



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:16 AM UTC

PDB ID : 9F9A / pdb_00009f9a
Title : Crystal structure of MUS81-EME1 bound by compound 12.
Authors : Collie, G.W.
Deposited on : 2024-05-07
Resolution : 2.91 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

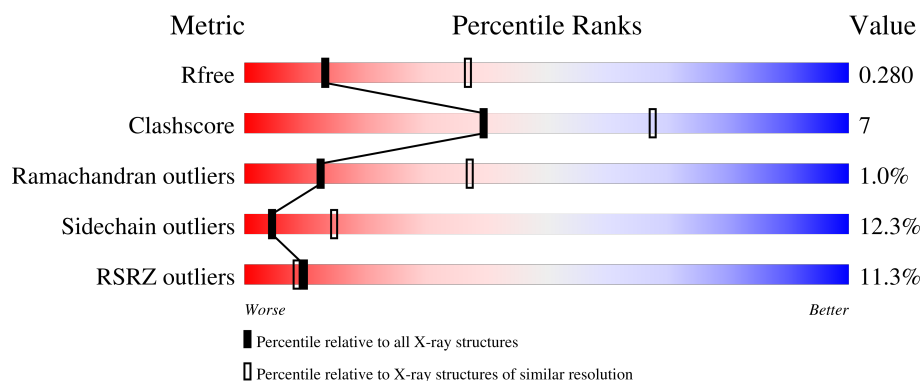
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	4% 48% 10% . 40%
1	C	308	3% 44% 13% . 40%
1	E	308	5% 47% 13% . 39%
1	G	308	3% 42% 15% . 40%
2	B	326	9% 38% . 58%

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Mol	Chain	Length	Quality of chain
2	D	326	
2	F	326	
2	H	326	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10093 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
			1458	924	265	265	4			
1	C	186	Total	C	N	O	S	0	0	0
			1468	929	267	268	4			
1	E	187	Total	C	N	O	S	0	0	0
			1472	933	267	268	4			
1	G	185	Total	C	N	O	S	0	0	0
			1458	924	265	265	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

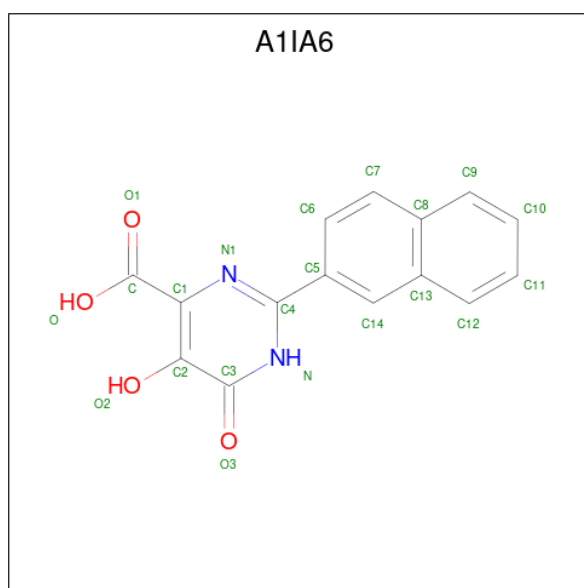
- Molecule 2 is a protein called Crossover junction endonuclease EME1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1031	653	170	200	8			
2	D	139	Total	C	N	O	S	0	0	0
			1045	664	172	201	8			
2	F	139	Total	C	N	O	S	0	0	0
			1045	664	172	201	8			
2	H	137	Total	C	N	O	S	0	0	0
			1024	648	169	199	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-naphthalen-2-yl-5-oxidanyl-6-oxidanylidene-1H-pyrimidine-4-carboxylic acid (CCD ID: A1IA6) (formula: C₁₅H₁₀N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			21	15	2	4		
3	C	1	Total	C	N	O	0	0
			21	15	2	4		
3	E	1	Total	C	N	O	0	0
			21	15	2	4		
3	G	1	Total	C	N	O	0	0
			21	15	2	4		

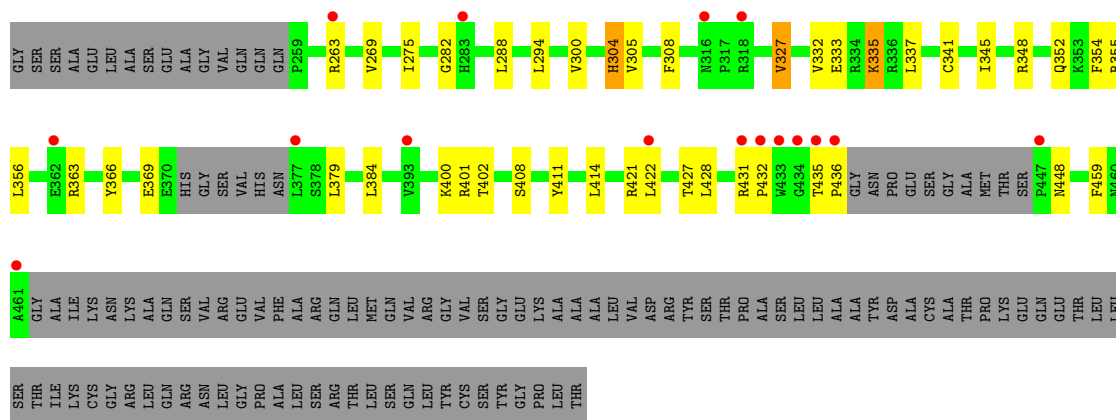
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

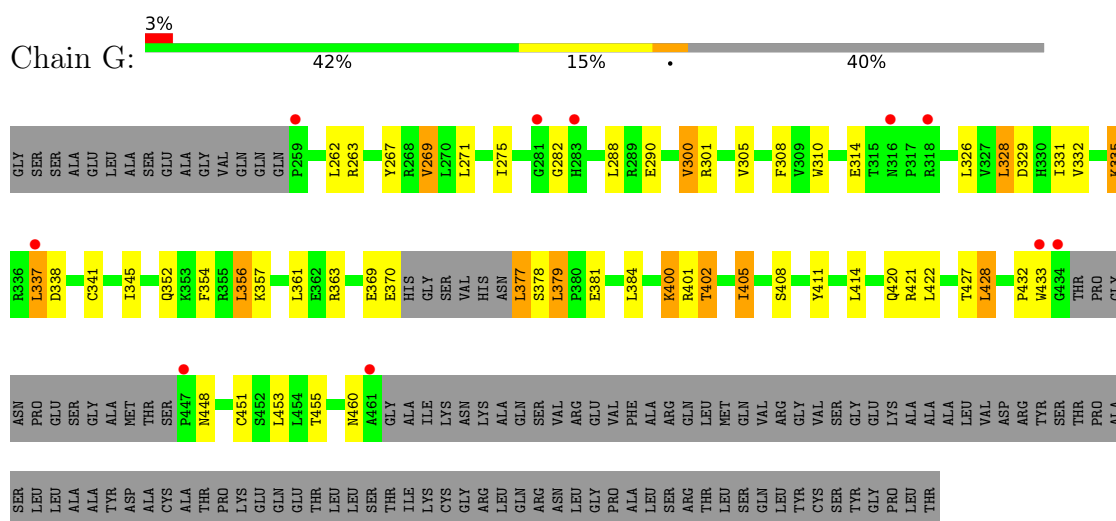
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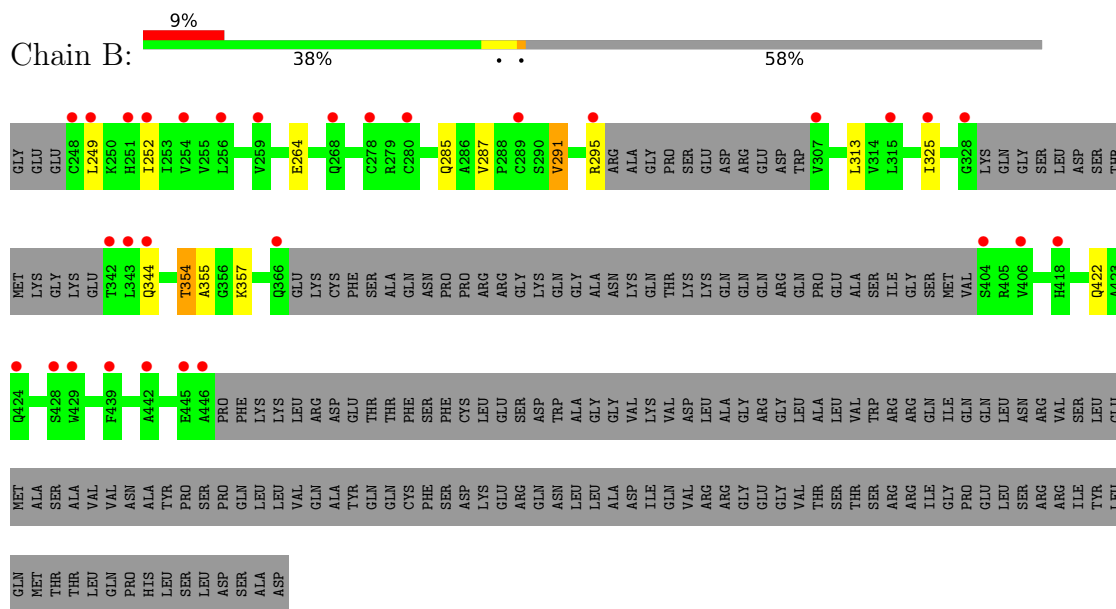
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total 2	Mg 2	0	0
4	G	2	Total 2	Mg 2	0	0



