



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:40 PM UTC

PDB ID : 9F99 / pdb_00009f99
Title : Crystal structure of MUS81-EME1 bound by compound 10.
Authors : Collie, G.W.
Deposited on : 2024-05-07
Resolution : 2.80 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

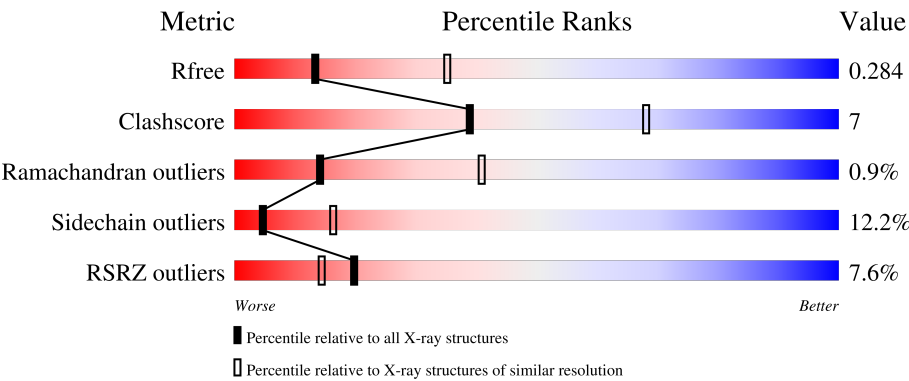
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	308	
1	C	308	
1	E	308	
1	G	308	
2	B	326	

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Mol	Chain	Length	Quality of chain
2	D	326	5% 34% 8% 57%
2	F	326	4% 33% 9% 57%
2	H	326	3% 31% 9% 57%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10145 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 Crossover junction endonuclease MUS81.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	185	Total	C	N	O	S	0	0	0
			1465	928	266	267	4			
1	C	186	Total	C	N	O	S	0	0	0
			1467	928	267	268	4			
1	E	187	Total	C	N	O	S	0	0	0
			1474	933	268	269	4			
1	G	187	Total	C	N	O	S	0	0	0
			1469	931	264	270	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP Q96NY9
A	245	SER	-	expression tag	UNP Q96NY9
C	244	GLY	-	expression tag	UNP Q96NY9
C	245	SER	-	expression tag	UNP Q96NY9
E	244	GLY	-	expression tag	UNP Q96NY9
E	245	SER	-	expression tag	UNP Q96NY9
G	244	GLY	-	expression tag	UNP Q96NY9
G	245	SER	-	expression tag	UNP Q96NY9

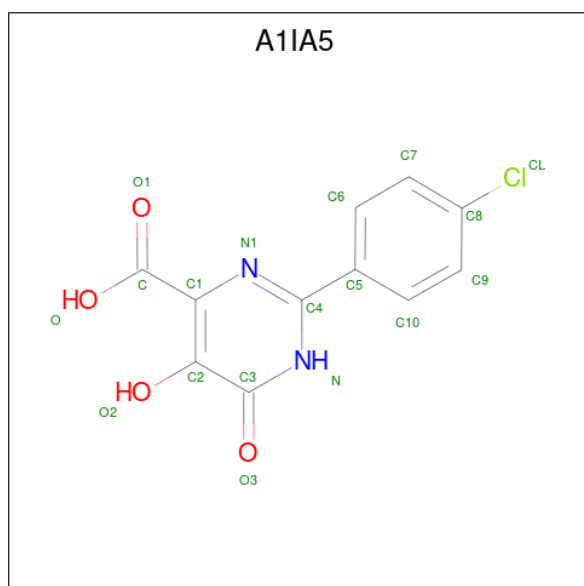
- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1048	666	173	201	8			
2	D	139	Total	C	N	O	S	0	0	0
			1048	666	173	201	8			
2	F	139	Total	C	N	O	S	0	0	0
			1050	666	175	201	8			
2	H	139	Total	C	N	O	S	0	0	0
			1044	663	172	201	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	245	GLY	-	expression tag	UNP Q96AY2
D	245	GLY	-	expression tag	UNP Q96AY2
F	245	GLY	-	expression tag	UNP Q96AY2
H	245	GLY	-	expression tag	UNP Q96AY2

- Molecule 3 is 2-(4-chlorophenyl)-5-oxidanyl-6-oxidanylidene-1H-pyrimidine-4-carboxylic acid (CCD ID: A1IA5) (formula: $C_{11}H_7ClN_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			18	11	1	2	4		
3	C	1	Total	C	Cl	N	O	0	0
			18	11	1	2	4		
3	E	1	Total	C	Cl	N	O	0	0
			18	11	1	2	4		
3	G	1	Total	C	Cl	N	O	0	0
			18	11	1	2	4		

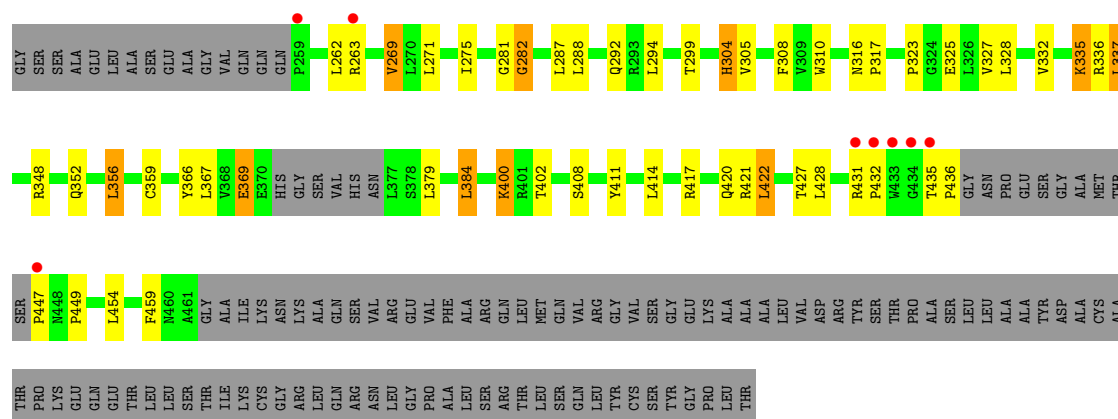
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

