



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:55 PM UTC

PDB ID : 4TL8 / pdb_00004tl8
Title : Crystal structure of N-terminal C1 domain of KaiC
Authors : Abe, J.; Hiyama, T.B.; Mukaiyama, A.; Son, S.; Akiyama, S.
Deposited on : 2014-05-29
Resolution : 1.86 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

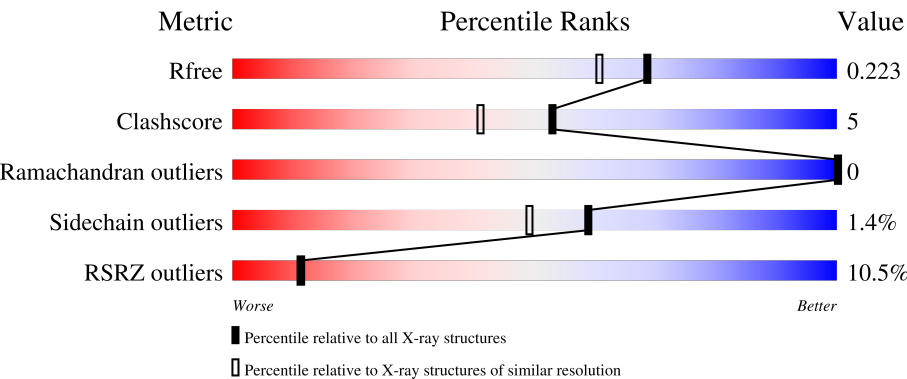
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	253	11% 72% 13% 15%
1	B	253	5% 76% 9% 15%
1	C	253	7% 80% 7% 13%
1	D	253	6% 76% 10% 14%
1	E	253	12% 75% 9% 15%

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Mol	Chain	Length	Quality of chain
1	F	253	12% 72% 11% • 16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11623 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 Circadian clock protein kinase KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	6	0
			1735	1101	304	326	4			
1	B	215	Total	C	N	O	S	0	6	0
			1737	1105	301	326	5			
1	C	221	Total	C	N	O	S	0	8	0
			1786	1136	312	334	4			
1	D	217	Total	C	N	O	S	0	5	0
			1760	1115	308	332	5			
1	E	216	Total	C	N	O	S	0	5	0
			1743	1110	303	326	4			
1	F	213	Total	C	N	O	S	0	6	0
			1732	1096	302	330	4			

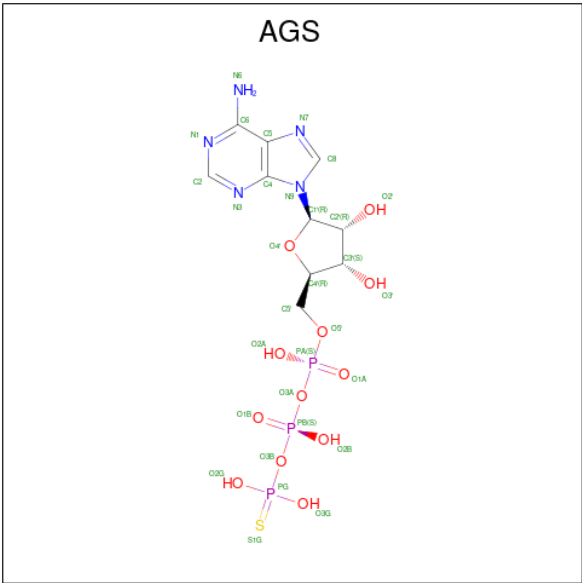
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		

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



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

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

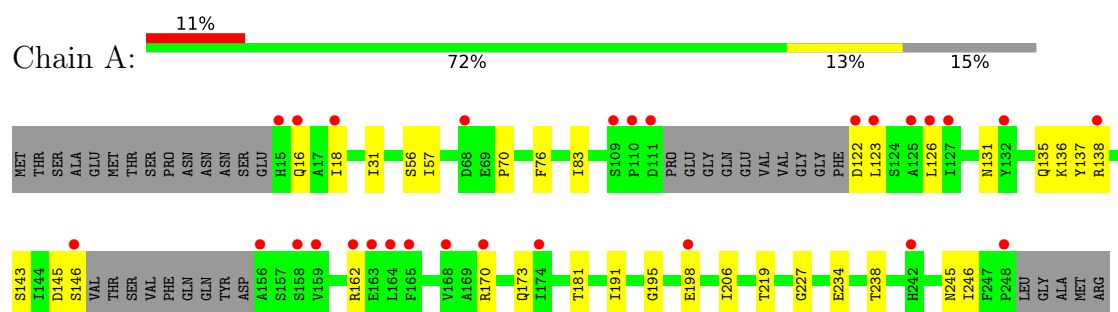
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	119	Total	O	0	0
			119	119		
5	B	181	Total	O	0	0
			181	181		
5	C	178	Total	O	0	0
			178	178		
5	D	178	Total	O	0	0
			178	178		
5	E	139	Total	O	0	0
			139	139		
5	F	137	Total	O	0	0
			137	137		

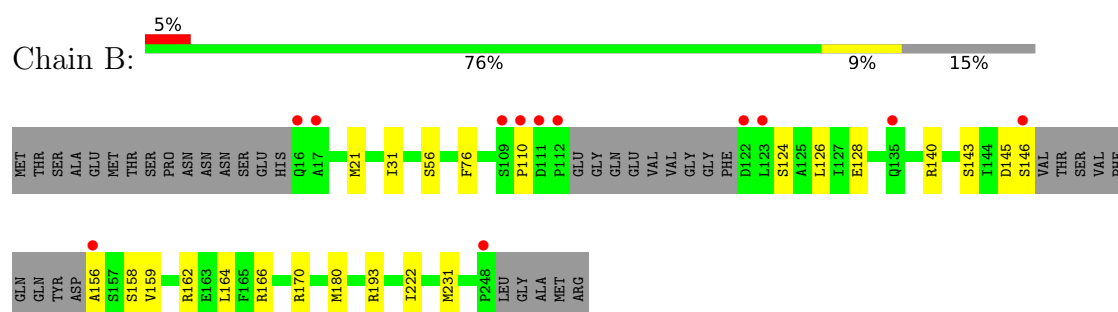
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

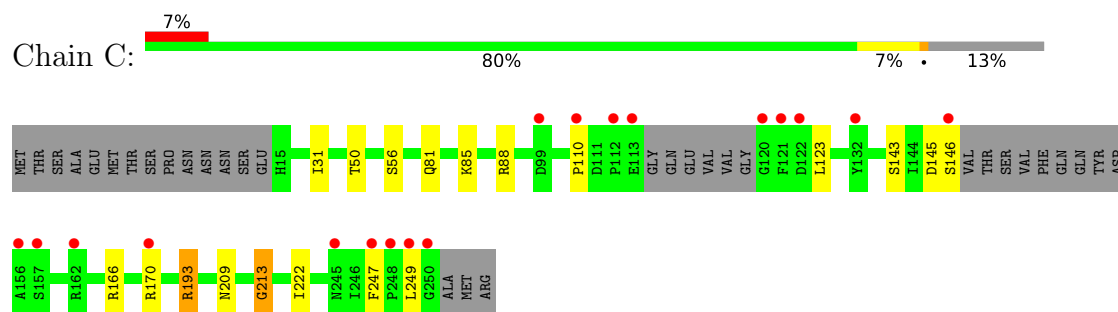
- Molecule 1: Circadian clock protein kinase KaiC



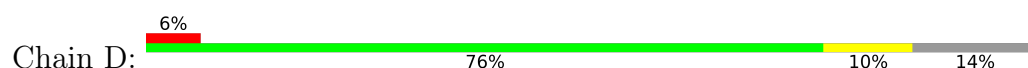
- Molecule 1: Circadian clock protein kinase KaiC