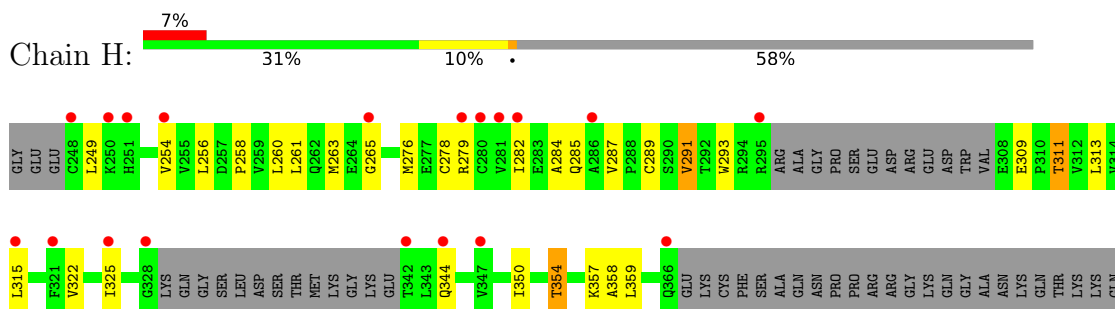
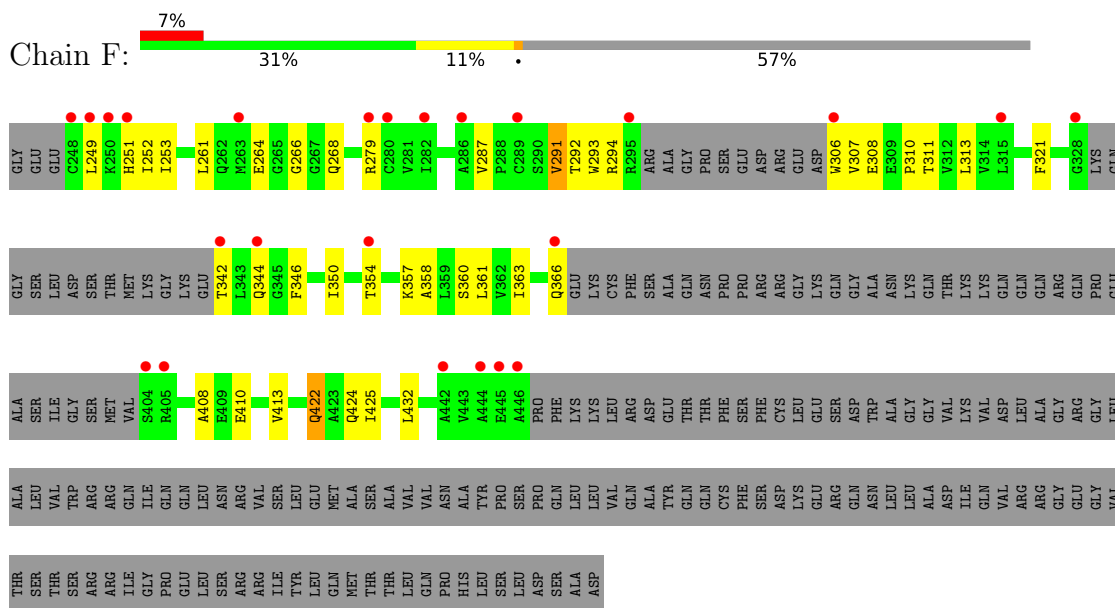
• Molecule 1: Crossover junction endonuclease MUS81

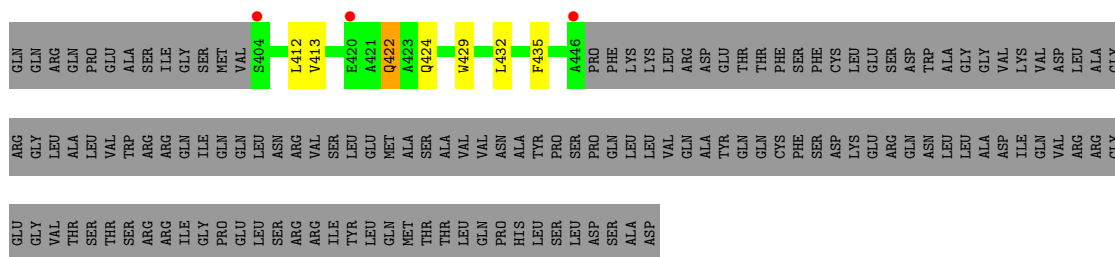


• Molecule 2: Crossover junction endonuclease EME1



• 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	111.87Å 124.35Å 217.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.17 – 2.91 83.17 – 2.91	Depositor EDS
% Data completeness (in resolution range)	60.8 (83.17-2.91) 60.7 (83.17-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.243 , 0.278 0.243 , 0.280	Depositor DCC
R_{free} test set	2051 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10093	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: A1IA6, 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	0.68	0/1486	1.12	4/2014 (0.2%)
1	C	0.71	0/1496	1.18	9/2028 (0.4%)
1	E	0.64	0/1501	1.10	0/2036
1	G	0.66	0/1486	1.09	4/2014 (0.2%)
2	B	0.59	0/1040	1.00	0/1413
2	D	0.65	0/1056	1.14	0/1436
2	F	0.62	0/1056	1.11	0/1436
2	H	0.63	0/1033	1.07	0/1403
All	All	0.65	0/10154	1.11	17/13780 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	LEU	N-CA-C	9.32	122.85	112.97
1	G	328	LEU	N-CA-C	7.29	121.83	113.15
1	A	269	VAL	N-CA-CB	6.16	118.42	111.21
1	A	369	GLU	CA-C-N	5.93	132.38	121.70
1	A	369	GLU	C-N-CA	5.93	132.38	121.70
1	C	327	VAL	CA-C-N	5.57	132.19	121.54
1	C	327	VAL	C-N-CA	5.57	132.19	121.54
1	C	300	VAL	N-CA-CB	5.54	117.69	111.21
1	G	300	VAL	N-CA-CB	5.54	116.76	110.72
1	C	328	LEU	N-CA-C	5.48	122.47	110.80
1	C	407	GLU	CA-C-N	5.46	127.87	120.44
1	C	407	GLU	C-N-CA	5.46	127.87	120.44
1	C	381	GLU	CA-C-N	5.38	127.44	120.44
1	C	381	GLU	C-N-CA	5.38	127.44	120.44
1	G	377	LEU	CA-C-N	5.16	127.71	120.28
1	G	377	LEU	C-N-CA	5.16	127.71	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	298	HIS	N-CA-C	5.03	116.70	108.76

