



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:00 PM UTC

PDB ID : 7EJW / pdb_00007ejw
Title : Crystal structure of FleN in complex with FleQ AAA+ domain
Authors : Chanchal; Banerjee, P.; Raghav, S.; Jain, D.
Deposited on : 2021-04-02
Resolution : 1.98 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

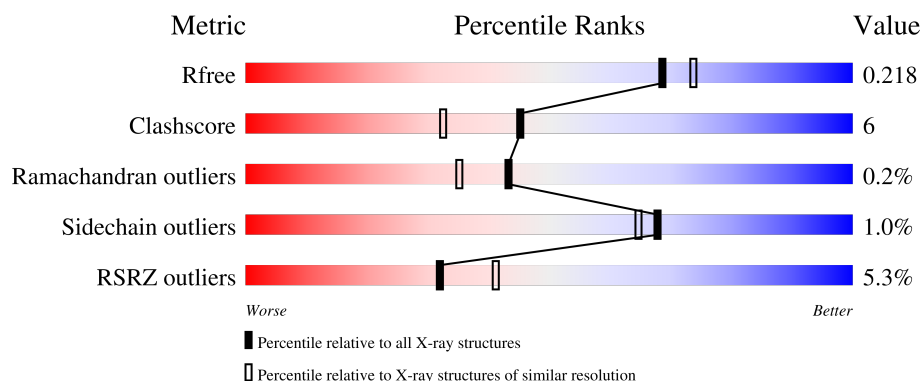
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	285	
1	B	285	
2	C	259	
2	D	259	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9213 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 Transcriptional antiactivator FleN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2065	1309	370	378	8			
1	B	265	Total	C	N	O	S	0	1	0
			2015	1278	361	369	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP G3XD64
A	-3	PRO	-	expression tag	UNP G3XD64
A	-2	LEU	-	expression tag	UNP G3XD64
A	-1	GLY	-	expression tag	UNP G3XD64
A	0	SER	-	expression tag	UNP G3XD64
B	-4	GLY	-	expression tag	UNP G3XD64
B	-3	PRO	-	expression tag	UNP G3XD64
B	-2	LEU	-	expression tag	UNP G3XD64
B	-1	GLY	-	expression tag	UNP G3XD64
B	0	SER	-	expression tag	UNP G3XD64

- Molecule 2 is a protein called Transcriptional regulator FleQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	252	Total	C	N	O	S	0	0	0
			1995	1256	367	361	11			
2	D	254	Total	C	N	O	S	0	0	0
			2011	1264	369	367	11			

There are 10 discrepancies between the modelled and reference sequences:

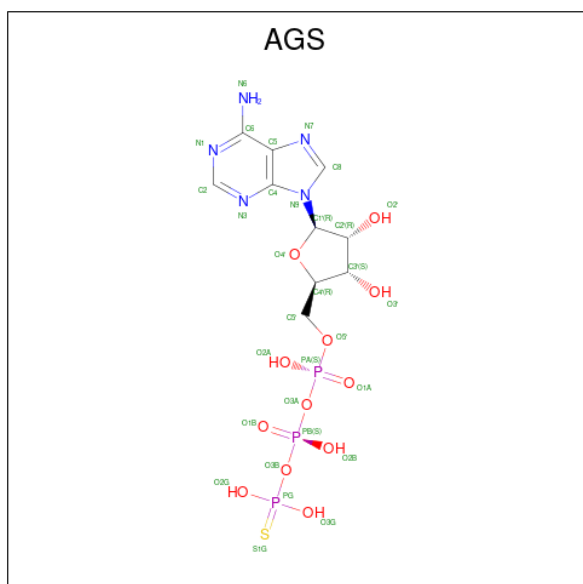
Chain	Residue	Modelled	Actual	Comment	Reference
C	137	GLY	-	expression tag	UNP G3XCV0
C	138	PRO	-	expression tag	UNP G3XCV0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	139	LEU	-	expression tag	UNP G3XCV0
C	140	GLY	-	expression tag	UNP G3XCV0
C	141	SER	-	expression tag	UNP G3XCV0
D	137	GLY	-	expression tag	UNP G3XCV0
D	138	PRO	-	expression tag	UNP G3XCV0
D	139	LEU	-	expression tag	UNP G3XCV0
D	140	GLY	-	expression tag	UNP G3XCV0
D	141	SER	-	expression tag	UNP G3XCV0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

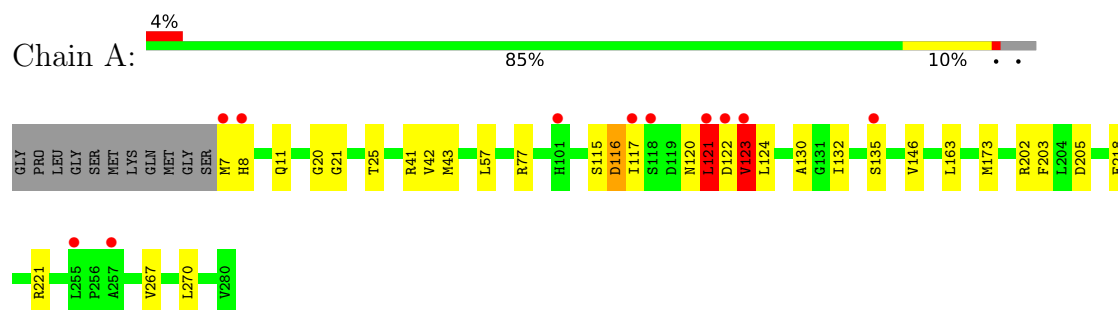
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	276	Total	O	0	0
			276	276		
6	B	323	Total	O	0	0
			323	323		
6	C	199	Total	O	0	0
			199	199		
6	D	257	Total	O	0	0
			257	257		

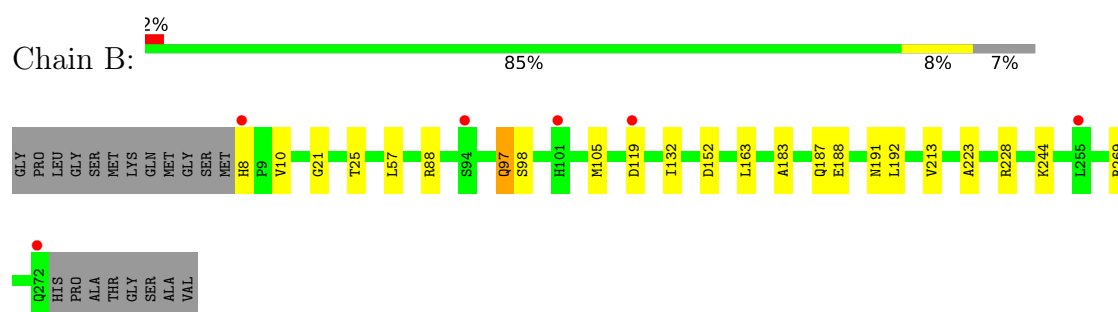
3 Residue-property plots

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.

