



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:50 AM UTC

PDB ID : 9RUS / pdb_00009rus
Title : Structure of WRN in complex with ATPgS and Compound 3
Authors : Fletcher, C.T.; Rucktoo, P.
Deposited on : 2025-07-04
Resolution : 2.19 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

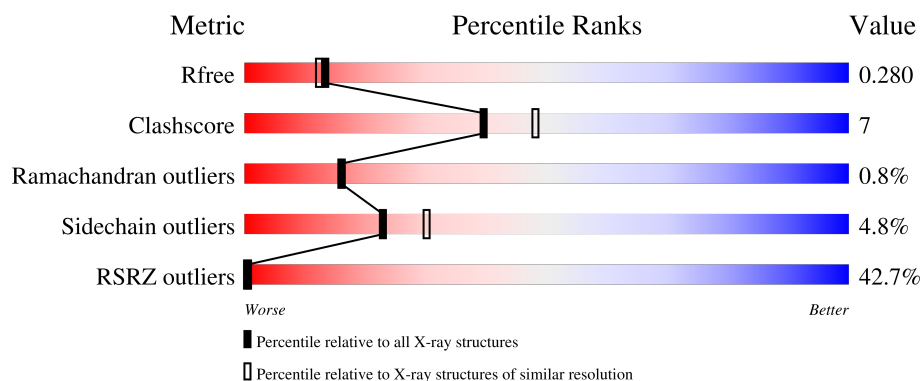
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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	38% 72% 21% 5%
1	B	427	42% 80% 14% 6%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 7456 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.

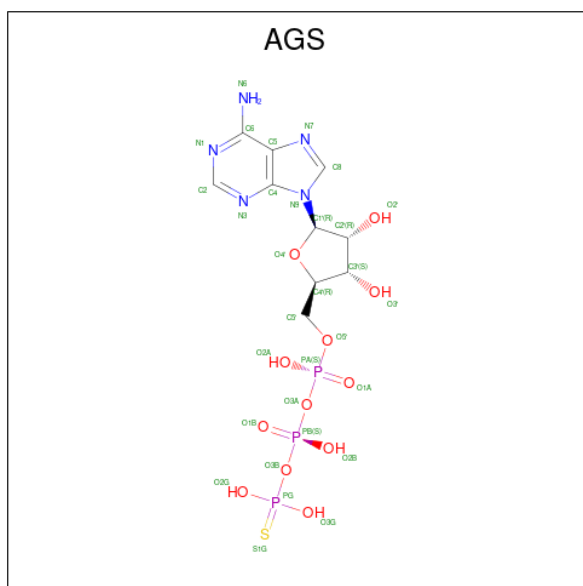
- Molecule 1 is a protein called Bifunctional 3'-5' exonuclease/ATP-dependent helicase WRN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total	C	N	O	S	0	102	0
			3902	2468	681	719	34			
1	B	400	Total	C	N	O	S	0	3	0
			3197	2021	569	578	29			

There are 4 discrepancies between the modelled and reference sequences:

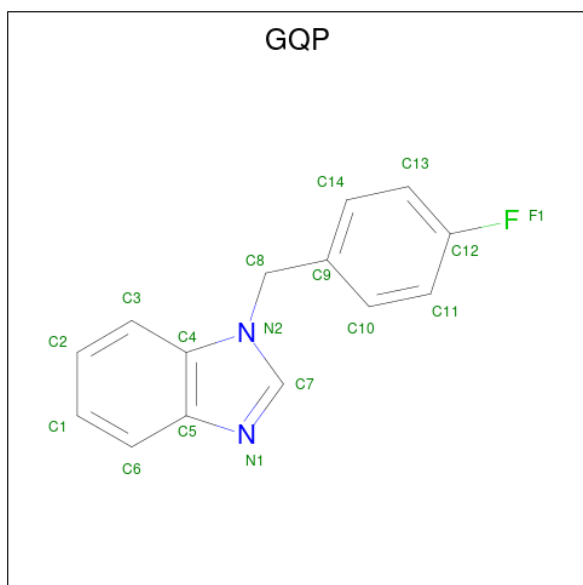
Chain	Residue	Modelled	Actual	Comment	Reference
A	515	GLY	-	expression tag	UNP Q14191
A	516	MET	-	expression tag	UNP Q14191
B	515	GLY	-	expression tag	UNP Q14191
B	516	MET	-	expression tag	UNP Q14191

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

- Molecule 3 is 1-[(4-fluorophenyl)methyl]benzimidazole (CCD ID: GQP) (formula: $C_{14}H_{11}FN_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N		
			34	28	2	4	0	1

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



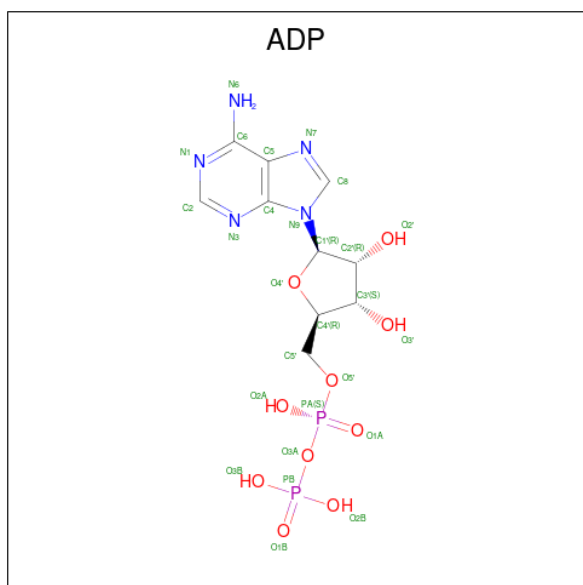
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

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

- 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		
6	B	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	Zn	0	0
			1	1		
7	B	1	Total	Zn	0	0
			1	1		

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

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

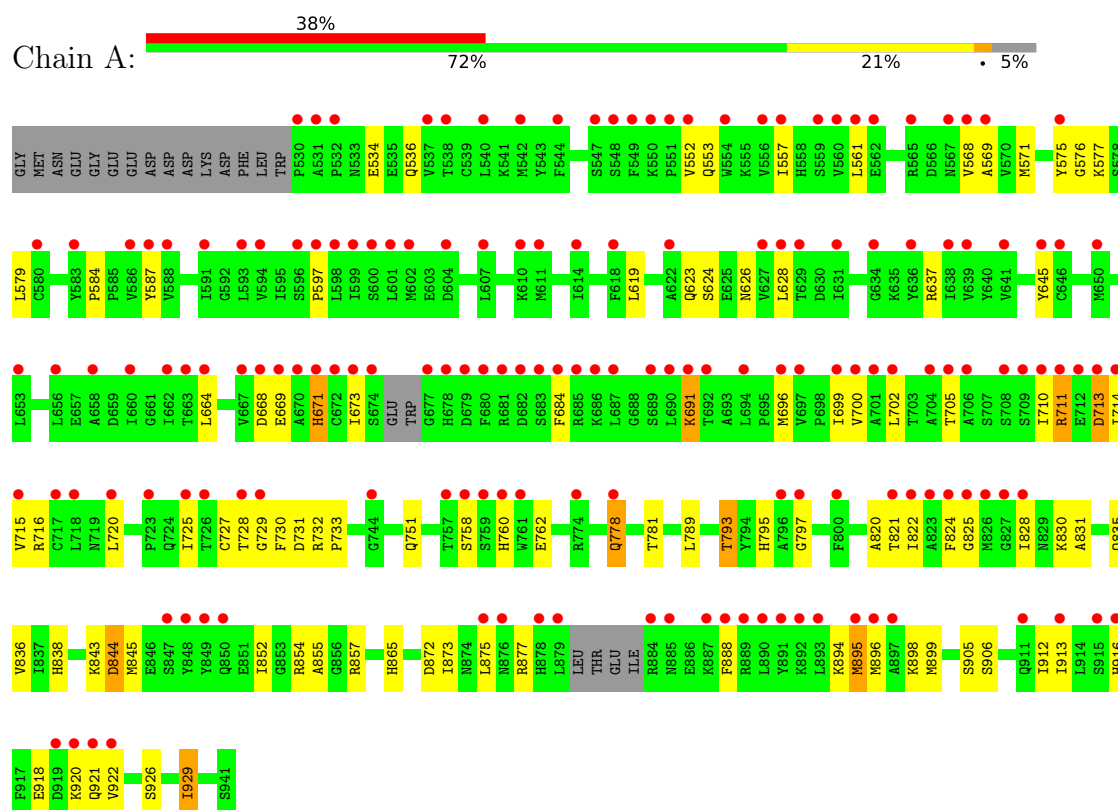
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	90	Total 90	O 90	0	0
9	B	90	Total 90	O 90	0	0