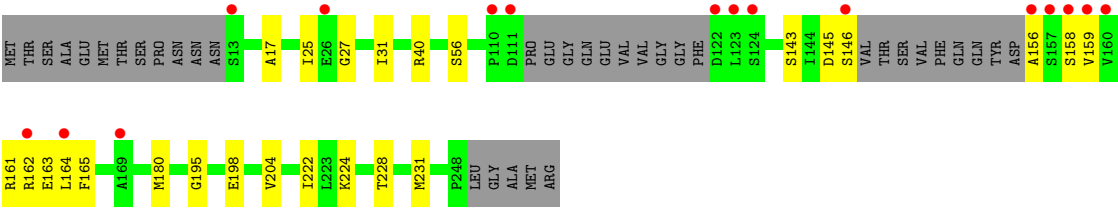


- Molecule 1: Circadian clock protein kinase KaiC

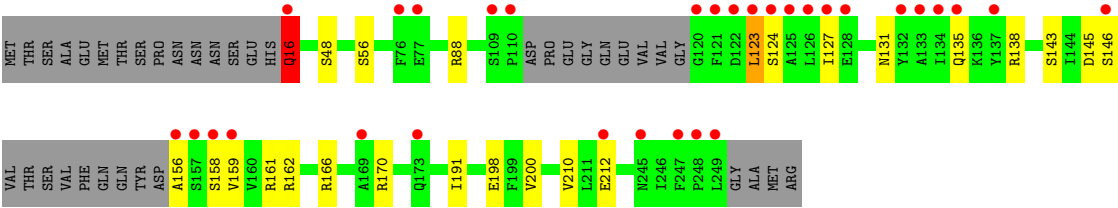
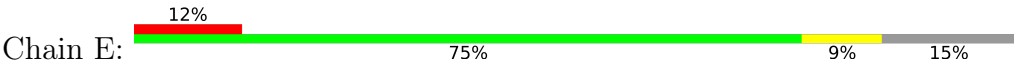