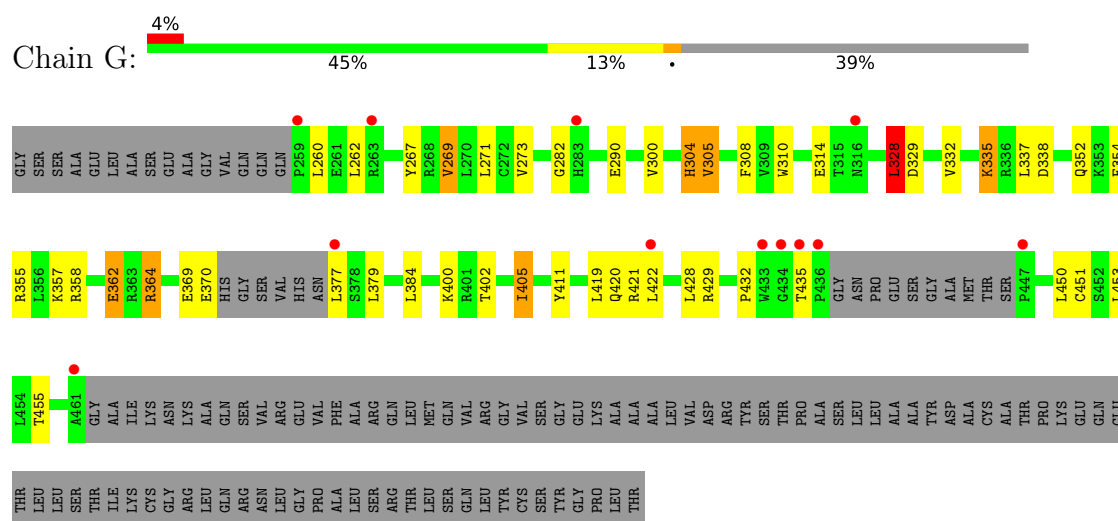
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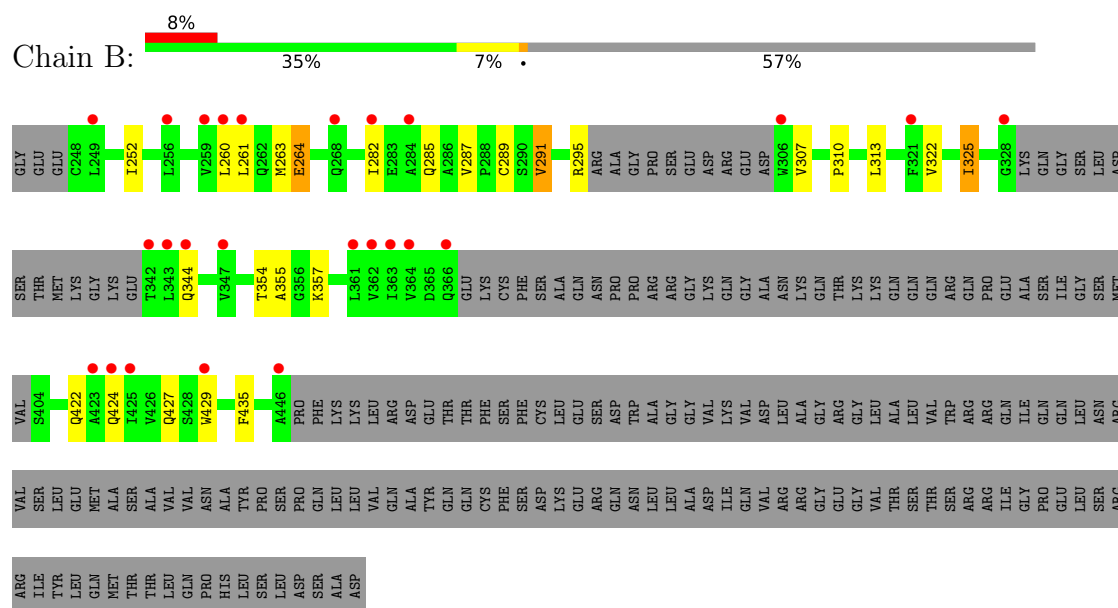
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total 2	Mg 2	0	0
4	G	2	Total 2	Mg 2	0	0



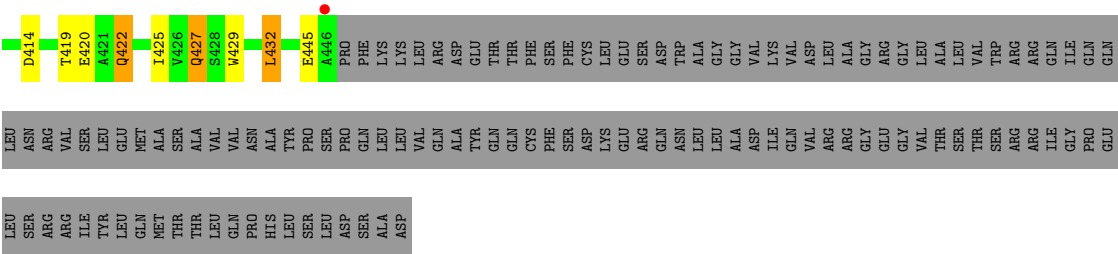
• Molecule 1: Crossover junction endonuclease MUS81



• Molecule 2: Crossover junction endonuclease EME1



• Molecule 2: Crossover junction endonuclease EME1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.35Å 125.10Å 218.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.95 – 2.80 38.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	51.1 (38.95-2.80) 51.1 (38.95-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.240 , 0.280 0.240 , 0.284	Depositor DCC
R_{free} test set	1932 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	78.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10145	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: A1IA5, 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	0.70	1/1493 (0.1%)	1.09	3/2022 (0.1%)
1	C	0.72	0/1495	1.20	7/2027 (0.3%)
1	E	0.67	0/1503	1.18	6/2039 (0.3%)
1	G	0.68	0/1498	1.09	1/2033 (0.0%)
2	B	0.60	0/1059	1.02	0/1439
2	D	0.65	0/1059	1.12	1/1439 (0.1%)
2	F	0.63	0/1061	1.10	0/1442
2	H	0.65	0/1055	1.08	0/1435
All	All	0.67	1/10223 (0.0%)	1.12	18/13876 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	345	ILE	CG1-CD1	-5.09	1.31	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	369	GLU	CA-C-N	7.44	135.09	121.70
1	A	369	GLU	C-N-CA	7.44	135.09	121.70
1	G	328	LEU	N-CA-C	7.12	121.63	113.15
1	C	327	VAL	CA-C-N	6.00	133.00	121.54
1	C	327	VAL	C-N-CA	6.00	133.00	121.54
1	C	300	VAL	N-CA-CB	5.92	118.09	110.99
1	E	328	LEU	CA-C-N	5.88	130.09	120.63
1	E	328	LEU	C-N-CA	5.88	130.09	120.63
1	A	328	LEU	N-CA-C	5.72	122.99	110.80
1	E	447	PRO	CA-C-N	5.22	127.67	120.67
1	E	447	PRO	C-N-CA	5.22	127.67	120.67
2	D	365	ASP	CA-CB-CG	5.08	117.68	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	407	GLU	CA-C-N	5.06	127.32	120.44
1	C	407	GLU	C-N-CA	5.06	127.32	120.44
1	E	369	GLU	CA-C-N	5.04	130.78	121.70
1	E	369	GLU	C-N-CA	5.04	130.78	121.70
1	C	369	GLU	CA-C-N	5.02	130.74	121.70
1	C	369	GLU	C-N-CA	5.02	130.74	121.70

