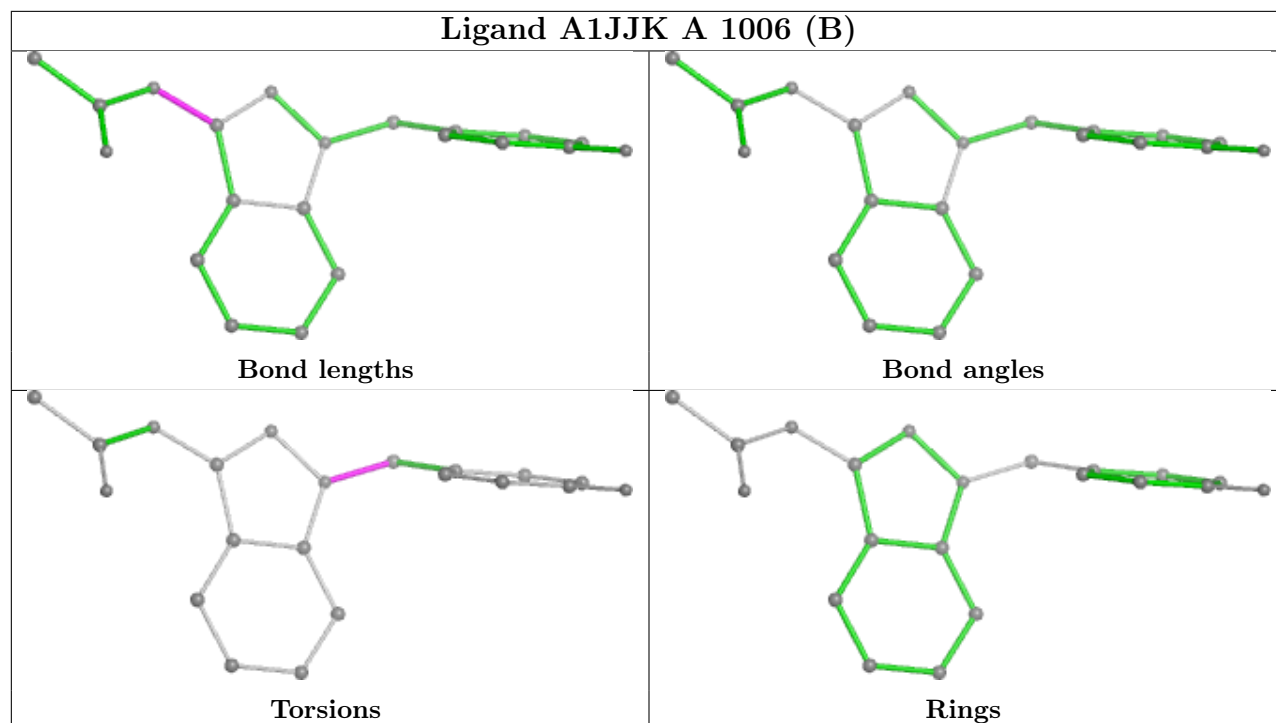
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand AGS A 1001 (A)



Ligand ADP A 1007 (B)





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	406/427 (95%)	1.09	70 (17%) 5 6	20, 64, 109, 124	5 (1%)
1	B	390/427 (91%)	1.51	133 (34%) 1 1	28, 77, 147, 174	2 (0%)
All	All	796/854 (93%)	1.29	203 (25%) 2 2	20, 66, 140, 174	7 (0%)