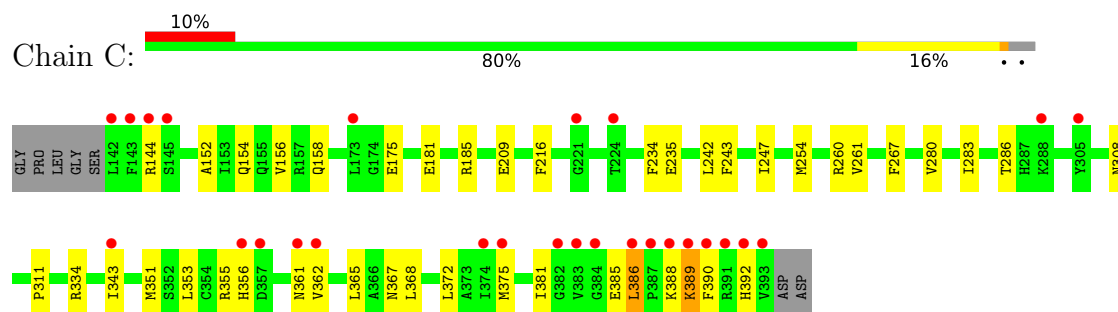
• Molecule 1: Transcriptional antiactivator FleN



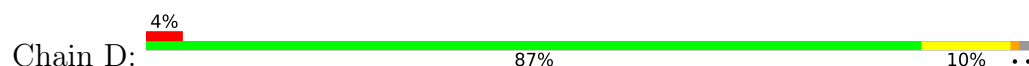
• Molecule 1: Transcriptional antiactivator FleN

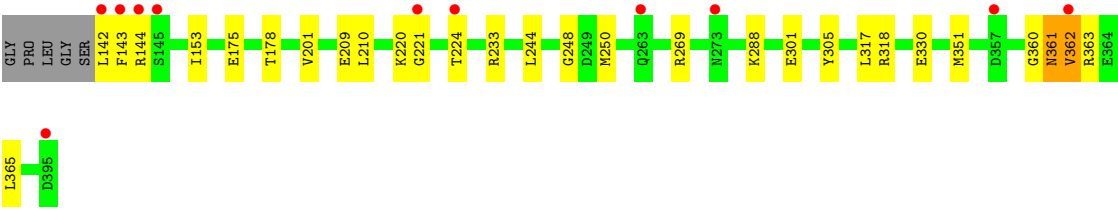


• Molecule 2: Transcriptional regulator FleQ



• Molecule 2: Transcriptional regulator FleQ





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.22Å 153.93Å 64.57Å 90.00° 95.03° 90.00°	Depositor
Resolution (Å)	64.32 – 1.98 64.32 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.4 (64.32-1.98) 99.5 (64.32-1.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.179 , 0.218 0.180 , 0.218	Depositor DCC
R_{free} test set	4363 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9213	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: AGS, GOL, MG

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	0.45	0/2099	0.66	4/2853 (0.1%)
1	B	0.37	0/2047	0.55	0/2781
2	C	0.31	0/2029	0.53	0/2733
2	D	0.39	2/2045 (0.1%)	0.63	6/2755 (0.2%)
All	All	0.38	2/8220 (0.0%)	0.60	10/11122 (0.1%)

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	A	0	1
2	C	0	1
2	D	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	361	ASN	C-O	-5.93	1.19	1.24
2	D	361	ASN	C-N	-5.52	1.26	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	361	ASN	CA-C-N	-8.76	108.68	121.65
2	D	361	ASN	C-N-CA	-8.76	108.68	121.65
2	D	362	VAL	N-CA-C	-8.71	103.35	111.45
2	D	361	ASN	N-CA-C	6.86	120.13	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	LEU	CA-CB-CG	6.09	137.61	116.30
1	A	123	VAL	CA-C-N	-5.89	114.74	123.11
1	A	123	VAL	C-N-CA	-5.89	114.74	123.11
1	A	123	VAL	CA-CB-CG2	-5.53	101.00	110.40
2	D	220	LYS	CA-C-N	-5.09	107.70	122.46
2	D	220	LYS	C-N-CA	-5.09	107.70	122.46

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	VAL	Peptide
2	C	386	LEU	Peptide
2	D	221	GLY	Peptide
2	D	360	GLY	Mainchain

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	2065	0	2129	32	0
1	B	2015	0	2079	18	0
2	C	1995	0	2027	29	0
2	D	2011	0	2035	18	0
3	A	31	0	12	2	0
3	B	31	0	12	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	B	6	0	8	2	0
6	A	276	0	0	1	0
6	B	323	0	0	4	0
6	C	199	0	0	1	1
6	D	257	0	0	4	1
All	All	9213	0	8302	97	1

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 6.