- Molecule 1: Circadian clock protein kinase KaiC

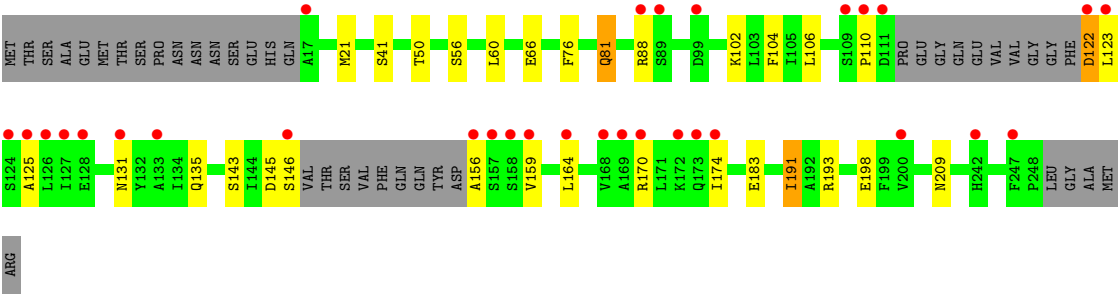




● Molecule 1: Circadian clock protein kinase KaiC



● Molecule 1: Circadian clock protein kinase KaiC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.93Å 133.22Å 150.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.59 – 1.86 37.59 – 1.86	Depositor EDS
% Data completeness (in resolution range)	97.8 (37.59-1.86) 97.8 (37.59-1.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.28 (at 1.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.180 , 0.222 0.183 , 0.223	Depositor DCC
R_{free} test set	6644 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11623	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: CL, MG, 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	0.71	0/1774	0.83	0/2388
1	B	0.84	0/1776	0.92	1/2391 (0.0%)
1	C	0.78	0/1827	0.93	1/2459 (0.0%)
1	D	0.83	0/1787	0.90	1/2405 (0.0%)
1	E	0.85	0/1776	0.95	2/2390 (0.1%)
1	F	0.85	0/1758	0.99	1/2366 (0.0%)
All	All	0.81	0/10698	0.92	6/14399 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	213	GLY	N-CA-C	-6.71	98.50	110.86
1	B	193	ARG	N-CA-C	5.48	117.33	111.36
1	F	60	LEU	N-CA-C	5.37	116.94	111.14
1	D	17	ALA	N-CA-C	5.08	118.74	112.54
1	E	16	GLN	CA-CB-CG	-5.07	103.96	114.10
1	E	123	LEU	N-CA-C	5.05	117.52	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	16	GLN	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1735	0	1754	24	0
1	B	1737	0	1765	17	0
1	C	1786	0	1808	16	0
1	D	1760	0	1765	17	0
1	E	1743	0	1767	21	0
1	F	1732	0	1737	20	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
4	E	31	0	12	2	0
4	F	31	0	12	0	0
5	A	119	0	0	2	0
5	B	181	0	0	2	0
5	C	178	0	0	4	0
5	D	178	0	0	2	0
5	E	139	0	0	1	0
5	F	137	0	0	2	0
All	All	11623	0	10668	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (107) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ARG:NH1	1:D:195:GLY:O	1.91	1.04
1:A:195:GLY:O	1:F:193:ARG:NH2	2.03	0.91
1:E:16:GLN:O	1:E:16:GLN:HG2	1.70	0.90
1:B:124:SER:OG	1:B:166:ARG:NH2	2.05	0.90
1:F:81:GLN:NE2	5:F:504:HOH:O	2.12	0.83
1:E:127:ILE:HG21	1:E:170:ARG:HD3	1.69	0.75
1:B:164:LEU:HD11	1:B:180:MET:HE1	1.74	0.69
1:F:41:SER:OG	5:F:536:HOH:O	1.96	0.68
1:A:238:THR:OG1	1:A:245[A]:ASN:OD1	2.14	0.66
1:D:158:SER:HA	1:D:161:ARG:HB3	1.78	0.65
1:D:198:GLU:OE1	5:D:545:HOH:O	2.15	0.65
1:E:131:ASN:OD1	1:E:135:GLN:NE2	2.26	0.64
1:E:123:LEU:HD13	1:E:127:ILE:HD11	1.82	0.62
1:B:158:SER:O	1:B:162:ARG:HG3	1.99	0.61
1:F:191:ILE:HG21	1:F:198:GLU:HB3	1.83	0.61
1:F:156:ALA:HB3	1:F:159:VAL:HG12	1.81	0.60
1:E:156:ALA:HB3	1:E:159:VAL:HG12	1.86	0.58
1:B:156:ALA:HB3	1:B:159:VAL:HG12	1.88	0.55
1:A:76:PHE:HZ	1:A:126:LEU:HD21	1.71	0.55
1:F:56[A]:SER:HB2	1:F:143:SER:HB3	1.90	0.54
1:A:122:ASP:OD1	1:A:123:LEU:N	2.40	0.54
1:D:31[A]:ILE:HG22	1:D:222:ILE:HD12	1.91	0.53
1:B:140:ARG:HD2	5:B:469:HOH:O	2.09	0.52
1:E:162:ARG:HH11	1:E:162:ARG:HG3	1.74	0.52
1:E:191:ILE:HG21	1:E:198:GLU:HB3	1.91	0.52
1:E:56[A]:SER:HB2	1:E:143:SER:HB3	1.92	0.52
1:C:146[B]:SER:OG	5:C:488:HOH:O	2.06	0.51
1:F:104:PHE:HE2	1:F:106:LEU:HD12	1.74	0.50
1:A:162:ARG:NH1	1:F:110:PRO:HG3	2.26	0.50
1:A:16:GLN:OE1	5:A:401:HOH:O	2.20	0.50
1:B:164:LEU:CD1	1:B:180:MET:HE1	2.40	0.49
1:C:110:PRO:HG2	1:D:165:PHE:CE1	2.48	0.49
1:D:31[B]:ILE:HG22	1:D:222:ILE:HD12	1.95	0.49
1:A:170:ARG:HD3	1:A:173:GLN:OE1	2.12	0.48
1:C:213:GLY:O	5:C:561:HOH:O	2.17	0.48
1:A:162:ARG:NE	1:A:162:ARG:HA	2.28	0.48
1:E:123:LEU:HD11	1:E:166:ARG:CZ	2.44	0.48
1:E:145[A]:ASP:HA	1:E:146[A]:SER:HA	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LYS:HE3	1:D:40:ARG:NH2	2.29	0.48
1:C:166:ARG:O	1:C:170:ARG:HG2	2.13	0.48
1:A:145[A]:ASP:HA	1:A:146[A]:SER:HA	1.67	0.47
1:F:170:ARG:O	1:F:174:ILE:HG13	2.14	0.47
1:D:145[A]:ASP:HA	1:D:146[A]:SER:HA	1.67	0.47
1:D:156:ALA:O	1:D:159:VAL:HG12	2.15	0.47
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.97	0.47
1:B:56[A]:SER:HB2	1:B:143:SER:HB3	1.97	0.46
1:C:170:ARG:NH1	5:C:512:HOH:O	2.30	0.46
1:D:56[A]:SER:HB2	1:D:143:SER:HB3	1.97	0.46
1:F:183:GLU:OE2	1:F:193:ARG:NH1	2.49	0.46
1:C:88[A]:ARG:HD3	5:C:418:HOH:O	2.14	0.46
1:F:122:ASP:HB2	1:F:125:ALA:CB	2.46	0.46
1:E:131:ASN:O	1:E:135:GLN:HG2	2.16	0.46
1:A:131:ASN:O	1:A:135:GLN:HG2	2.16	0.45
1:D:25:ILE:O	5:D:551:HOH:O	2.21	0.45
1:F:145[A]:ASP:HA	1:F:146[A]:SER:HA	1.71	0.45
1:B:166:ARG:O	1:B:170:ARG:HG2	2.17	0.45
1:F:122:ASP:HB2	1:F:125:ALA:HB3	1.97	0.45
1:C:31:ILE:HG22	1:C:222:ILE:HD12	1.97	0.45
1:E:162:ARG:HH11	1:E:162:ARG:CG	2.29	0.45
1:A:16:GLN:HB2	1:F:88:ARG:HB3	2.00	0.44
1:F:76:PHE:O	1:F:110:PRO:HD3	2.18	0.44
1:A:18:ILE:HD13	1:A:227:GLY:O	2.17	0.44
1:D:164:LEU:CD1	1:D:180[B]:MET:HE1	2.48	0.44
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.99	0.44
1:E:161:ARG:HG3	1:E:200:VAL:HG11	1.99	0.44
1:B:31[A]:ILE:HG22	1:B:222:ILE:HD12	2.00	0.43
1:C:247:PHE:O	1:C:249:LEU:HD23	2.18	0.43
1:C:145[A]:ASP:HA	1:C:146[A]:SER:HA	1.57	0.43
1:E:88:ARG:NE	5:E:401:HOH:O	2.44	0.43
1:B:76:PHE:HZ	1:B:126:LEU:HD21	1.83	0.43
1:D:31[B]:ILE:HD13	1:D:231:MET:SD	2.59	0.43
1:D:159:VAL:O	1:D:163:GLU:HG2	2.18	0.43
1:B:140:ARG:NH1	5:B:525:HOH:O	2.50	0.43
1:D:204:VAL:HG23	1:D:224:LYS:HE2	2.01	0.43
1:B:124:SER:O	1:B:128:GLU:HG2	2.18	0.43
1:A:70:PRO:HG2	1:A:138:ARG:O	2.17	0.43
1:B:145[A]:ASP:HA	1:B:146[A]:SER:HA	1.67	0.43
1:E:158:SER:O	1:E:162:ARG:HG3	2.19	0.43
1:A:162:ARG:HA	1:A:162:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146[A]:SER:HA	1:A:181:THR:OG1	2.19	0.42
1:E:56[B]:SER:HB3	1:E:143:SER:HB3	2.01	0.42
1:F:191:ILE:CG2	1:F:198:GLU:HB3	2.48	0.42
1:A:56[A]:SER:HB2	1:A:143:SER:HB3	2.00	0.42
1:E:48[B]:SER:HA	4:E:303:AGS:S1G	2.60	0.42
1:B:56[B]:SER:HB3	1:B:143:SER:HB3	2.00	0.42
1:C:50:THR:HG22	1:C:209:ASN:HB2	2.00	0.42
1:E:123:LEU:HD11	1:E:166:ARG:NH2	2.35	0.42
1:C:56[B]:SER:HB3	1:C:143:SER:HB3	2.01	0.42
1:A:16:GLN:OE1	1:F:88:ARG:HD3	2.20	0.41
1:D:27:GLY:O	1:D:31[B]:ILE:HG12	2.19	0.41
1:E:123:LEU:HD12	1:E:124:SER:HA	2.02	0.41
1:F:131:ASN:O	1:F:135:GLN:HG2	2.20	0.41
1:E:48[A]:SER:HA	4:E:303:AGS:S1G	2.60	0.41
1:B:76:PHE:O	1:B:110:PRO:HD3	2.20	0.41
1:B:31[B]:ILE:HG23	1:B:231[B]:MET:HB2	2.02	0.41
1:A:136:LYS:NZ	5:A:509:HOH:O	2.54	0.41
1:A:191:ILE:HB	1:A:198:GLU:HB3	2.03	0.41
1:E:127:ILE:HD12	1:E:170:ARG:HD2	2.03	0.41
1:C:85:LYS:HE3	1:D:40:ARG:HH21	1.84	0.41
1:C:123:LEU:HA	1:C:123:LEU:HD12	1.77	0.41
1:A:57:ILE:HD11	1:A:83:ILE:HG23	2.02	0.40
1:A:191:ILE:HD12	1:A:206:ILE:HD11	2.02	0.40
1:C:56[A]:SER:HB2	1:C:143:SER:HB3	2.02	0.40
1:A:137:TYR:O	1:A:138:ARG:HB2	2.21	0.40
1:A:219:THR:HB	1:A:234:GLU:HB3	2.03	0.40
1:B:31[A]:ILE:HD13	1:B:31[A]:ILE:HG21	1.87	0.40
1:F:102:LYS:HA	1:F:102:LYS:HD3	1.96	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	214/253 (85%)	210 (98%)	4 (2%)	0	100	100
1	B	214/253 (85%)	208 (97%)	6 (3%)	0	100	100
1	C	220/253 (87%)	214 (97%)	6 (3%)	0	100	100
1	D	215/253 (85%)	211 (98%)	4 (2%)	0	100	100
1	E	214/253 (85%)	211 (99%)	3 (1%)	0	100	100
1	F	212/253 (84%)	208 (98%)	4 (2%)	0	100	100
All	All	1289/1518 (85%)	1262 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/217 (88%)	190 (100%)	0	100	100
1	B	191/217 (88%)	190 (100%)	1 (0%)	81	77
1	C	195/217 (90%)	193 (99%)	2 (1%)	68	60
1	D	191/217 (88%)	189 (99%)	2 (1%)	68	60
1	E	190/217 (88%)	186 (98%)	4 (2%)	47	33
1	F	189/217 (87%)	182 (96%)	7 (4%)	30	15
All	All	1146/1302 (88%)	1130 (99%)	16 (1%)	59	49

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

Mol	Chain	Res	Type
1	B	21	MET
1	C	81	GLN
1	C	193	ARG
1	D	162	ARG
1	D	228	THR
1	E	16	GLN
1	E	138	ARG

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Mol	Chain	Res	Type
1	E	210	VAL
1	E	212	GLU
1	F	21	MET
1	F	66	GLU
1	F	81	GLN
1	F	122	ASP
1	F	123	LEU
1	F	164	LEU
1	F	191	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	135	GLN
1	C	131	ASN
1	D	131	ASN
1	D	242	HIS
1	F	81	GLN

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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	AGS	D	303	2	32,33,33	0.78	1 (3%)	45,52,52	0.70	1 (2%)
4	AGS	C	303	2	32,33,33	1.07	2 (6%)	45,52,52	0.84	2 (4%)
4	AGS	B	303	2	32,33,33	1.09	3 (9%)	45,52,52	0.81	2 (4%)
4	AGS	E	303	2	32,33,33	0.70	1 (3%)	45,52,52	1.02	2 (4%)
4	AGS	F	301	2	32,33,33	1.26	2 (6%)	45,52,52	0.95	1 (2%)
4	AGS	A	303	2	32,33,33	0.76	2 (6%)	45,52,52	0.68	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AGS	D	303	2	-	5/21/38/38	0/3/3/3
4	AGS	C	303	2	-	4/21/38/38	0/3/3/3
4	AGS	B	303	2	-	4/21/38/38	0/3/3/3
4	AGS	E	303	2	-	5/21/38/38	0/3/3/3
4	AGS	F	301	2	-	5/21/38/38	0/3/3/3
4	AGS	A	303	2	-	6/21/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	301	AGS	PB-O3A	4.58	1.64	1.59
4	C	303	AGS	PB-O3A	4.25	1.64	1.59
4	F	301	AGS	PA-O3A	-4.19	1.55	1.59
4	C	303	AGS	PG-S1G	3.38	1.98	1.90
4	B	303	AGS	PB-O3A	3.20	1.63	1.59
4	D	303	AGS	PG-S1G	3.12	1.97	1.90
4	B	303	AGS	PB-O3B	3.02	1.62	1.59
4	A	303	AGS	PG-S1G	2.86	1.96	1.90
4	A	303	AGS	PA-O3A	-2.61	1.56	1.59
4	E	303	AGS	O5'-C5'	-2.51	1.35	1.44
4	B	303	AGS	PG-S1G	2.27	1.95	1.90