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	690	LEU	7.9
1	A	880	LEU	6.9
1	B	883	ILE	5.7
1	B	653	LEU	5.5
1	A	758	SER	5.5
1	B	700	VAL	5.4
1	B	561	LEU	5.3
1	B	530	PRO	5.2
1	A	680	PHE	5.1
1	B	808[A]	HIS	4.9
1	B	631	ILE	4.8
1	A	883	ILE	4.7
1	B	699	ILE	4.6
1	B	693	ALA	4.6
1	B	664	LEU	4.5
1	B	760	HIS	4.4
1	A	714	ILE	4.4
1	B	880	LEU	4.3
1	A	670	ALA	4.3
1	B	627	VAL	4.2
1	B	588	VAL	4.2
1	B	656	LEU	4.2
1	A	600	SER	4.2
1	B	633	LEU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	879	LEU	4.1
1	A	879	LEU	4.1
1	A	672	CYS	4.1
1	B	646	CYS	4.1
1	B	710	ILE	4.1
1	B	714	ILE	4.1
1	B	662	ILE	4.1
1	B	761	TRP	4.1
1	B	586	VAL	4.0
1	B	696	MET	3.9
1	A	826	MET	3.9
1	B	702	LEU	3.8
1	B	660	ILE	3.8
1	B	888	PHE	3.8
1	A	919	ASP	3.8
1	B	638	ILE	3.8
1	A	893	LEU	3.7
1	A	715	VAL	3.7
1	B	755	VAL	3.7
1	B	560	VAL	3.6
1	B	694	LEU	3.6
1	B	617	CYS	3.6
1	B	890	LEU	3.6
1	A	671	HIS	3.6
1	B	619	LEU	3.6
1	B	645	TYR	3.5
1	A	881	THR	3.5
1	B	562	GLU	3.5
1	B	531	ALA	3.5
1	B	725	ILE	3.5
1	B	891	TYR	3.5
1	B	692	THR	3.5
1	B	715	VAL	3.4
1	A	683	SER	3.4
1	B	718	LEU	3.4
1	B	593	LEU	3.4
1	A	720	LEU	3.3
1	A	684	PHE	3.3
1	B	549	PHE	3.3
1	B	697	VAL	3.3
1	A	890	LEU	3.3
1	B	941	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	763	PHE	3.2
1	B	667	VAL	3.2
1	A	885	ASN	3.2
1	B	658	ALA	3.2
1	B	544	PHE	3.2
1	A	827	GLY	3.2
1	B	639	VAL	3.1
1	B	591	ILE	3.1
1	A	529	TRP	3.1
1	B	563	GLU	3.1
1	B	628	LEU	3.1
1	B	709	SER	3.1
1	B	552	VAL	3.1
1	B	542	MET	3.1
1	A	531	ALA	3.1
1	B	691	LYS	3.1
1	A	710	ILE	3.0
1	B	698	PRO	3.0
1	A	660	ILE	3.0
1	B	595	ILE	3.0
1	A	540	LEU	3.0
1	A	687	LEU	3.0
1	B	634	GLY	3.0
1	B	568	VAL	3.0
1	B	887	LYS	3.0
1	B	614	ILE	3.0
1	A	702	LEU	3.0
1	B	543	TYR	2.9
1	B	554	TRP	2.9
1	B	567	ASN	2.9
1	B	624	SER	2.9
1	A	824	PHE	2.9
1	B	701	ALA	2.9
1	B	640	TYR	2.9
1	B	650	MET	2.8
1	B	581	PHE	2.8
1	A	694	LEU	2.8
1	A	682	ASP	2.8
1	B	720	LEU	2.8
1	B	539	CYS	2.8
1	B	665	ILE	2.7
1	B	587	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	580	CYS	2.7
1	B	756	LYS	2.7
1	B	815	ILE	2.7
1	B	674	SER	2.7
1	B	643	PRO	2.7
1	B	636	TYR	2.7
1	A	634	GLY	2.7
1	A	825	GLY	2.7
