Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2025 – 10:31 AM EST

PDB ID	:	9MJG
Title	:	Crystal structure of HAT1 in complex with XS380871
Authors	:	Zeng, H.; Li, F.; Wang, X.; Sun, J.; Dong, A.; Peng, H.; Arrowsmith, C.H.; Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium (SGC)
Deposited on	:	2024-12-15
Resolution	:	2.58 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 (i) 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 (i)) were used in the production of this report:

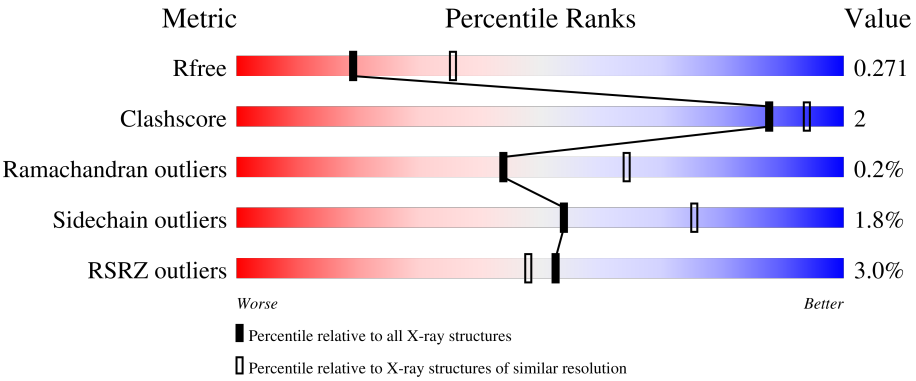
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.58 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}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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 <=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	322	92% 5%
1	B	322	4% 91% 7%
1	C	322	3% 91% 6%
1	D	322	3% 95%
1	E	322	2% 92% 5%

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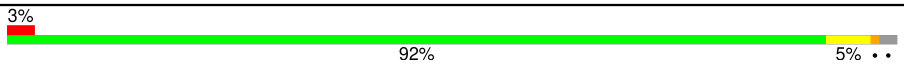
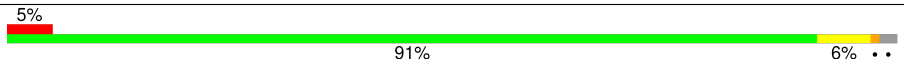
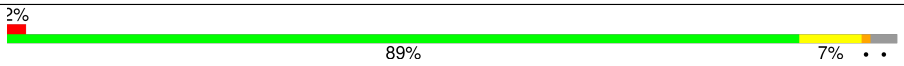
Mol	Chain	Length	Quality of chain
1	F	322	
1	G	322	
1	H	322	

2 Entry composition (i)

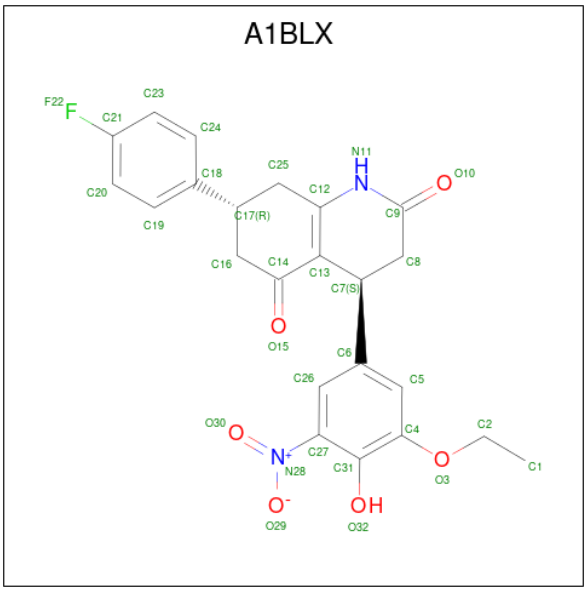
There are 3 unique types of molecules in this entry. The entry contains 20479 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Histone acetyltransferase type B catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2541	1653	401	474	13			
1	B	315	Total	C	N	O	S	0	0	0
			2507	1636	396	463	12			
1	C	313	Total	C	N	O	S	0	0	0
			2507	1634	402	459	12			
1	D	318	Total	C	N	O	S	0	0	0
			2528	1639	401	475	13			
1	E	311	Total	C	N	O	S	0	1	0
			2513	1638	396	467	12			
1	F	314	Total	C	N	O	S	0	2	0
			2518	1638	402	466	12			
1	G	314	Total	C	N	O	S	0	2	0
			2516	1631	403	468	14			
1	H	313	Total	C	N	O	S	0	2	0
			2500	1627	399	462	12			

- Molecule 2 is (4S,7R)-4-(3-ethoxy-4-hydroxy-5-nitrophenyl)-7-(4-fluorophenyl)-4,6,7,8-tetrahydroquinoline-2,5(1H,3H)-dione (three-letter code: A1BLX) (formula: $C_{23}H_{21}FN_2O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			32	23	1	2	6		
2	B	1	Total	C	F	N	O	0	0
			32	23	1	2	6		
2	C	1	Total	C	F	N	O	0	0
			32	23	1	2	6		
2	D	1	Total	C	F	N	O	0	0
			32	23	1	2	6		
2	E	1	Total	C	F	N	O	0	0
			32	23	1	2	6		
2	F	1	Total	C	F	N	O	0	0
			32	23	1	2	6		
2	G	1	Total	C	F	N	O	0	0
			32	23	1	2	6		
2	H	1	Total	C	F	N	O	0	0
			32	23	1	2	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	1
			21	21		
3	B	10	Total	O	0	0
			10	10		
3	C	9	Total	O	0	0
			9	9		
3	D	17	Total	O	0	0
			17	17		