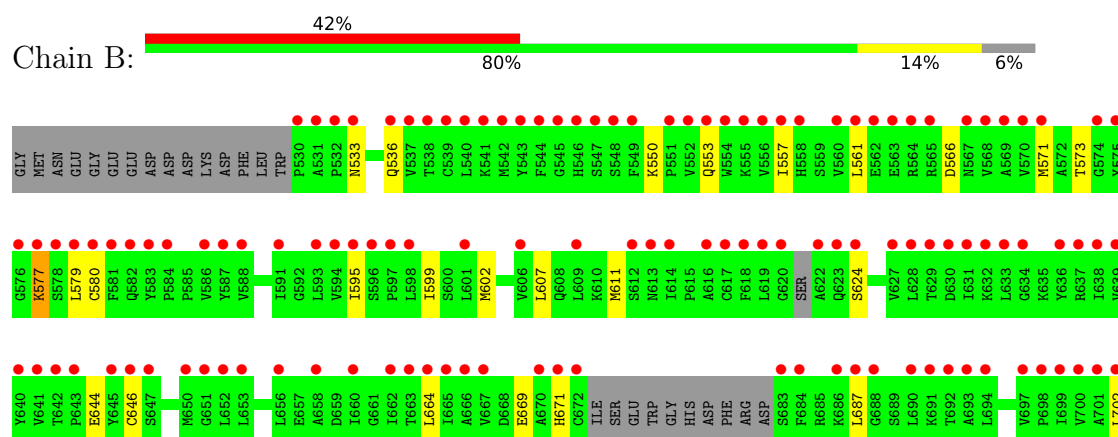
3 Residue-property plots

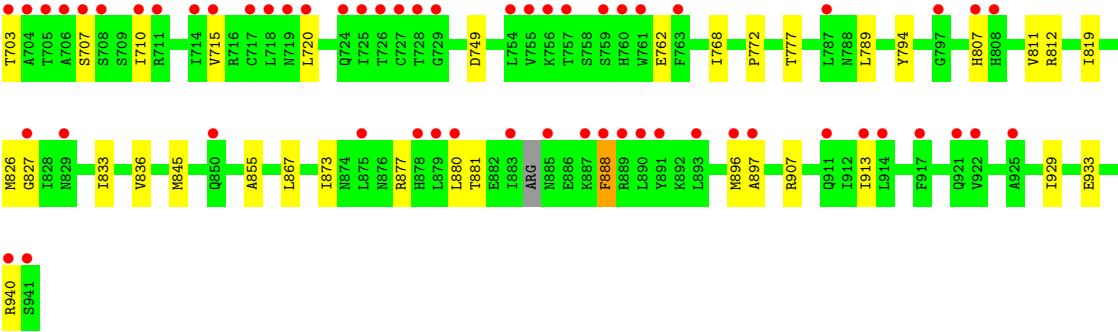
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	91.17Å 91.17Å 242.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.32 – 2.19 85.32 – 2.19	Depositor EDS
% Data completeness (in resolution range)	69.8 (85.32-2.19) 69.8 (85.32-2.19)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.267 , 0.298 (Not available) , 0.280	Depositor DCC
R_{free} test set	1838 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7456	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: EDO, DMS, ZN, MG, GQP, ADP, AGS

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	0.65	0/3976	0.99	9/5366 (0.2%)
1	B	0.71	0/3256	1.06	1/4386 (0.0%)
All	All	0.68	0/7232	1.02	10/9752 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	758	SER	CA-C-N	7.48	131.69	120.17
1	A	758	SER	C-N-CA	7.48	131.69	120.17
1	A	844	ASP	CA-CB-CG	7.10	119.70	112.60
1	B	888	PHE	CA-CB-CG	7.03	120.83	113.80
1	A	758	SER	N-CA-C	-6.71	102.94	112.13
1	A	713	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	872	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	905	SER	N-CA-C	5.28	117.11	110.24
1	A	645	TYR	CA-C-N	5.20	127.56	120.54
1	A	645	TYR	C-N-CA	5.20	127.56	120.54

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	3902	0	3913	68	0
1	B	3197	0	3242	31	0
2	A	31	0	12	3	0
2	B	31	0	12	4	0
3	A	34	0	0	0	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
5	A	8	0	12	2	0
5	B	4	0	6	0	0
6	A	27	0	12	3	0
6	B	27	0	12	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	1	0	0	0	0
9	A	90	0	0	1	0
9	B	90	0	0	0	0
All	All	7456	0	7239	98	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 7.

All (98) 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:711[A]:ARG:HE	1:A:725:ILE:HG21	1.38	0.88
1:A:568[B]:VAL:HG23	1:A:725:ILE:HG12	1.59	0.83
1:A:710[B]:ILE:HA	1:A:713:ASP:HB3	1.59	0.83
1:B:553:GLN:HE22	2:B:1001[A]:AGS:HN61	1.32	0.76
1:A:713:ASP:HA	1:A:716:ARG:HG2	1.67	0.76
1:A:571[B]:MET:HB3	1:A:577:LYS:HE3	1.71	0.72
1:A:831[B]:ALA:HA	1:A:857:ARG:HB2	1.72	0.71
1:A:795:HIS:HD2	1:A:797:GLY:H	1.39	0.70
1:A:673:ILE:HG13	1:A:684:PHE:HB3	1.72	0.70
1:A:713:ASP:HA	1:A:716:ARG:CG	2.21	0.70
1:B:577:LYS:HB2	2:B:1001[A]:AGS:O2B	1.93	0.68
1:A:857:ARG:NH1	2:A:1001[A]:AGS:O3G	2.29	0.65
1:A:577:LYS:NZ	6:A:1006[B]:ADP:O2B	2.28	0.63
1:A:821[B]:THR:HG22	1:A:822[B]:ILE:H	1.65	0.61
1:A:835:GLN:HE22	1:A:865:HIS:CD2	2.17	0.61
1:B:836:VAL:HG23	1:B:855:ALA:HB2	1.84	0.60
1:B:845:MET:HE1	1:B:913:ILE:HG12	1.83	0.59
1:A:835:GLN:HE22	1:A:865:HIS:HD2	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:MET:HE1	1:A:916[A]:HIS:HB3	1.86	0.58
1:A:727[A]:CYS:SG	1:A:730[A]:PHE:HZ	2.27	0.57
1:A:691:LYS:HG2	1:A:699[B]:ILE:HD12	1.86	0.57
1:B:550:LYS:H	1:B:553:GLN:HE21	1.51	0.57
1:B:762:GLU:HA	1:B:789:LEU:HD21	1.87	0.57
1:A:760:HIS:CE1	1:B:873:ILE:HD12	2.41	0.55
1:A:575[B]:TYR:O	6:A:1006[B]:ADP:O2B	2.24	0.55
1:A:569[A]:ALA:HB1	1:A:571[A]:MET:HE3	1.89	0.55
1:B:933:GLU:HA	1:B:940[B]:ARG:HG2	1.89	0.55
1:A:795:HIS:HD2	1:A:797:GLY:N	2.05	0.55
1:A:710[B]:ILE:O	1:A:714:ILE:HG13	2.07	0.55
1:A:733[B]:PRO:HB2	1:A:929:ILE:HD13	1.89	0.54
1:B:573:THR:HA	2:B:1001[A]:AGS:S1G	2.47	0.54
1:B:772:PRO:HB2	1:B:873:ILE:HD11	1.90	0.53
1:A:710[B]:ILE:CA	1:A:713:ASP:HB3	2.37	0.53
1:A:577:LYS:HG3	6:A:1006[B]:ADP:O2B	2.09	0.52
1:A:894:LYS:O	1:A:898:LYS:HG2	2.07	0.52
1:A:845[A]:MET:HE1	1:A:913[A]:ILE:HG12	1.92	0.52
1:B:566:ASP:HB3	1:B:720:LEU:HD13	1.91	0.52
1:A:838:HIS:HD2	5:A:1005:EDO:H21	1.75	0.51
1:A:710[B]:ILE:HA	1:A:713:ASP:CB	2.38	0.51
1:A:778:GLN:HE22	1:A:795:HIS:HE1	1.58	0.51
1:A:553:GLN:O	1:A:557:ILE:HG13	2.10	0.51
1:A:731[B]:ASP:O	1:A:732[B]:ARG:HB2	2.11	0.51
1:B:599:ILE:HA	1:B:602:MET:HE2	1.93	0.51
1:A:912:ILE:HG22	1:A:916[A]:HIS:NE2	2.27	0.50
1:A:673:ILE:CG1	1:A:684:PHE:HB3	2.39	0.50
1:B:715:VAL:HG13	1:B:720:LEU:HB2	1.93	0.50
1:B:533:ASN:ND2	1:B:536:GLN:HE21	2.11	0.49
1:A:877:ARG:HA	1:A:896:MET:HE1	1.95	0.49
1:A:828[B]:ILE:HD12	1:A:854:ARG:HD2	1.95	0.49
1:A:922[B]:VAL:CG2	1:A:926:SER:HB2	2.43	0.49
1:B:707:SER:HB2	1:B:710:ILE:HD12	1.95	0.49
1:A:854:ARG:NH1	2:A:1001[A]:AGS:O3G	2.46	0.49
1:B:607:LEU:O	1:B:611:MET:HG3	2.12	0.48
1:A:713:ASP:HA	1:A:716:ARG:CD	2.43	0.48
1:A:715:VAL:HG13	1:A:720:LEU:HB2	1.94	0.48
1:A:845[A]:MET:HE2	1:A:916[A]:HIS:CD2	2.48	0.48
1:B:812:ARG:HA	1:B:812:ARG:HE	1.78	0.47
1:A:711[A]:ARG:NE	1:A:725:ILE:HG21	2.20	0.46
1:A:597[A]:PRO:HD2	9:A:1114:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:MET:HE1	1:B:580:CYS:SG	2.55	0.46
1:A:552:VAL:HG12	1:A:571[A]:MET:HE2	1.96	0.46
1:A:705[B]:THR:HB	1:A:710[B]:ILE:HD11	1.97	0.46
1:A:669[A]:GLU:OE1	1:A:671[A]:HIS:HE1	1.99	0.46
1:B:749:ASP:HB3	1:B:867:LEU:HD13	1.98	0.46
1:A:857:ARG:HH12	2:A:1001[A]:AGS:PG	2.38	0.46
1:B:557:ILE:O	1:B:561:LEU:HB2	2.15	0.46
1:A:781:THR:HG21	1:A:793:THR:HG22	1.97	0.46
1:A:536:GLN:HG3	1:A:587:TYR:CZ	2.51	0.45
1:A:557:ILE:HG23	1:A:584:PRO:HG3	1.99	0.45
1:A:623:GLN:HE21	1:A:624:SER:H	1.63	0.45
1:A:711[A]:ARG:NE	1:A:725:ILE:HD13	2.32	0.45
1:A:728[A]:THR:HG22	1:A:729[A]:GLY:N	2.32	0.44
1:B:553:GLN:NE2	2:B:1001[A]:AGS:HN61	2.09	0.44
1:B:877:ARG:HH22	1:B:897:ALA:HB2	1.81	0.44
1:A:713:ASP:CA	1:A:716:ARG:HG2	2.44	0.44
1:A:561:LEU:HD13	1:A:584:PRO:HB3	2.00	0.43
1:B:768:ILE:HD11	1:B:833:ILE:HD13	1.99	0.43
1:B:794:TYR:CE1	1:B:827:GLY:HA3	2.53	0.43
1:A:727[A]:CYS:SG	1:A:730[A]:PHE:CZ	3.09	0.43
1:A:845[B]:MET:HG2	1:A:899:MET:SD	2.58	0.43
1:A:762:GLU:HA	1:A:789:LEU:HD21	2.00	0.43
1:B:807:HIS:NE2	1:B:811:VAL:HG21	2.34	0.43
1:A:836:VAL:HG23	1:A:855:ALA:HB2	2.02	0.42
1:A:898:LYS:HB3	1:A:916[A]:HIS:CE1	2.54	0.42
1:A:619:LEU:HD11	1:A:628:LEU:HD13	2.01	0.42
1:A:795:HIS:CD2	1:A:797:GLY:H	2.29	0.42
1:A:557:ILE:O	1:A:561:LEU:HB2	2.19	0.42
1:A:912:ILE:O	1:A:916[A]:HIS:CD2	2.73	0.42
1:B:595:ILE:HG21	1:B:687:LEU:HD21	2.01	0.42
1:B:777:THR:HG23	1:B:819:ILE:HG22	2.00	0.42
1:A:820:ALA:HB1	1:A:824[B]:PHE:HB2	2.02	0.42
1:B:807:HIS:HD2	1:B:826:MET:O	2.03	0.41
1:B:896:MET:HE3	1:B:896:MET:HB2	1.94	0.41
1:B:671:HIS:HD2	1:B:703:THR:OG1	2.04	0.41
1:A:668[B]:ASP:HA	1:A:702[B]:LEU:HB2	2.03	0.41
1:A:852:ILE:HD11	5:A:1007:EDO:H11	2.03	0.41
1:A:673:ILE:HG22	1:A:714:ILE:HG12	2.03	0.40
1:B:807:HIS:CD2	1:B:826:MET:O	2.74	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	492/427 (115%)	457 (93%)	25 (5%)	10 (2%)	6	4
1	B	395/427 (92%)	379 (96%)	16 (4%)	0	100	100
All	All	887/854 (104%)	836 (94%)	41 (5%)	10 (1%)	16	10

