



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2025 – 01:56 pm BST

PDB ID : 9RTI / pdb_00009rti
Title : Structure of WRN in complex with ATPgS and covalent ligand Compound 7
Authors : Fletcher, C.T.; Rucktooa, P.
Deposited on : 2025-07-02
Resolution : 2.20 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

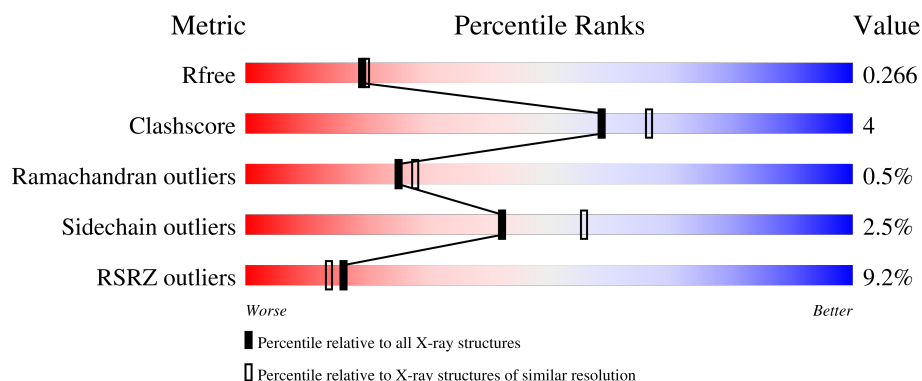
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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>9%</div> <div>82%</div> <div>11%</div> <div>6%</div> </div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3645 atoms, of which 33 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.

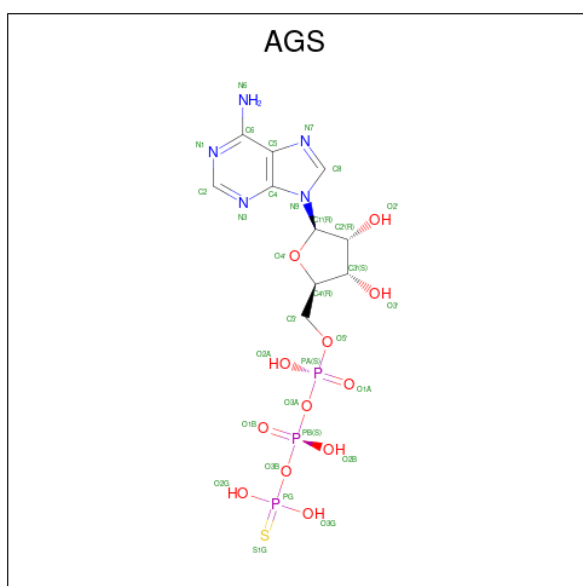
- Molecule 1 is a protein called Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	4	0
			3219	2036	569	582	32			

There are 2 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

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



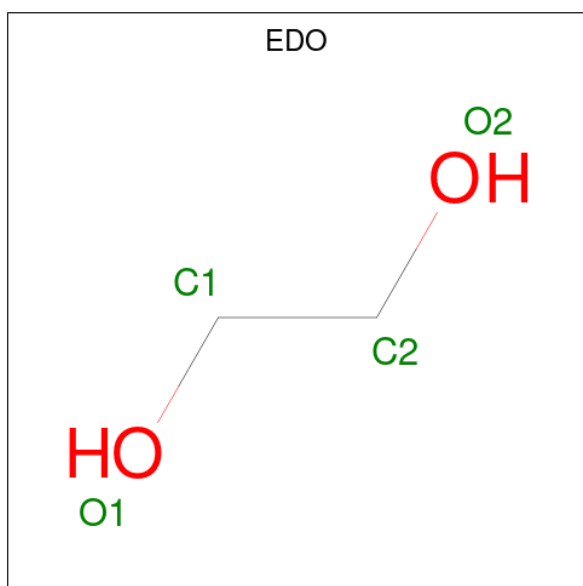
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- 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		

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



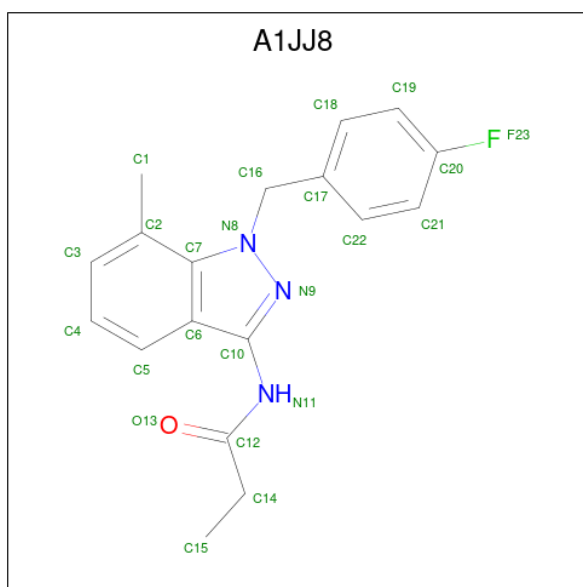
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