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	303	AGS	O2G-PG-O3B	4.08	118.26	104.64
4	F	301	AGS	O2G-PG-O3B	3.88	117.61	104.64
4	C	303	AGS	O2G-PG-O3B	3.10	114.98	104.64
4	D	303	AGS	O2G-PG-O3B	3.00	114.65	104.64
4	B	303	AGS	O2G-PG-O3B	2.72	113.71	104.64
4	E	303	AGS	O3A-PB-O1B	-2.27	103.86	110.70
4	B	303	AGS	O3A-PB-O1B	-2.22	104.03	110.70
4	A	303	AGS	O2G-PG-O3B	2.22	112.04	104.64
4	C	303	AGS	O2B-PB-O3B	2.10	112.94	107.27

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	303	AGS	C5'-O5'-PA-O2A
4	B	303	AGS	PB-O3B-PG-O2G
4	B	303	AGS	PB-O3B-PG-O3G
4	C	303	AGS	PB-O3B-PG-O2G
4	C	303	AGS	PB-O3B-PG-O3G
4	D	303	AGS	PB-O3B-PG-O2G
4	D	303	AGS	PB-O3B-PG-O3G
4	D	303	AGS	C5'-O5'-PA-O2A
4	E	303	AGS	PB-O3B-PG-O2G
4	E	303	AGS	PB-O3B-PG-O3G
4	F	301	AGS	PB-O3B-PG-O2G
4	F	301	AGS	PB-O3B-PG-O3G
4	B	303	AGS	PA-O3A-PB-O1B
4	C	303	AGS	PA-O3A-PB-O1B
4	D	303	AGS	PA-O3A-PB-O1B
4	F	301	AGS	PA-O3A-PB-O2B
4	A	303	AGS	C5'-O5'-PA-O3A
4	B	303	AGS	PA-O3A-PB-O2B
4	E	303	AGS	PA-O3A-PB-O2B
4	D	303	AGS	PG-O3B-PB-O2B
4	F	301	AGS	PG-O3B-PB-O2B
4	A	303	AGS	PA-O3A-PB-O1B
4	E	303	AGS	PA-O3A-PB-O1B
4	A	303	AGS	PB-O3B-PG-O2G
4	A	303	AGS	PB-O3B-PG-O3G
4	E	303	AGS	PG-O3B-PB-O1B
4	A	303	AGS	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
4	C	303	AGS	PA-O3A-PB-O2B
4	F	301	AGS	PA-O3A-PB-O1B

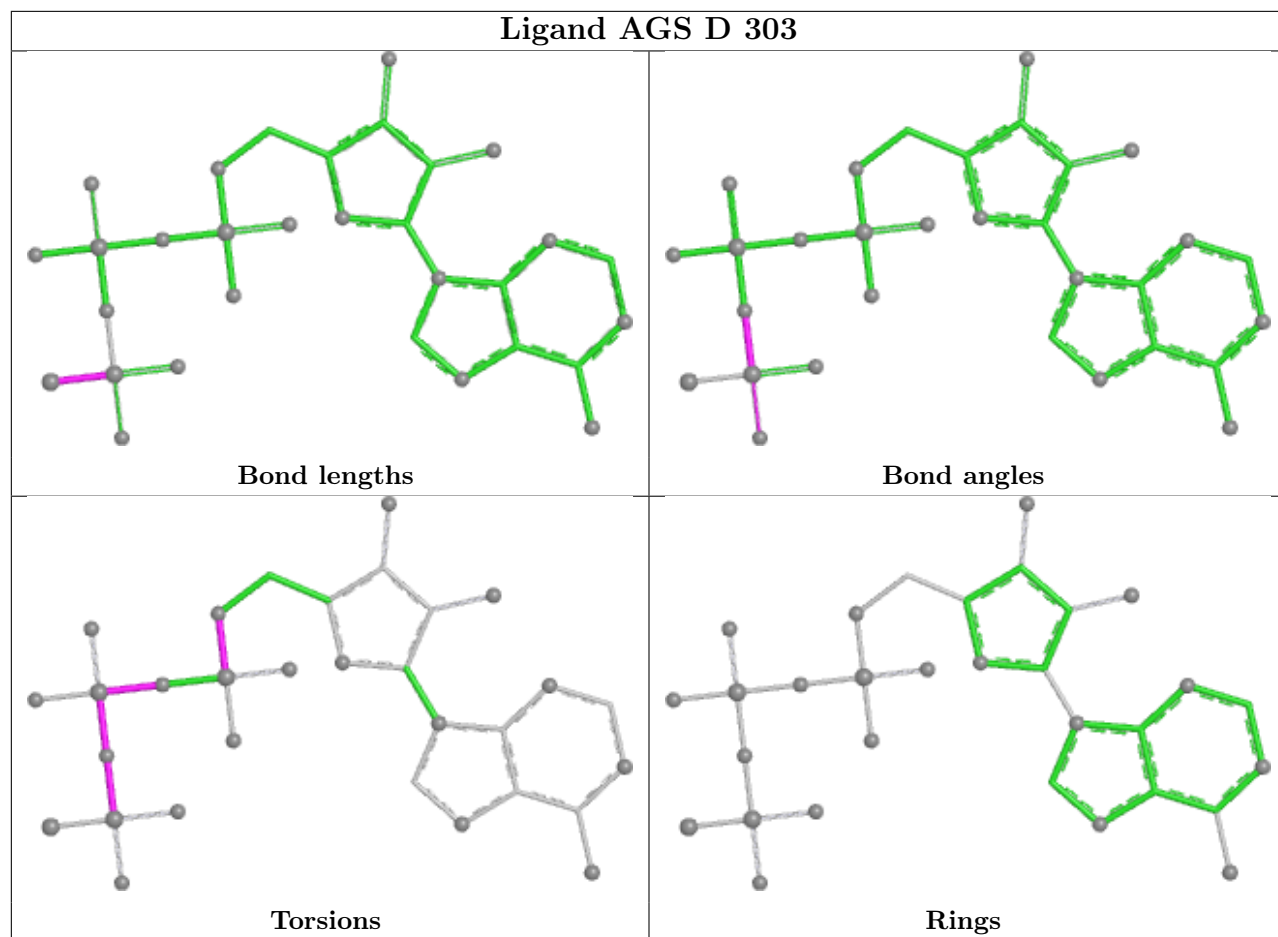
There are no ring outliers.

1 monomer is involved in 2 short contacts:

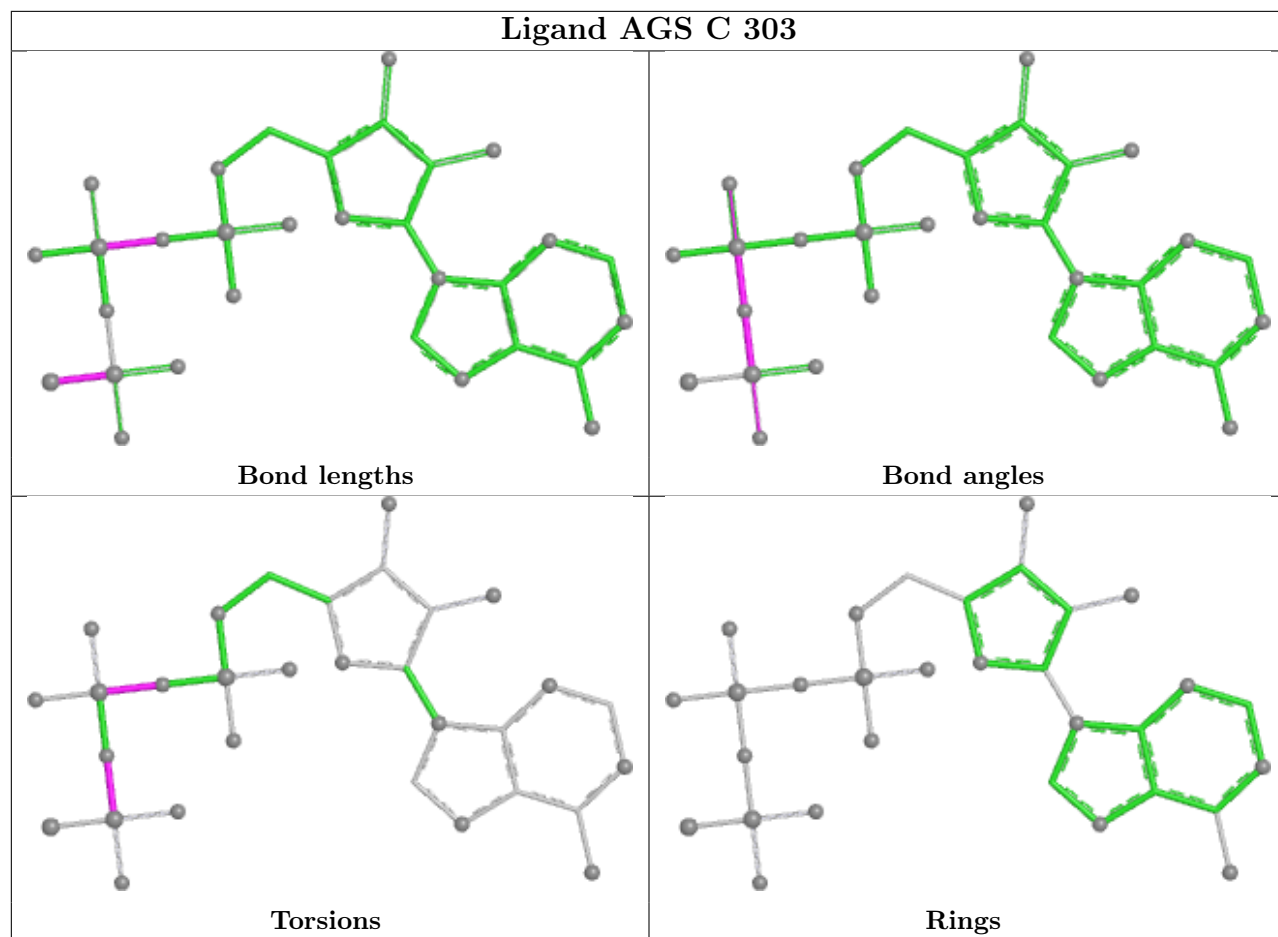
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	303	AGS	2	0

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.