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	671[A]	HIS
1	A	576[A]	GLY
1	A	576[B]	GLY
1	A	830[A]	LYS
1	A	830[B]	LYS
1	A	843	LYS
1	A	920[A]	LYS
1	A	920[B]	LYS
1	A	825[A]	GLY
1	A	825[B]	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	432/377 (115%)	407 (94%)	25 (6%)	18	22
1	B	356/377 (94%)	342 (96%)	14 (4%)	28	39
All	All	788/754 (104%)	749 (95%)	39 (5%)	23	29

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	534	GLU
1	A	579	LEU
1	A	626	ASN
1	A	637	ARG
1	A	664	LEU
1	A	691	LYS
1	A	696	MET
1	A	700[A]	VAL
1	A	700[B]	VAL
1	A	711[A]	ARG
1	A	711[B]	ARG
1	A	751	GLN
1	A	778	GLN
1	A	793	THR
1	A	844	ASP
1	A	873	ILE
1	A	875	LEU
1	A	888	PHE
1	A	895	MET
1	A	906	SER
1	A	918[A]	GLU
1	A	918[B]	GLU
1	A	921[A]	GLN
1	A	921[B]	GLN
1	A	929	ILE
1	B	577	LYS
1	B	579	LEU
1	B	624	SER
1	B	644	GLU
1	B	646	CYS
1	B	664	LEU
1	B	669	GLU
1	B	702	LEU
1	B	880	LEU
1	B	881	THR
1	B	888	PHE
1	B	907[A]	ARG
1	B	907[B]	ARG
1	B	929	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	558	HIS
1	A	623	GLN
1	A	655	GLN
1	A	678[A]	HIS
1	A	751	GLN
1	A	760	HIS
1	A	778	GLN
1	A	795	HIS
1	A	835	GLN
1	A	874	ASN
1	A	876	ASN
1	A	885	ASN
1	A	904	HIS
1	B	533	ASN
1	B	536	GLN
1	B	553	GLN
1	B	671	HIS
1	B	778	GLN
1	B	807	HIS
1	B	850	GLN
1	B	904	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 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	1007	-	3,3,3	0.21	0	2,2,2	0.95	0
2	AGS	A	1001[A]	8	32,33,33	0.72	1 (3%)	45,52,52	0.62	0
5	EDO	B	1002	-	3,3,3	0.17	0	2,2,2	0.74	0
2	AGS	B	1001[A]	-	32,33,33	0.66	1 (3%)	45,52,52	0.53	0
5	EDO	A	1005	-	3,3,3	0.12	0	2,2,2	0.65	0
3	GQP	A	1002[B]	-	19,19,19	0.21	0	26,26,26	0.32	0
3	GQP	A	1002[C]	-	19,19,19	0.22	0	26,26,26	0.28	0
6	ADP	A	1006[B]	-	28,29,29	0.42	0	43,45,45	0.42	0
4	DMS	B	1004	-	3,3,3	0.71	0	3,3,3	0.47	0
6	ADP	B	1003[B]	-	28,29,29	0.39	0	43,45,45	0.44	0
4	DMS	A	1003	-	3,3,3	0.46	0	3,3,3	0.67	0
4	DMS	A	1004	-	3,3,3	0.65	0	3,3,3	0.44	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
5	EDO	A	1007	-	-	1/1/1/1	-
2	AGS	A	1001[A]	8	-	4/21/38/38	0/3/3/3
5	EDO	B	1002	-	-	1/1/1/1	-
2	AGS	B	1001[A]	-	-	1/21/38/38	0/3/3/3
5	EDO	A	1005	-	-	1/1/1/1	-
3	GQP	A	1002[B]	-	-	0/4/4/4	0/3/3/3
3	GQP	A	1002[C]	-	-	1/4/4/4	0/3/3/3
6	ADP	A	1006[B]	-	-	5/16/32/32	0/3/3/3
6	ADP	B	1003[B]	-	-	4/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001[A]	AGS	PG-S1G	2.44	1.96	1.90
2	B	1001[A]	AGS	PG-S1G	2.17	1.95	1.90