All (97) 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:41:ARG:O	1:A:123:VAL:HG21	1.59	1.03
1:A:11:GLN:HB3	1:A:122:ASP:HA	1.46	0.97
3:B:302:AGS:S1G	6:B:458:HOH:O	2.34	0.86
1:A:42:VAL:HA	1:A:123:VAL:HB	1.59	0.84
1:A:121:LEU:C	1:A:123:VAL:HG22	2.06	0.81
1:A:41:ARG:HH21	1:A:121:LEU:HG	1.48	0.78
1:A:43:MET:HE1	1:A:117:ILE:HG21	1.69	0.72
1:A:130:ALA:HB2	3:A:501:AGS:S1G	2.30	0.71
2:D:201:VAL:HG22	2:D:233:ARG:HD2	1.73	0.71
2:D:362:VAL:O	2:D:365:LEU:N	2.24	0.70
2:D:142:LEU:N	6:D:403:HOH:O	2.24	0.69
1:A:11:GLN:CB	1:A:122:ASP:HA	2.20	0.68
1:B:97[A]:GLN:NE2	6:B:401:HOH:O	2.24	0.66
1:A:11:GLN:HB3	1:A:122:ASP:CA	2.24	0.64
1:A:42:VAL:HA	1:A:123:VAL:CB	2.26	0.64
1:A:20:GLY:HA2	3:A:501:AGS:S1G	2.38	0.63
1:B:10:VAL:HG23	1:B:269:ARG:HE	1.64	0.63
2:C:385:GLU:OE1	2:C:385:GLU:N	2.32	0.61
2:D:244:LEU:HD21	2:D:250:MET:HE1	1.82	0.61
1:B:8:HIS:O	1:B:269:ARG:NH2	2.33	0.61
2:C:343:ILE:HD11	2:C:381:ILE:HD11	1.83	0.60
2:C:353:LEU:HD21	2:C:386:LEU:HD11	1.84	0.60
2:C:216:PHE:CE2	2:C:254:MET:HE1	2.38	0.58
1:A:42:VAL:HG22	1:A:123:VAL:HG11	1.86	0.57
2:D:317:LEU:H	2:D:361:ASN:HD22	1.51	0.57
1:A:123:VAL:HG23	1:A:123:VAL:O	2.04	0.57
2:D:209:GLU:HG3	2:D:210:LEU:HD13	1.88	0.56
2:C:368:LEU:O	2:C:372:LEU:HG	2.06	0.55
2:C:356:HIS:CD2	2:C:389:LYS:O	2.60	0.55
1:B:88:ARG:HG2	5:B:301:GOL:H32	1.88	0.54
5:B:301:GOL:H2	6:B:499:HOH:O	2.08	0.52
1:B:97[A]:GLN:H	1:B:97[A]:GLN:CD	2.18	0.51
1:B:187:GLN:NE2	1:B:191:ASN:OD1	2.43	0.51
2:D:351:MET:HG3	6:D:588:HOH:O	2.11	0.51
2:D:362:VAL:O	2:D:363:ARG:C	2.54	0.51
1:A:218:GLU:OE2	1:A:221:ARG:HD3	2.11	0.50
2:C:235:GLU:HG3	2:C:267:PHE:HZ	1.76	0.50
2:C:260:ARG:HD3	6:C:537:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:144:ARG:HD2	2:C:334:ARG:CZ	2.41	0.50
1:B:132:ILE:HG22	1:B:163:LEU:HD13	1.93	0.49
1:A:21:GLY:HA3	1:B:21:GLY:HA3	1.94	0.49
1:B:152:ASP:HA	1:B:192:LEU:HD13	1.94	0.49
2:D:144:ARG:HD3	2:D:330:GLU:OE2	2.14	0.48
2:D:317:LEU:H	2:D:361:ASN:ND2	2.10	0.48
2:C:154:GLN:O	2:C:158:GLN:HG3	2.14	0.48
1:B:269:ARG:NH2	6:B:413:HOH:O	2.47	0.47
2:C:216:PHE:CE1	2:C:261:VAL:HG21	2.49	0.47
2:C:247:ILE:HG22	2:C:286:THR:HB	1.97	0.47
2:D:248:GLY:HA3	2:D:288:LYS:HD2	1.98	0.46
1:A:7:MET:HB3	1:A:8:HIS:H	1.64	0.46
1:A:42:VAL:HG22	1:A:123:VAL:CG1	2.45	0.45
1:A:116:ASP:C	1:A:117:ILE:HD13	2.40	0.45
1:B:25:THR:HG22	1:B:57:LEU:HD12	1.98	0.45
1:A:42:VAL:HA	1:A:123:VAL:CG1	2.46	0.45
1:A:146:VAL:HG21	1:A:173:MET:HE1	1.98	0.45
1:A:120:ASN:HB2	1:A:123:VAL:HG23	1.97	0.45
1:A:25:THR:HG22	1:A:57:LEU:HD12	1.98	0.44
1:B:183:ALA:HA	1:B:188:GLU:OE1	2.18	0.44
1:B:244:LYS:HB3	1:B:244:LYS:HE2	1.79	0.44
2:D:269:ARG:NH2	6:D:417:HOH:O	2.41	0.44
1:B:183:ALA:HB3	1:B:213:VAL:HG21	1.98	0.44
2:D:209:GLU:HG2	6:D:526:HOH:O	2.17	0.44
1:A:122:ASP:C	1:A:123:VAL:HG13	2.43	0.44
2:C:152:ALA:O	2:C:156:VAL:HG23	2.18	0.44
2:C:386:LEU:HG	2:C:390:PHE:HB2	2.00	0.43
1:A:202:ARG:HG2	1:A:203:PHE:CE2	2.53	0.43
1:B:223:ALA:HB1	1:B:228:ARG:O	2.19	0.43
1:B:97[A]:GLN:CD	1:B:97[A]:GLN:N	2.75	0.43
2:C:361:ASN:HB3	2:C:362:VAL:H	1.64	0.43
2:C:209:GLU:H	2:C:209:GLU:CD	2.27	0.43
2:D:209:GLU:HG3	2:D:210:LEU:CD1	2.49	0.43
1:A:120:ASN:HB2	1:A:123:VAL:CG2	2.49	0.43
6:A:744:HOH:O	2:C:367:ASN:HB3	2.17	0.42
2:C:362:VAL:O	2:C:365:LEU:N	2.53	0.42
2:C:308:ASN:OD1	2:C:311:PRO:HB3	2.17	0.42
2:C:175:GLU:HB2	2:C:361:ASN:HD21	1.83	0.42
1:A:132:ILE:HG22	1:A:163:LEU:HD13	2.01	0.42
1:B:269:ARG:HG2	1:B:269:ARG:HH11	1.84	0.42
2:C:351:MET:HE3	2:C:355:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:375:MET:HE3	2:C:375:MET:HB2	1.91	0.42
1:A:7:MET:HE3	1:A:8:HIS:ND1	2.35	0.41
2:C:242:LEU:HB2	2:C:280:VAL:HG21	2.02	0.41
2:D:153:ILE:HD12	2:D:153:ILE:HA	1.85	0.41
1:A:267:VAL:HA	1:A:270:LEU:HD12	2.03	0.41
2:C:181:GLU:O	2:C:185:ARG:HG3	2.20	0.41
2:C:234:PHE:CD1	2:C:280:VAL:HG11	2.56	0.41
1:A:42:VAL:HA	1:A:123:VAL:HG11	2.03	0.41
1:B:105:MET:HE3	1:B:105:MET:HA	2.02	0.41
2:D:301:GLU:HG2	2:D:305:TYR:CE2	2.55	0.41
1:A:115:SER:C	1:A:117:ILE:H	2.29	0.41
1:A:124:LEU:HA	1:A:124:LEU:HD12	1.69	0.41
2:D:143:PHE:O	2:D:143:PHE:CG	2.74	0.41
2:C:388:LYS:HD2	2:C:389:LYS:N	2.36	0.40
2:C:355:ARG:HD2	2:C:392:HIS:CG	2.57	0.40
2:D:175:GLU:OE2	2:D:318:ARG:NH2	2.34	0.40
1:A:205:ASP:OD2	2:C:389:LYS:NZ	2.55	0.40
2:C:243:PHE:HA	2:C:283:ILE:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:697:HOH:O	6:D:538:HOH:O[1_454]	2.14	0.06