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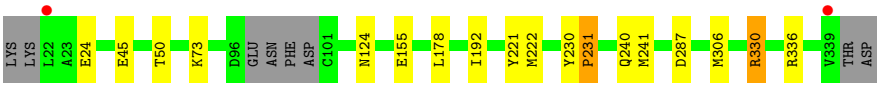
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	12	Total O 12 12	0	0
3	F	9	Total O 9 9	0	0
3	G	6	Total O 6 6	0	0
3	H	9	Total O 9 9	0	0

3 Residue-property plots (i)

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

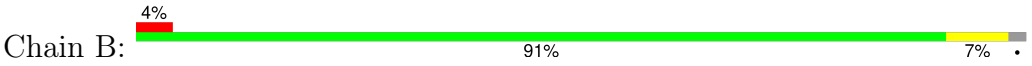
• Molecule 1: Histone acetyltransferase type B catalytic subunit

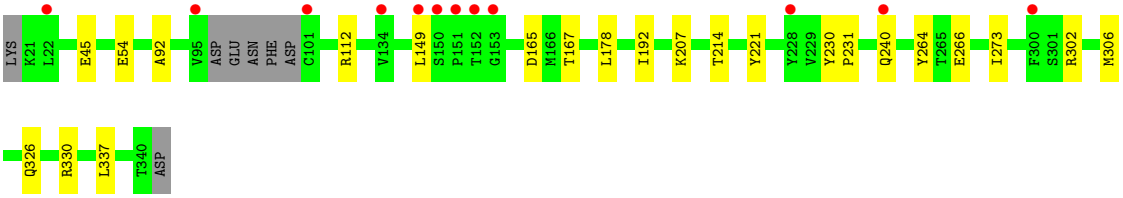
Chain A:



• Molecule 1: Histone acetyltransferase type B catalytic subunit

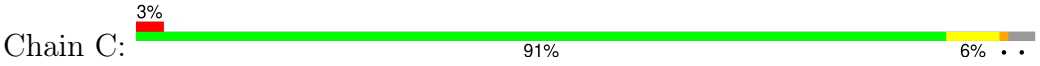
Chain B:

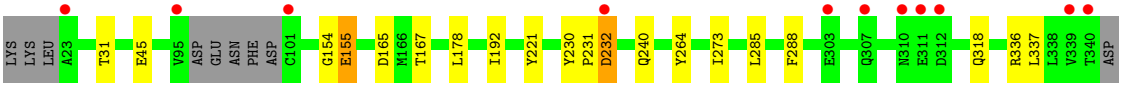




• Molecule 1: Histone acetyltransferase type B catalytic subunit

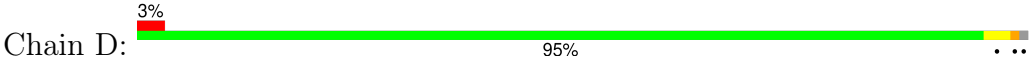
Chain C:





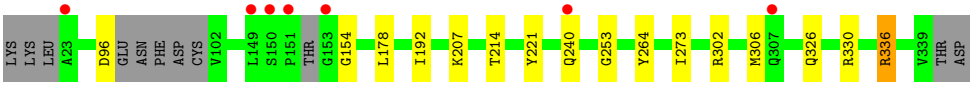
• Molecule 1: Histone acetyltransferase type B catalytic subunit

Chain D:

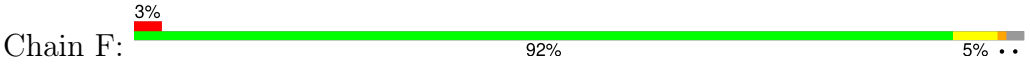


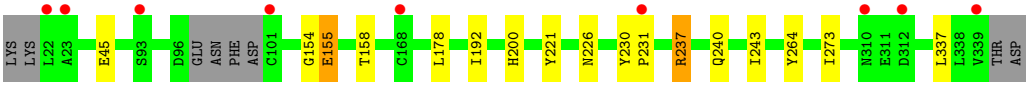
• Molecule 1: Histone acetyltransferase type B catalytic subunit

Chain E:

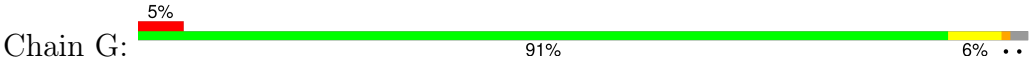


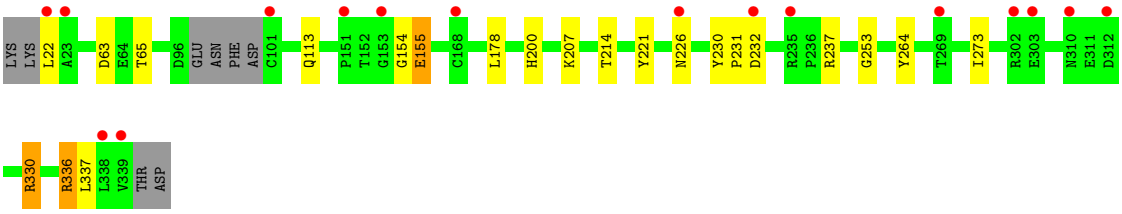
• Molecule 1: Histone acetyltransferase type B catalytic subunit