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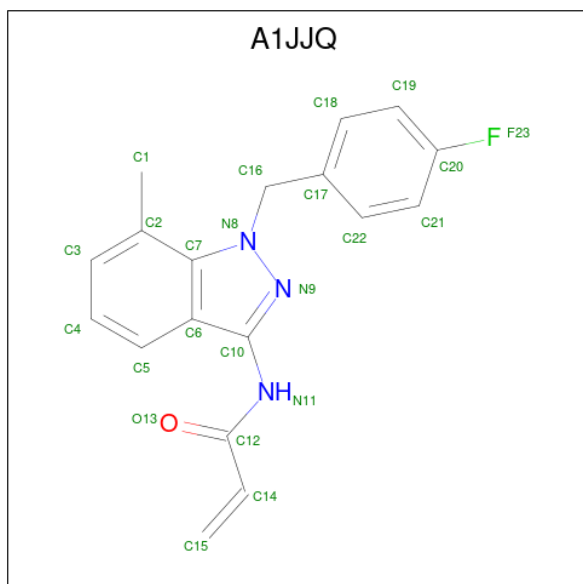
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total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

- Molecule 5 is {N}-[1-[(4-fluorophenyl)methyl]-7-methyl-indazol-3-yl]propanamide (CCD ID: A1JJ8) (formula: C₁₈H₁₈FN₃O) (labeled as "Ligand of Interest" by depositor).



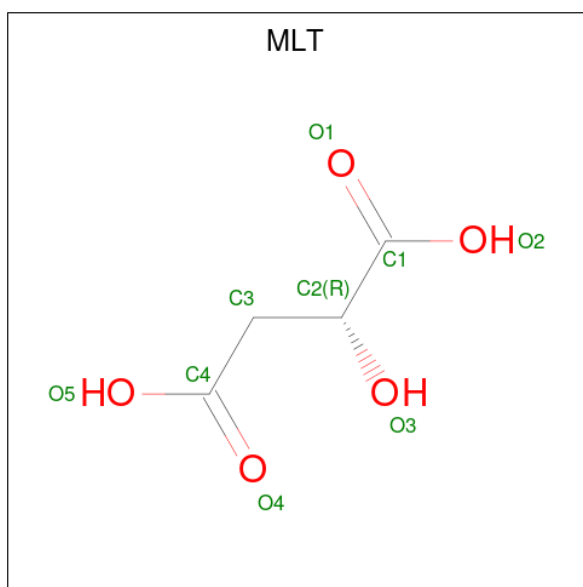
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	F	H	N	O	17	1
			40	18	1	17	3	1		

- Molecule 6 is {N}-[1-[(4-fluorophenyl)methyl]-7-methyl-indazol-3-yl]prop-2-enamide (CCD ID: A1JJQ) (formula: $C_{18}H_{16}FN_3O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	F	H	N	O	16	1
			39	18	1	16	3	1		

- Molecule 7 is D-MALATE (CCD ID: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

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

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		

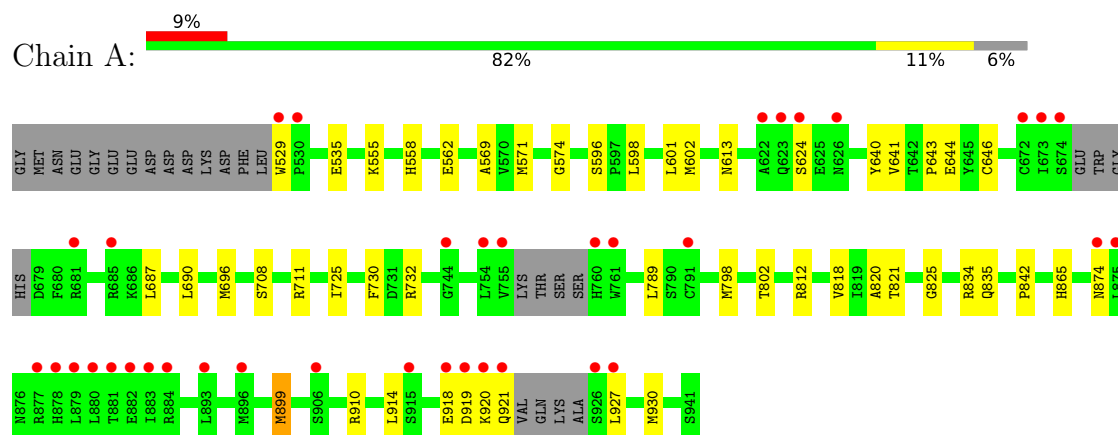
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	203	Total	O	0	0
			203	203		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.02Å 122.02Å 104.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.85 – 2.20 17.85 – 2.20	Depositor EDS
% Data completeness (in resolution range)	71.2 (17.85-2.20) 71.0 (17.85-2.20)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.21Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.246 , 0.274 0.242 , 0.266	Depositor DCC
R_{free} test set	1591 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3645	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: A1JJ8, ZN, PEG, EDO, DMS, AGS, MLT, A1JJQ