1	A	728	THR	2.7
1	A	602	MET	2.7
1	B	555	LYS	2.7
1	B	812	ARG	2.6
1	B	663	THR	2.6
1	A	711	ARG	2.6
1	B	616	ALA	2.6
1	B	717	CYS	2.6
1	B	721	ARG	2.6
1	B	657	GLU	2.6
1	A	941	SER	2.6
1	A	882	GLU	2.5
1	A	537	VAL	2.5
1	B	557	ILE	2.5
1	A	744	GLY	2.5
1	B	537	VAL	2.5
1	B	618	PHE	2.5
1	B	873	ILE	2.5
1	A	696	MET	2.5
1	A	718	LEU	2.5
1	B	532	PRO	2.5
1	B	791	CYS	2.5
1	B	726	THR	2.5
1	B	611	MET	2.4
1	A	549	PHE	2.4
1	A	570	VAL	2.4
1	A	667	VAL	2.4
1	B	570	VAL	2.4
1	B	673	ILE	2.4
1	B	647	SER	2.4
1	B	652	LEU	2.4
1	B	695	PRO	2.3
1	B	659	ASP	2.3
1	B	893	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	704	ALA	2.3
1	A	877	ARG	2.3
1	B	651	GLY	2.3
1	B	569	ALA	2.3
1	A	530	PRO	2.3
1	A	532	PRO	2.3
1	B	881	THR	2.3
1	A	626	ASN	2.3
1	B	897	ALA	2.3
1	B	564	ARG	2.3
1	B	558	HIS	2.3
1	B	654	GLN	2.3
1	B	590	LYS	2.2
1	A	542	MET	2.2
1	B	829	ASN	2.2
1	A	568	VAL	2.2
1	B	556	VAL	2.2
1	B	594	VAL	2.2
1	A	690	LEU	2.2
1	B	540	LEU	2.2
1	B	672	CYS	2.2
1	A	571	MET	2.2
1	A	681	ARG	2.2
1	B	754	LEU	2.2
1	A	647	SER	2.2
1	B	708	SER	2.2
1	A	554	TRP	2.2
1	A	876	ASN	2.2
1	A	917	PHE	2.2
1	B	917	PHE	2.2
1	A	547	SER	2.1
1	A	760	HIS	2.1
1	A	560	VAL	2.1
1	B	565	ARG	2.1
1	A	598	LEU	2.1
1	A	656	LEU	2.1
1	B	533	ASN	2.1
1	B	622	ALA	2.1
1	B	716	ARG	2.1
1	A	887	LYS	2.1
1	A	572	ALA	2.1
1	B	705	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	878	HIS	2.1
1	A	920	LYS	2.1
1	A	601	LEU	2.1
1	B	589	GLY	2.0
1	B	548	SER	2.0
1	A	686	LYS	2.0
1	A	829[A]	ASN	2.0
1	B	547	SER	2.0
1	B	894	LYS	2.0
1	B	536	GLN	2.0
1	B	585	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
4	EDO	B	1007	4/4	0.76	0.20	65,66,67,67	0
4	EDO	A	1005	4/4	0.77	0.20	72,72,72,72	0
3	DMS	A	1008	4/4	0.77	0.25	83,83,84,84	0
3	DMS	B	1004	4/4	0.82	0.24	103,104,104,105	0
3	DMS	B	1003	4/4	0.84	0.26	103,104,104,105	0
6	ADP	A	1007[B]	27/27	0.84	0.14	57,61,67,68	27
4	EDO	A	1010	4/4	0.85	0.20	95,96,96,97	0
4	EDO	B	1006	4/4	0.86	0.17	81,81,81,81	0
3	DMS	A	1003	4/4	0.86	0.20	96,97,97,97	0
4	EDO	B	1002	4/4	0.86	0.19	47,47,48,48	0
8	MG	B	1009	1/1	0.86	0.22	58,58,58,58	0
5	A1JJK	A	1006[B]	21/24	0.89	0.15	57,59,66,69	21