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	272/285 (95%)	264 (97%)	6 (2%)	2 (1%)	18 9
1	B	264/285 (93%)	256 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	250/259 (96%)	243 (97%)	7 (3%)	0	100	100
2	D	252/259 (97%)	246 (98%)	6 (2%)	0	100	100
All	All	1038/1088 (95%)	1009 (97%)	27 (3%)	2 (0%)	43	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	VAL
1	A	116	ASP

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	222/230 (96%)	219 (99%)	3 (1%)	59	54
1	B	217/230 (94%)	213 (98%)	4 (2%)	51	46
2	C	214/219 (98%)	213 (100%)	1 (0%)	81	79
2	D	216/219 (99%)	214 (99%)	2 (1%)	70	67
All	All	869/898 (97%)	859 (99%)	10 (1%)	68	58

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	121	LEU
1	A	135	SER
1	B	97[A]	GLN
1	B	97[B]	GLN
1	B	98	SER
1	B	119	ASP
2	C	389	LYS
2	D	178	THR
2	D	224	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	225	GLN
1	A	272	GLN
1	A	273	HIS
1	B	53	ASN
1	B	248	GLN
2	C	155	GLN
2	C	161	GLN
2	D	361	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 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
3	AGS	B	302	4	32,33,33	0.40	0	45,52,52	0.65	1 (2%)
5	GOL	B	301	-	5,5,5	0.78	0	5,5,5	1.27	0
3	AGS	A	501	4	32,33,33	0.85	1 (3%)	45,52,52	0.92	3 (6%)

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
3	AGS	B	302	4	-	0/21/38/38	0/3/3/3
5	GOL	B	301	-	-	1/4/4/4	-
3	AGS	A	501	4	-	1/21/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	AGS	PB-O3B	-4.41	1.54	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	AGS	PB-O3B-PG	-3.89	118.94	133.17
3	A	501	AGS	O2G-PG-O3B	2.65	113.47	104.64
3	B	302	AGS	PB-O3B-PG	-2.21	125.09	133.17
3	A	501	AGS	O3G-PG-O3B	2.16	111.84	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	AGS	PB-O3B-PG-O2G
5	B	301	GOL	O1-C1-C2-O2

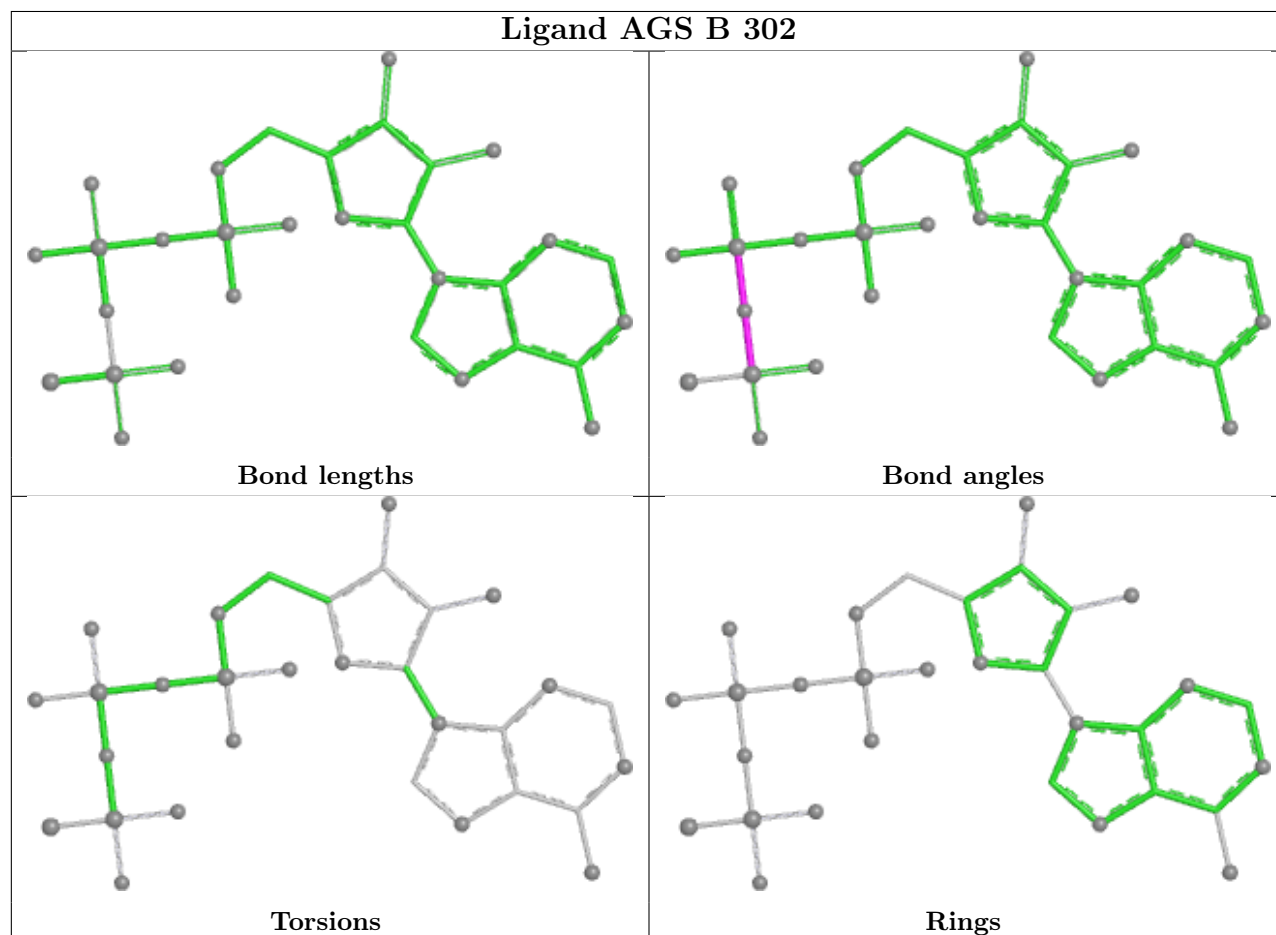
There are no ring outliers.