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	1465	0	1459	15	0
1	C	1467	0	1455	20	0
1	E	1474	0	1462	30	0
1	G	1469	0	1451	26	0
2	B	1048	0	1055	10	0
2	D	1048	0	1055	16	0
2	F	1050	0	1055	11	0
2	H	1044	0	1044	17	0
3	A	18	0	0	0	0
3	C	18	0	0	0	0
3	E	18	0	0	0	0
3	G	18	0	0	0	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
All	All	10145	0	10036	137	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 (137) 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:335:LYS:NZ	1:A:352:GLN:HE22	1.58	1.00
1:A:335:LYS:HZ1	1:A:352:GLN:HE22	1.01	0.96
1:E:431:ARG:HD3	1:E:435:THR:HA	1.56	0.86
1:A:335:LYS:HZ1	1:A:352:GLN:NE2	1.71	0.86
2:D:258:PRO:HD2	2:D:284:ALA:HA	1.60	0.83
1:G:304:HIS:CD2	1:G:305:VAL:HG12	2.18	0.78
1:A:335:LYS:NZ	1:A:352:GLN:NE2	2.30	0.75
1:G:304:HIS:NE2	1:G:305:VAL:HG12	2.01	0.74
1:G:308:PHE:HB2	1:G:332:VAL:HB	1.68	0.74
2:B:291:VAL:HG13	2:B:313:LEU:HB3	1.69	0.73
1:E:304:HIS:CD2	1:E:305:VAL:HG12	2.26	0.70
2:H:291:VAL:HG13	2:H:313:LEU:HB3	1.73	0.69
1:G:335:LYS:NZ	1:G:352:GLN:NE2	2.43	0.67
2:H:249:LEU:HD22	2:H:278:CYS:HB3	1.77	0.67
2:D:292:THR:HG22	2:D:293:TRP:H	1.60	0.67
2:B:252:ILE:HG13	2:B:295:ARG:HG2	1.78	0.65
1:E:369:GLU:HA	1:E:402:THR:HG23	1.79	0.64
2:F:263:MET:HE1	2:F:315:LEU:HD22	1.79	0.64
2:F:291:VAL:HG13	2:F:313:LEU:HB3	1.79	0.64
1:G:335:LYS:NZ	1:G:352:GLN:HE22	1.95	0.64
1:A:282:GLY:HA2	1:G:362:GLU:HG2	1.79	0.63
1:E:335:LYS:NZ	1:E:352:GLN:HE22	1.97	0.63
1:G:335:LYS:HZ1	1:G:352:GLN:NE2	1.97	0.62
1:E:348:ARG:O	1:E:352:GLN:HG3	2.00	0.61
2:D:310:PRO:HA	2:D:357:LYS:HG2	1.82	0.61
1:E:308:PHE:HB2	1:E:332:VAL:HB	1.81	0.61
2:D:292:THR:HG21	2:D:357:LYS:NZ	2.17	0.60
1:E:335:LYS:NZ	1:E:352:GLN:NE2	2.50	0.60
1:G:369:GLU:HA	1:G:402:THR:HG23	1.83	0.60
1:C:333:GLU:HB2	1:C:356:LEU:HD21	1.84	0.60
2:D:315:LEU:HD11	2:D:432:LEU:HD21	1.84	0.59
1:G:335:LYS:HZ1	1:G:352:GLN:HE22	1.50	0.59
2:F:310:PRO:HA	2:F:357:LYS:HD3	1.84	0.59
1:E:335:LYS:HZ1	1:E:352:GLN:NE2	2.01	0.59
2:B:263:MET:HE2	2:B:429:TRP:HH2	1.68	0.58
1:C:332:VAL:HG22	1:C:365:VAL:HB	1.84	0.58
1:E:269:VAL:HG13	1:E:420:GLN:HG2	1.85	0.57
2:B:261:LEU:HD11	2:B:282:ILE:HD12	1.86	0.57
1:A:297:THR:H	1:C:316:ASN:HD21	1.52	0.57
1:A:341:CYS:O	1:A:345:ILE:HG12	2.04	0.57
1:E:327:VAL:HG11	1:E:459:PHE:HB2	1.88	0.56
1:E:414:LEU:HB3	2:F:413:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:LEU:HD13	1:C:449:PRO:HB3	1.88	0.56
1:A:364:ARG:NH1	1:A:395:ASP:O	2.39	0.56
1:E:400:LYS:HG3	1:E:411:TYR:CE1	2.41	0.56
2:H:294:ARG:HG2	2:H:306:TRP:HB3	1.88	0.55
2:B:260:LEU:HB2	2:B:289:CYS:HA	1.88	0.55
2:D:258:PRO:CD	2:D:284:ALA:HA	2.33	0.55
1:G:354:PHE:HE2	1:G:355:ARG:NH2	2.05	0.54
1:C:333:GLU:CB	1:C:356:LEU:HD21	2.38	0.54
2:H:260:LEU:HD11	2:H:315:LEU:HD13	1.90	0.53
1:A:283:HIS:HE1	1:G:329:ASP:OD1	1.91	0.52
2:F:252:ILE:HG13	2:F:295:ARG:HG2	1.91	0.52
2:D:354:THR:HG23	2:D:357:LYS:H	1.75	0.52
1:G:354:PHE:HE2	1:G:355:ARG:HH21	1.58	0.52
1:C:335:LYS:HG3	1:C:366:TYR:OH	2.09	0.52
1:G:405:ILE:HD12	1:G:405:ILE:H	1.74	0.52
1:E:317:PRO:HG3	1:E:323:PRO:HB3	1.92	0.51
1:G:450:LEU:HD23	1:G:453:LEU:HD23	1.91	0.51
1:G:428:LEU:HD12	1:G:451:CYS:HA	1.93	0.50
1:E:281:GLY:O	1:E:282:GLY:O	2.29	0.50
1:C:414:LEU:HB3	2:D:413:VAL:HG21	1.93	0.50
2:D:276:MET:HE3	2:D:278:CYS:SG	2.51	0.49
2:H:261:LEU:HD11	2:H:282:ILE:HD12	1.94	0.49
2:H:258:PRO:HD2	2:H:284:ALA:HA	1.94	0.49
1:C:331:ILE:HB	1:C:361:LEU:HD23	1.94	0.49
1:G:262:LEU:HD22	1:G:267:TYR:HB3	1.95	0.49
1:A:348:ARG:O	1:A:352:GLN:HG3	2.13	0.49
1:E:422:LEU:HD22	1:E:449:PRO:HB3	1.94	0.49
1:C:287:LEU:HD12	1:C:409:ALA:HB2	1.94	0.48
1:E:335:LYS:HG3	1:E:366:TYR:OH	2.14	0.48
1:E:400:LYS:HG3	1:E:411:TYR:CZ	2.49	0.48
2:H:311:THR:HG23	2:H:358:ALA:HB3	1.95	0.48
1:E:271:LEU:HD13	1:E:310:TRP:CE2	2.48	0.48
1:G:369:GLU:O	1:G:370:GLU:HB2	2.13	0.48
1:C:379:LEU:HG	1:C:380:PRO:HD2	1.94	0.47
1:G:400:LYS:HG3	1:G:411:TYR:CE1	2.49	0.47
1:E:262:LEU:HB2	1:E:428:LEU:HB2	1.96	0.47
2:D:292:THR:HG21	2:D:357:LYS:HZ3	1.78	0.47
2:F:346:PHE:O	2:F:350:ILE:HG13	2.15	0.47
1:G:335:LYS:HZ3	1:G:352:GLN:NE2	2.13	0.47
1:C:283:HIS:HD2	1:E:436:PRO:HD2	1.79	0.47
1:G:269:VAL:HG13	1:G:420:GLN:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:328:LEU:HD23	1:G:419:LEU:HD22	1.97	0.47
2:H:365:ASP:HB3	2:H:427:GLN:HG3	1.97	0.47
1:G:354:PHE:CE2	1:G:355:ARG:NH2	2.83	0.46
1:C:269:VAL:HG13	1:C:420:GLN:HG2	1.97	0.46
1:C:308:PHE:HB2	1:C:332:VAL:HB	1.98	0.46
2:H:363:ILE:HB	2:H:425:ILE:HG12	1.97	0.46
1:A:305:VAL:HG11	1:A:359:CYS:HB2	1.97	0.46
1:C:341:CYS:O	1:C:345:ILE:HG12	2.16	0.46
2:H:315:LEU:HD21	2:H:432:LEU:HD21	1.98	0.46
1:A:345:ILE:HD11	1:A:379:LEU:HD13	1.98	0.45
1:E:304:HIS:NE2	1:E:305:VAL:HG12	2.30	0.45
1:E:271:LEU:HD11	1:E:308:PHE:HB3	1.97	0.45
2:B:310:PRO:HA	2:B:357:LYS:HG2	1.97	0.45
2:H:344:GLN:HE21	2:H:419:THR:HG23	1.83	0.44
1:E:367:LEU:HD21	1:E:408:SER:HB3	1.99	0.44
1:C:283:HIS:CD2	1:E:436:PRO:HD2	2.52	0.44
2:H:422:GLN:HE21	2:H:422:GLN:HB2	1.66	0.44
1:E:352:GLN:O	1:E:356:LEU:HB2	2.18	0.44
2:H:265:GLY:HA3	2:H:429:TRP:CD2	2.53	0.44
2:B:313:LEU:HD11	2:B:435:PHE:HE2	1.82	0.44
1:C:299:THR:HG21	1:C:301:ARG:HE	1.83	0.44
2:F:292:THR:HG22	2:F:293:TRP:H	1.83	0.44
1:E:305:VAL:HG11	1:E:359:CYS:HB2	2.00	0.44
1:A:423:TYR:CZ	1:A:449:PRO:HB2	2.53	0.43
2:D:276:MET:HE1	2:D:440:THR:HB	1.99	0.43
2:H:354:THR:HG23	2:H:357:LYS:HB2	2.01	0.43
1:E:336:ARG:HG2	1:E:369:GLU:HB3	2.00	0.43
2:F:292:THR:HG21	2:F:357:LYS:HZ3	1.84	0.43
2:H:276:MET:HE3	2:H:278:CYS:SG	2.59	0.42
2:H:354:THR:CG2	2:H:357:LYS:HB2	2.49	0.42
1:G:271:LEU:HD13	1:G:310:TRP:NE1	2.33	0.42
2:D:440:THR:HA	2:D:443:VAL:HG22	2.01	0.42
2:D:291:VAL:HG13	2:D:313:LEU:HB3	2.01	0.42
1:E:417:ARG:NH2	2:F:410:GLU:OE2	2.53	0.42
1:C:271:LEU:O	1:C:298:HIS:HA	2.20	0.41
2:D:422:GLN:HE21	2:D:422:GLN:HB2	1.69	0.41
2:F:257:ASP:O	2:F:260:LEU:HB2	2.21	0.41
1:G:357:LYS:HA	1:G:364:ARG:HE	1.85	0.41
1:E:263:ARG:HA	1:E:427:THR:HG23	2.02	0.41
2:D:310:PRO:CA	2:D:357:LYS:HG2	2.48	0.41
2:B:322:VAL:O	2:B:325:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:LEU:HD12	1:E:384:LEU:HG	2.01	0.41
1:A:332:VAL:HG22	1:A:365:VAL:HB	2.03	0.41
1:C:405:ILE:HA	1:C:408:SER:HB2	2.03	0.41
2:B:264:GLU:CD	2:B:264:GLU:H	2.29	0.41
1:C:400:LYS:HG3	1:C:411:TYR:CZ	2.56	0.41
1:C:422:LEU:HD22	1:C:449:PRO:HG3	2.03	0.41
1:G:267:TYR:HA	1:G:314:GLU:HA	2.01	0.41
1:A:335:LYS:HG3	1:A:366:TYR:OH	2.20	0.40
2:D:255:VAL:HG13	2:D:281:VAL:HG23	2.03	0.40
2:B:261:LEU:CD1	2:B:282:ILE:HD12	2.51	0.40
1:G:273:VAL:HG22	1:G:308:PHE:HE1	1.86	0.40
2:F:257:ASP:HB2	2:F:285:GLN:HB2	2.04	0.40
2:H:253:ILE:HG23	2:H:279:ARG:HB3	2.03	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	179/308 (58%)	172 (96%)	6 (3%)	1 (1%)	21	51
1	C	180/308 (58%)	172 (96%)	7 (4%)	1 (1%)	21	51
1	E	181/308 (59%)	176 (97%)	3 (2%)	2 (1%)	11	36
1	G	181/308 (59%)	170 (94%)	9 (5%)	2 (1%)	11	36
2	B	131/326 (40%)	127 (97%)	2 (2%)	2 (2%)	8	28
2	D	131/326 (40%)	120 (92%)	10 (8%)	1 (1%)	16	44
2	F	131/326 (40%)	122 (93%)	8 (6%)	1 (1%)	16	44
2	H	131/326 (40%)	122 (93%)	8 (6%)	1 (1%)	16	44
All	All	1245/2536 (49%)	1181 (95%)	53 (4%)	11 (1%)	14	41