Continued on next page...

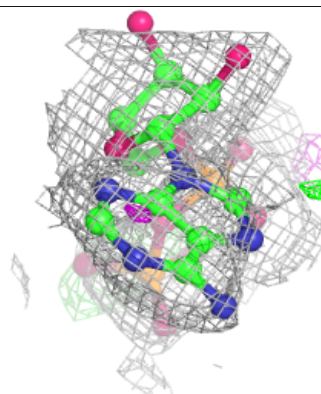
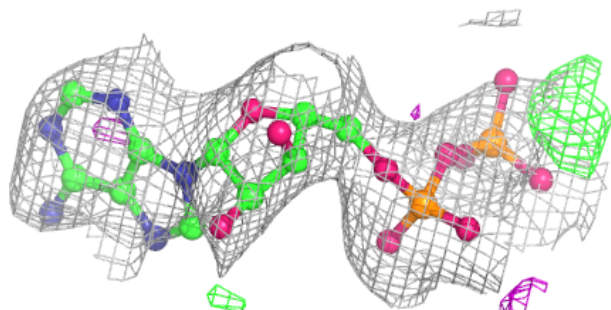
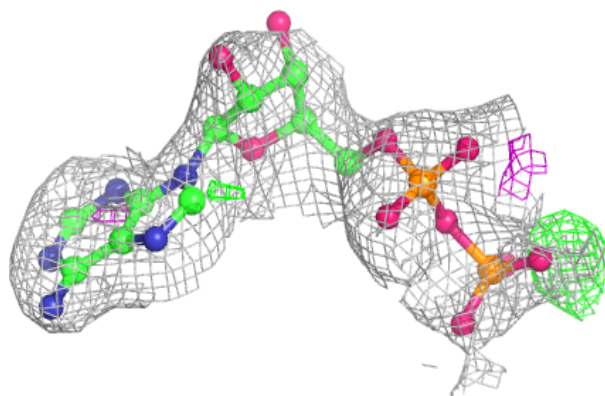
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	B	1005	4/4	0.90	0.13	67,68,69,69	0
2	AGS	B	1001	31/31	0.92	0.11	64,80,91,92	0
4	EDO	A	1009	4/4	0.92	0.18	73,74,74,74	0
2	AGS	A	1001[A]	31/31	0.93	0.09	28,39,48,49	31
4	EDO	A	1004	4/4	0.93	0.13	50,51,51,51	0
3	DMS	A	1002	4/4	0.94	0.23	61,62,62,62	0
7	ZN	B	1008	1/1	0.98	0.04	41,41,41,41	0
7	ZN	A	1011	1/1	0.99	0.06	45,45,45,45	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.

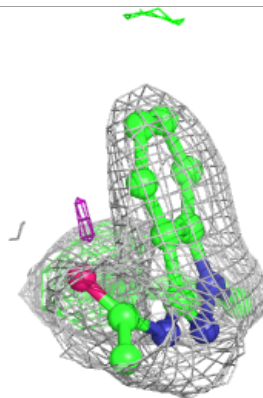
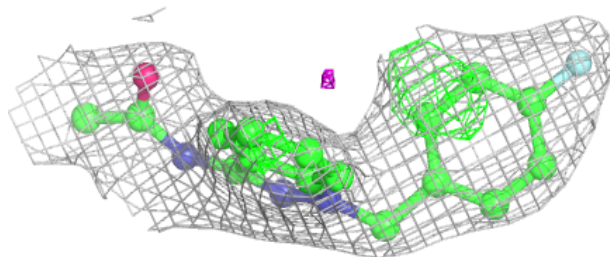
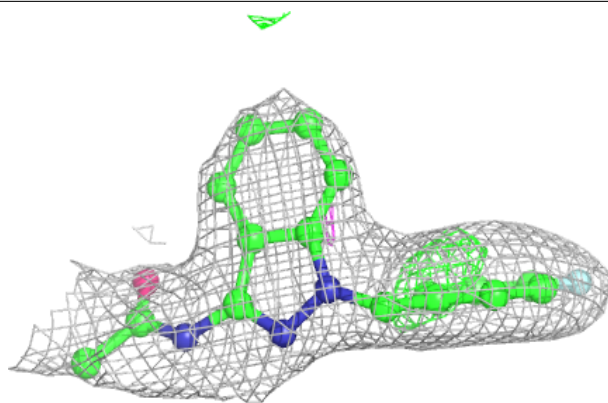
Electron density around ADP A 1007 (B):