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	1458	0	1446	17	0
1	C	1468	0	1457	17	0
1	E	1472	0	1460	24	0
1	G	1458	0	1446	26	0
2	B	1031	0	1036	3	0
2	D	1045	0	1046	19	0
2	F	1045	0	1046	15	0
2	H	1024	0	1027	20	0
3	A	21	0	0	0	0
3	C	21	0	0	0	0
3	E	21	0	0	0	0
3	G	21	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	10093	0	9964	134	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 (134) 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:304:HIS:CD2	1:C:305:VAL:HG12	2.10	0.85
1:E:335:LYS:NZ	1:E:352:GLN:HE22	1.73	0.84
2:D:258:PRO:HD2	2:D:284:ALA:HA	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:310:PRO:HA	2:D:357:LYS:HG2	1.64	0.78
2:F:253:ILE:HD11	2:F:306:TRP:CE2	2.22	0.75
1:G:308:PHE:HB2	1:G:332:VAL:HB	1.69	0.74
1:G:341:CYS:O	1:G:345:ILE:HG12	1.87	0.74
2:D:258:PRO:CD	2:D:284:ALA:HA	2.16	0.74
1:E:335:LYS:NZ	1:E:352:GLN:NE2	2.35	0.74
2:H:254:VAL:HG22	2:H:293:TRP:CD1	2.27	0.70
2:D:252:ILE:HD11	2:D:293:TRP:CD1	2.27	0.70
2:B:291:VAL:HG13	2:B:313:LEU:HB3	1.74	0.68
2:H:254:VAL:HG22	2:H:293:TRP:NE1	2.08	0.68
2:F:291:VAL:HG13	2:F:313:LEU:HB3	1.76	0.66
1:E:304:HIS:CD2	1:E:305:VAL:HG12	2.31	0.66
1:E:341:CYS:O	1:E:345:ILE:HG12	1.96	0.65
2:H:258:PRO:HD2	2:H:284:ALA:HA	1.78	0.65
1:E:431:ARG:HD3	1:E:435:THR:HA	1.79	0.65
2:D:315:LEU:HD11	2:D:432:LEU:HD11	1.78	0.64
2:H:254:VAL:HG22	2:H:293:TRP:HE1	1.63	0.64
1:E:308:PHE:HB2	1:E:332:VAL:HB	1.81	0.62
1:E:335:LYS:HZ1	1:E:352:GLN:NE2	1.96	0.60
1:E:348:ARG:O	1:E:352:GLN:HG3	2.00	0.60
1:E:414:LEU:HB3	2:F:413:VAL:HG21	1.83	0.60
1:A:364:ARG:NH2	1:A:395:ASP:O	2.35	0.60
1:E:335:LYS:HZ3	1:E:352:GLN:HE22	1.48	0.59
2:D:354:THR:HG23	2:D:357:LYS:H	1.68	0.57
1:E:335:LYS:HZ1	1:E:352:GLN:HE22	1.49	0.57
1:E:335:LYS:HZ3	1:E:352:GLN:NE2	2.01	0.57
2:B:252:ILE:HG13	2:B:295:ARG:HG2	1.86	0.57
1:C:335:LYS:HG3	1:C:366:TYR:OH	2.04	0.57
2:H:315:LEU:HD21	2:H:432:LEU:HD21	1.85	0.57
2:F:363:ILE:HB	2:F:425:ILE:HG12	1.86	0.56
2:D:364:VAL:HG13	2:D:426:VAL:HG23	1.87	0.56
1:G:305:VAL:HG22	1:G:356:LEU:HD12	1.85	0.56
1:G:345:ILE:HD11	1:G:379:LEU:HD13	1.88	0.56
1:C:269:VAL:HG13	1:C:420:GLN:HG2	1.87	0.56
1:A:345:ILE:HD11	1:A:379:LEU:HD13	1.86	0.56
1:E:400:LYS:HG3	1:E:411:TYR:CE1	2.42	0.55
1:E:304:HIS:NE2	1:E:305:VAL:HG12	2.22	0.55
1:G:405:ILE:HD12	1:G:405:ILE:H	1.72	0.54
2:D:252:ILE:HD11	2:D:293:TRP:HD1	1.71	0.52
2:F:346:PHE:O	2:F:350:ILE:HG13	2.09	0.52
1:A:341:CYS:O	1:A:345:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:GLU:HA	1:E:402:THR:HG23	1.92	0.52
1:G:363:ARG:HH21	1:G:448:ASN:HD22	1.56	0.52
1:E:263:ARG:HA	1:E:427:THR:HG23	1.90	0.52
2:H:249:LEU:HD13	2:H:278:CYS:HB3	1.92	0.52
1:C:308:PHE:HB2	1:C:332:VAL:HB	1.91	0.51
2:H:291:VAL:HG13	2:H:313:LEU:HB3	1.92	0.51
1:C:332:VAL:HG22	1:C:365:VAL:HB	1.92	0.51
2:D:292:THR:HG22	2:D:293:TRP:H	1.75	0.51
1:E:363:ARG:NH1	1:E:448:ASN:ND2	2.59	0.51
1:C:287:LEU:HD12	1:C:409:ALA:HB2	1.92	0.50
1:E:333:GLU:HB2	1:E:356:LEU:HD11	1.94	0.50
1:A:297:THR:H	1:C:316:ASN:HD21	1.60	0.49
1:A:305:VAL:HG11	1:A:359:CYS:HB2	1.94	0.49
2:D:261:LEU:HD12	2:D:282:ILE:HG21	1.93	0.49
1:G:363:ARG:HH21	1:G:448:ASN:ND2	2.10	0.49
1:A:335:LYS:HZ1	1:A:352:GLN:HE22	1.60	0.49
1:C:327:VAL:HG22	1:C:361:LEU:HD21	1.95	0.49
2:H:350:ILE:HG21	2:H:359:LEU:HD13	1.95	0.48
1:E:327:VAL:HG11	1:E:459:PHE:HB2	1.94	0.48
1:G:402:THR:HG21	1:G:408:SER:OG	2.14	0.48
2:D:291:VAL:HG13	2:D:313:LEU:HB3	1.96	0.48
2:H:260:LEU:HD11	2:H:315:LEU:HD13	1.96	0.48
1:A:335:LYS:NZ	1:A:352:GLN:NE2	2.62	0.47
1:G:263:ARG:HA	1:G:427:THR:HG23	1.97	0.47
1:A:369:GLU:O	1:A:370:GLU:HB2	2.15	0.47
2:H:260:LEU:HD13	2:H:289:CYS:HA	1.97	0.47
1:A:340:LEU:HD23	1:A:384:LEU:HD12	1.97	0.46
1:C:345:ILE:HD11	1:C:379:LEU:HD13	1.96	0.46
2:D:347:VAL:HG21	2:D:415:LEU:HD11	1.98	0.46
2:F:253:ILE:HB	2:F:294:ARG:HB2	1.98	0.46
2:D:363:ILE:HB	2:D:425:ILE:HG12	1.97	0.46
1:A:338:ASP:HA	1:A:377:LEU:HD21	1.98	0.46
1:C:369:GLU:HA	1:C:402:THR:HG22	1.96	0.46
2:D:315:LEU:HD21	2:D:432:LEU:HD21	1.97	0.46
1:A:335:LYS:NZ	1:A:352:GLN:HE22	2.14	0.46
1:G:269:VAL:HG13	1:G:420:GLN:HG2	1.98	0.46
1:E:354:PHE:HE1	1:E:355:ARG:NH1	2.13	0.45
1:G:428:LEU:HD12	1:G:451:CYS:HA	1.99	0.45
1:C:333:GLU:HB2	1:C:356:LEU:HD21	1.98	0.45
2:H:261:LEU:HD11	2:H:282:ILE:HD12	1.98	0.45
1:G:331:ILE:HB	1:G:361:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369:GLU:O	1:G:370:GLU:HB2	2.17	0.45
1:C:392:GLN:NE2	2:D:422:GLN:HG2	2.32	0.45
2:F:253:ILE:HD11	2:F:306:TRP:CD2	2.51	0.45
1:G:400:LYS:HG3	1:G:411:TYR:CE1	2.51	0.45
1:G:337:LEU:HB3	1:G:377:LEU:HD11	1.98	0.44
1:C:336:ARG:HG3	1:C:369:GLU:HB3	1.98	0.44
1:C:304:HIS:HD2	1:C:305:VAL:HG12	1.76	0.44
2:D:441:LYS:O	2:D:445:GLU:OE2	2.35	0.44
1:E:335:LYS:HG3	1:E:366:TYR:OH	2.18	0.44
2:F:321:PHE:HE2	2:F:408:ALA:HB1	1.82	0.44
1:G:271:LEU:HD13	1:G:310:TRP:NE1	2.33	0.44
1:C:329:ASP:HA	1:C:361:LEU:HG	2.00	0.44
1:G:354:PHE:HA	1:G:357:LYS:HG2	2.00	0.43
1:C:283:HIS:CD2	1:E:436:PRO:HD2	2.53	0.43
1:C:335:LYS:NZ	1:C:352:GLN:HE22	2.17	0.43
2:B:354:THR:OG1	2:B:357:LYS:HD2	2.17	0.43
1:A:317:PRO:HG2	1:A:320:PRO:HA	2.01	0.43
2:D:322:VAL:O	2:D:325:ILE:HG13	2.18	0.43
1:E:327:VAL:HG11	1:E:459:PHE:CB	2.49	0.43
1:G:400:LYS:HG3	1:G:411:TYR:CZ	2.55	0.42
2:H:260:LEU:HD11	2:H:315:LEU:HD22	2.00	0.42
2:H:422:GLN:HE21	2:H:422:GLN:HB2	1.65	0.42
1:A:335:LYS:HZ1	1:A:352:GLN:NE2	2.17	0.42
2:H:256:LEU:HD22	2:H:260:LEU:HD23	2.01	0.42
2:F:308:GLU:CD	2:F:357:LYS:HZ3	2.27	0.42
2:F:354:THR:HG23	2:F:357:LYS:H	1.85	0.42
1:G:369:GLU:HA	1:G:402:THR:HG22	2.00	0.42
2:F:311:THR:HG23	2:F:358:ALA:HB3	2.01	0.42
1:A:287:LEU:HD12	1:A:409:ALA:HB2	2.02	0.42
1:E:400:LYS:HG3	1:E:411:TYR:CZ	2.55	0.42
2:F:310:PRO:HA	2:F:357:LYS:HG2	2.02	0.41
2:H:354:THR:HG23	2:H:357:LYS:H	1.85	0.41
1:A:423:TYR:CZ	1:A:449:PRO:HB2	2.56	0.41
2:D:310:PRO:CA	2:D:357:LYS:HG2	2.42	0.41
2:F:261:LEU:HA	2:F:266:GLY:HA3	2.03	0.41
2:H:265:GLY:HA3	2:H:429:TRP:CD2	2.55	0.41
2:H:311:THR:HG23	2:H:358:ALA:HB3	2.02	0.41
2:H:322:VAL:O	2:H:325:ILE:HG13	2.20	0.41
1:G:262:LEU:HD22	1:G:267:TYR:HB3	2.02	0.41
1:G:335:LYS:NZ	1:G:352:GLN:HE22	2.18	0.41
2:F:292:THR:HG22	2:F:293:TRP:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:326:LEU:HB3	1:G:453:LEU:HB2	2.01	0.41
1:A:283:HIS:CE1	1:G:329:ASP:OD1	2.74	0.41
1:G:414:LEU:HB3	2:H:413:VAL:HG21	2.02	0.41
1:A:400:LYS:HG3	1:A:411:TYR:CZ	2.55	0.41
2:D:260:LEU:HD11	2:D:315:LEU:HD22	2.03	0.41
1:G:401:ARG:HH22	2:H:435:PHE:HE1	1.68	0.41
1:G:267:TYR:HA	1:G:314:GLU:HA	2.02	0.40
2:F:422:GLN:HE21	2:F:422:GLN:HB2	1.56	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	179/308 (58%)	172 (96%)	5 (3%)	2 (1%)	11	35
1	C	180/308 (58%)	169 (94%)	10 (6%)	1 (1%)	21	50
1	E	181/308 (59%)	172 (95%)	7 (4%)	2 (1%)	11	35
1	G	179/308 (58%)	164 (92%)	13 (7%)	2 (1%)	11	35
2	B	130/326 (40%)	125 (96%)	4 (3%)	1 (1%)	16	43
2	D	131/326 (40%)	121 (92%)	7 (5%)	3 (2%)	5	18
2	F	131/326 (40%)	118 (90%)	12 (9%)	1 (1%)	16	43
2	H	129/326 (40%)	121 (94%)	8 (6%)	0	100	100
All	All	1240/2536 (49%)	1162 (94%)	66 (5%)	12 (1%)	12	37