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1006[B]	ADP	C5'-O5'-PA-O1A
6	A	1006[B]	ADP	O4'-C4'-C5'-O5'
5	B	1002	EDO	O1-C1-C2-O2
6	A	1006[B]	ADP	C3'-C4'-C5'-O5'
5	A	1005	EDO	O1-C1-C2-O2
2	A	1001[A]	AGS	PG-O3B-PB-O1B
6	A	1006[B]	ADP	PA-O3A-PB-O3B
2	A	1001[A]	AGS	C5'-O5'-PA-O1A
6	A	1006[B]	ADP	C5'-O5'-PA-O3A
6	B	1003[B]	ADP	C5'-O5'-PA-O1A
6	B	1003[B]	ADP	PB-O3A-PA-O2A
6	B	1003[B]	ADP	O4'-C4'-C5'-O5'
5	A	1007	EDO	O1-C1-C2-O2
2	A	1001[A]	AGS	PG-O3B-PB-O2B
6	B	1003[B]	ADP	PB-O3A-PA-O1A
2	A	1001[A]	AGS	O4'-C4'-C5'-O5'
2	B	1001[A]	AGS	O4'-C4'-C5'-O5'
3	A	1002[C]	GQP	C9-C8-N2-C4

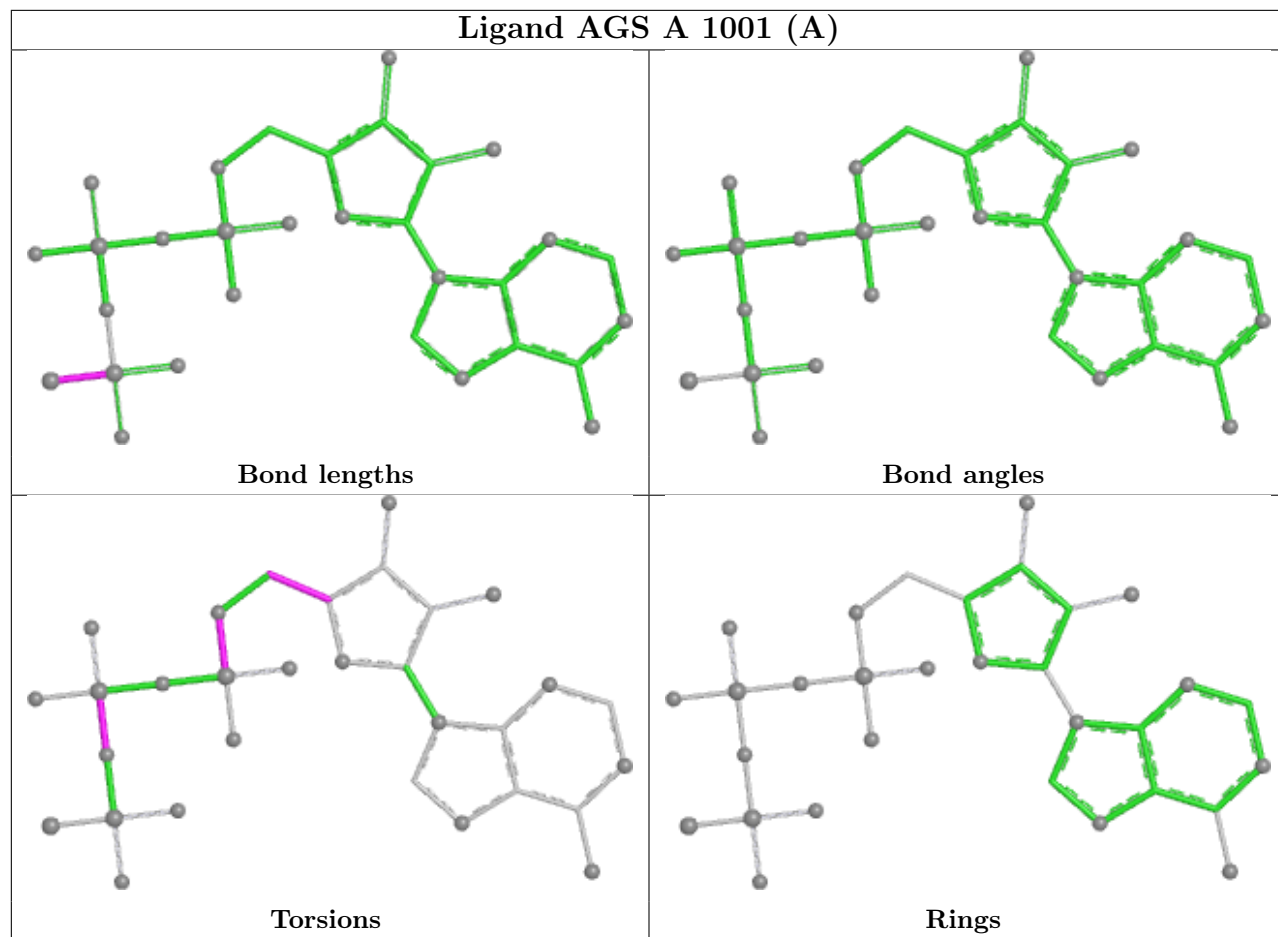
There are no ring outliers.

5 monomers are involved in 12 short contacts:

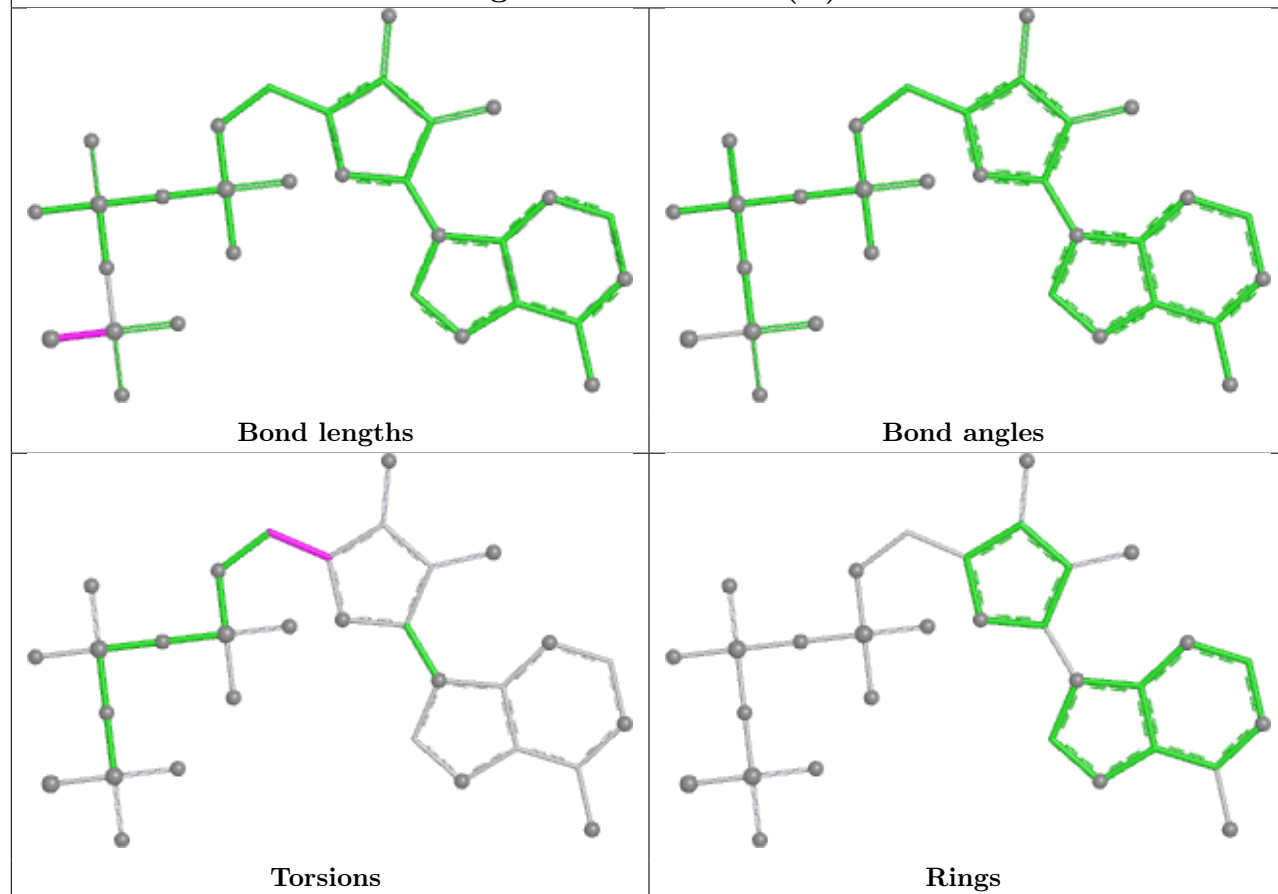
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1007	EDO	1	0
2	A	1001[A]	AGS	3	0
2	B	1001[A]	AGS	4	0
5	A	1005	EDO	1	0
6	A	1006[B]	ADP	3	0