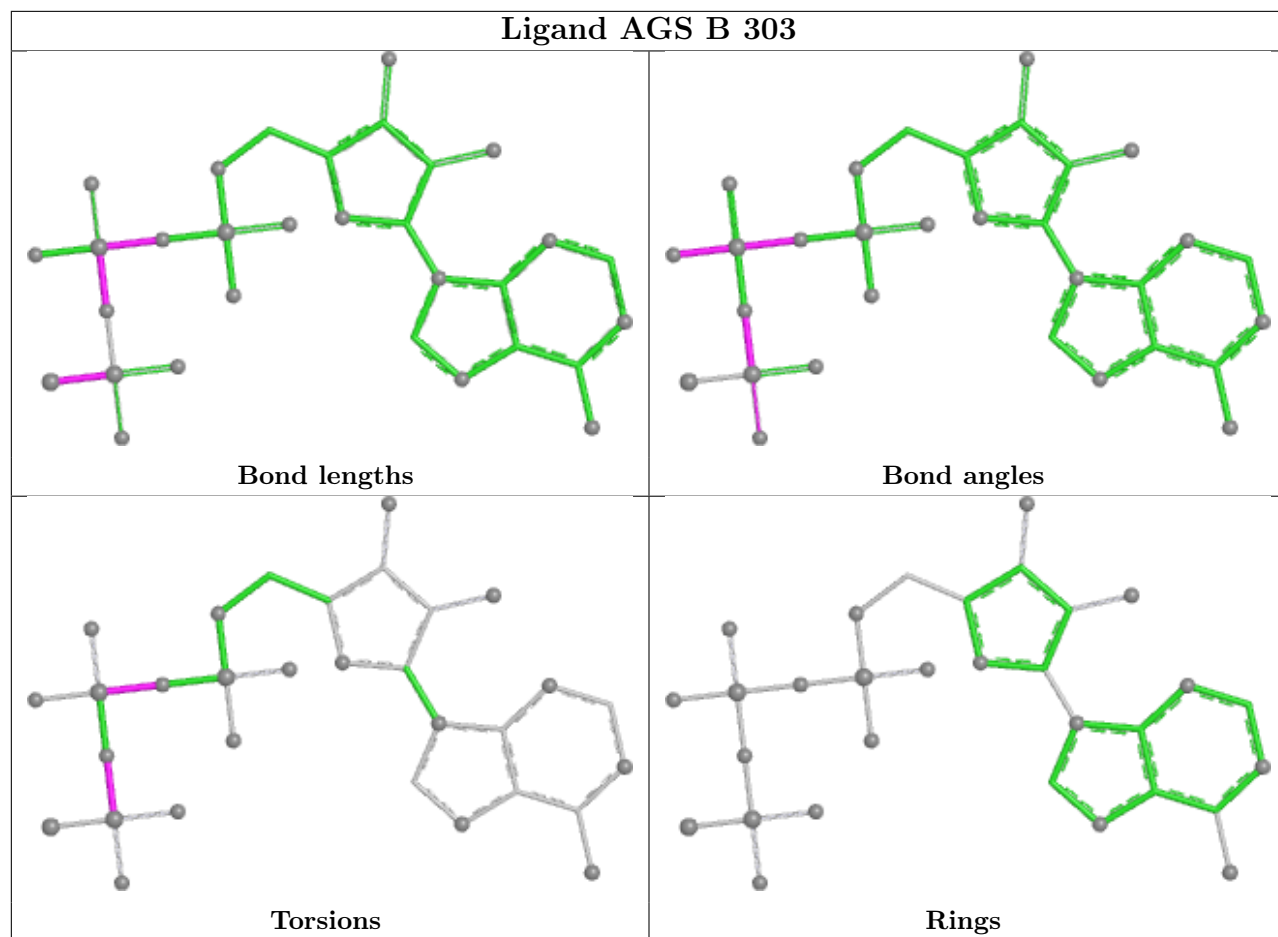
Ligand AGS D 303



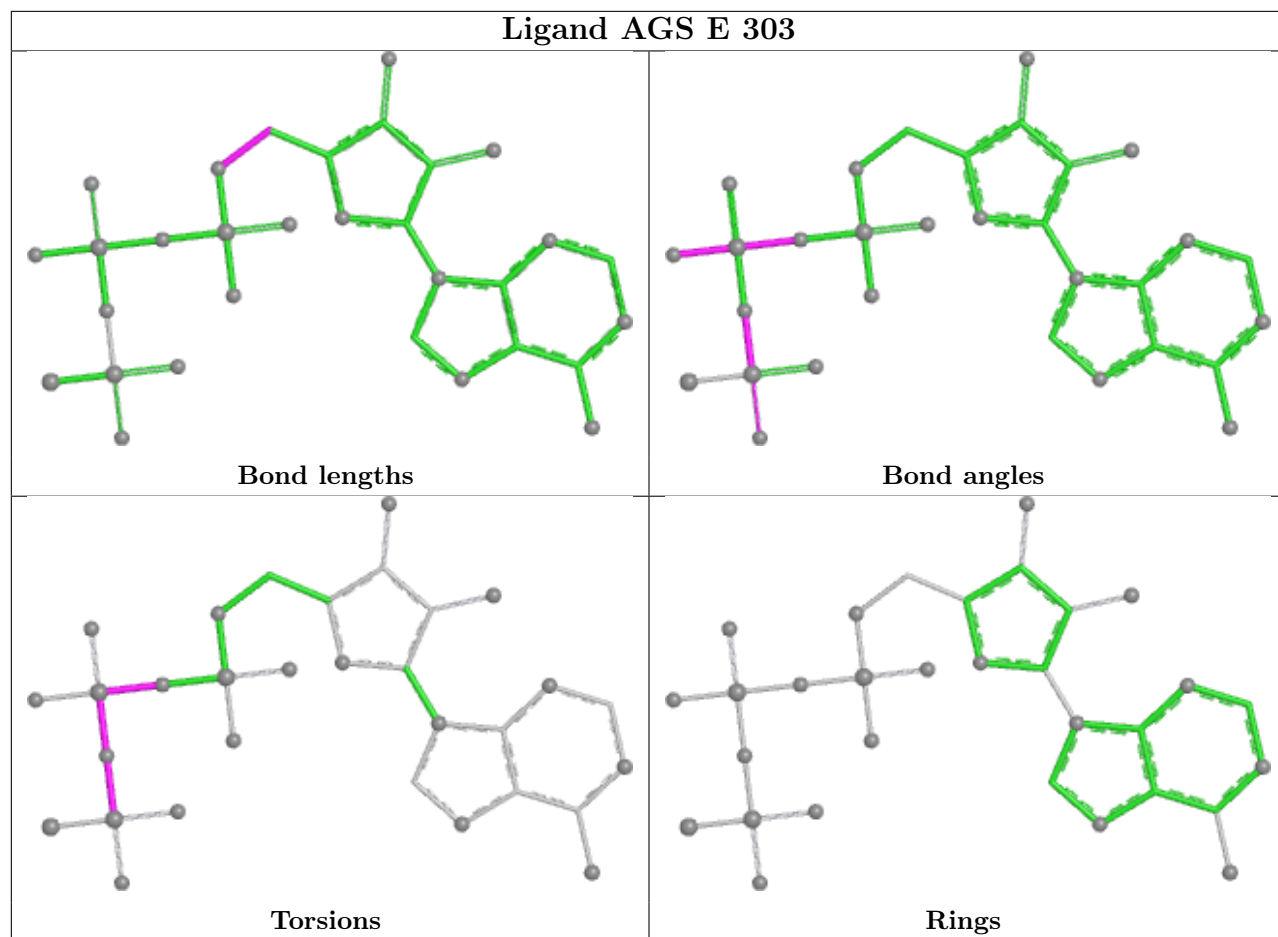
Ligand AGS C 303



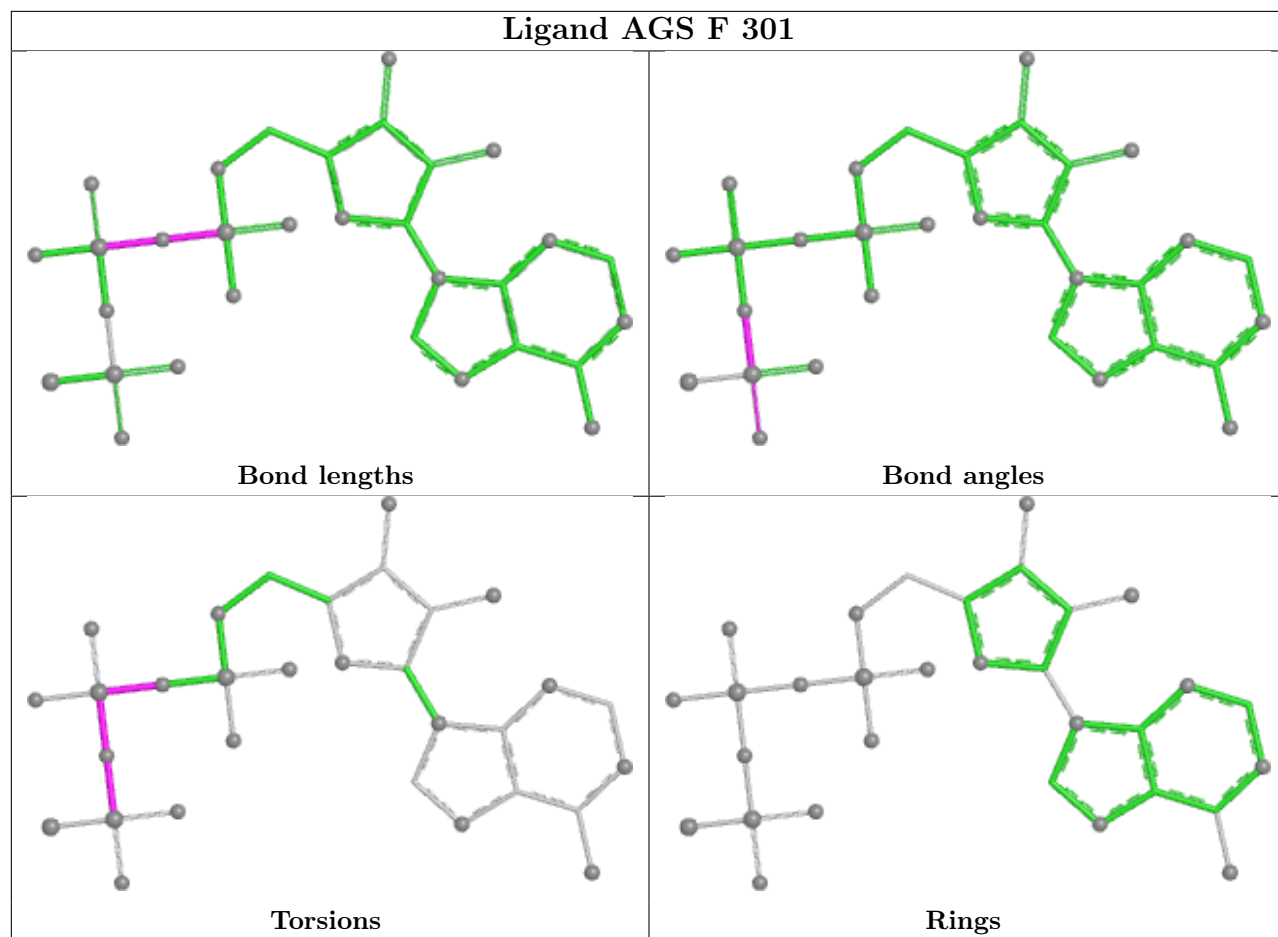
Ligand AGS B 303

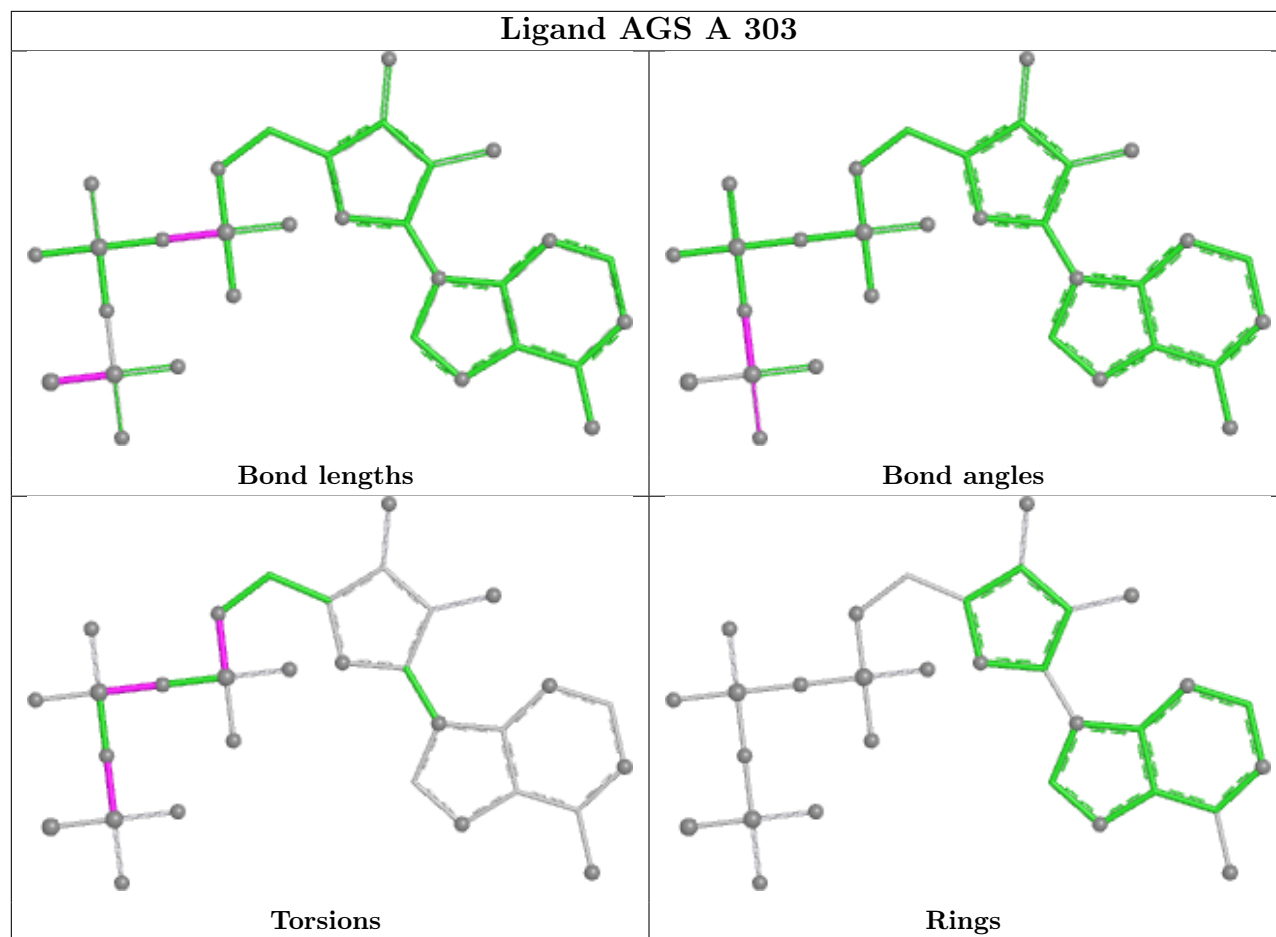


Ligand AGS E 303



Ligand AGS F 301





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	215/253 (84%)	0.67	28 (13%) 7 7	13, 35, 68, 94	6 (2%)
1	B	215/253 (84%)	0.24	12 (5%) 30 33	11, 26, 52, 88	6 (2%)
1	C	221/253 (87%)	0.22	18 (8%) 18 19	9, 26, 50, 104	6 (2%)
1	D	217/253 (85%)	0.19	16 (7%) 20 22	8, 25, 52, 90	5 (2%)
1	E	216/253 (85%)	0.58	31 (14%) 6 6	10, 28, 65, 103	5 (2%)
1	F	213/253 (84%)	0.69	31 (14%) 6 5	8, 28, 59, 95	6 (2%)
All	All	1297/1518 (85%)	0.43	136 (10%) 11 11	8, 28, 60, 104	34 (2%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	123	LEU	6.5
1	E	123	LEU	6.5
1	B	248	PRO	6.0
1	F	125	ALA	5.9
1	C	250	GLY	5.8
1	E	110	PRO	5.5
1	F	17	ALA	5.4
1	A	156	ALA	4.9
1	B	156	ALA	4.9
1	E	121	PHE	4.8
1	A	248	PRO	4.8
1	D	156	ALA	4.7
1	E	249	LEU	4.7
1	F	124	SER	4.7
1	F	159	VAL	4.6
1	A	125	ALA	4.6
1	F	158	SER	4.5
1	E	125	ALA	4.5
1	C	247	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	112	PRO	4.3
1	A	109	SER	4.2
1	D	13	SER	4.2
1	A	16	GLN	4.1
1	E	132	TYR	4.1
1	E	156	ALA	4.0
1	F	146[A]	SER	4.0
1	E	120	GLY	3.9
1	E	126	LEU	3.9
1	C	248	PRO	3.9
1	F	156	ALA	3.9
1	F	126	LEU	3.9
1	D	122	ASP	3.8
1	C	157	SER	3.8
1	F	110	PRO	3.8
1	E	247	PHE	3.8
1	F	174	ILE	3.7
1	A	162	ARG	3.7
1	A	159	VAL	3.7
1	F	200	VAL	3.6
1	C	156	ALA	3.6
1	E	16	GLN	3.6
1	F	122	ASP	3.4
1	B	146[A]	SER	3.3
1	B	111	ASP	3.3
1	E	158	SER	3.3
1	A	126	LEU	3.3
1	A	110	PRO	3.2
1	C	132	TYR	3.2
1	D	110	PRO	3.2
1	D	123	LEU	3.2
1	D	146[A]	SER	3.2
1	D	169	ALA	3.2
1	C	110	PRO	3.2
1	F	128	GLU	3.1
1	E	146[A]	SER	3.1
1	F	170	ARG	3.0
1	A	123	LEU	2.9
1	A	198	GLU	2.9
1	B	135	GLN	2.9
1	B	109	SER	2.9
1	E	127	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	157	SER	2.9
1	A	122	ASP	2.9
1	F	111	ASP	2.9
1	F	127	ILE	2.9
1	A	163	GLU	2.8
1	C	113	GLU	2.8
1	F	109	SER	2.8
1	A	111	ASP	2.8
1	A	158	SER	2.8
1	E	77	GLU	2.8