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	432	PRO
2	D	307	VAL
1	E	282	GLY
1	E	432	PRO
1	G	282	GLY
1	A	432	PRO
2	B	307	VAL
2	F	307	VAL
2	B	355	ALA
1	G	432	PRO
2	H	307	VAL

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	158/260 (61%)	143 (90%)	15 (10%)	8	26
1	C	158/260 (61%)	136 (86%)	22 (14%)	3	12
1	E	159/260 (61%)	140 (88%)	19 (12%)	5	17
1	G	158/260 (61%)	136 (86%)	22 (14%)	3	12
2	B	113/275 (41%)	103 (91%)	10 (9%)	9	29
2	D	113/275 (41%)	102 (90%)	11 (10%)	8	25
2	F	113/275 (41%)	95 (84%)	18 (16%)	2	9
2	H	112/275 (41%)	97 (87%)	15 (13%)	4	13
All	All	1084/2140 (51%)	952 (88%)	132 (12%)	5	16

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	ILE
1	A	279	ARG
1	A	288	LEU

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Mol	Chain	Res	Type
1	A	299	THR
1	A	300	VAL
1	A	335	LYS
1	A	337	LEU
1	A	355	ARG
1	A	362	GLU
1	A	370	GLU
1	A	379	LEU
1	A	381	GLU
1	A	384	LEU
1	A	422	LEU
1	A	424	GLN
2	B	264	GLU
2	B	285	GLN
2	B	287	VAL
2	B	291	VAL
2	B	325	ILE
2	B	344	GLN
2	B	354	THR
2	B	422	GLN
2	B	424	GLN
2	B	427	GLN
1	C	269	VAL
1	C	275	ILE
1	C	279	ARG
1	C	299	THR
1	C	300	VAL
1	C	304	HIS
1	C	311	VAL
1	C	315	THR
1	C	335	LYS
1	C	361	LEU
1	C	362	GLU
1	C	384	LEU
1	C	402	THR
1	C	405	ILE
1	C	408	SER
1	C	415	LEU
1	C	417	ARG
1	C	421	ARG
1	C	422	LEU
1	C	426	HIS

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Mol	Chain	Res	Type
1	C	429	ARG
1	C	455	THR
2	D	260	LEU
2	D	261	LEU
2	D	285	GLN
2	D	287	VAL
2	D	291	VAL
2	D	315	LEU
2	D	322	VAL
2	D	326	ASP
2	D	344	GLN
2	D	412	LEU
2	D	422	GLN
1	E	269	VAL
1	E	275	ILE
1	E	287	LEU
1	E	288	LEU
1	E	292	GLN
1	E	294	LEU
1	E	299	THR
1	E	304	HIS
1	E	316	ASN
1	E	325	GLU
1	E	335	LYS
1	E	337	LEU
1	E	356	LEU
1	E	379	LEU
1	E	384	LEU
1	E	400	LYS
1	E	421	ARG
1	E	422	LEU
1	E	454	LEU
2	F	249	LEU
2	F	251	HIS
2	F	252	ILE
2	F	264	GLU
2	F	268	GLN
2	F	276	MET
2	F	279	ARG
2	F	287	VAL
2	F	290	SER
2	F	291	VAL