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

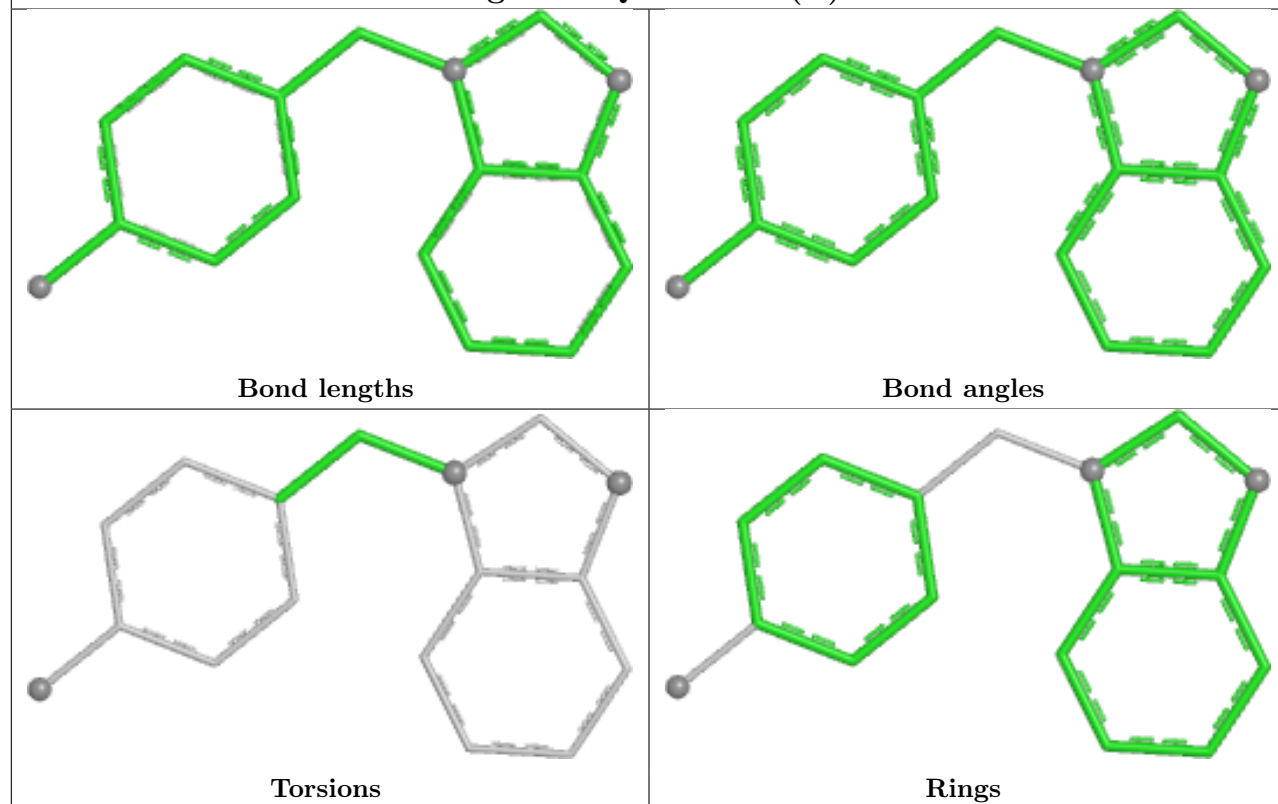
equivalents in the CSD to analyse the geometry.



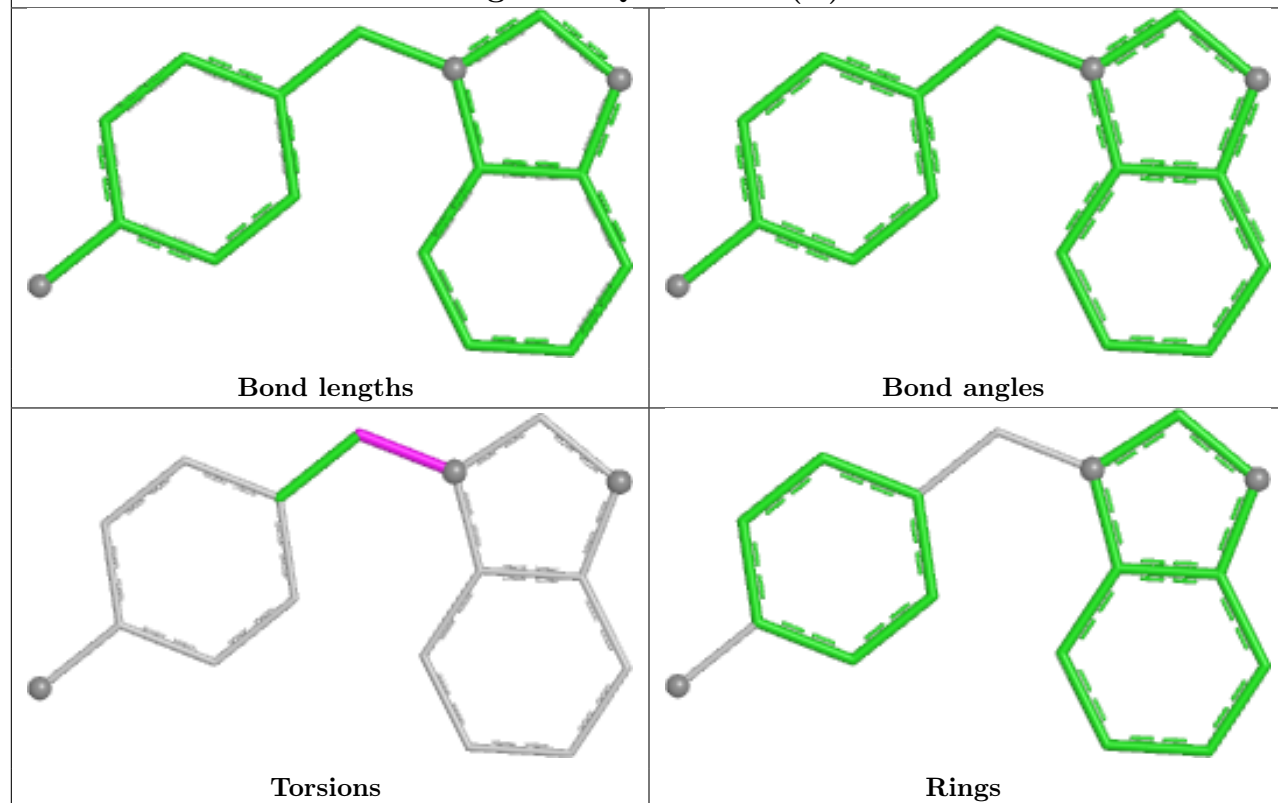
Ligand AGS B 1001 (A)



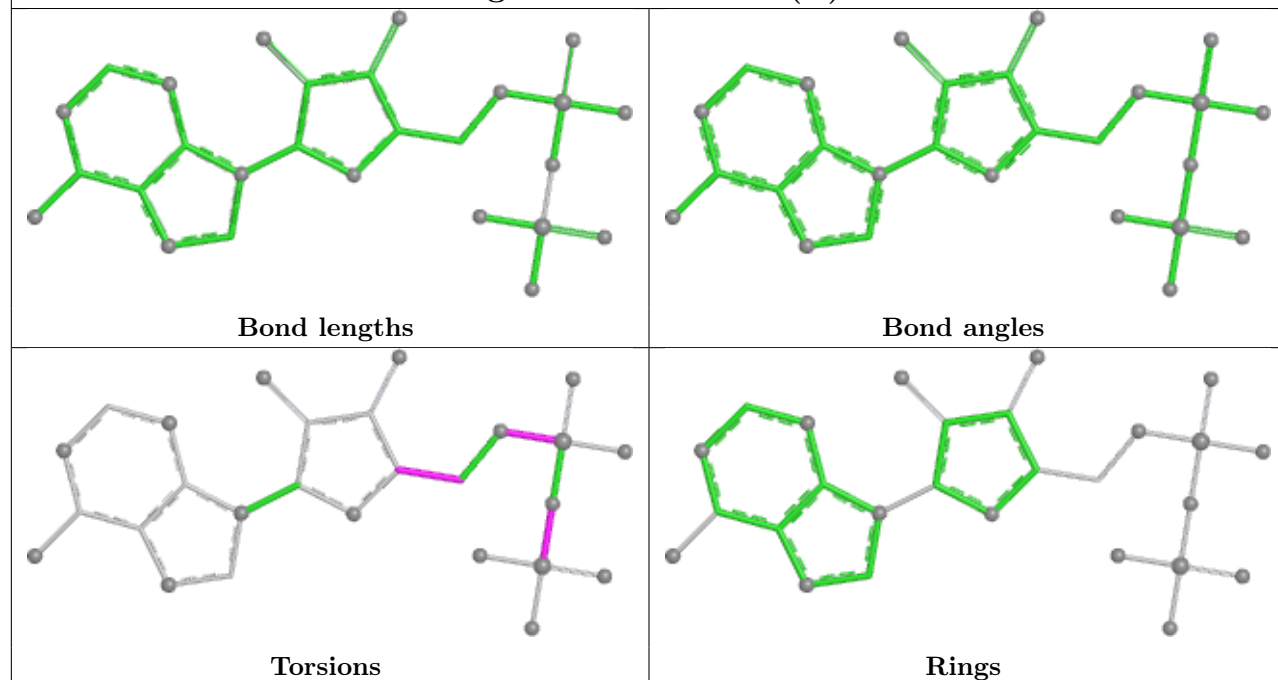
Ligand GQP A 1002 (B)