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	432	PRO
1	A	282	GLY

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Mol	Chain	Res	Type
2	D	307	VAL
1	E	282	GLY
1	E	432	PRO
1	A	432	PRO
2	F	307	VAL
1	G	432	PRO
2	B	355	ALA
1	G	282	GLY
2	D	445	GLU
2	D	282	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	156/260 (60%)	144 (92%)	12 (8%)	12	34
1	C	158/260 (61%)	133 (84%)	25 (16%)	2	8
1	E	158/260 (61%)	142 (90%)	16 (10%)	7	23
1	G	156/260 (60%)	132 (85%)	24 (15%)	2	9
2	B	111/275 (40%)	102 (92%)	9 (8%)	11	31
2	D	112/275 (41%)	96 (86%)	16 (14%)	3	10
2	F	112/275 (41%)	95 (85%)	17 (15%)	3	9
2	H	110/275 (40%)	97 (88%)	13 (12%)	5	16
All	All	1073/2140 (50%)	941 (88%)	132 (12%)	4	15

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

Mol	Chain	Res	Type
1	A	269	VAL
1	A	275	ILE
1	A	279	ARG
1	A	288	LEU
1	A	300	VAL

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Mol	Chain	Res	Type
1	A	343	SER
1	A	355	ARG
1	A	370	GLU
1	A	384	LEU
1	A	400	LYS
1	A	402	THR
1	A	422	LEU
2	B	249	LEU
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
1	C	269	VAL
1	C	275	ILE
1	C	288	LEU
1	C	299	THR
1	C	300	VAL
1	C	304	HIS
1	C	315	THR
1	C	328	LEU
1	C	335	LYS
1	C	351	GLU
1	C	355	ARG
1	C	356	LEU
1	C	358	ARG
1	C	377	LEU
1	C	384	LEU
1	C	400	LYS
1	C	401	ARG
1	C	402	THR
1	C	405	ILE
1	C	408	SER
1	C	417	ARG
1	C	422	LEU
1	C	426	HIS
1	C	433	TRP
1	C	448	ASN
2	D	249	LEU