1	E	124	SER	2.7
1	B	16	GLN	2.7
1	E	248	PRO	2.7
1	E	133	ALA	2.7
1	E	159	VAL	2.7
1	C	120	GLY	2.6
1	F	133	ALA	2.6
1	F	169	ALA	2.6
1	B	122	ASP	2.6
1	E	122	ASP	2.6
1	B	123	LEU	2.6
1	E	157	SER	2.6
1	C	249	LEU	2.6
1	F	89	SER	2.6
1	A	170	ARG	2.6
1	F	164	LEU	2.6
1	A	174	ILE	2.6
1	E	128	GLU	2.6
1	F	247	PHE	2.5
1	E	212	GLU	2.5
1	D	111	ASP	2.5
1	A	132	TYR	2.4
1	A	165	PHE	2.4
1	C	121	PHE	2.4
1	A	68	ASP	2.4
1	D	157	SER	2.3
1	F	173	GLN	2.3
1	A	242	HIS	2.3
1	A	18	ILE	2.3
1	C	162	ARG	2.3
1	A	164	LEU	2.3
1	B	17	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	110	PRO	2.3
1	E	109	SER	2.3
1	E	135	GLN	2.3
1	C	170	ARG	2.2
1	F	88	ARG	2.2
1	C	112	PRO	2.2
1	F	168	VAL	2.2
1	F	172	LYS	2.2
1	F	99	ASP	2.2
1	C	146[A]	SER	2.2
1	D	158	SER	2.2
1	E	245	ASN	2.2
1	C	122	ASP	2.2
1	D	164	LEU	2.2
1	A	15	HIS	2.1
1	C	245	ASN	2.1
1	D	26	GLU	2.1
1	E	173	GLN	2.1
1	C	99	ASP	2.1
1	E	76	PHE	2.1
1	E	134	ILE	2.1
1	A	146[A]	SER	2.1
1	D	159	VAL	2.1
1	F	131	ASN	2.1
1	A	127	ILE	2.1
1	A	168	VAL	2.1
1	D	160	VAL	2.1
1	A	138	ARG	2.0
1	D	162	ARG	2.0
1	E	169	ALA	2.0
1	D	124	SER	2.0
1	F	242	HIS	2.0
1	E	137	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

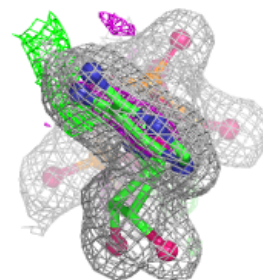
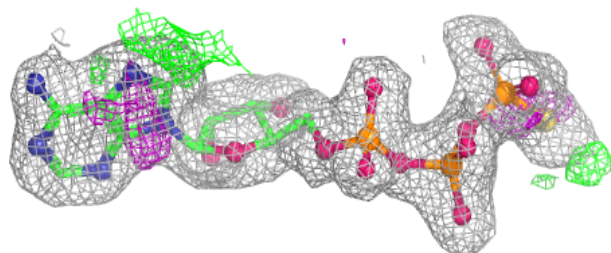
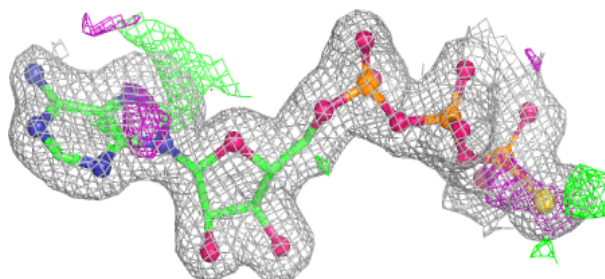
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	AGS	E	303	31/31	0.97	0.07	13,18,26,32	0
4	AGS	B	303	31/31	0.98	0.05	15,18,25,26	0
4	AGS	C	303	31/31	0.98	0.05	14,18,23,25	0
4	AGS	A	303	31/31	0.98	0.06	19,24,29,32	0
4	AGS	F	301	31/31	0.98	0.05	15,20,29,30	0
2	MG	F	302	1/1	0.99	0.02	20,20,20,20	0
3	CL	B	302	1/1	0.99	0.06	24,24,24,24	0
3	CL	E	302	1/1	0.99	0.09	22,22,22,22	0
3	CL	F	303	1/1	0.99	0.04	19,19,19,19	0
2	MG	A	301	1/1	0.99	0.04	25,25,25,25	0
2	MG	B	301	1/1	0.99	0.02	17,17,17,17	0
2	MG	C	301	1/1	0.99	0.05	19,19,19,19	0
4	AGS	D	303	31/31	0.99	0.04	14,17,24,26	0
2	MG	D	301	1/1	0.99	0.03	18,18,18,18	0
2	MG	E	301	1/1	0.99	0.07	19,19,19,19	0
3	CL	D	302	1/1	1.00	0.02	17,17,17,17	0
3	CL	A	302	1/1	1.00	0.03	25,25,25,25	0
3	CL	C	302	1/1	1.00	0.03	20,20,20,20	0