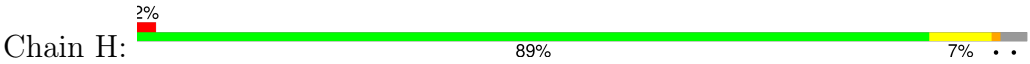


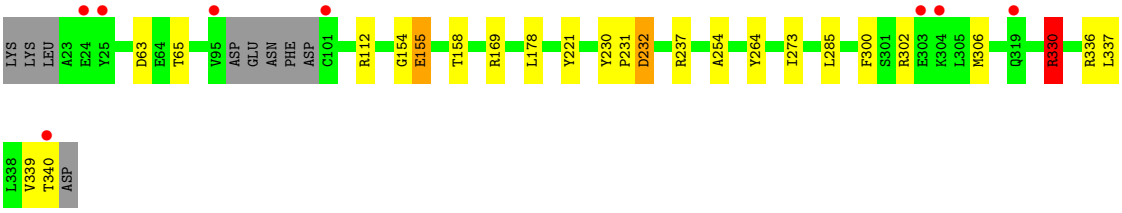
• Molecule 1: Histone acetyltransferase type B catalytic subunit





• Molecule 1: Histone acetyltransferase type B catalytic subunit





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.89Å 87.84Å 118.03Å 84.38° 80.07° 76.76°	Depositor
Resolution (Å)	49.45 – 2.58 49.45 – 2.58	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.45-2.58) 96.1 (49.45-2.58)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.235 , 0.270 0.236 , 0.271	Depositor DCC
R_{free} test set	4754 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20479	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A1BLX

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	0.37	0/2607	0.66	0/3536
1	B	0.37	0/2573	0.70	3/3498 (0.1%)
1	C	0.36	0/2573	0.64	0/3495
1	D	0.36	0/2595	0.66	0/3526
1	E	0.36	0/2578	0.69	0/3498
1	F	0.35	0/2584	0.67	1/3514 (0.0%)
1	G	0.34	0/2582	0.65	1/3509 (0.0%)
1	H	0.36	0/2564	0.66	0/3485
All	All	0.36	0/20656	0.67	5/28061 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	2
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	266	GLU	CB-CG-CD	-7.29	94.53	114.20
1	F	237	ARG	CG-CD-NE	6.02	124.43	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	54	GLU	CG-CD-OE2	5.32	128.94	118.30
1	B	54	GLU	CG-CD-OE1	-5.28	107.75	118.30
1	G	237	ARG	CB-CG-CD	5.03	124.67	111.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ARG	Sidechain
1	B	112	ARG	Sidechain
1	E	336	ARG	Sidechain
1	F	237	ARG	Sidechain
1	G	336	ARG	Sidechain
1	H	237	ARG	Sidechain
1	H	330	ARG	Sidechain

5.2 Too-close contacts (i)

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	2541	0	2403	9	0
1	B	2507	0	2337	8	0
1	C	2507	0	2356	14	0
1	D	2528	0	2334	11	0
1	E	2513	0	2352	9	0
1	F	2518	0	2343	9	0
1	G	2516	0	2326	11	0
1	H	2500	0	2321	18	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
2	E	32	0	0	1	0
2	F	32	0	0	1	0
2	G	32	0	0	1	0
2	H	32	0	0	0	0
3	A	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	0	0	0
3	C	9	0	0	0	0
3	D	17	0	0	0	0
3	E	12	0	0	0	0
3	F	9	0	0	1	0
3	G	6	0	0	0	0
3	H	9	0	0	0	0
All	All	20479	0	18772	76	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 2.