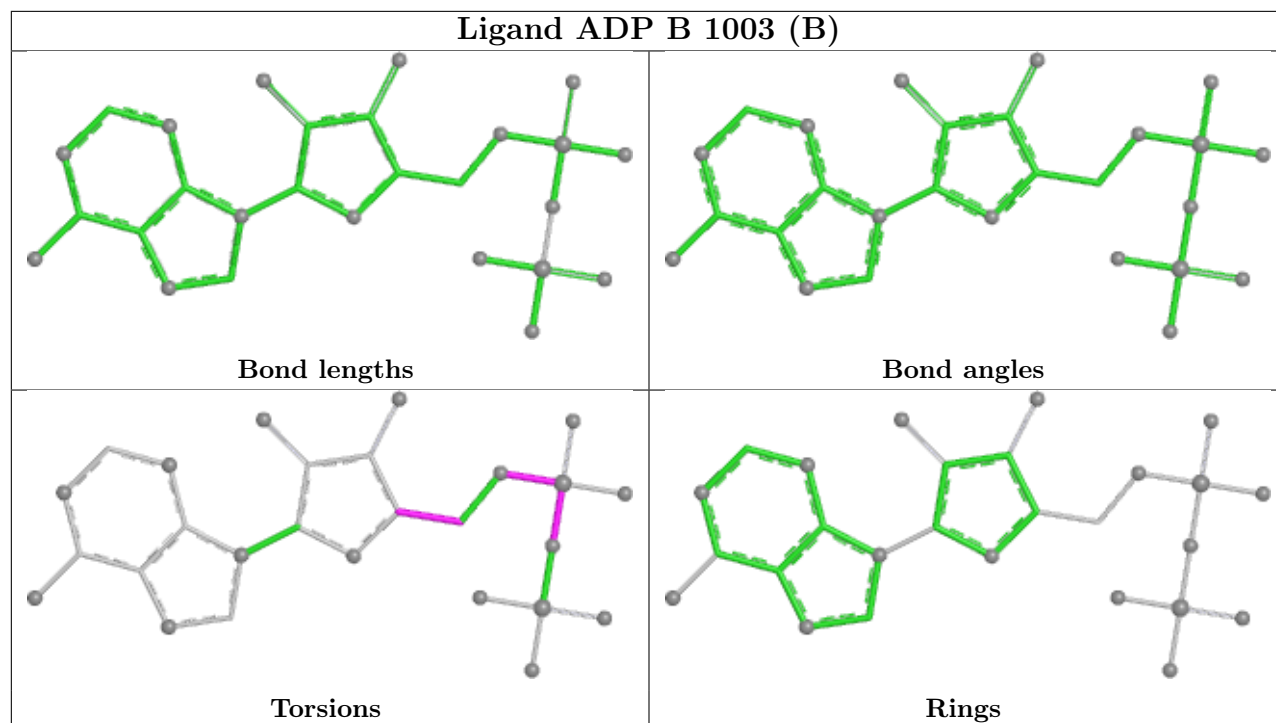


Ligand GQP A 1002 (C)



Ligand ADP A 1006 (B)





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	406/427 (95%)	1.85	163 (40%) 0 0	14, 46, 92, 120	105 (25%)
1	B	400/427 (93%)	1.99	181 (45%) 0 0	20, 67, 115, 133	3 (0%)
All	All	806/854 (94%)	1.92	344 (42%) 0 0	14, 56, 109, 133	108 (13%)