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Mol	Chain	Res	Type
2	F	309	GLU
2	F	344	GLN
2	F	361	LEU
2	F	366	GLN
2	F	410	GLU
2	F	422	GLN
2	F	432	LEU
2	F	443	VAL
1	G	260	LEU
1	G	269	VAL
1	G	290	GLU
1	G	300	VAL
1	G	304	HIS
1	G	305	VAL
1	G	328	LEU
1	G	335	LYS
1	G	337	LEU
1	G	338	ASP
1	G	358	ARG
1	G	362	GLU
1	G	364	ARG
1	G	377	LEU
1	G	379	LEU
1	G	384	LEU
1	G	405	ILE
1	G	421	ARG
1	G	422	LEU
1	G	429	ARG
1	G	435	THR
1	G	455	THR
2	H	264	GLU
2	H	276	MET
2	H	287	VAL
2	H	291	VAL
2	H	309	GLU
2	H	311	THR
2	H	344	GLN
2	H	354	THR
2	H	364	VAL
2	H	414	ASP
2	H	420	GLU
2	H	422	GLN

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Mol	Chain	Res	Type
2	H	427	GLN
2	H	432	LEU
2	H	445	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
1	A	304	HIS
1	A	322	ASN
1	A	352	GLN
1	A	392	GLN
1	A	424	GLN
2	B	344	GLN
1	C	295	HIS
1	C	316	ASN
1	C	322	ASN
1	C	352	GLN
1	C	448	ASN
2	D	251	HIS
1	E	295	HIS
1	E	352	GLN
1	E	448	ASN
2	F	268	GLN
1	G	292	GLN
1	G	295	HIS
1	G	330	HIS
1	G	352	GLN
2	H	268	GLN
2	H	344	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	A1IA5	A	601	4	17,19,19	0.47	0	20,27,27	0.50	0
3	A1IA5	G	601	4	17,19,19	0.35	0	20,27,27	0.43	0
3	A1IA5	C	601	4	17,19,19	0.25	0	20,27,27	0.60	0
3	A1IA5	E	601	4	17,19,19	0.28	0	20,27,27	0.43	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
3	A1IA5	A	601	4	-	3/8/8/8	0/2/2/2
3	A1IA5	G	601	4	-	2/8/8/8	0/2/2/2
3	A1IA5	C	601	4	-	4/8/8/8	0/2/2/2
3	A1IA5	E	601	4	-	0/8/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	A1IA5	O1-C-C1-C2
3	A	601	A1IA5	O-C-C1-C2

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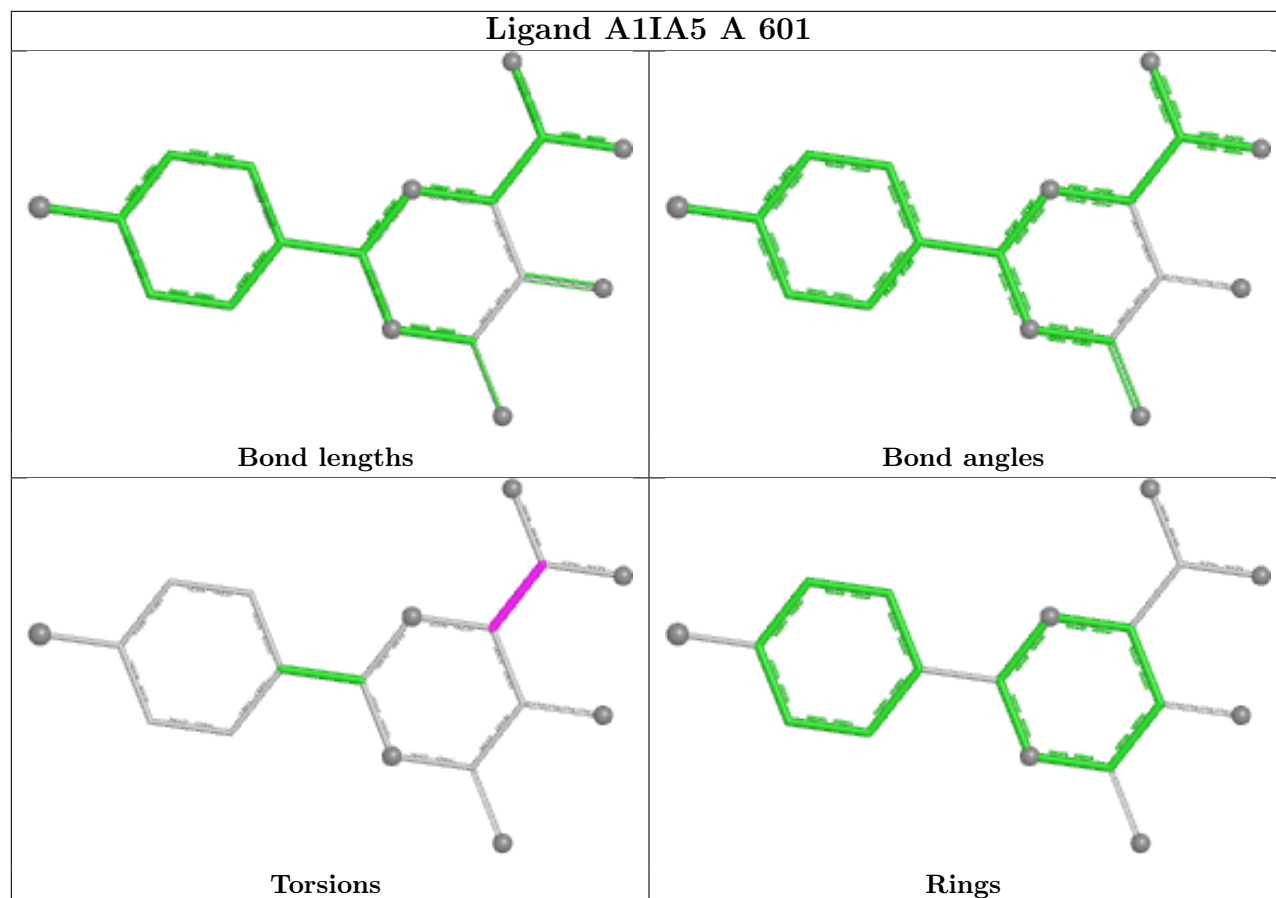
Mol	Chain	Res	Type	Atoms
3	A	601	A1IA5	O-C-C1-N1
3	C	601	A1IA5	O-C-C1-C2
3	C	601	A1IA5	O-C-C1-N1
3	C	601	A1IA5	N-C4-C5-C6
3	G	601	A1IA5	N-C4-C5-C6
3	C	601	A1IA5	N-C4-C5-C10
3	G	601	A1IA5	N-C4-C5-C10

There are no ring outliers.