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	0.71	1/3281 (0.0%)	1.08	1/4423 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	899	MET	SD-CE	-7.10	1.61	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	821	THR	N-CA-C	-5.61	102.45	110.59

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	3219	0	3239	28	0
2	A	31	0	12	0	0
3	A	8	0	12	2	0
4	A	60	0	90	6	0
5	A	23	17	0	0	0
6	A	23	16	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	9	0	4	0	0
8	A	35	0	50	3	0
9	A	1	0	0	0	0
10	A	203	0	0	0	0
All	All	3612	33	3407	29	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 (29) 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:798:MET:HE3	1:A:802:THR:HG22	1.41	0.98
1:A:730:PHE:HA	1:A:921:GLN:HG2	1.72	0.72
1:A:798:MET:CE	1:A:802:THR:HG22	2.22	0.66
1:A:644:GLU:HB2	4:A:1012:EDO:H22	1.82	0.62
1:A:798:MET:HE3	1:A:802:THR:CG2	2.22	0.61
1:A:643:PRO:HD2	4:A:1012:EDO:H21	1.84	0.60
1:A:598:LEU:HD13	4:A:1013:EDO:H21	1.87	0.57
1:A:711:ARG:HD2	1:A:725:ILE:HD12	1.89	0.53
1:A:529:TRP:NE1	1:A:555:LYS:HE3	2.25	0.52
1:A:730:PHE:HA	1:A:921:GLN:CG	2.39	0.52
1:A:842:PRO:HD2	1:A:899:MET:HE2	1.91	0.52
1:A:529:TRP:HE1	1:A:555:LYS:HE3	1.76	0.50
1:A:569:ALA:HB1	1:A:571:MET:HE2	1.94	0.49
1:A:601:LEU:HD13	4:A:1013:EDO:H22	1.95	0.48
1:A:835:GLN:NE2	1:A:865:HIS:ND1	2.57	0.47
1:A:918:GLU:HG3	1:A:920:LYS:H	1.80	0.47
1:A:812:ARG:HB3	8:A:1026:PEG:H41	1.99	0.45
1:A:818:VAL:HG12	1:A:820:ALA:HB2	1.98	0.44
1:A:574:GLY:HA3	4:A:1008:EDO:H11	2.00	0.42
4:A:1004:EDO:H21	8:A:1020:PEG:H31	2.00	0.42
1:A:602[A]:MET:SD	1:A:640:TYR:HB3	2.60	0.42
1:A:910:ARG:O	1:A:914:LEU:HG	2.19	0.42
1:A:732:ARG:HD3	3:A:1002:DMS:O	2.19	0.42
1:A:732:ARG:H	3:A:1002:DMS:H12	1.86	0.41
1:A:596:SER:HB3	1:A:602[A]:MET:SD	2.61	0.41
1:A:641:VAL:HG21	1:A:646[B]:CYS:SG	2.61	0.41
1:A:834:ARG:HD3	8:A:1020:PEG:H42	2.03	0.41
1:A:558:HIS:CE1	1:A:562:GLU:HG3	2.56	0.40
1:A:687:LEU:HB3	1:A:690:LEU:HD12	2.03	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	397/427 (93%)	388 (98%)	7 (2%)	2 (0%)	25 28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	624	SER
1	A	825	GLY

5.3.2 Protein sidechains [i](#)

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	359/377 (95%)	350 (98%)	9 (2%)	42 56

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	535	GLU
1	A	613	ASN
1	A	696	MET
1	A	708	SER
1	A	789	LEU
1	A	874	ASN

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Mol	Chain	Res	Type
1	A	919	ASP
1	A	927	LEU
1	A	930	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	558	HIS
1	A	671	HIS
1	A	795	HIS
1	A	885	ASN