All (76) 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:H:300:PHE:CD1	1:H:300:PHE:CZ	2.41	0.95
1:C:285:LEU:HD13	1:D:230:TYR:OH	1.90	0.72
1:E:330:ARG:HG2	1:E:330:ARG:HH11	1.54	0.70
1:C:288:PHE:CE1	1:D:231:PRO:HD3	2.31	0.65
1:D:59:LEU:HA	1:H:330:ARG:HH11	1.63	0.62
1:A:124:ASN:ND2	1:B:92:ALA:O	2.31	0.62
1:G:330:ARG:HH11	1:G:330:ARG:CG	2.18	0.56
1:C:285:LEU:CD1	1:D:230:TYR:OH	2.57	0.53
1:C:288:PHE:CE2	1:D:231:PRO:HG3	2.44	0.52
1:E:330:ARG:HG2	1:E:330:ARG:NH1	2.25	0.52
1:H:339:VAL:O	1:H:340:THR:C	2.49	0.50
1:A:155:GLU:HG3	1:F:158:THR:OG1	2.11	0.50
1:E:154:GLY:C	1:H:158:THR:HG21	2.32	0.49
1:H:231:PRO:O	1:H:232:ASP:OD1	2.30	0.49
1:C:231:PRO:O	1:C:232:ASP:OD1	2.30	0.48
1:E:264:TYR:HB2	1:E:273:ILE:HD11	1.94	0.48
1:C:288:PHE:CE1	1:D:231:PRO:CD	2.96	0.48
1:H:63:ASP:OD2	1:H:65:THR:HG22	2.13	0.48
1:G:63[B]:ASP:OD2	1:G:65:THR:HG22	2.13	0.48
1:H:178:LEU:HD21	1:H:221:TYR:CD1	2.50	0.47
1:C:178:LEU:HD21	1:C:221:TYR:CD1	2.50	0.47
1:A:50:THR:HB	1:H:169:ARG:HH12	1.79	0.46
1:D:178:LEU:HD21	1:D:221:TYR:CD1	2.50	0.46
1:G:178:LEU:HD21	1:G:221:TYR:CD1	2.50	0.46
1:F:264:TYR:HB2	1:F:273:ILE:HD11	1.98	0.46
1:C:154:GLY:O	1:C:155:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:TYR:HA	1:D:231:PRO:HA	1.75	0.46
1:H:154:GLY:O	1:H:155:GLU:HB2	2.15	0.46
1:A:178:LEU:HD21	1:A:221:TYR:CD1	2.51	0.46
1:B:230:TYR:HA	1:B:231:PRO:HA	1.73	0.46
1:F:178:LEU:HD21	1:F:221:TYR:CD1	2.51	0.46
1:B:302:ARG:O	1:B:306:MET:HG2	2.17	0.45
1:B:178:LEU:HD21	1:B:221:TYR:CD1	2.51	0.45
1:C:31:THR:HG21	1:H:231:PRO:HB2	1.97	0.45
1:G:264:TYR:HB2	1:G:273:ILE:HD11	1.99	0.45
1:H:230:TYR:HA	1:H:231:PRO:HA	1.79	0.45
1:B:264:TYR:HB2	1:B:273:ILE:HD11	1.97	0.45
1:E:178:LEU:HD21	1:E:221:TYR:CD1	2.51	0.45
1:H:231:PRO:C	1:H:232:ASP:OD1	2.54	0.45
1:H:264:TYR:HB2	1:H:273:ILE:HD11	1.99	0.45
1:A:230:TYR:HA	1:A:231:PRO:HA	1.74	0.45
1:C:231:PRO:C	1:C:232:ASP:OD1	2.54	0.45
1:F:243:ILE:HG13	2:F:401:A1BLX:O29	2.16	0.45
1:E:302:ARG:O	1:E:306:MET:HG2	2.17	0.44
1:G:230:TYR:HA	1:G:231:PRO:HA	1.80	0.44
1:C:230:TYR:HA	1:C:231:PRO:HA	1.79	0.44
1:F:154:GLY:O	1:F:155:GLU:HB2	2.17	0.44
1:C:264:TYR:HB2	1:C:273:ILE:HD11	2.00	0.44
1:A:24:GLU:OE2	1:H:112:ARG:NH2	2.51	0.44
1:G:63[B]:ASP:HB2	1:G:65:THR:HG22	2.00	0.44
1:E:207:LYS:HE2	1:E:214:THR:HG21	2.00	0.44
1:G:154:GLY:O	1:G:155:GLU:HB2	2.16	0.44
1:A:287:ASP:OD2	1:A:330:ARG:NH2	2.51	0.43
1:C:165:ASP:OD1	1:C:167:THR:OG1	2.28	0.43
1:D:330:ARG:CG	1:D:330:ARG:HH21	2.32	0.43
1:C:192:ILE:HG23	1:C:240:GLN:HE22	1.84	0.42
1:F:230:TYR:HA	1:F:231:PRO:HA	1.72	0.42
1:B:192:ILE:HG23	1:B:240:GLN:HE22	1.85	0.42
1:F:200:HIS:CE1	1:F:226:ASN:ND2	2.88	0.42
1:G:200:HIS:CE1	1:G:226:ASN:ND2	2.88	0.42
1:B:165:ASP:OD1	1:B:167:THR:OG1	2.28	0.42
1:F:200:HIS:HA	3:F:505:HOH:O	2.19	0.41
1:G:63[B]:ASP:OD2	1:G:65:THR:CG2	2.69	0.41
1:H:63:ASP:OD2	1:H:65:THR:CG2	2.68	0.41
1:E:192:ILE:HG23	1:E:240:GLN:HE22	1.86	0.41
1:A:192:ILE:HG23	1:A:240:GLN:HE22	1.84	0.41
1:A:222:MET:CE	1:A:241:MET:HE3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:GLY:HA3	2:E:401:A1BLX:O30	2.21	0.41
1:F:192:ILE:HG23	1:F:240:GLN:HE22	1.86	0.41
1:G:207:LYS:HE2	1:G:214:THR:HG21	2.02	0.41
1:B:207:LYS:HE2	1:B:214:THR:HG21	2.03	0.40
1:D:59:LEU:HA	1:H:330:ARG:NH1	2.31	0.40
1:D:161:ILE:HA	1:D:203:LEU:O	2.22	0.40
1:G:253:GLY:HA3	2:G:401:A1BLX:O29	2.22	0.40
1:H:254:ALA:HA	1:H:285:LEU:HD11	2.04	0.40
1:H:302:ARG:O	1:H:306:MET:HG2	2.21	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	310/322 (96%)	304 (98%)	6 (2%)	0	100	100
1	B	311/322 (97%)	306 (98%)	5 (2%)	0	100	100
1	C	309/322 (96%)	303 (98%)	5 (2%)	1 (0%)	37	57
1	D	316/322 (98%)	310 (98%)	6 (2%)	0	100	100
1	E	306/322 (95%)	300 (98%)	6 (2%)	0	100	100
1	F	312/322 (97%)	308 (99%)	3 (1%)	1 (0%)	37	57
1	G	312/322 (97%)	305 (98%)	6 (2%)	1 (0%)	37	57
1	H	311/322 (97%)	306 (98%)	4 (1%)	1 (0%)	37	57
All	All	2487/2576 (96%)	2442 (98%)	41 (2%)	4 (0%)	44	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	155	GLU