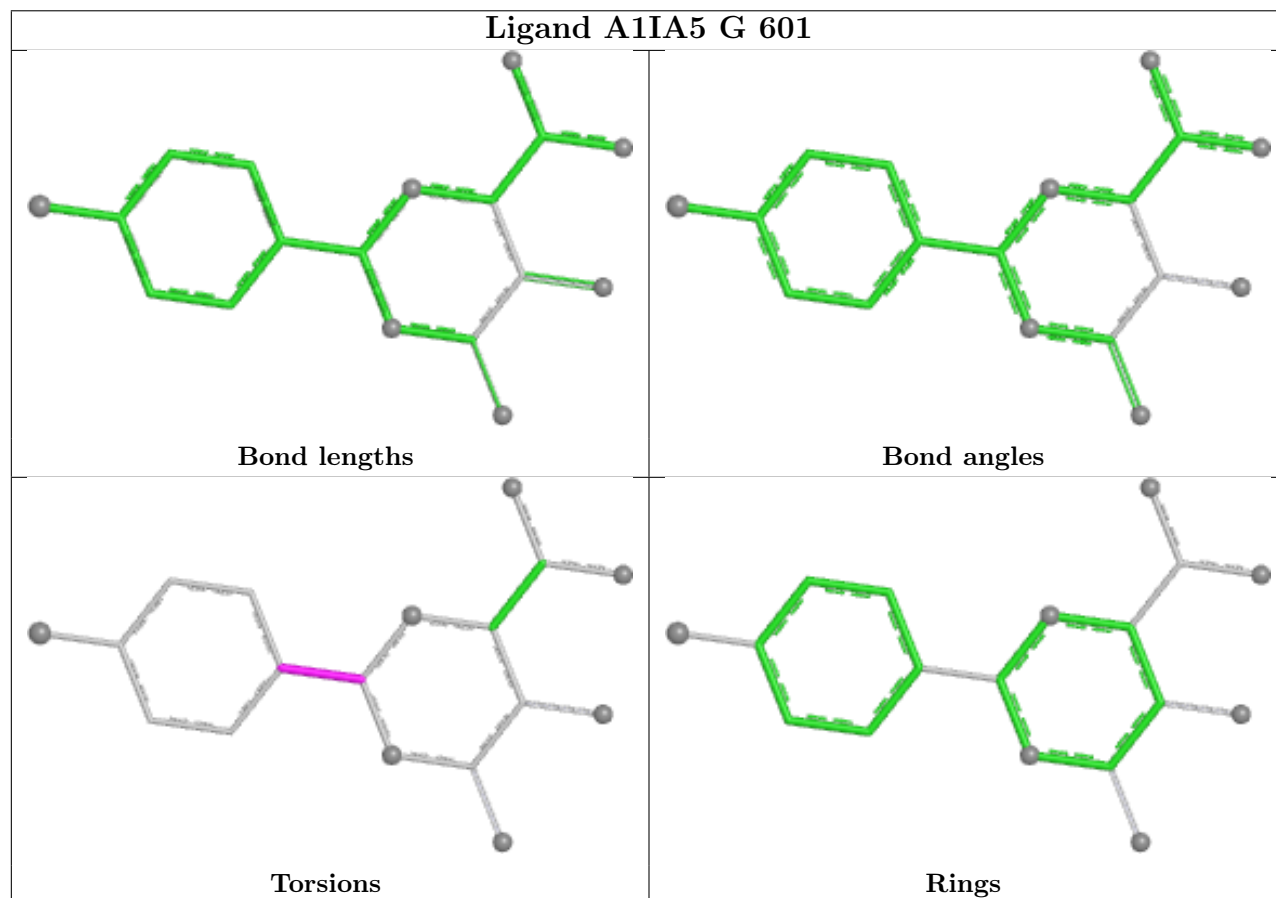
No monomer is involved in short contacts.

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.