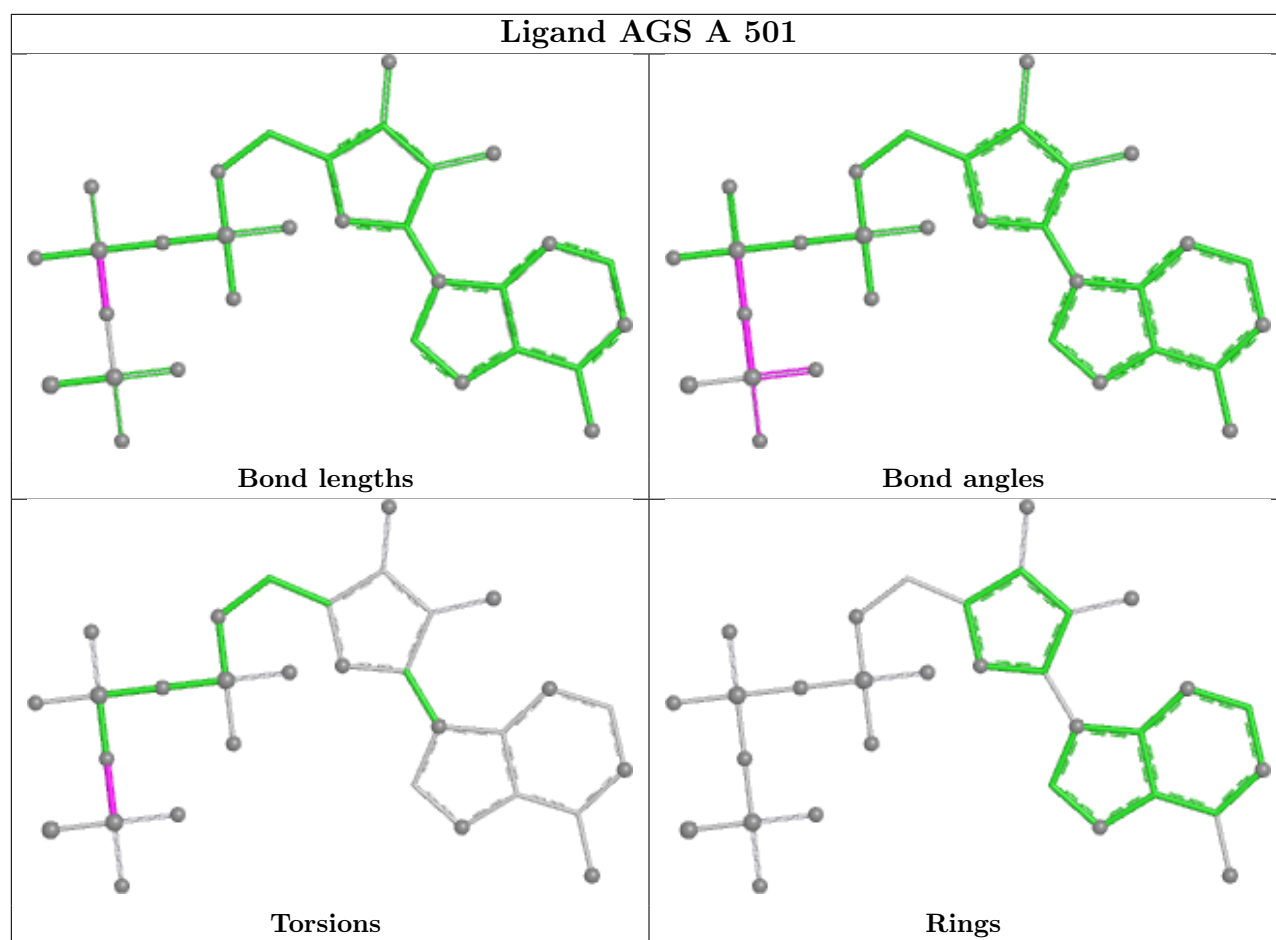
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	AGS	1	0
5	B	301	GOL	2	0
3	A	501	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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	274/285 (96%)	-0.06	11 (4%)	42	52	13, 21, 39, 78	0
1	B	265/285 (92%)	-0.25	6 (2%)	61	70	12, 20, 37, 74	1 (0%)
2	C	252/259 (97%)	0.71	27 (10%)	11	15	19, 35, 71, 115	0
2	D	254/259 (98%)	0.27	11 (4%)	40	49	18, 31, 50, 106	0
All	All	1045/1088 (96%)	0.16	55 (5%)	32	41	12, 27, 51, 115	1 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	VAL	12.8
2	D	143	PHE	8.6
1	A	122	ASP	8.2
1	A	121	LEU	8.1
2	C	142	LEU	7.6
2	C	386	LEU	7.6
2	C	143	PHE	7.0
2	D	362	VAL	6.9
2	C	387	PRO	6.8
1	A	117	ILE	6.1
2	C	392	HIS	5.5
2	C	393	VAL	5.2
1	A	118	SER	5.1
2	C	144	ARG	4.5
2	C	382	GLY	4.2
1	A	7	MET	4.2
2	C	390	PHE	4.1
2	D	221	GLY	4.1
2	C	361	ASN	4.0
2	C	145	SER	3.9
2	C	389	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	221	GLY	3.6
2	D	145	SER	3.5
2	C	388	LYS	3.5
1	B	272	GLN	3.4
2	D	144	ARG	3.3
2	D	273	ASN	3.2
2	C	362	VAL	3.1
2	D	224	THR	3.0
2	C	305	TYR	2.9
2	C	383	VAL	2.9
1	A	257	ALA	2.9
2	D	142	LEU	2.9
2	C	224	THR	2.8
1	B	94	SER	2.8
1	B	8	HIS	2.8
1	B	101	HIS	2.7
2	C	391	ARG	2.6
2	C	288	LYS	2.6
2	C	374	ILE	2.6
2	C	173	LEU	2.5
2	D	357	ASP	2.4
2	C	384	GLY	2.4
2	D	395	ASP	2.3
2	C	357	ASP	2.3
1	A	8	HIS	2.3
1	B	119	ASP	2.2
2	C	356	HIS	2.2
2	C	375	MET	2.2
1	A	101	HIS	2.2
1	B	255	LEU	2.2
2	D	263	GLN	2.1
1	A	135	SER	2.1
1	A	255	LEU	2.0
2	C	343	ILE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