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	677[A]	GLY	9.5
1	B	653	LEU	9.3
1	A	681[A]	ARG	8.2
1	B	560	VAL	7.7
1	A	680[A]	PHE	7.6
1	B	561	LEU	7.4
1	A	683[A]	SER	7.3
1	B	700	VAL	7.3
1	B	701	ALA	7.2
1	A	888	PHE	6.9
1	A	684	PHE	6.8
1	B	699	ILE	6.7
1	B	702	LEU	6.5
1	B	697	VAL	6.2
1	B	593	LEU	6.2
1	A	678[A]	HIS	5.9
1	B	628	LEU	5.9
1	A	824[A]	PHE	5.9
1	A	601[A]	LEU	5.9
1	B	883	ILE	5.8
1	A	687	LEU	5.8
1	B	718	LEU	5.8
1	B	638	ILE	5.8
1	A	822[A]	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	825[A]	GLY	5.6
1	B	698	PRO	5.4
1	B	639	VAL	5.4
1	A	714	ILE	5.4
1	A	891	TYR	5.3
1	B	665	ILE	5.3
1	A	682[A]	ASP	5.3
1	B	687	LEU	5.1
1	B	595	ILE	5.1
1	A	673	ILE	5.0
1	B	631	ILE	5.0
1	A	679[A]	ASP	4.9
1	B	715	VAL	4.9
1	B	714	ILE	4.9
1	A	893	LEU	4.9
1	B	588	VAL	4.9
1	A	879	LEU	4.8
1	A	674[A]	SER	4.8
1	A	702[A]	LEU	4.8
1	B	640	TYR	4.7
1	A	726[A]	THR	4.7
1	B	664	LEU	4.7
1	B	632	LYS	4.6
1	B	684	PHE	4.6
1	B	888	PHE	4.6
1	B	941	SER	4.6
1	B	704	ALA	4.5
1	A	890	LEU	4.5
1	B	670	ALA	4.5
1	B	530	PRO	4.5
1	B	725	ILE	4.4
1	B	663	THR	4.4
1	B	890	LEU	4.4
1	B	662	ILE	4.4
1	B	710	ILE	4.4
1	A	916[A]	HIS	4.3
1	A	597[A]	PRO	4.3
1	B	594	VAL	4.3
1	B	549	PHE	4.3
1	A	827[A]	GLY	4.3
1	A	757	THR	4.3
1	A	568[A]	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	672[A]	CYS	4.2
1	A	575[A]	TYR	4.2
1	A	668[A]	ASP	4.2
1	B	622	ALA	4.2
1	A	588	VAL	4.2
1	B	694	LEU	4.2
1	B	552	VAL	4.2
1	A	710[A]	ILE	4.2
1	B	667	VAL	4.2
1	B	596	SER	4.1
1	A	875	LEU	4.1
1	A	823[A]	ALA	4.1
1	B	706	ALA	4.1
1	B	671	HIS	4.1
1	B	569	ALA	4.0
1	B	880	LEU	4.0
1	A	826[A]	MET	4.0
1	A	560	VAL	4.0
1	A	711[A]	ARG	4.0
1	B	580	CYS	4.0
1	A	708[A]	SER	4.0
1	B	531	ALA	3.9
1	A	653	LEU	3.9
1	A	690	LEU	3.9
1	B	683	SER	3.9
1	B	705	THR	3.9
1	A	549	PHE	3.9
1	A	656	LEU	3.9
1	A	547	SER	3.9
1	B	879	LEU	3.9
1	A	667[A]	VAL	3.8
1	A	892	LYS	3.8
1	B	666	ALA	3.8
1	A	598[A]	LEU	3.8
1	B	656	LEU	3.8
1	B	567	ASN	3.8
1	B	690	LEU	3.8
1	B	568	VAL	3.8
1	A	670[A]	ALA	3.8
1	A	761	TRP	3.7
1	B	627	VAL	3.7
1	A	913[A]	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	563	GLU	3.7
1	A	728[A]	THR	3.7
1	A	530	PRO	3.6
1	B	646	CYS	3.6
1	B	564	ARG	3.6
1	A	537	VAL	3.6
1	A	720	LEU	3.6
1	A	922[A]	VAL	3.6
1	A	618	PHE	3.6
1	B	720	LEU	3.6
1	B	556	VAL	3.5
1	B	557	ILE	3.5
1	B	618	PHE	3.5
1	B	619	LEU	3.5
1	B	574	GLY	3.5
1	A	552	VAL	3.5
1	B	755	VAL	3.5
1	B	651	GLY	3.5
1	A	556	VAL	3.5
1	A	921[A]	GLN	3.5
1	A	593[A]	LEU	3.4
1	A	600[A]	SER	3.4
1	A	694	LEU	3.4
1	A	758	SER	3.4
1	A	542	MET	3.4
1	B	917	PHE	3.4
1	B	633	LEU	3.4
1	B	850	GLN	3.4
1	A	692	THR	3.4
1	B	537	VAL	3.4
1	B	641	VAL	3.4
1	A	699[A]	ILE	3.4
1	B	634	GLY	3.4
1	B	540	LEU	3.4
1	B	893	LEU	3.4
1	B	660	ILE	3.3
1	A	696	MET	3.3
1	A	760	HIS	3.3
1	B	645	TYR	3.3
1	A	591[A]	ILE	3.3
1	B	922	VAL	3.2
1	B	584	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	717	CYS	3.2
1	A	594[A]	VAL	3.2
1	B	808	HIS	3.2
1	B	554	TRP	3.1
1	A	540	LEU	3.1
1	A	664	LEU	3.1
1	A	915[A]	SER	3.1
1	B	558	HIS	3.1
1	A	610	LYS	3.1
1	B	544	PHE	3.1
1	A	531	ALA	3.1
1	A	715	VAL	3.1
1	B	601	LEU	3.1
1	A	631	ILE	3.1
1	A	587	TYR	3.1
1	B	597	PRO	3.1
1	B	652	LEU	3.1
1	A	895	MET	3.1
1	B	581	PHE	3.0
1	A	569[A]	ALA	3.0
1	B	543	TYR	3.0
1	A	671[A]	HIS	3.0
1	A	704[A]	ALA	3.0
1	A	599[A]	ILE	3.0
1	B	925	ALA	3.0
1	A	639	VAL	3.0
1	B	885	ASN	3.0
1	A	691	LYS	3.0
1	A	544	PHE	3.0
1	A	885	ASN	2.9
1	A	638	ILE	2.9
1	A	821[A]	THR	2.9
1	B	624	SER	2.9
1	A	718	LEU	2.9
1	B	913	ILE	2.9
1	A	723	PRO	2.9
1	A	897	ALA	2.9
1	B	598	LEU	2.9
1	B	555	LYS	2.9
1	B	636	TYR	2.9
1	A	685	ARG	2.8
1	B	571	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	583	TYR	2.8
1	B	688	GLY	2.8
1	B	761	TRP	2.8
1	A	725	ILE	2.8
1	A	700[A]	VAL	2.8
1	A	849[A]	TYR	2.8
1	B	693	ALA	2.8
1	B	703	THR	2.8
1	A	660	ILE	2.8
1	B	591	ILE	2.8
1	A	911	GLN	2.7
1	B	576	GLY	2.7
1	B	897	ALA	2.7
1	A	705[A]	THR	2.7
1	B	692	THR	2.7
1	B	532	PRO	2.7
1	A	627	VAL	2.7
1	A	554	TRP	2.7
1	B	691	LYS	2.7
1	B	616	ALA	2.7
1	B	642	THR	2.7
1	B	914	LEU	2.7
1	B	724	GLN	2.7
1	A	580	CYS	2.7
1	A	611	MET	2.7
1	A	636	TYR	2.7
1	A	586	VAL	2.7
1	A	713	ASP	2.7
1	B	575	TYR	2.6
1	B	582	GLN	2.6
1	B	546	HIS	2.6
1	A	538	THR	2.6
1	A	551	PRO	2.6
1	B	583	TYR	2.6
1	B	614	ILE	2.6
1	B	538	THR	2.6
1	A	561	LEU	2.6
1	B	763	PHE	2.6
1	B	891	TYR	2.6
1	B	672	CYS	2.6
1	B	878	HIS	2.6
1	B	829	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	756	LYS	2.6
1	A	629	THR	2.6
1	B	647	SER	2.6
1	B	921[A]	GLN	2.5
1	A	662	ILE	2.5
1	B	729	GLY	2.5
1	A	559	SER	2.5
1	A	896	MET	2.5
1	A	634	GLY	2.5
1	A	729[A]	GLY	2.5
1	B	570	VAL	2.5
1	B	760	HIS	2.5
1	A	565	ARG	2.5
1	A	919[A]	ASP	2.5
1	A	567[A]	ASN	2.5
1	B	533	ASN	2.5
1	B	587	TYR	2.5
1	A	548	SER	2.5
1	B	707	SER	2.5
1	B	757	THR	2.5
1	A	887	LYS	2.5
1	A	604[A]	ASP	2.4
1	A	712[A]	GLU	2.4
1	B	911	GLN	2.4
1	B	629	THR	2.4
1	B	658	ALA	2.4
1	A	686	LYS	2.4
1	A	557	ILE	2.4
1	B	586	VAL	2.4
1	A	646	CYS	2.4
1	B	539	CYS	2.4
1	A	532	PRO	2.4
1	A	650	MET	2.4
1	A	658	ALA	2.4
1	A	706[A]	ALA	2.4
1	B	623	GLN	2.4
1	A	828[A]	ILE	2.4
1	A	689	SER	2.4
1	B	612	SER	2.4
1	B	541	LYS	2.4
1	B	577	LYS	2.4
1	B	889	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	645	TYR	2.4
1	A	701[A]	ALA	2.4
1	A	889	ARG	2.4
1	B	578	SER	2.4
1	B	536	GLN	2.3
1	B	630	ASP	2.3
1	A	774	ARG	2.3
1	B	542	MET	2.3
1	A	709[A]	SER	2.3
1	A	878	HIS	2.3
1	A	641	VAL	2.3
1	A	697[A]	VAL	2.3
1	B	726	THR	2.3
1	B	717	CYS	2.3
1	A	628	LEU	2.3
1	A	848[A]	TYR	2.3
1	B	686	LYS	2.3
1	A	800[A]	PHE	2.3
1	A	778	GLN	2.3
1	B	643	PRO	2.3
1	A	884	ARG	2.3
1	B	940[A]	ARG	2.3
1	B	887	LYS	2.3
1	B	650	MET	2.3
1	B	562	GLU	2.2
1	A	596[A]	SER	2.2
1	B	620	GLY	2.2
1	B	727	CYS	2.2
1	B	579	LEU	2.2
1	B	754	LEU	2.2
1	A	550	LYS	2.2
1	A	669[A]	GLU	2.2
1	B	547	SER	2.2
1	B	548	SER	2.2
1	B	551	PRO	2.2
1	B	617	CYS	2.2
1	B	787	LEU	2.2
1	B	711	ARG	2.2
1	B	719	ASN	2.2
1	A	614	ILE	2.1
1	B	875	LEU	2.1
1	A	562	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	606	VAL	2.1
1	B	827	GLY	2.1
1	A	847[A]	SER	2.1
1	A	602[A]	MET	2.1
1	A	876	ASN	2.1
1	A	796	ALA	2.1
1	A	607[A]	LEU	2.1
1	B	759	SER	2.1
1	B	896	MET	2.1
1	B	637	ARG	2.1
1	B	728	THR	2.1
1	A	744	GLY	2.1
1	B	545	GLY	2.1
1	A	920[A]	LYS	2.1
1	A	622	ALA	2.1
1	A	850[A]	GLN	2.0
1	B	553	GLN	2.0
1	A	663	THR	2.0
1	B	797	GLY	2.0
1	A	759	SER	2.0
1	B	708	SER	2.0
1	B	613	ASN	2.0
1	B	609	LEU	2.0
1	B	565	ARG	2.0
1	B	807	HIS	2.0
1	A	797	GLY	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](#)

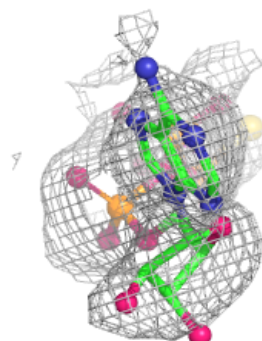
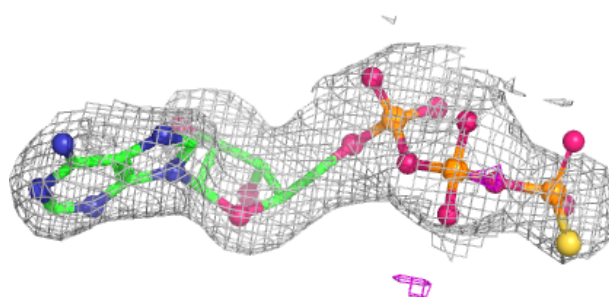
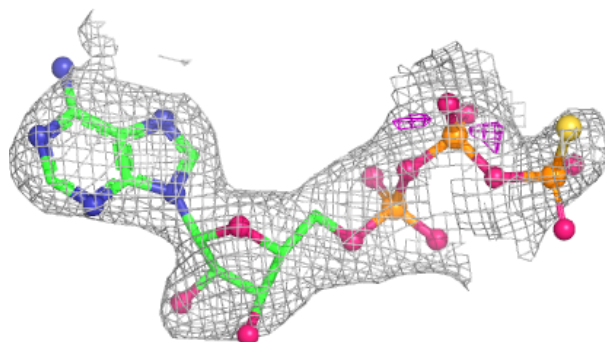
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	AGS	B	1001[A]	31/31	0.75	0.20	143,143,144,144	31
5	EDO	B	1002	4/4	0.77	0.32	48,48,49,49	0
2	AGS	A	1001[A]	31/31	0.78	0.16	62,65,66,66	31
3	GQP	A	1002[C]	17/17	0.83	0.29	26,27,28,28	17
3	GQP	A	1002[B]	17/17	0.83	0.29	44,45,45,45	17
8	MG	A	1009	1/1	0.83	0.15	59,59,59,59	0
4	DMS	B	1004	4/4	0.85	0.21	81,81,81,81	0
6	ADP	B	1003[B]	27/27	0.88	0.11	38,40,41,42	27
5	EDO	A	1005	4/4	0.89	0.18	49,49,50,51	0
4	DMS	A	1004	4/4	0.91	0.18	64,65,65,65	0
6	ADP	A	1006[B]	27/27	0.92	0.10	57,62,64,64	27
4	DMS	A	1003	4/4	0.94	0.13	90,90,90,90	0
5	EDO	A	1007	4/4	0.95	0.10	32,32,32,33	0
7	ZN	B	1005	1/1	0.99	0.04	37,37,37,37	0
7	ZN	A	1008	1/1	0.99	0.06	42,42,42,42	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.