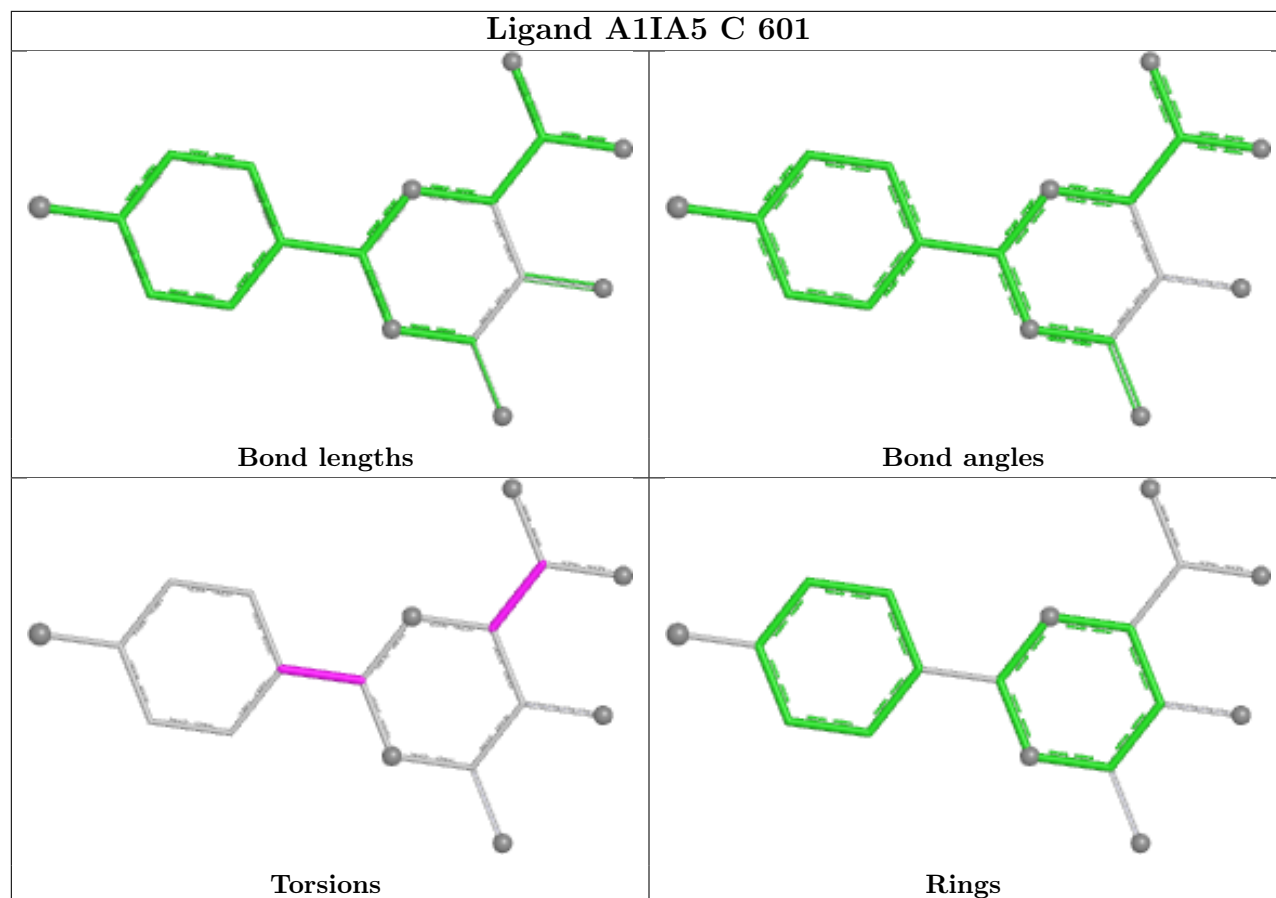
Ligand A1IA5 A 601



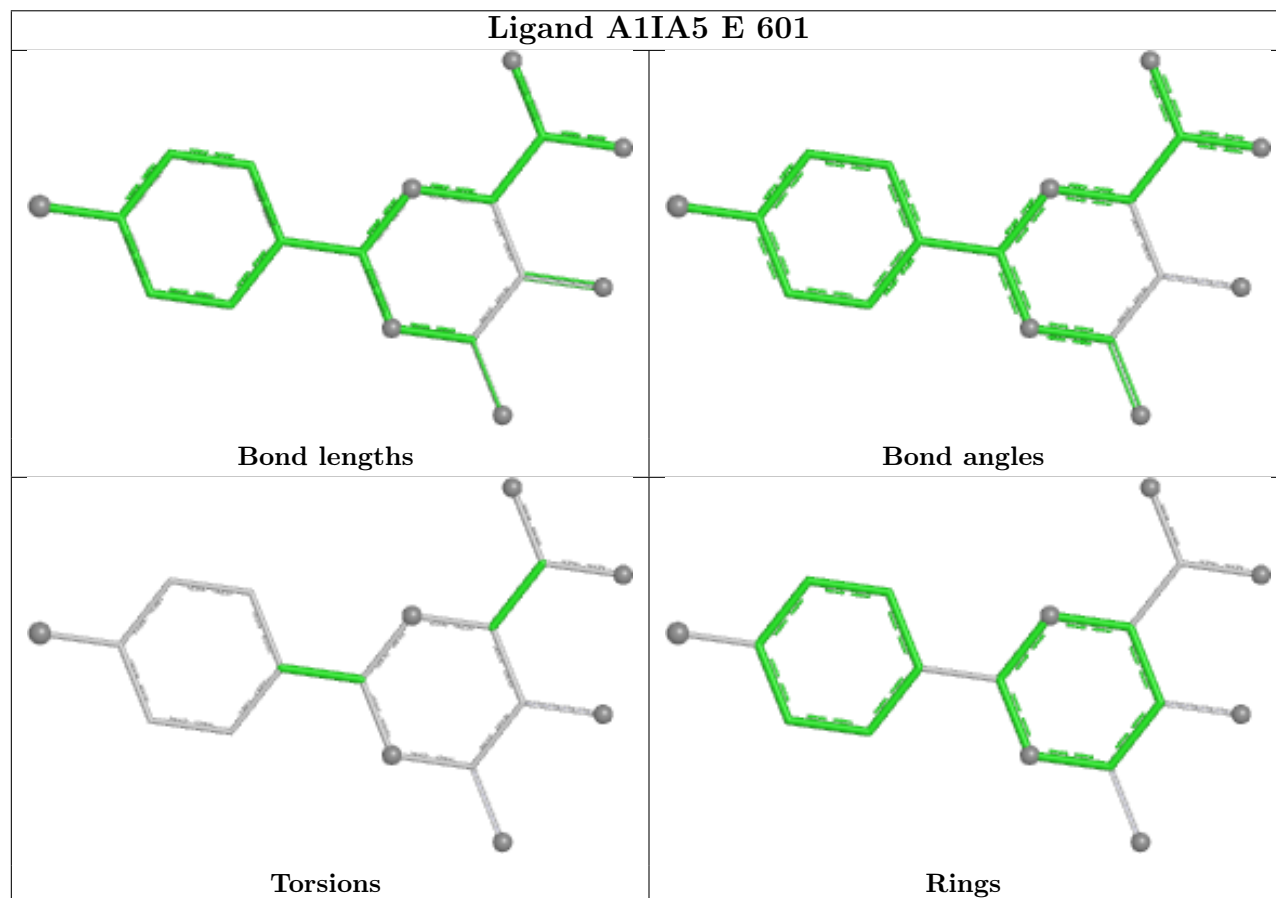
Ligand A1IA5 G 601



Ligand A1IA5 C 601



Ligand A1IA5 E 601



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	185/308 (60%)	0.21	5 (2%) 56 46	46, 68, 88, 97	0
1	C	186/308 (60%)	0.16	10 (5%) 31 24	49, 66, 88, 100	0
1	E	187/308 (60%)	0.39	8 (4%) 40 31	54, 79, 104, 113	0
1	G	187/308 (60%)	0.38	12 (6%) 25 18	53, 82, 105, 111	0
2	B	139/326 (42%)	1.16	25 (17%) 3 3	74, 99, 125, 130	0
2	D	139/326 (42%)	0.86	15 (10%) 11 8	70, 97, 118, 121	0
2	F	139/326 (42%)	0.80	13 (9%) 14 10	70, 95, 112, 116	0
2	H	139/326 (42%)	0.68	11 (7%) 18 13	75, 97, 117, 125	0
All	All	1301/2536 (51%)	0.54	99 (7%) 20 14	46, 85, 114, 130	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	GLY	6.8
2	B	328	GLY	6.7
1	E	435	THR	5.6
1	G	436	PRO	5.6
1	G	447	PRO	4.8
1	C	435	THR	4.8
1	E	447	PRO	4.6
2	D	328	GLY	4.5
2	B	424	GLN	4.5
1	G	435	THR	4.3
2	H	446	ALA	4.2
2	D	446	ALA	3.8
2	F	342	THR	3.8
2	H	366	GLN	3.7
2	B	425	ILE	3.6
2	B	446	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	434	GLY	3.6
2	F	366	GLN	3.5
2	H	342	THR	3.4
2	D	261	LEU	3.4
2	D	342	THR	3.3
2	B	343	LEU	3.3
1	E	433	TRP	3.2
2	D	289	CYS	3.2
1	G	259	PRO	3.2
2	B	249	LEU	3.2
1	G	461	ALA	3.1
1	C	461	ALA	3.0
2	B	261	LEU	3.0
2	H	328	GLY	2.9
2	D	363	ILE	2.9
2	F	249	LEU	2.9
2	H	248	CYS	2.9
2	D	262	GLN	2.8
2	B	344	GLN	2.8
2	B	366	GLN	2.8
1	C	377	LEU	2.8
2	B	342	THR	2.8
2	F	279	ARG	2.8
1	E	263	ARG	2.8
2	B	259	VAL	2.7
1	A	282	GLY	2.7
2	D	249	LEU	2.6
2	H	315	LEU	2.6
2	D	321	PHE	2.6
2	F	286	ALA	2.6
2	B	347	VAL	2.5
2	B	423	ALA	2.5
1	C	259	PRO	2.5
2	B	260	LEU	2.5
2	F	321	PHE	2.5
1	E	431	ARG	2.5
2	B	268	GLN	2.5
1	A	447	PRO	2.4
1	G	434	GLY	2.4
1	G	283	HIS	2.4
1	G	422	LEU	2.4
2	H	249	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	278	CYS	2.4
1	C	434	GLY	2.4
2	D	362	VAL	2.4
2	D	445	GLU	2.4
2	B	429	TRP	2.4
2	D	361	LEU	2.4
1	G	316	ASN	2.4
2	H	279	ARG	2.4
1	G	433	TRP	2.4
2	F	281	VAL	2.3
1	E	432	PRO	2.3
2	B	321	PHE	2.3
2	D	366	GLN	2.3
2	H	280	CYS	2.3
1	A	433	TRP	2.3
2	B	361	LEU	2.3
2	B	284	ALA	2.2
2	D	344	GLN	2.2
2	B	306	TRP	2.2
2	B	256	LEU	2.2
2	B	282	ILE	2.2
2	D	405	ARG	2.2
2	F	446	ALA	2.2
1	A	300	VAL	2.2
1	G	377	LEU	2.2
2	F	289	CYS	2.1
2	F	442	ALA	2.1
1	C	284	ARG	2.1
1	G	263	ARG	2.1
2	F	253	ILE	2.1
2	H	362	VAL	2.1
1	C	433	TRP	2.1
1	C	318	ARG	2.1
1	C	283	HIS	2.0
1	C	447	PRO	2.0
2	H	361	LEU	2.0
2	F	405	ARG	2.0
2	B	363	ILE	2.0
2	B	362	VAL	2.0
2	B	364	VAL	2.0
1	E	259	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