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Mol	Chain	Res	Type
1	G	155	GLU
1	C	155	GLU
1	H	155	GLU

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	265/291 (91%)	260 (98%)	5 (2%)	52	74
1	B	253/291 (87%)	248 (98%)	5 (2%)	50	73
1	C	255/291 (88%)	250 (98%)	5 (2%)	50	73
1	D	257/291 (88%)	251 (98%)	6 (2%)	45	69
1	E	257/291 (88%)	254 (99%)	3 (1%)	67	84
1	F	255/291 (88%)	253 (99%)	2 (1%)	79	91
1	G	256/291 (88%)	250 (98%)	6 (2%)	45	69
1	H	252/291 (87%)	248 (98%)	4 (2%)	58	78
All	All	2050/2328 (88%)	2014 (98%)	36 (2%)	54	75

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	73	LYS
1	A	231	PRO
1	A	306	MET
1	A	330	ARG
1	B	45	GLU
1	B	149	LEU
1	B	326	GLN
1	B	330	ARG
1	B	337	LEU
1	C	45	GLU
1	C	232	ASP

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Mol	Chain	Res	Type
1	C	318	GLN
1	C	336	ARG
1	C	337	LEU
1	D	45	GLU
1	D	73	LYS
1	D	100	ASP
1	D	169	ARG
1	D	231	PRO
1	D	330	ARG
1	E	96	ASP
1	E	326	GLN
1	E	336	ARG
1	F	45	GLU
1	F	337	LEU
1	G	22	LEU
1	G	113	GLN
1	G	232	ASP
1	G	330	ARG
1	G	336	ARG
1	G	337	LEU
1	H	232	ASP
1	H	330	ARG
1	H	336	ARG
1	H	337	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	28	ASN
1	F	226	ASN
1	G	226	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)

8 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	A1BLX	G	401	-	35,35,35	0.66	1 (2%)	44,51,51	0.61	0
2	A1BLX	F	401	-	35,35,35	0.59	0	44,51,51	0.83	0
2	A1BLX	B	401	-	35,35,35	0.60	0	44,51,51	0.67	1 (2%)
2	A1BLX	H	401	-	35,35,35	0.58	0	44,51,51	0.71	1 (2%)
2	A1BLX	C	401	-	35,35,35	0.56	0	44,51,51	0.63	0
2	A1BLX	A	401	-	35,35,35	0.66	0	44,51,51	0.86	1 (2%)
2	A1BLX	E	401	-	35,35,35	0.50	0	44,51,51	0.68	0
2	A1BLX	D	401	-	35,35,35	0.60	0	44,51,51	0.83	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1BLX	G	401	-	-	2/13/43/43	0/4/4/4
2	A1BLX	F	401	-	-	3/13/43/43	0/4/4/4
2	A1BLX	B	401	-	-	0/13/43/43	0/4/4/4
2	A1BLX	H	401	-	-	3/13/43/43	0/4/4/4
2	A1BLX	C	401	-	-	3/13/43/43	0/4/4/4
2	A1BLX	A	401	-	-	0/13/43/43	0/4/4/4
2	A1BLX	E	401	-	-	1/13/43/43	0/4/4/4
2	A1BLX	D	401	-	-	0/13/43/43	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	A1BLX	C16-C17	-2.44	1.43	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	A1BLX	O32-C31-C27	3.10	125.01	120.89
2	H	401	A1BLX	O32-C31-C27	2.95	124.82	120.89
2	B	401	A1BLX	C17-C16-C14	-2.21	108.34	114.17
2	A	401	A1BLX	O32-C31-C27	2.03	123.60	120.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	A1BLX	C26-C27-N28-O30
2	C	401	A1BLX	C31-C27-N28-O30
2	E	401	A1BLX	C31-C27-N28-O30
2	F	401	A1BLX	C26-C27-N28-O30
2	F	401	A1BLX	C31-C27-N28-O30
2	H	401	A1BLX	C31-C27-N28-O30
2	F	401	A1BLX	C1-C2-O3-C4
2	C	401	A1BLX	C1-C2-O3-C4
2	H	401	A1BLX	C1-C2-O3-C4
2	G	401	A1BLX	C26-C27-N28-O30
2	H	401	A1BLX	C26-C27-N28-O30
2	G	401	A1BLX	C31-C27-N28-O30

There are no ring outliers.

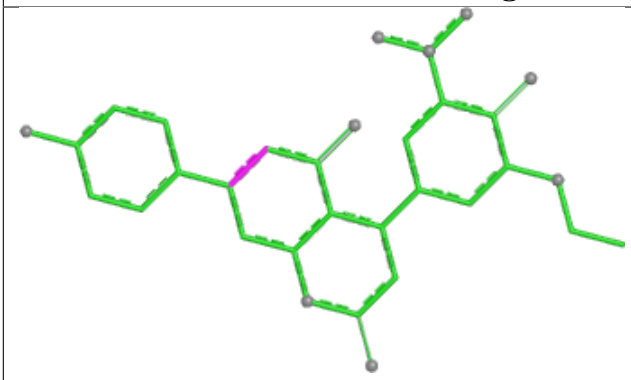
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	401	A1BLX	1	0
2	F	401	A1BLX	1	0
2	E	401	A1BLX	1	0