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Mol	Chain	Res	Type
2	D	252	ILE
2	D	260	LEU
2	D	287	VAL
2	D	291	VAL
2	D	315	LEU
2	D	319	GLU
2	D	344	GLN
2	D	354	THR
2	D	361	LEU
2	D	364	VAL
2	D	406	VAL
2	D	410	GLU
2	D	422	GLN
2	D	424	GLN
2	D	445	GLU
1	E	269	VAL
1	E	275	ILE
1	E	288	LEU
1	E	294	LEU
1	E	300	VAL
1	E	304	HIS
1	E	327	VAL
1	E	335	LYS
1	E	337	LEU
1	E	379	LEU
1	E	384	LEU
1	E	401	ARG
1	E	408	SER
1	E	421	ARG
1	E	422	LEU
1	E	428	LEU
2	F	249	LEU
2	F	251	HIS
2	F	252	ILE
2	F	264	GLU
2	F	268	GLN
2	F	279	ARG
2	F	287	VAL
2	F	291	VAL
2	F	342	THR
2	F	344	GLN
2	F	360	SER

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Mol	Chain	Res	Type
2	F	361	LEU
2	F	366	GLN
2	F	410	GLU
2	F	422	GLN
2	F	424	GLN
2	F	432	LEU
1	G	269	VAL
1	G	275	ILE
1	G	288	LEU
1	G	290	GLU
1	G	300	VAL
1	G	301	ARG
1	G	328	LEU
1	G	335	LYS
1	G	337	LEU
1	G	338	ASP
1	G	356	LEU
1	G	378	SER
1	G	379	LEU
1	G	381	GLU
1	G	384	LEU
1	G	400	LYS
1	G	402	THR
1	G	405	ILE
1	G	421	ARG
1	G	422	LEU
1	G	428	LEU
1	G	433	TRP
1	G	455	THR
1	G	460	ASN
2	H	263	MET
2	H	276	MET
2	H	279	ARG
2	H	285	GLN
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	412	LEU
2	H	422	GLN

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Mol	Chain	Res	Type
2	H	424	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	HIS
1	A	295	HIS
1	A	304	HIS
1	A	322	ASN
1	A	352	GLN
1	A	392	GLN
1	A	448	ASN
2	B	344	GLN
1	C	283	HIS
1	C	304	HIS
1	C	316	ASN
1	C	352	GLN
1	C	392	GLN
1	C	448	ASN
2	D	416	GLN
1	E	352	GLN
1	E	392	GLN
1	E	448	ASN
1	G	330	HIS
1	G	352	GLN
1	G	448	ASN
2	H	251	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	A1IA6	E	601	4	21,23,23	0.35	0	26,33,33	0.45	0
3	A1IA6	G	601	4	21,23,23	0.26	0	26,33,33	0.41	0
3	A1IA6	A	601	4	21,23,23	0.35	0	26,33,33	0.45	0
3	A1IA6	C	601	4	21,23,23	0.25	0	26,33,33	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	A1IA6	E	601	4	-	3/8/8/8	0/3/3/3
3	A1IA6	G	601	4	-	5/8/8/8	0/3/3/3
3	A1IA6	A	601	4	-	1/8/8/8	0/3/3/3
3	A1IA6	C	601	4	-	3/8/8/8	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	601	A1IA6	N-C4-C5-C14
3	G	601	A1IA6	N-C4-C5-C6
3	G	601	A1IA6	N1-C4-C5-C6
3	G	601	A1IA6	N1-C4-C5-C14
3	G	601	A1IA6	O1-C-C1-N1
3	C	601	A1IA6	N-C4-C5-C6
3	E	601	A1IA6	N-C4-C5-C6

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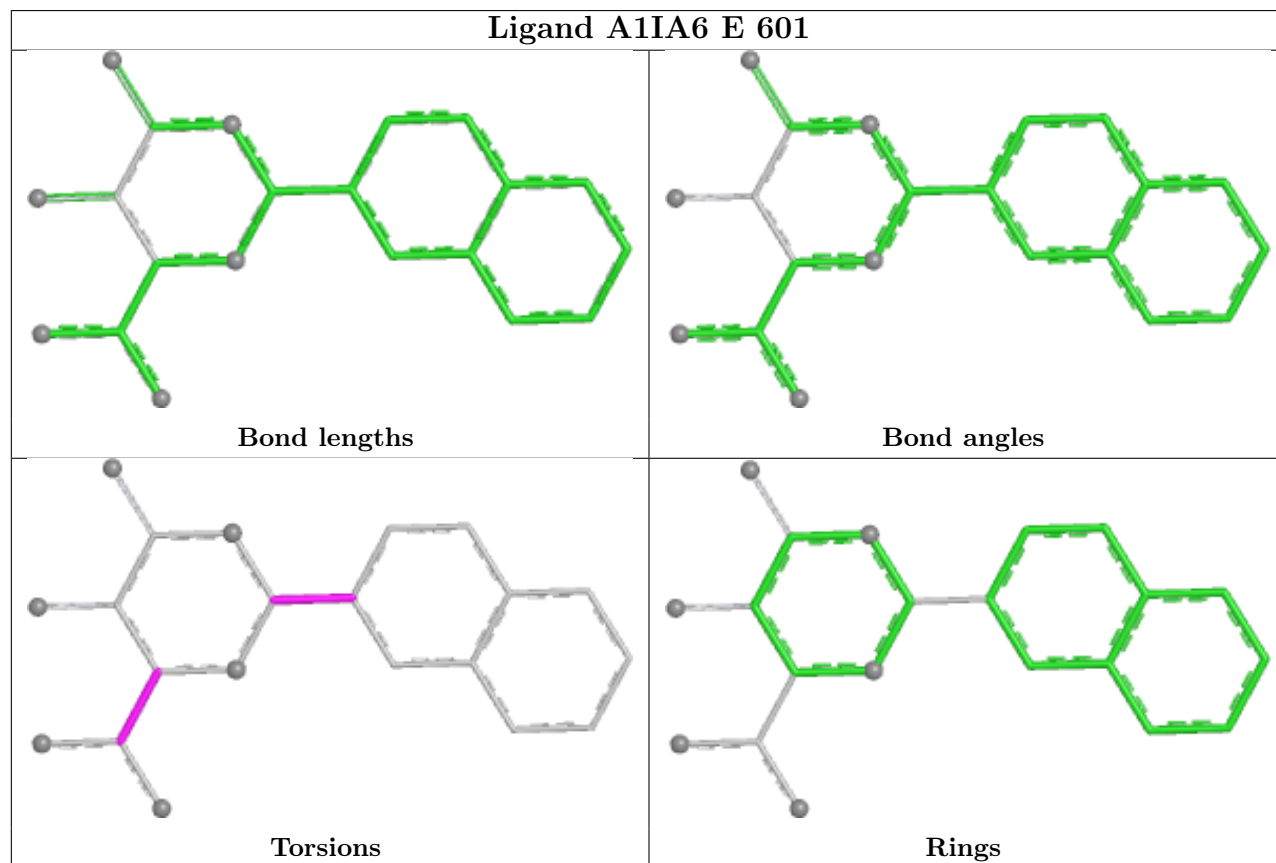
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Mol	Chain	Res	Type	Atoms
3	C	601	A1IA6	O1-C-C1-C2
3	C	601	A1IA6	N-C4-C5-C14
3	E	601	A1IA6	N-C4-C5-C14
3	A	601	A1IA6	O1-C-C1-N1
3	E	601	A1IA6	O1-C-C1-N1