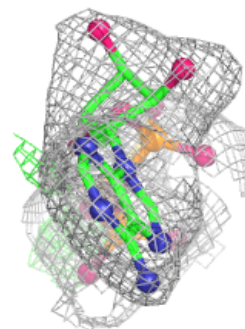
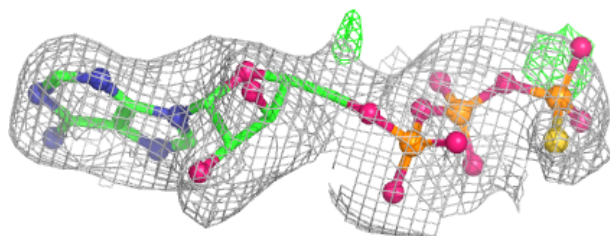
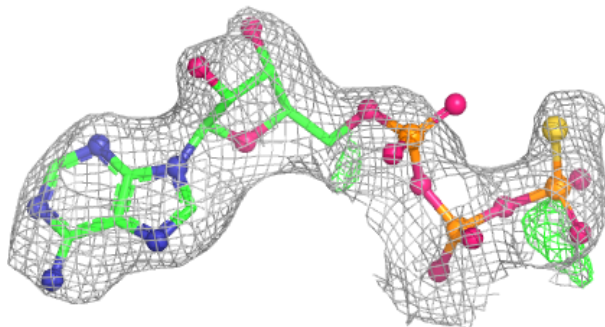
Electron density around AGS B 1001 (A):

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

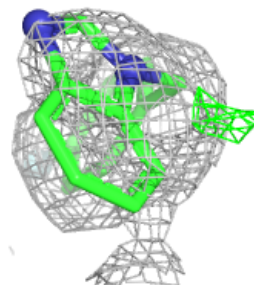
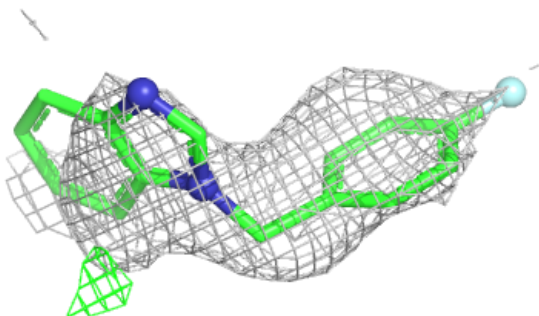
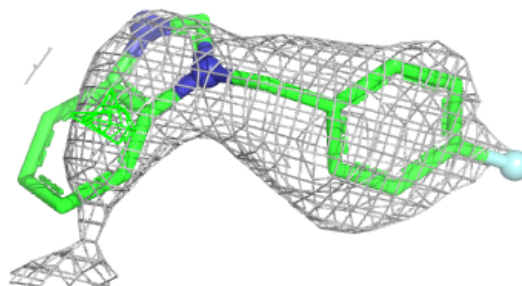


Electron density around AGS A 1001 (A):

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

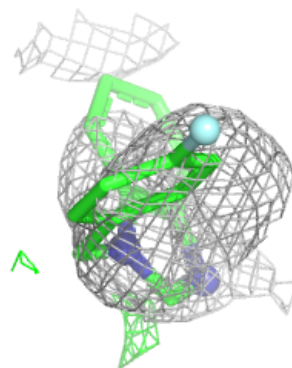
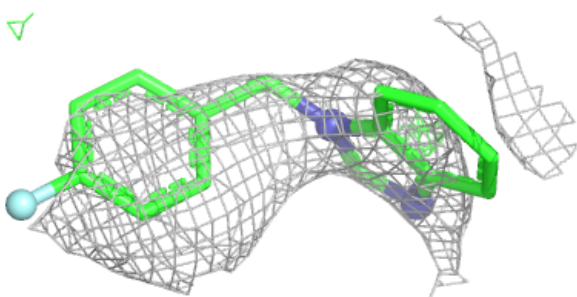
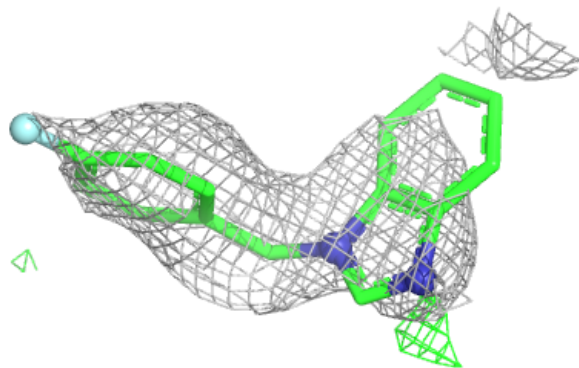
**Electron density around GQP A 1002 (C):**

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

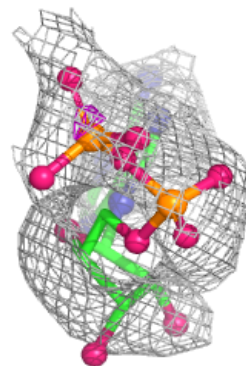
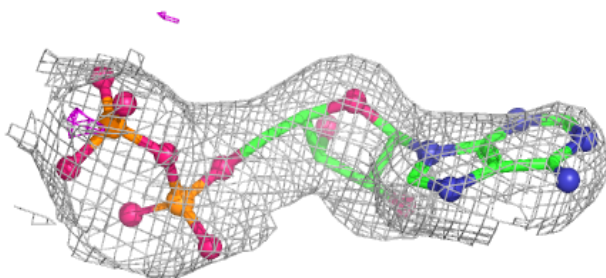
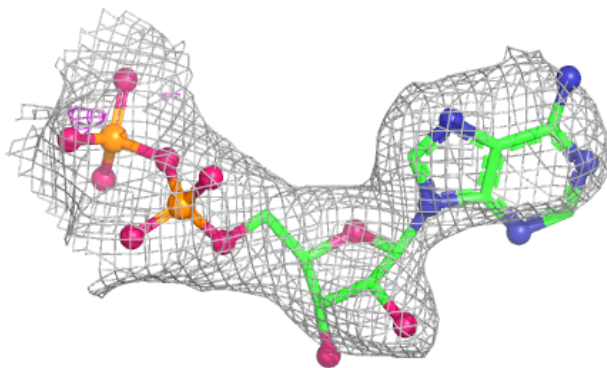


Electron density around GQP A 1002 (B):

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

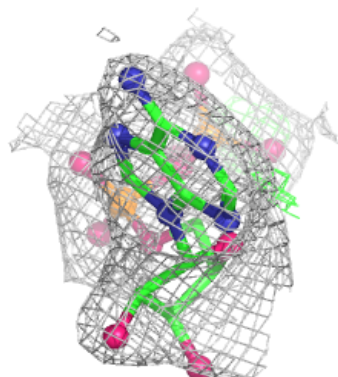
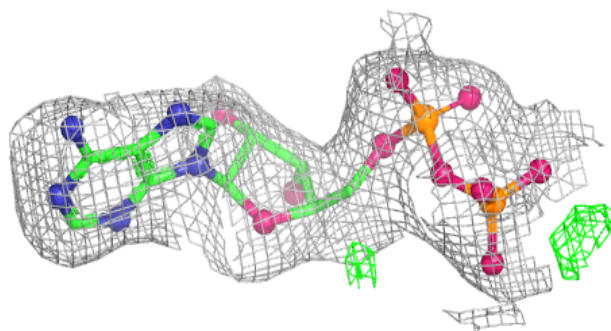
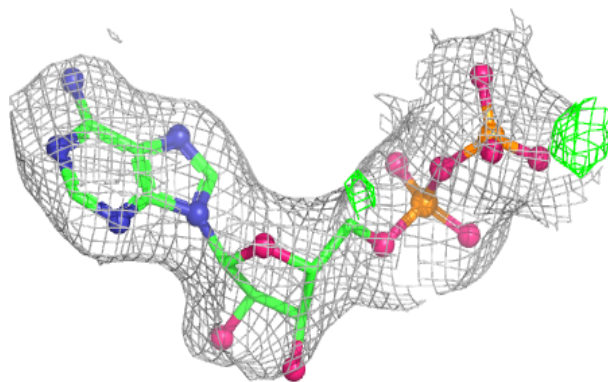
**Electron density around ADP B 1003 (B):**

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



Electron density around ADP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.