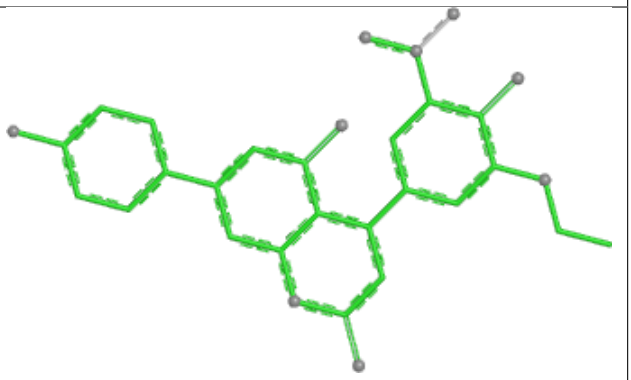
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

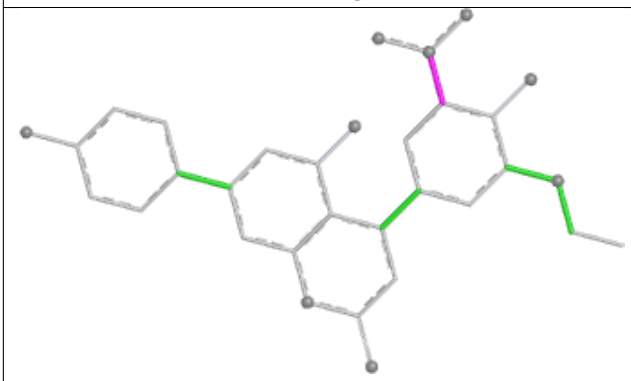
Ligand A1BLX G 401



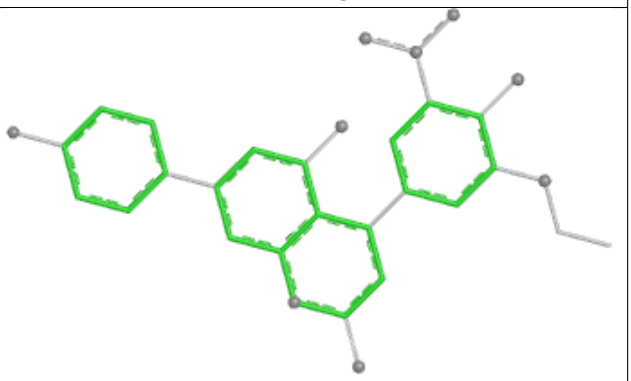
Bond lengths



Bond angles

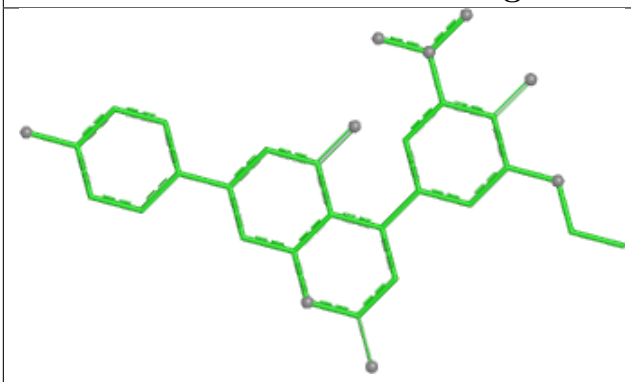


Torsions



Rings

Ligand A1BLX F 401



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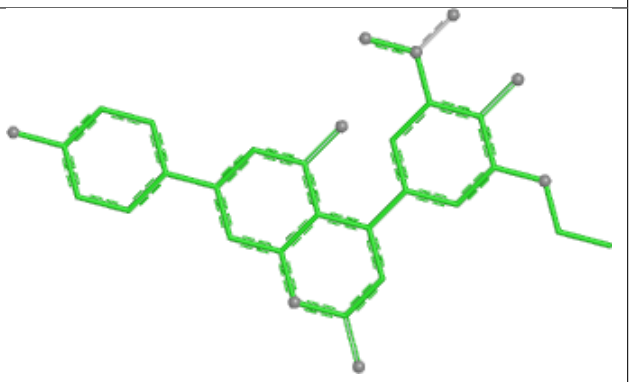

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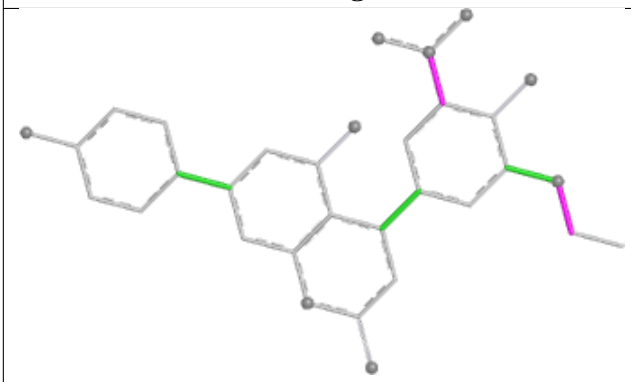