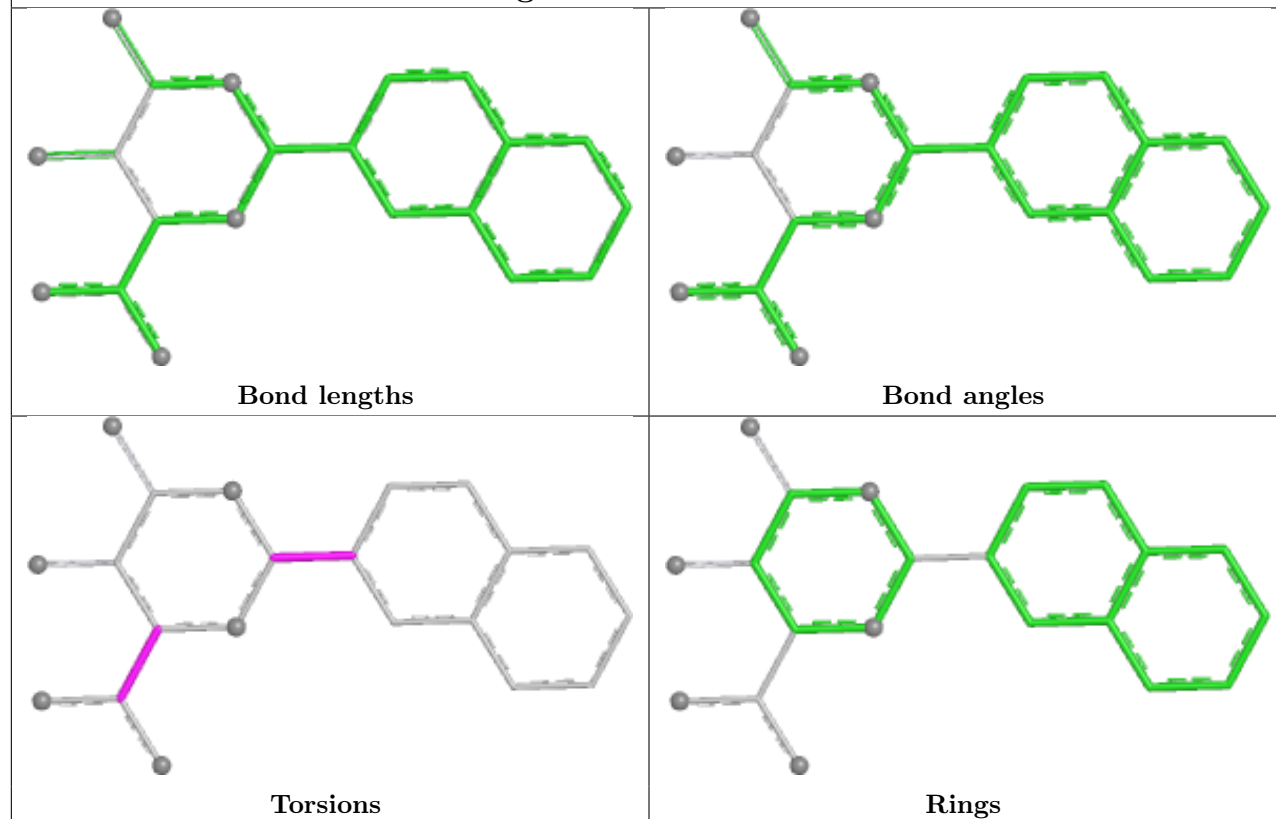
There are no ring outliers.

No monomer is involved in short contacts.

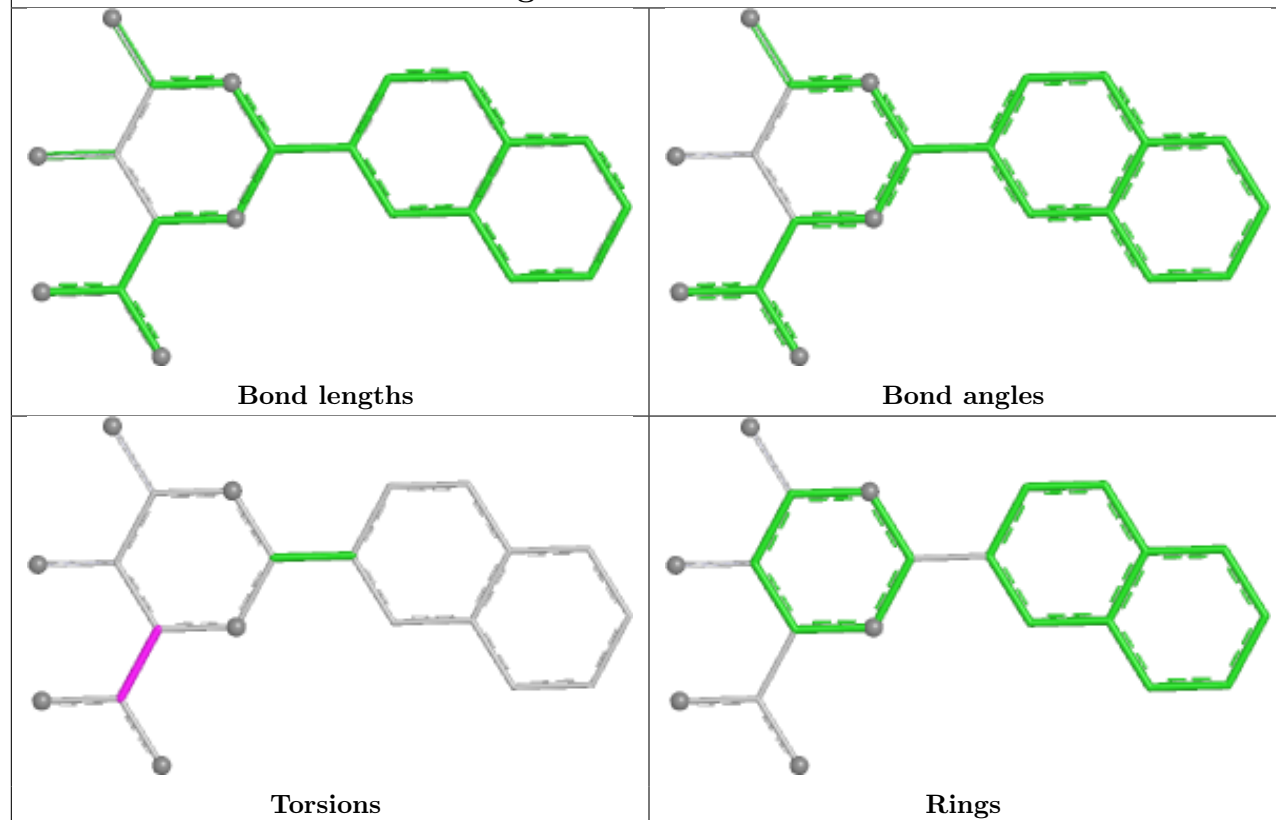
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