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 27 ligands modelled in this entry, 1 is monoatomic - leaving 26 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	1003	-	3,3,3	0.10	0	2,2,2	0.41	0
4	EDO	A	1023	-	3,3,3	0.43	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	1012	-	3,3,3	0.21	0	2,2,2	0.14	0
4	EDO	A	1011	-	3,3,3	0.35	0	2,2,2	0.17	0
4	EDO	A	1022	-	3,3,3	0.37	0	2,2,2	0.18	0
6	A1JJQ	A	1014[A]	-	22,25,25	1.05	2 (9%)	23,35,35	1.41	3 (13%)
4	EDO	A	1017	-	3,3,3	0.36	0	2,2,2	0.14	0
4	EDO	A	1018	-	3,3,3	0.21	0	2,2,2	0.37	0
4	EDO	A	1004	-	3,3,3	0.26	0	2,2,2	0.10	0
4	EDO	A	1008	-	3,3,3	0.17	0	2,2,2	0.46	0
5	A1JJ8	A	1010[B]	1	22,25,25	0.79	1 (4%)	22,35,35	0.73	1 (4%)
4	EDO	A	1009	-	3,3,3	0.26	0	2,2,2	0.34	0
3	DMS	A	1002	-	3,3,3	0.57	0	3,3,3	1.02	0
8	PEG	A	1020	-	6,6,6	0.23	0	5,5,5	0.10	0
8	PEG	A	1024	-	6,6,6	0.16	0	5,5,5	0.04	0
4	EDO	A	1019	-	3,3,3	0.40	0	2,2,2	0.16	0
7	MLT	A	1015	-	8,8,8	1.09	0	10,10,10	1.38	2 (20%)
4	EDO	A	1013	-	3,3,3	0.25	0	2,2,2	0.24	0
8	PEG	A	1016	-	6,6,6	0.16	0	5,5,5	0.11	0
4	EDO	A	1005	-	3,3,3	0.15	0	2,2,2	0.56	0
8	PEG	A	1021	-	6,6,6	0.18	0	5,5,5	0.06	0
4	EDO	A	1006	-	3,3,3	0.58	0	2,2,2	0.18	0
4	EDO	A	1007	-	3,3,3	0.16	0	2,2,2	0.31	0
3	DMS	A	1025	-	3,3,3	0.65	0	3,3,3	0.37	0
2	AGS	A	1001	-	26,33,33	0.72	0	26,52,52	0.86	1 (3%)
8	PEG	A	1026	-	6,6,6	0.18	0	5,5,5	0.08	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
4	EDO	A	1003	-	-	0/1/1/1	-
4	EDO	A	1023	-	-	1/1/1/1	-
4	EDO	A	1012	-	-	1/1/1/1	-
4	EDO	A	1011	-	-	0/1/1/1	-
4	EDO	A	1022	-	-	1/1/1/1	-
6	A1JJQ	A	1014[A]	-	-	2/8/10/10	0/3/3/3
4	EDO	A	1017	-	-	0/1/1/1	-
4	EDO	A	1018	-	-	0/1/1/1	-
4	EDO	A	1004	-	-	1/1/1/1	-
4	EDO	A	1008	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A1JJ8	A	1010[B]	1	-	0/8/10/10	0/3/3/3
4	EDO	A	1009	-	-	1/1/1/1	-
8	PEG	A	1020	-	-	3/4/4/4	-
8	PEG	A	1024	-	-	2/4/4/4	-
4	EDO	A	1019	-	-	0/1/1/1	-
7	MLT	A	1015	-	-	4/8/8/8	-
4	EDO	A	1013	-	-	0/1/1/1	-
8	PEG	A	1016	-	-	2/4/4/4	-
4	EDO	A	1005	-	-	0/1/1/1	-
8	PEG	A	1021	-	-	1/4/4/4	-
4	EDO	A	1006	-	-	1/1/1/1	-
4	EDO	A	1007	-	-	1/1/1/1	-
2	AGS	A	1001	-	-	0/17/38/38	0/3/3/3
8	PEG	A	1026	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1014[A]	A1JJQ	C10-N11	2.92	1.41	1.36
6	A	1014[A]	A1JJQ	C12-N11	2.66	1.40	1.35
5	A	1010[B]	A1JJ8	C10-N11	2.59	1.40	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1014[A]	A1JJQ	C14-C12-N11	5.14	117.22	113.84
7	A	1015	MLT	O1-C1-C2	-2.40	117.86	122.54
6	A	1014[A]	A1JJQ	C10-N11-C12	2.39	133.17	127.23
2	A	1001	AGS	C5-C6-N6	2.32	123.88	120.35
6	A	1014[A]	A1JJQ	O13-C12-N11	-2.30	120.41	123.05
5	A	1010[B]	A1JJ8	C5-C6-C7	2.18	120.81	116.73
7	A	1015	MLT	O2-C1-C2	2.04	117.20	112.72