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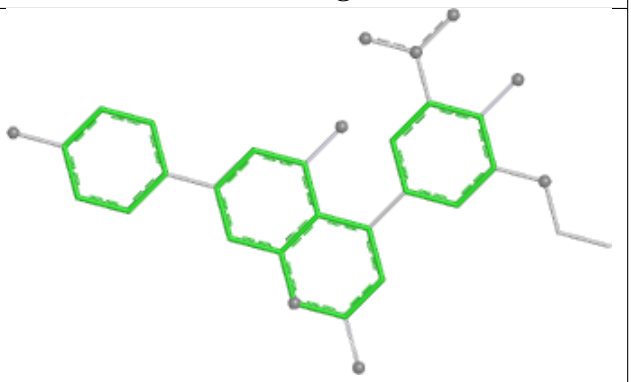
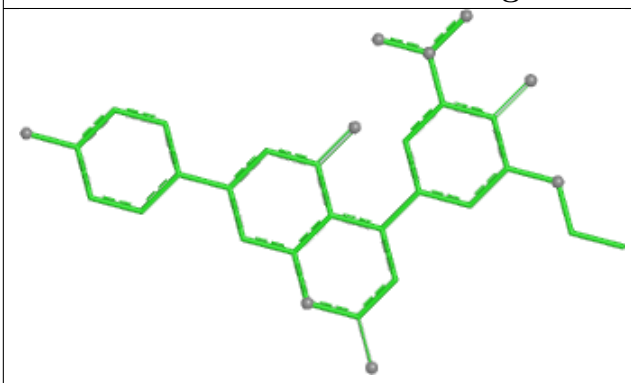


Rings

Ligand A1BLX B 401



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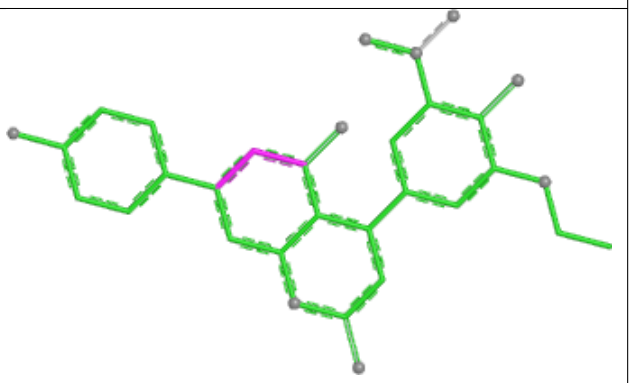
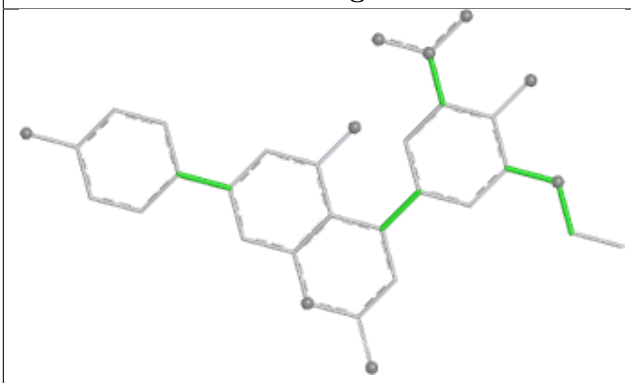


Bond angles



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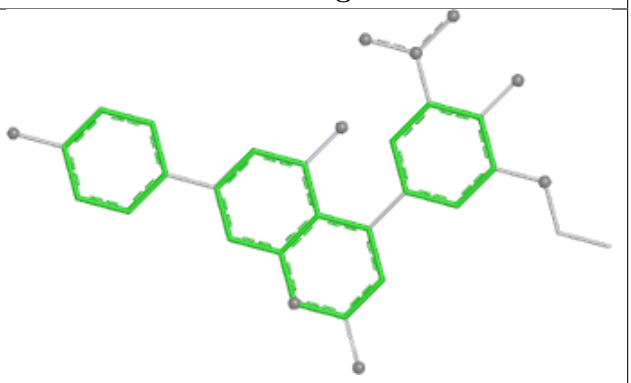
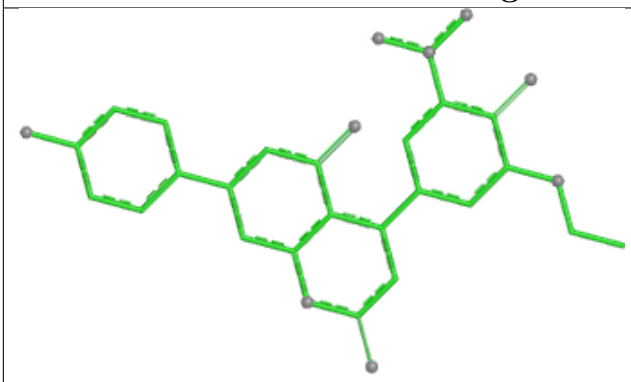
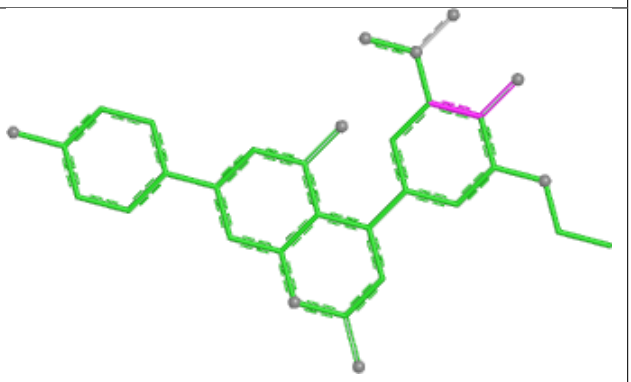