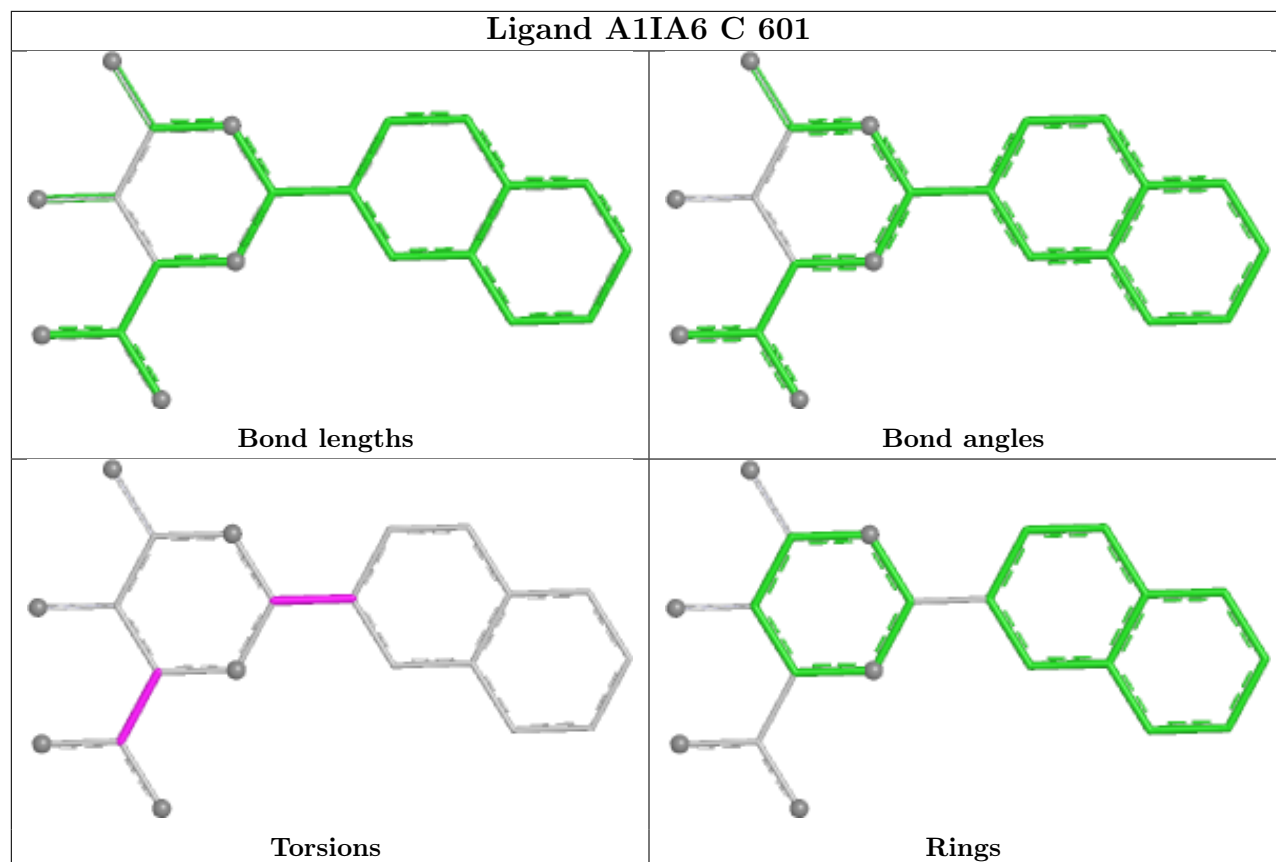


Ligand A1IA6 G 601



Ligand A1IA6 A 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%)	0.38	12 (6%) 25 20	35, 57, 80, 88	0
1	C	186/308 (60%)	0.34	9 (4%) 35 28	39, 58, 76, 82	0
1	E	187/308 (60%)	0.58	16 (8%) 16 13	40, 67, 93, 101	0
1	G	185/308 (60%)	0.60	10 (5%) 31 24	43, 70, 95, 101	0
2	B	138/326 (42%)	1.48	30 (21%) 2 2	66, 87, 111, 122	0
2	D	139/326 (42%)	1.10	23 (16%) 4 3	60, 85, 104, 108	0
2	F	139/326 (42%)	1.07	24 (17%) 4 3	62, 87, 104, 109	0
2	H	137/326 (42%)	1.07	22 (16%) 4 4	64, 90, 106, 113	0
All	All	1296/2536 (51%)	0.78	146 (11%) 10 8	35, 76, 102, 122	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	434	GLY	7.2
1	G	434	GLY	6.7
1	E	435	THR	6.0
2	B	328	GLY	5.8
1	E	447	PRO	5.7
2	D	328	GLY	5.3
1	E	434	GLY	5.2
2	B	249	LEU	4.6
2	H	248	CYS	4.4
2	H	420	GLU	4.2
2	D	342	THR	4.0
2	F	342	THR	4.0
2	H	366	GLN	4.0
1	A	316	ASN	4.0
2	F	279	ARG	4.0
2	H	279	ARG	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	276	MET	3.9
2	B	342	THR	3.9
2	H	280	CYS	3.8
2	H	342	THR	3.8
1	A	447	PRO	3.7
1	G	259	PRO	3.6
1	E	433	TRP	3.6
2	F	366	GLN	3.5
2	B	366	GLN	3.5
2	B	446	ALA	3.5
1	A	448	ASN	3.4
1	C	390	ASN	3.3
1	G	447	PRO	3.3
1	G	281	GLY	3.3
2	D	445	GLU	3.3
2	D	278	CYS	3.3
2	D	366	GLN	3.3
2	B	429	TRP	3.3
2	H	282	ILE	3.2
2	F	249	LEU	3.2
2	B	344	GLN	3.2
2	F	286	ALA	3.1
2	F	344	GLN	3.1
1	C	447	PRO	3.1
1	C	461	ALA	3.1
1	A	259	PRO	3.1
1	C	435	THR	3.1
2	F	251	HIS	3.1
2	B	259	VAL	3.1
2	B	307	VAL	3.1
2	H	254	VAL	3.0
1	G	318	ARG	3.0
2	F	445	GLU	3.0
1	E	318	ARG	3.0
2	F	328	GLY	3.0
1	G	283	HIS	3.0
2	B	278	CYS	2.9
2	D	289	CYS	2.9
2	H	446	ALA	2.9
2	H	344	GLN	2.9
2	D	279	ARG	2.9
1	E	316	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	263	ARG	2.9
2	B	404	SER	2.9
2	F	248	CYS	2.8
2	D	263	MET	2.8
2	H	404	SER	2.8
2	B	424	GLN	2.7
2	B	428	SER	2.7
2	B	248	CYS	2.7
2	F	250	LYS	2.7
1	G	316	ASN	2.7
2	D	446	ALA	2.7
2	F	280	CYS	2.7
2	F	295	ARG	2.7
2	H	281	VAL	2.7
2	B	280	CYS	2.6
2	H	286	ALA	2.6
2	B	295	ARG	2.6
2	F	289	CYS	2.6
2	B	406	VAL	2.6
2	D	286	ALA	2.6
2	F	442	ALA	2.6
2	D	429	TRP	2.6
2	H	328	GLY	2.5
2	F	282	ILE	2.5
2	F	444	ALA	2.5
2	F	446	ALA	2.5
1	E	436	PRO	2.5
2	D	249	LEU	2.5
1	E	362	GLU	2.5
1	C	259	PRO	2.5
2	B	325	ILE	2.5
2	D	405	ARG	2.5
1	E	432	PRO	2.5
2	B	439	PHE	2.4
2	F	354	THR	2.4
2	H	325	ILE	2.4
2	B	445	GLU	2.4
2	B	256	LEU	2.4
1	C	433	TRP	2.4
2	D	362	VAL	2.4
2	D	344	GLN	2.4
1	C	377	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	315	LEU	2.3
2	B	268	GLN	2.3
1	G	433	TRP	2.3
2	D	404	SER	2.3
1	C	318	ARG	2.3
1	A	420	GLN	2.3
2	D	424	GLN	2.3
2	F	315	LEU	2.3
1	E	283	HIS	2.3
2	B	251	HIS	2.3
1	E	431	ARG	2.3
2	B	254	VAL	2.3
2	H	315	LEU	2.3
2	H	250	LYS	2.2
2	D	348	THR	2.2
2	D	321	PHE	2.2
1	E	422	LEU	2.2
2	D	420	GLU	2.2
1	A	381	GLU	2.2
1	G	461	ALA	2.2
2	F	306	TRP	2.2
2	H	265	GLY	2.2
2	B	289	CYS	2.2
2	F	404	SER	2.2
1	A	421	ARG	2.1
1	E	377	LEU	2.1
1	G	337	LEU	2.1
2	B	343	LEU	2.1
2	B	252	ILE	2.1
1	A	377	LEU	2.1
2	H	321	PHE	2.1
2	H	295	ARG	2.1
2	H	251	HIS	2.1
1	A	451	CYS	2.1
1	C	378	SER	2.1
1	E	393	VAL	2.1
2	D	265	GLY	2.1
2	D	345	GLY	2.1
1	A	318	ARG	2.1
2	B	418	HIS	2.0
1	E	461	ALA	2.0
2	B	442	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	263	MET	2.0
1	A	393	VAL	2.0
2	H	347	VAL	2.0
2	F	405	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