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1014[A]	A1JJQ	N11-C12-C14-C15
6	A	1014[A]	A1JJQ	O13-C12-C14-C15
7	A	1015	MLT	O1-C1-C2-O3

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Mol	Chain	Res	Type	Atoms
7	A	1015	MLT	O2-C1-C2-O3
8	A	1016	PEG	O2-C3-C4-O4
4	A	1009	EDO	O1-C1-C2-O2
8	A	1020	PEG	O2-C3-C4-O4
8	A	1024	PEG	O2-C3-C4-O4
8	A	1020	PEG	O1-C1-C2-O2
4	A	1004	EDO	O1-C1-C2-O2
4	A	1006	EDO	O1-C1-C2-O2
4	A	1023	EDO	O1-C1-C2-O2
8	A	1021	PEG	O2-C3-C4-O4
8	A	1016	PEG	O1-C1-C2-O2
7	A	1015	MLT	O1-C1-C2-C3
7	A	1015	MLT	O2-C1-C2-C3
4	A	1012	EDO	O1-C1-C2-O2
4	A	1022	EDO	O1-C1-C2-O2
8	A	1026	PEG	O1-C1-C2-O2
8	A	1024	PEG	C1-C2-O2-C3
8	A	1020	PEG	C4-C3-O2-C2
8	A	1026	PEG	C1-C2-O2-C3
4	A	1007	EDO	O1-C1-C2-O2

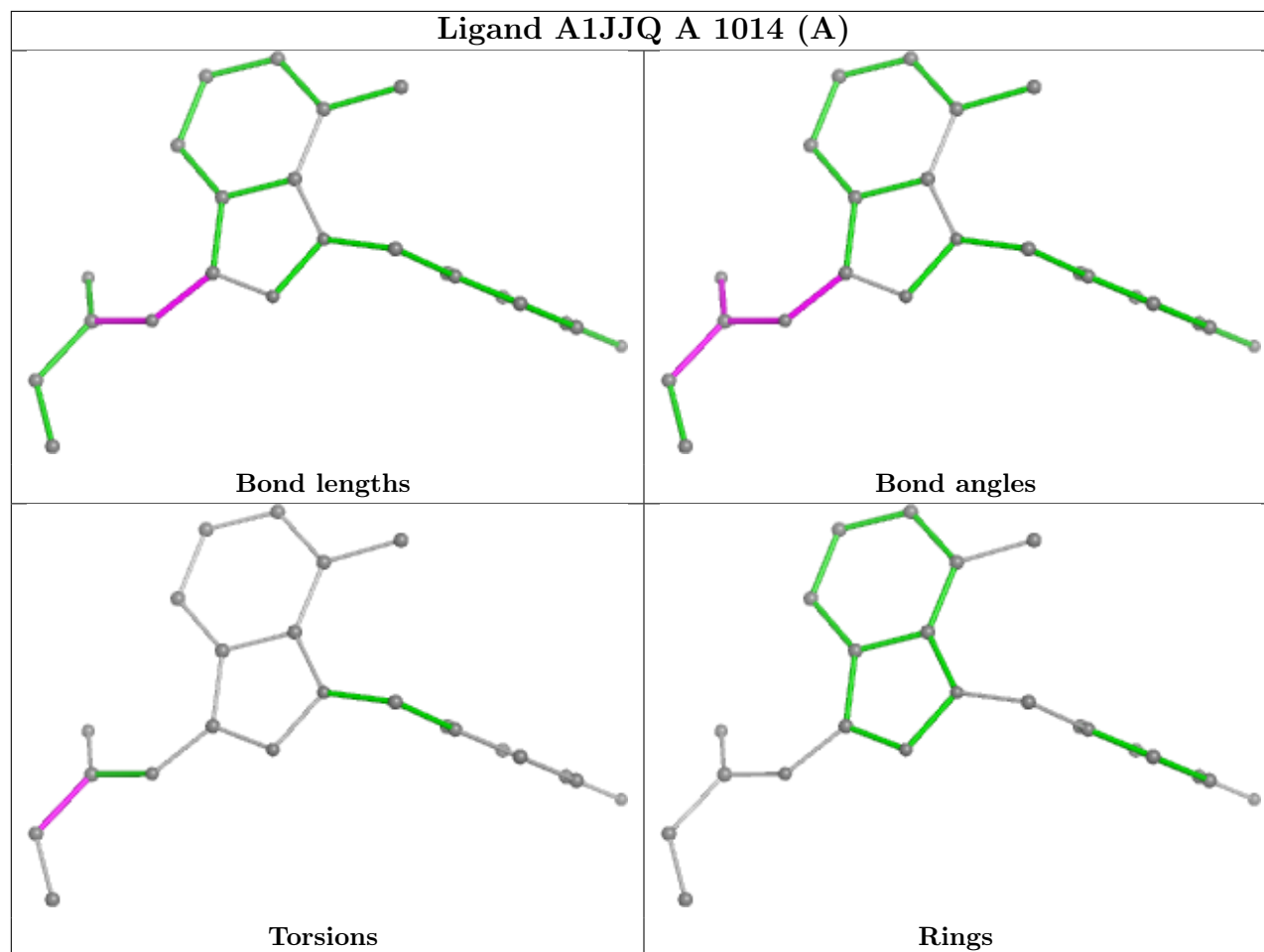
There are no ring outliers.