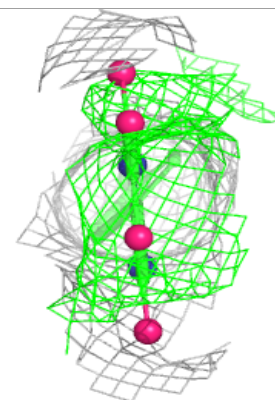
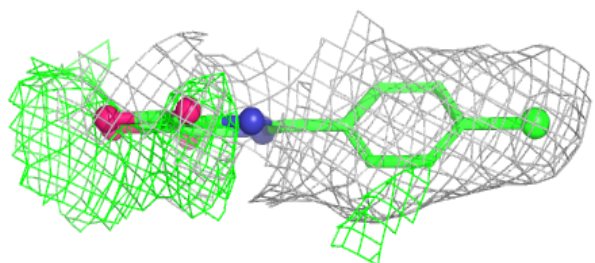
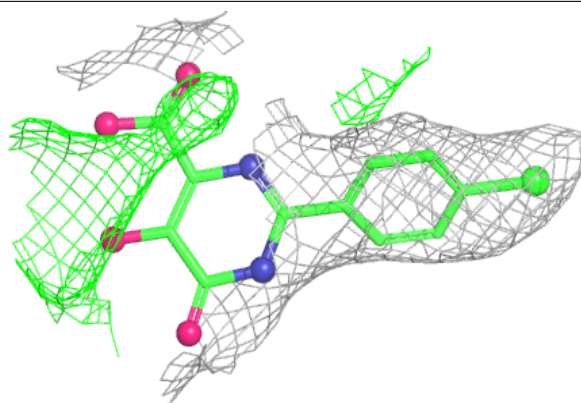
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	602	1/1	0.72	0.32	57,57,57,57	0
3	A1IA5	C	601	18/18	0.94	0.10	72,73,74,74	0
3	A1IA5	G	601	18/18	0.94	0.10	73,75,76,76	0
3	A1IA5	A	601	18/18	0.94	0.11	66,67,67,67	0
3	A1IA5	E	601	18/18	0.95	0.08	63,64,64,65	0
4	MG	E	602	1/1	0.95	0.20	54,54,54,54	0
4	MG	E	603	1/1	0.95	0.08	51,51,51,51	0
4	MG	C	602	1/1	0.96	0.20	57,57,57,57	0
4	MG	C	603	1/1	0.97	0.10	35,35,35,35	0
4	MG	G	602	1/1	0.97	0.13	43,43,43,43	0
4	MG	G	603	1/1	0.97	0.06	49,49,49,49	0
4	MG	A	603	1/1	0.98	0.08	34,34,34,34	0

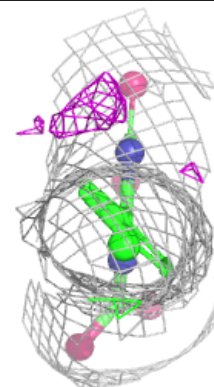
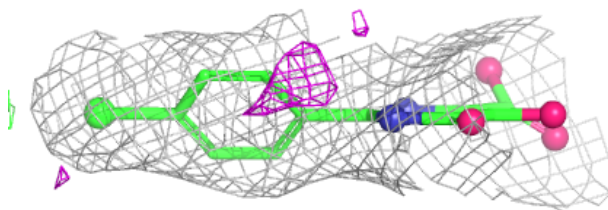
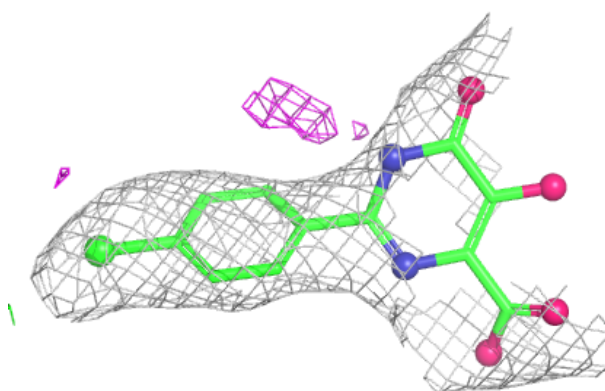
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IA5 C 601:

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

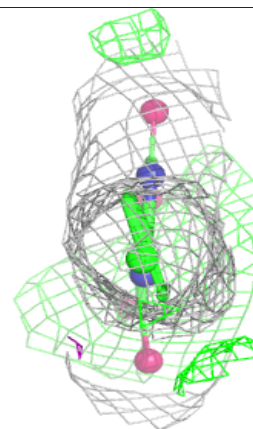
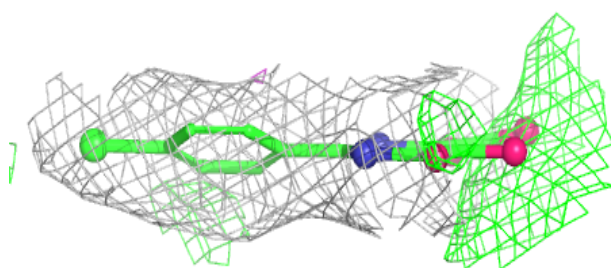
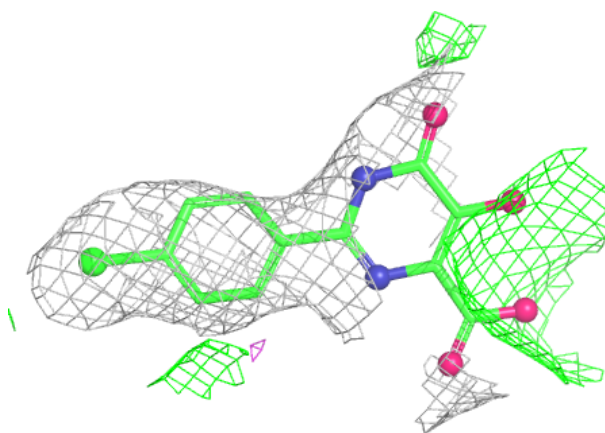
**Electron density around A1IA5 G 601:**

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

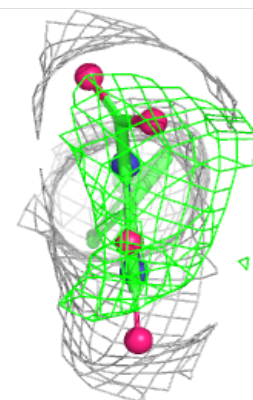
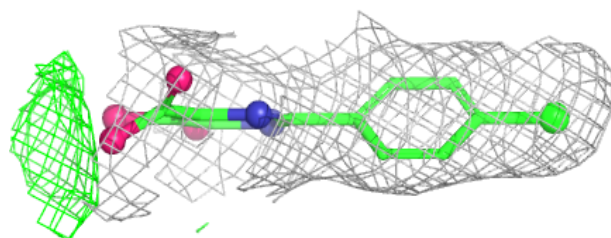
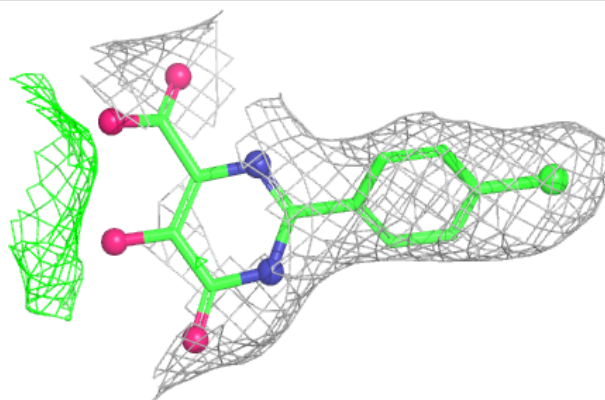


Electron density around A1IA5 A 601:

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

**Electron density around A1IA5 E 601:**

$2mF_o - DF_c$ (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.