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

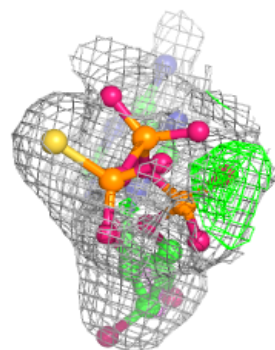
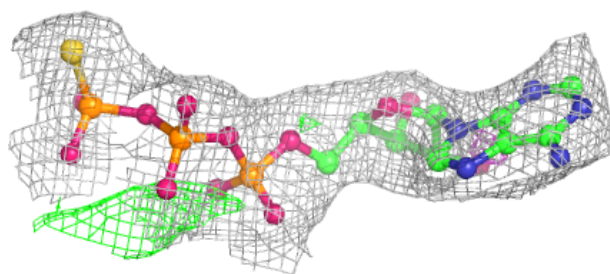
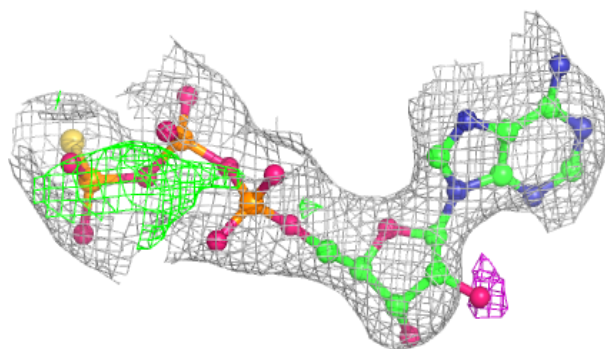


Electron density around A1JJK A 1006 (B):

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

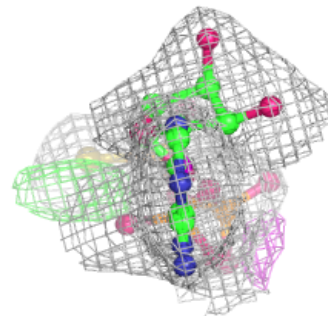
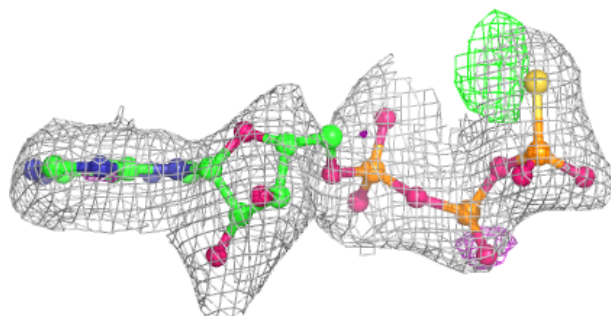
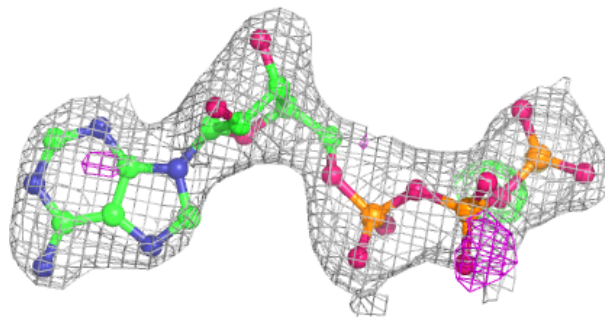
**Electron density around AGS B 1001:**

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



Electron density around AGS A 1001 (A):

$2mF_o-DF_c$ (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.