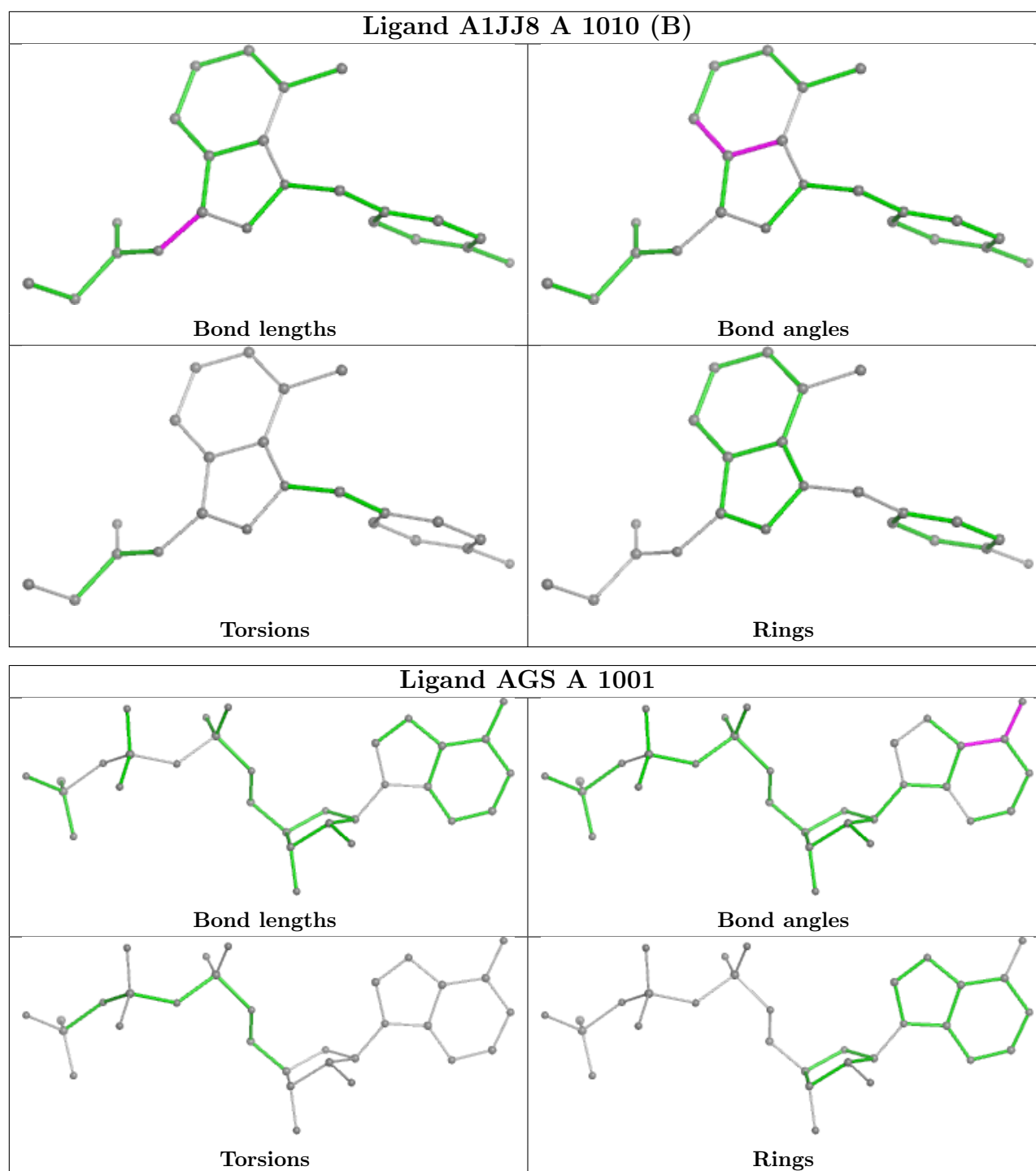
7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1012	EDO	2	0
4	A	1004	EDO	1	0
4	A	1008	EDO	1	0
3	A	1002	DMS	2	0
8	A	1020	PEG	2	0
4	A	1013	EDO	2	0
8	A	1026	PEG	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 ⓘ