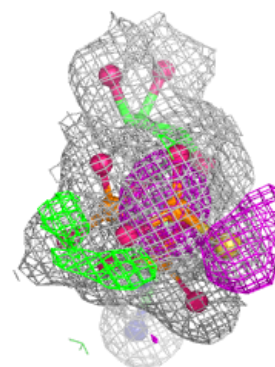
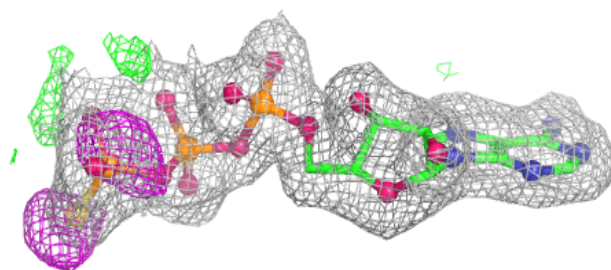
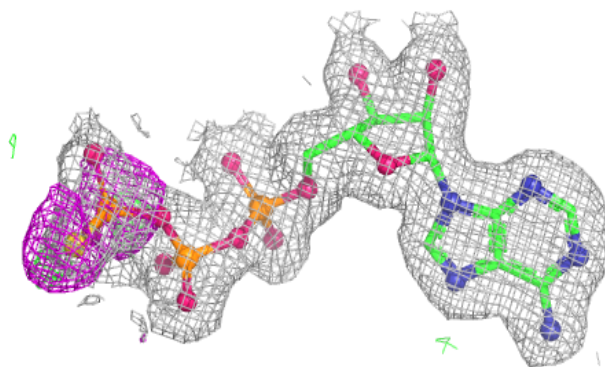
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	301	6/6	0.85	0.13	28,36,39,42	0
3	AGS	A	501	31/31	0.96	0.07	13,18,29,36	0
3	AGS	B	302	31/31	0.97	0.06	12,17,26,50	0
4	MG	C	401	1/1	0.98	0.05	34,34,34,34	0
4	MG	A	503	1/1	0.99	0.06	11,11,11,11	0
4	MG	B	303	1/1	0.99	0.05	3,3,3,3	0
4	MG	A	502	1/1	1.00	0.05	3,3,3,3	0

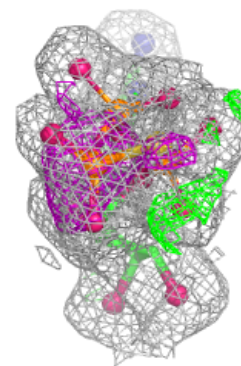
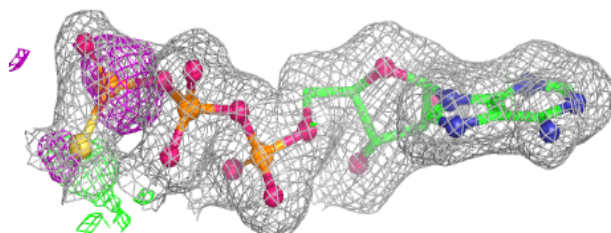
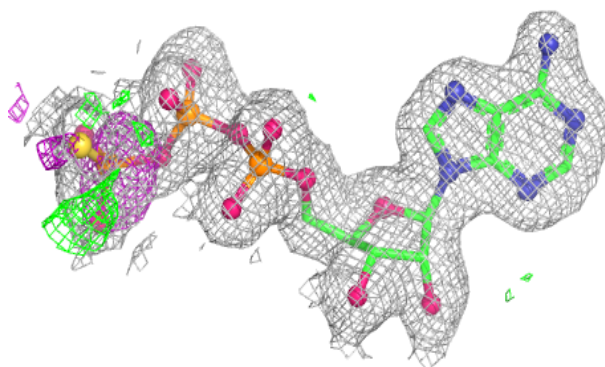
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS A 501:

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

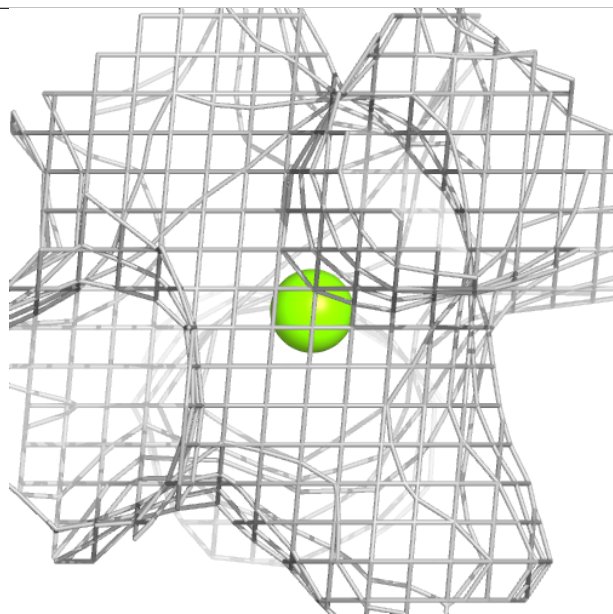
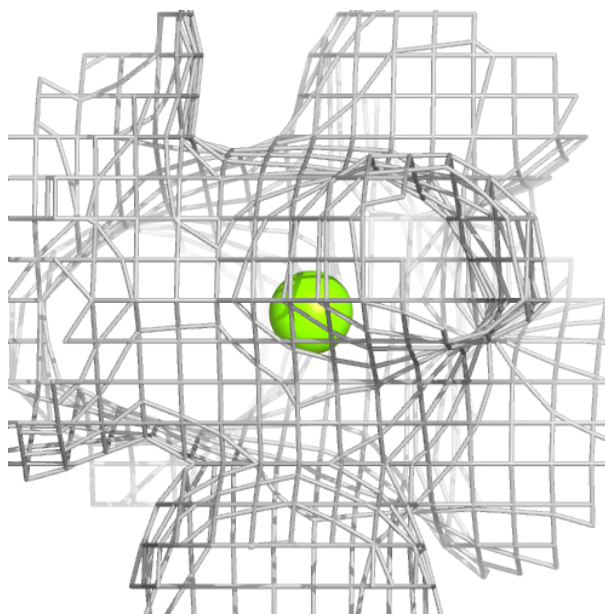
**Electron density around AGS B 302:**