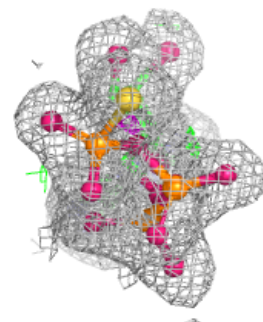
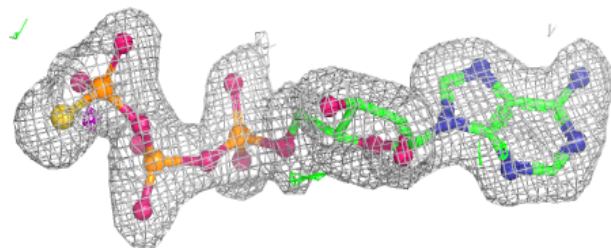
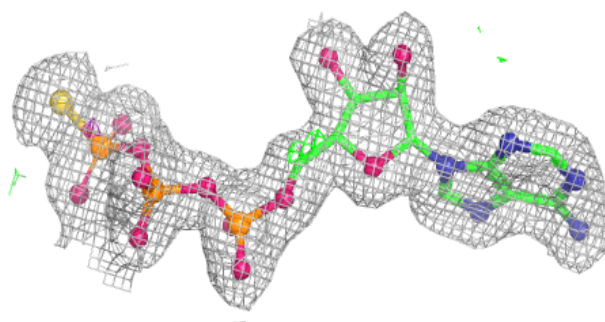
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AGS E 303:

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

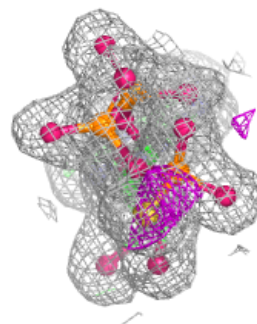
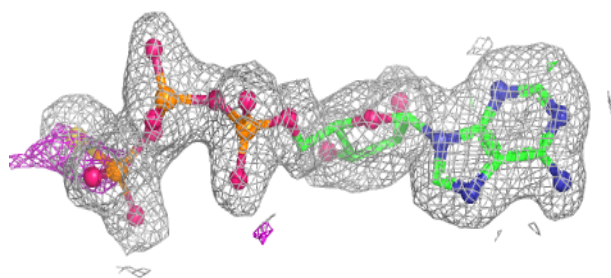
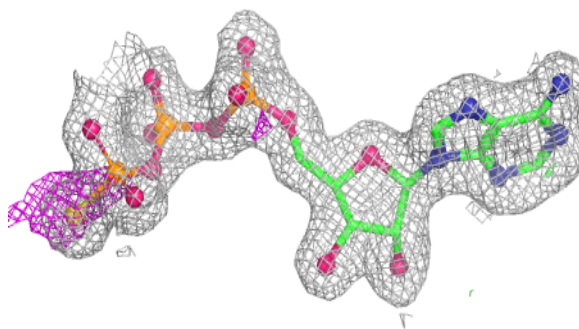
**Electron density around AGS B 303:**

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

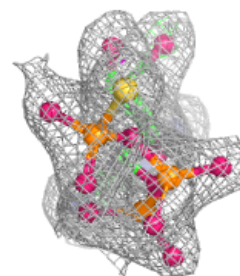
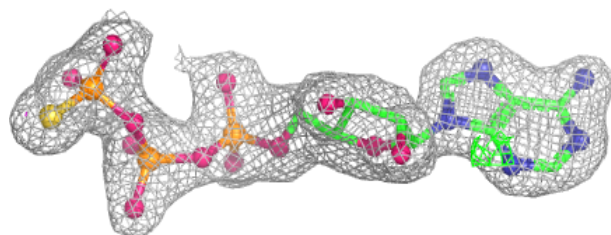
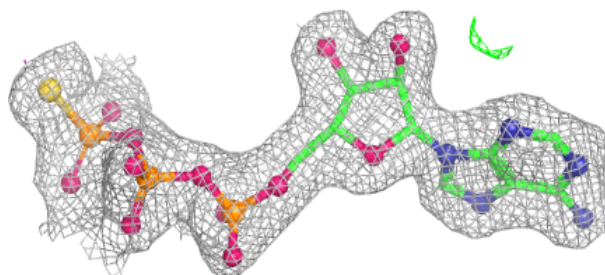


Electron density around AGS C 303:

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

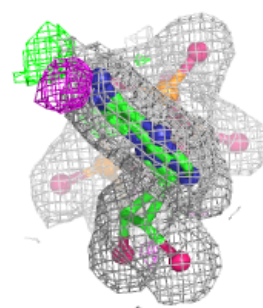
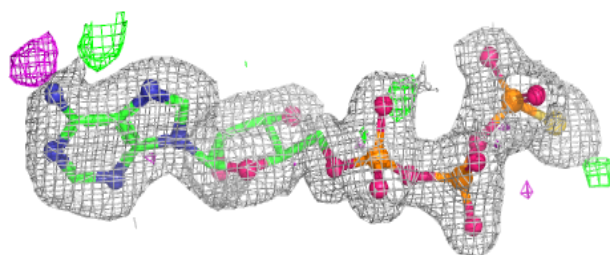
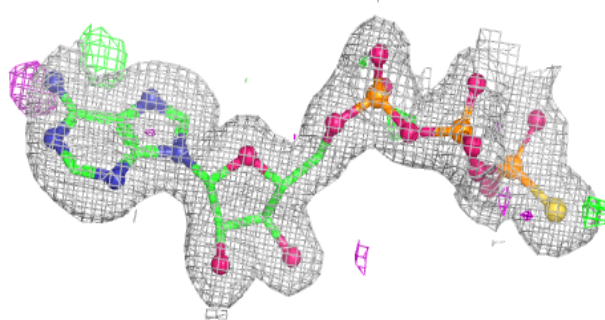
**Electron density around AGS A 303:**

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

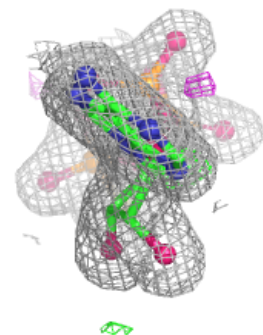
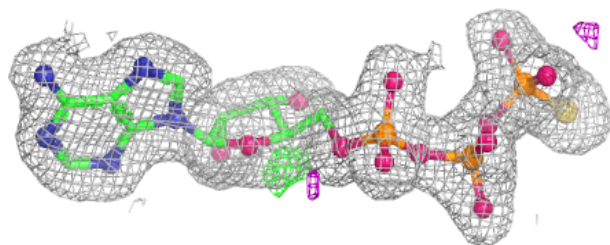
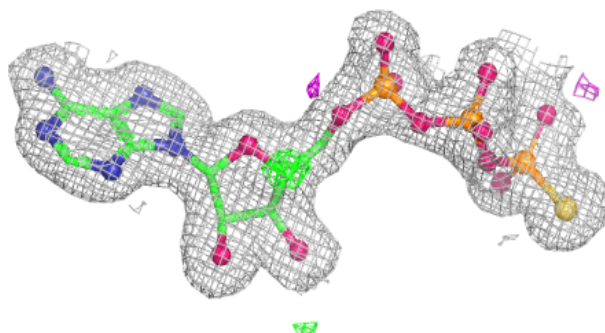


Electron density around AGS F 301:

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

**Electron density around AGS D 303:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.