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	401/427 (93%)	0.36	37 (9%) 16 14	14, 39, 69, 86	4 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	529	TRP	7.7
1	A	927	LEU	6.7
1	A	622	ALA	5.3
1	A	881	THR	4.9
1	A	673	ILE	4.6
1	A	761	TRP	4.4
1	A	744	GLY	4.0
1	A	879	LEU	4.0
1	A	880	LEU	3.8
1	A	760	HIS	3.6
1	A	921	GLN	3.5
1	A	883	ILE	3.4
1	A	623	GLN	3.3
1	A	875	LEU	3.3
1	A	530	PRO	3.2
1	A	882	GLU	3.2
1	A	878	HIS	3.2
1	A	755	VAL	3.1
1	A	893	LEU	2.9
1	A	877	ARG	2.9
1	A	926	SER	2.8
1	A	626	ASN	2.7
1	A	918	GLU	2.6
1	A	884	ARG	2.6
1	A	874	ASN	2.5
1	A	791	CYS	2.4
1	A	685	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	920	LYS	2.2
1	A	896	MET	2.2
1	A	754	LEU	2.1
1	A	919	ASP	2.1
1	A	672	CYS	2.1
1	A	915	SER	2.1
1	A	624	SER	2.0
1	A	674	SER	2.0
1	A	906	SER	2.0
1	A	681	ARG	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(\AA^2)	Q<0.9
8	PEG	A	1026	7/7	0.68	0.24	73,73,73,73	0
4	EDO	A	1006	4/4	0.69	0.26	56,57,57,57	0
8	PEG	A	1021	7/7	0.74	0.19	62,63,64,64	0
4	EDO	A	1019	4/4	0.78	0.18	51,51,51,52	0
4	EDO	A	1013	4/4	0.79	0.25	86,86,86,86	0
8	PEG	A	1024	7/7	0.79	0.20	76,76,77,77	0
4	EDO	A	1023	4/4	0.79	0.26	68,68,68,68	0
7	MLT	A	1015	9/9	0.80	0.22	84,84,84,84	0
8	PEG	A	1020	7/7	0.84	0.26	44,46,48,49	0
4	EDO	A	1011	4/4	0.84	0.22	53,53,53,54	0
4	EDO	A	1009	4/4	0.85	0.13	47,47,47,47	0
4	EDO	A	1004	4/4	0.85	0.17	40,40,41,41	0
4	EDO	A	1022	4/4	0.85	0.20	73,73,73,73	0

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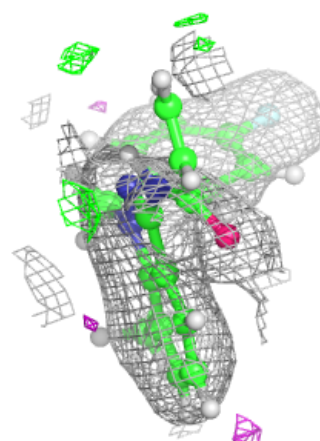
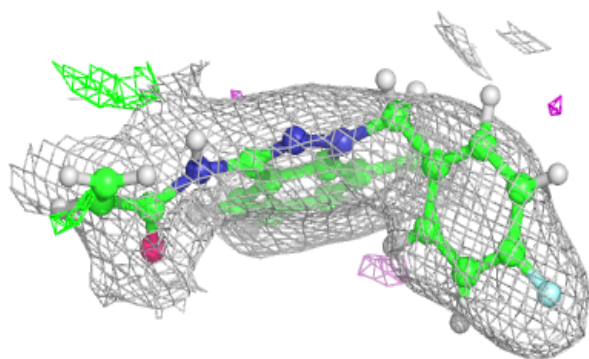
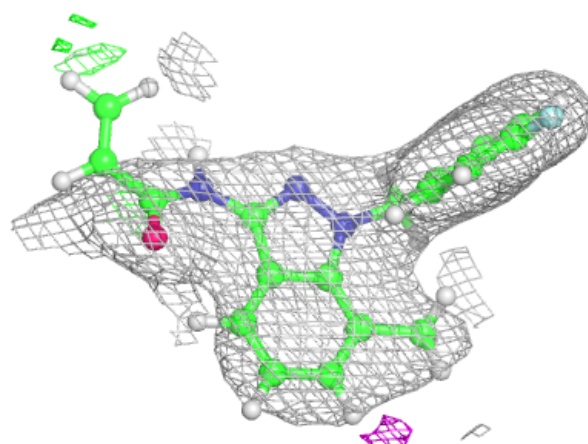
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PEG	A	1016	7/7	0.87	0.17	62,62,63,64	0
4	EDO	A	1017	4/4	0.88	0.12	52,52,52,52	0
3	DMS	A	1002	4/4	0.88	0.18	45,46,47,47	0
3	DMS	A	1025	4/4	0.89	0.23	102,102,102,102	0
4	EDO	A	1008	4/4	0.91	0.15	47,47,48,48	0
6	A1JJQ	A	1014[A]	23/23	0.92	0.10	27,29,37,38	39
5	A1JJ8	A	1010[B]	23/23	0.93	0.09	30,33,43,44	40
4	EDO	A	1018	4/4	0.93	0.11	58,58,58,59	0
4	EDO	A	1003	4/4	0.94	0.09	36,36,36,37	0
4	EDO	A	1012	4/4	0.95	0.09	41,42,42,42	0
4	EDO	A	1007	4/4	0.95	0.09	42,42,42,42	0
4	EDO	A	1005	4/4	0.95	0.10	37,38,38,39	0
2	AGS	A	1001	31/31	0.99	0.05	27,37,39,39	0
9	ZN	A	1027	1/1	0.99	0.04	31,31,31,31	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.