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



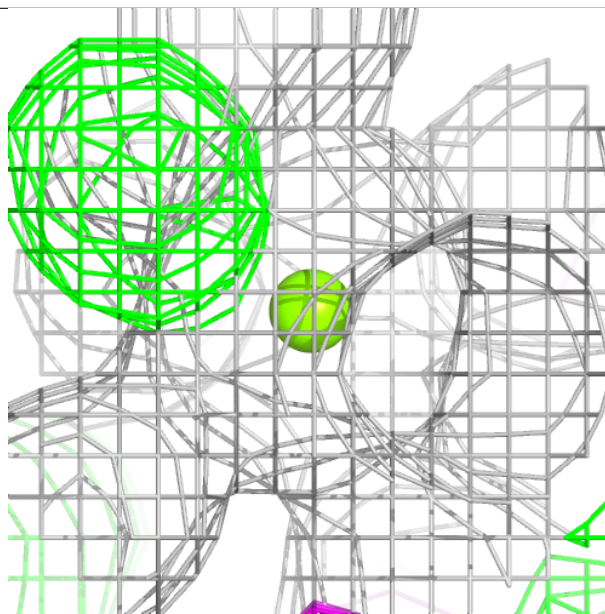
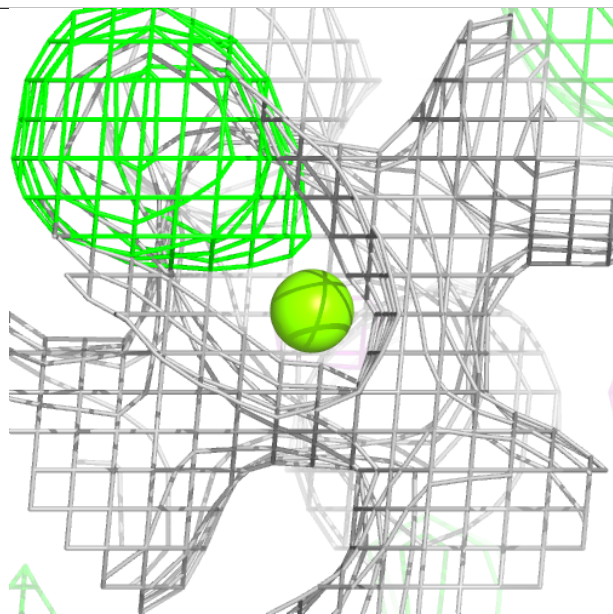
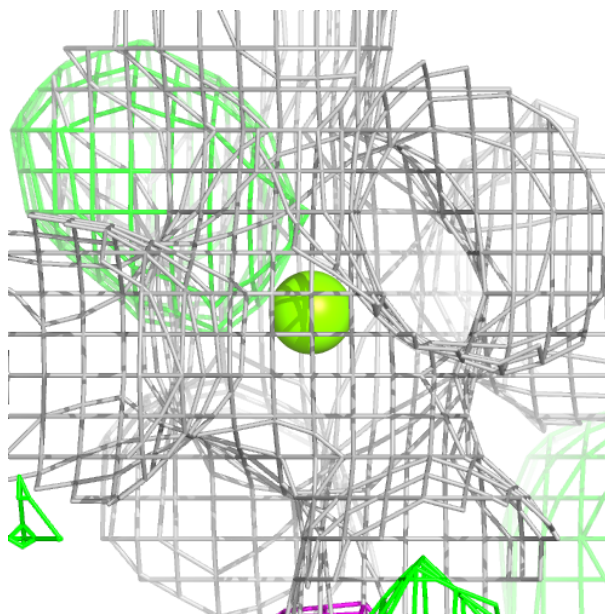
Electron density around MG C 401:

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



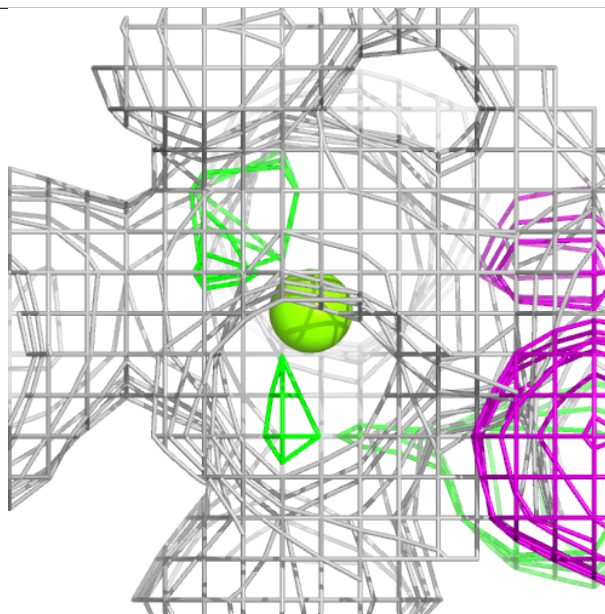
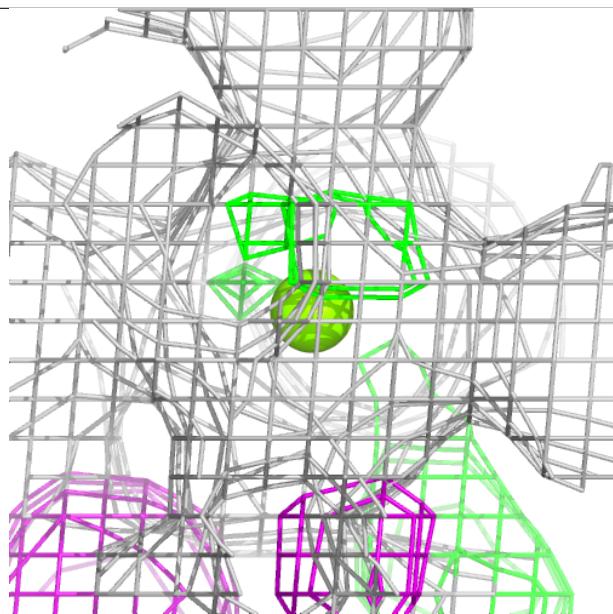
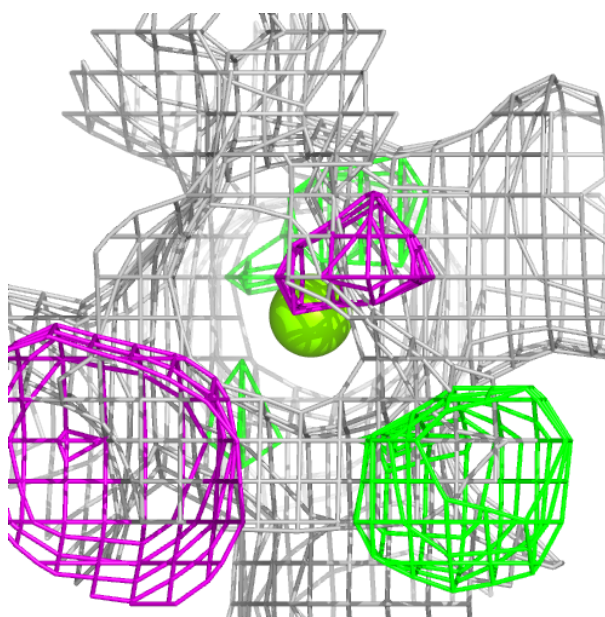
Electron density around MG A 503:

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



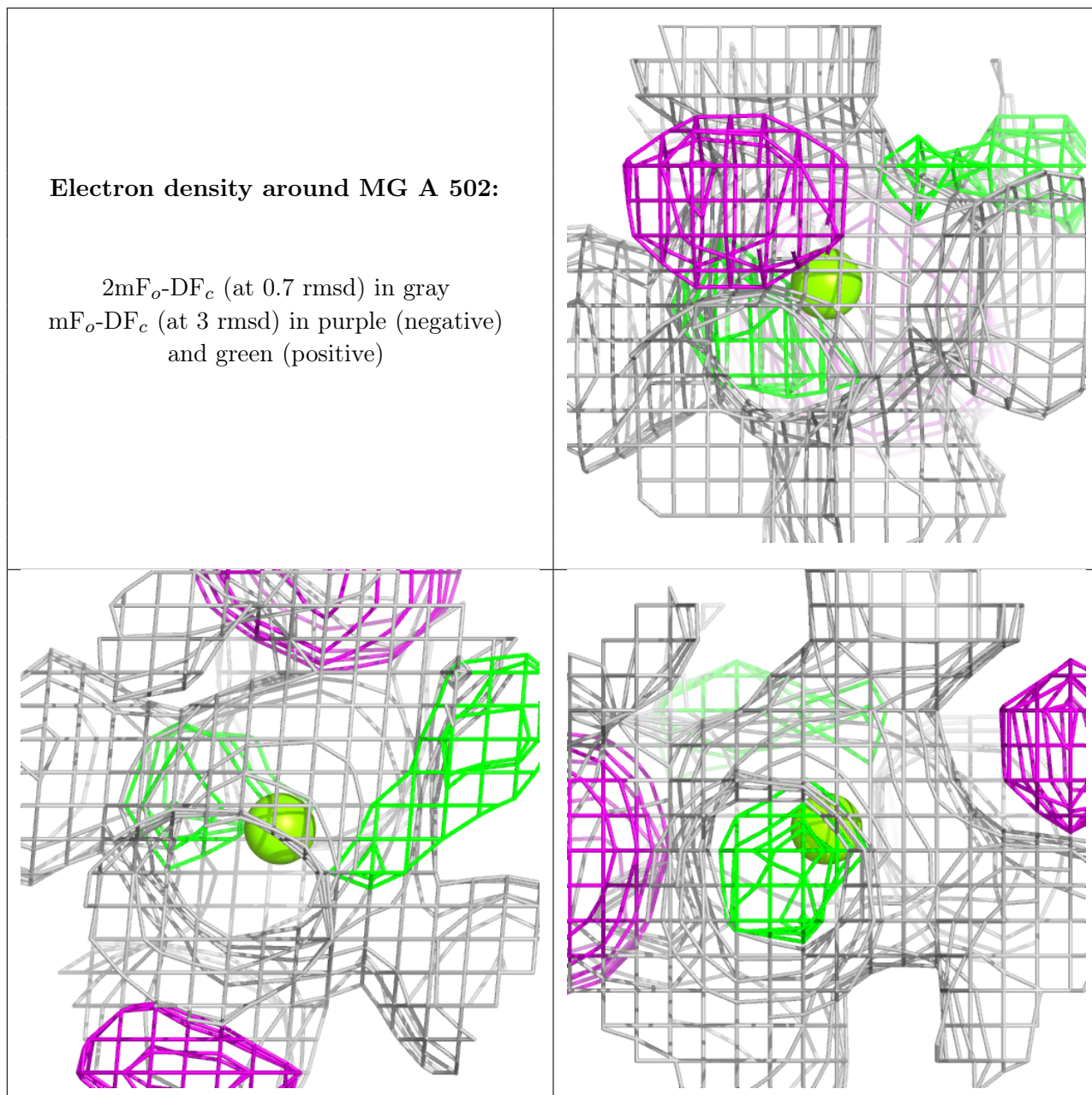
Electron density around MG B 303:

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



Electron density around MG A 502:

$2mF_o-DF_c$ (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.