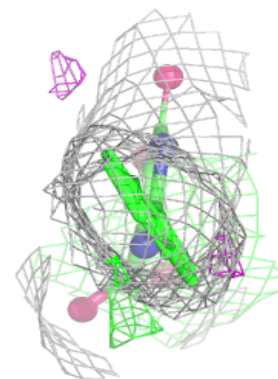
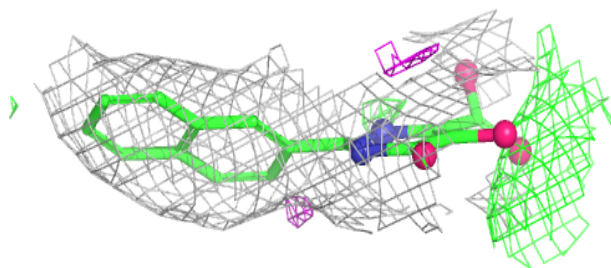
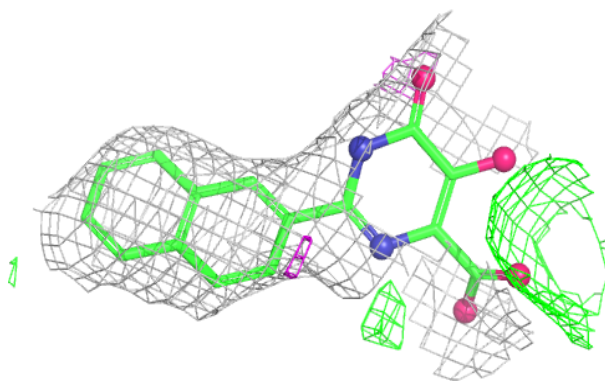
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	A1IA6	A	601	21/21	0.92	0.12	53,54,54,54	0
4	MG	C	602	1/1	0.93	0.17	51,51,51,51	0
3	A1IA6	C	601	21/21	0.94	0.12	66,67,67,67	0
3	A1IA6	G	601	21/21	0.95	0.10	61,62,64,64	0
4	MG	A	602	1/1	0.95	0.20	37,37,37,37	0
3	A1IA6	E	601	21/21	0.95	0.10	60,61,63,63	0
4	MG	C	603	1/1	0.97	0.07	38,38,38,38	0
4	MG	E	603	1/1	0.97	0.10	29,29,29,29	0
4	MG	G	602	1/1	0.97	0.10	42,42,42,42	0
4	MG	E	602	1/1	0.98	0.16	33,33,33,33	0
4	MG	A	603	1/1	0.99	0.08	27,27,27,27	0
4	MG	G	603	1/1	0.99	0.04	24,24,24,24	0

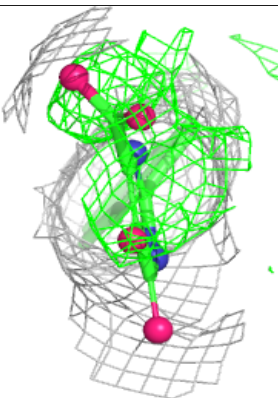
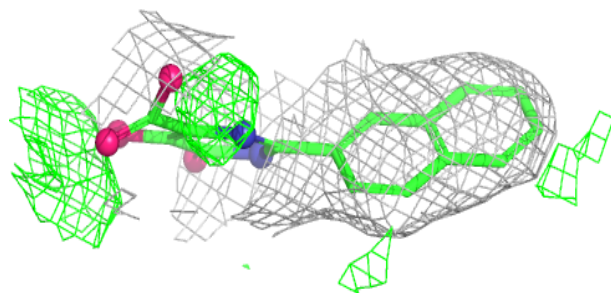
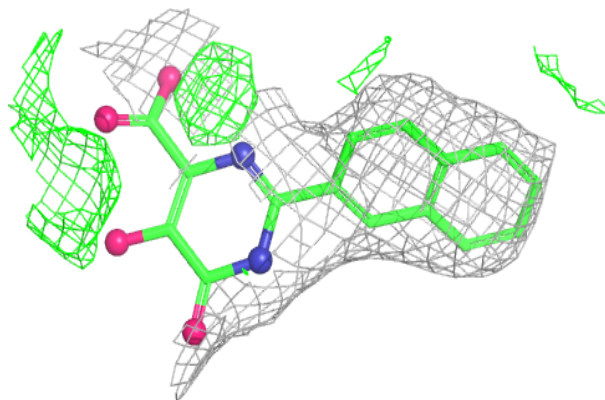
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IA6 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)

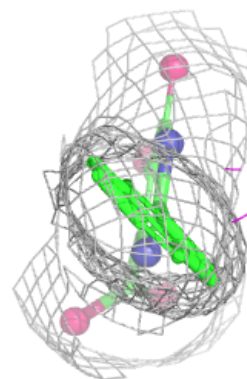
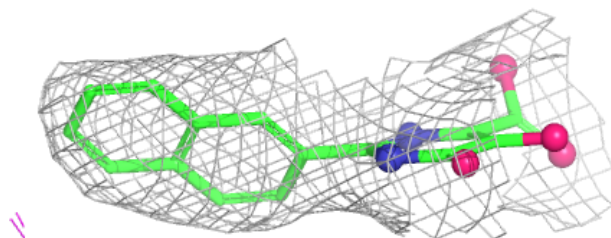
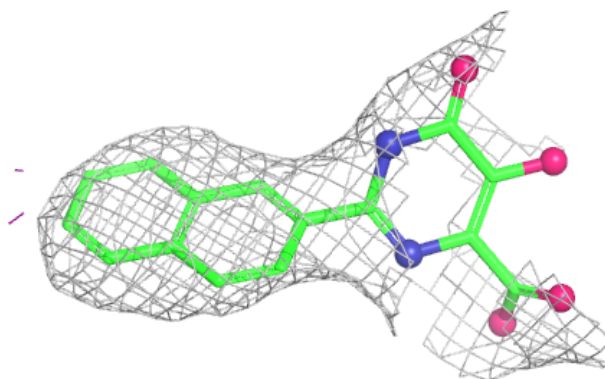
**Electron density around A1IA6 C 601:**

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

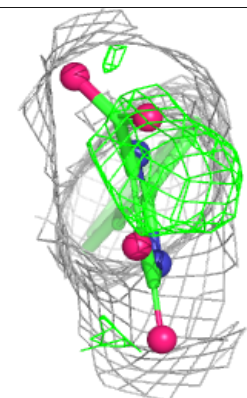
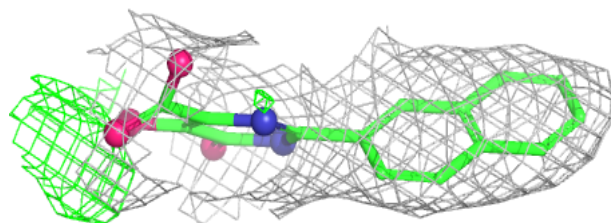
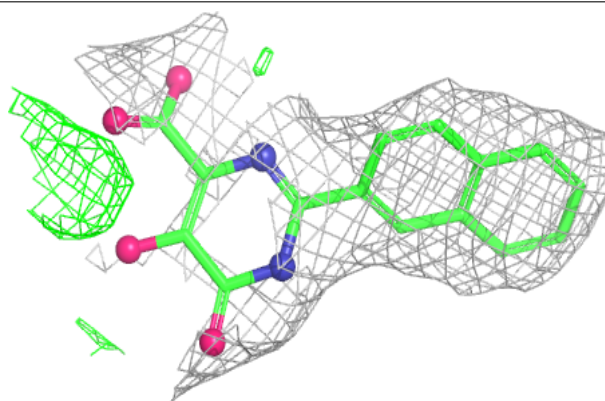


Electron density around A1IA6 G 601:

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

**Electron density around A1IA6 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.