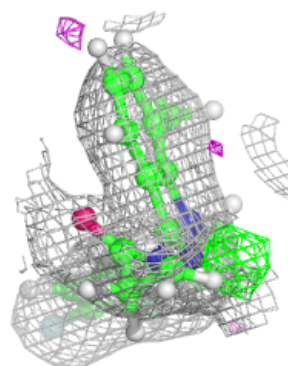
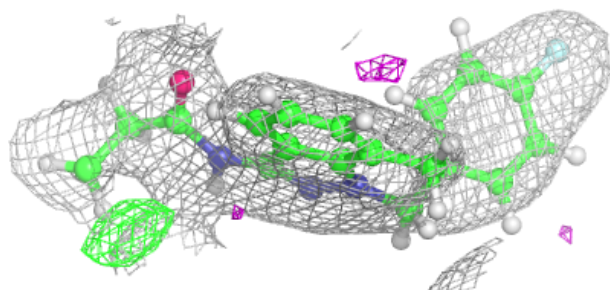
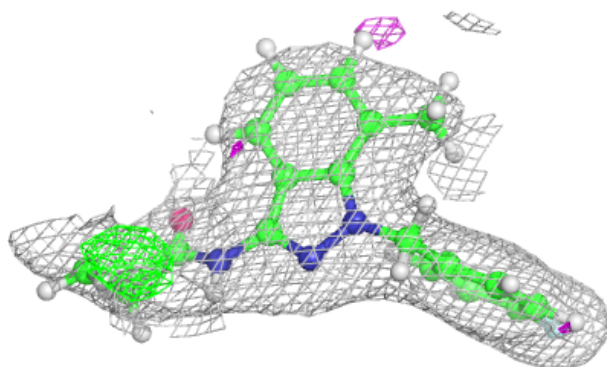
Electron density around A1JJQ A 1014 (A):

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

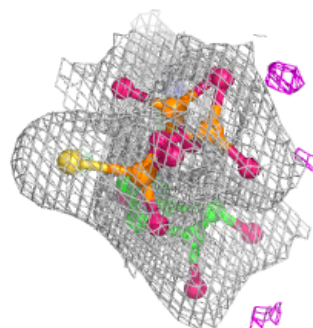
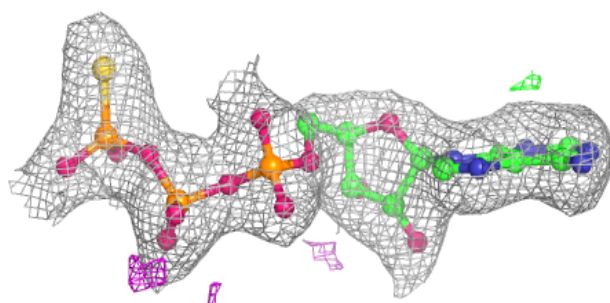
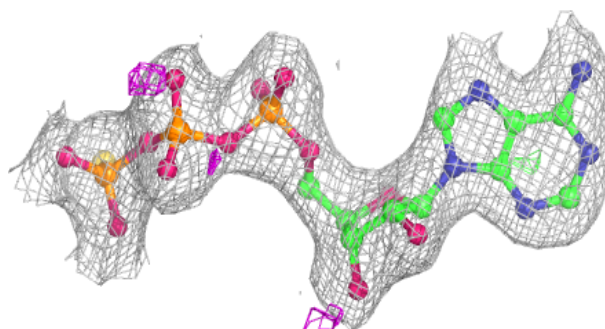


Electron density around A1JJ8 A 1010 (B):

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

**Electron density around AGS A 1001:**

$2mF_o-DF_c$ (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.