Rings

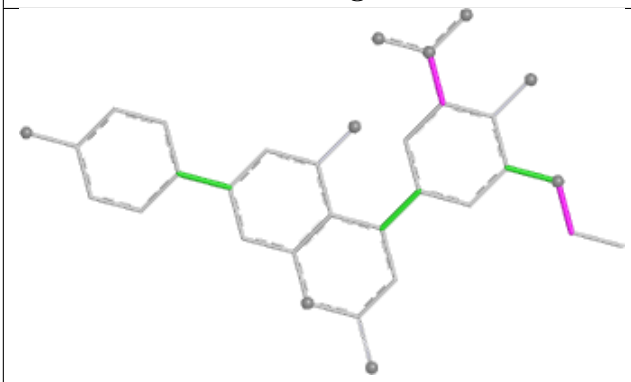
Ligand A1BLX H 401



Bond lengths



Bond angles



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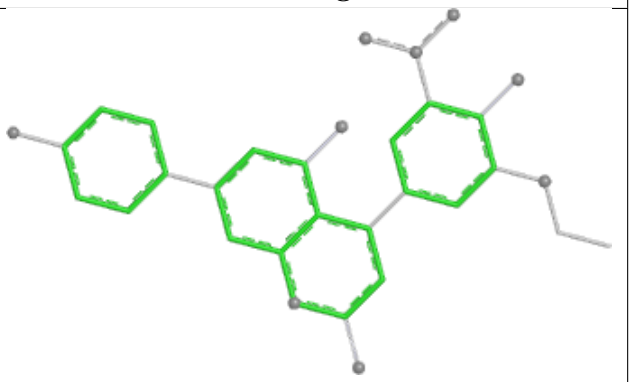
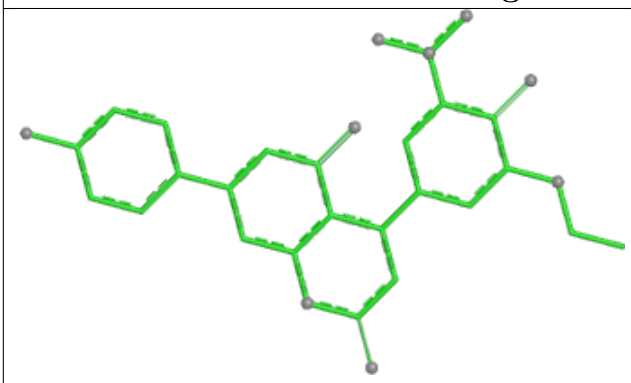


Rings

Ligand A1BLX C 401



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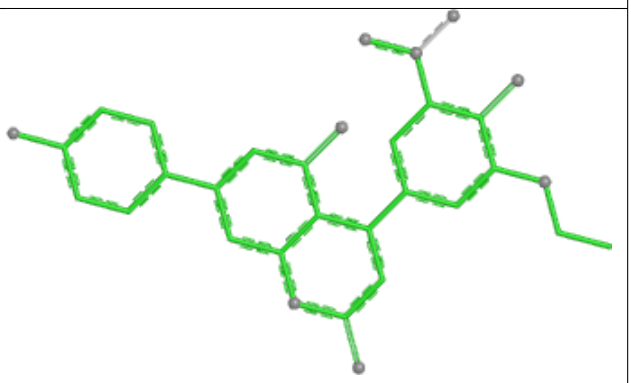

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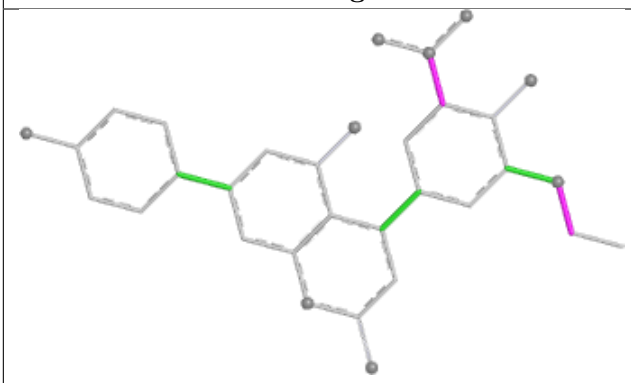
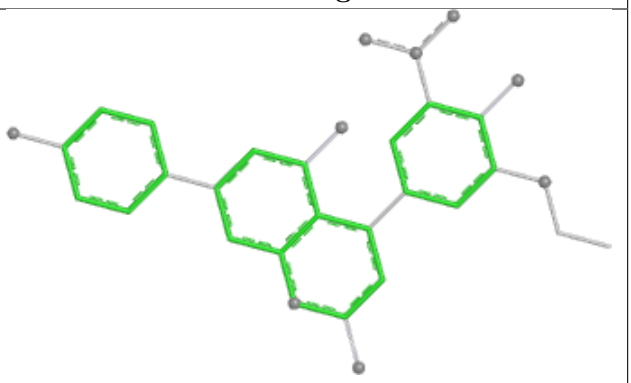
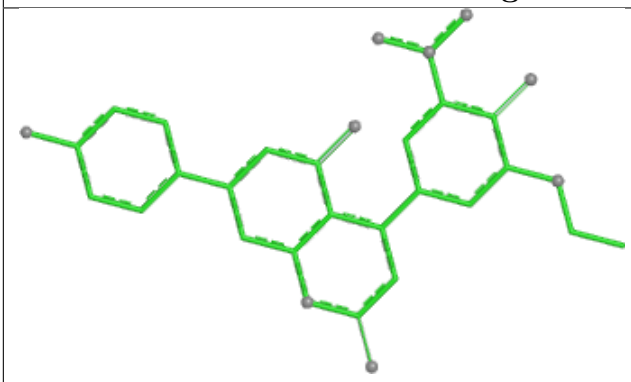


Torsions



Rings

Ligand A1BLX A 401



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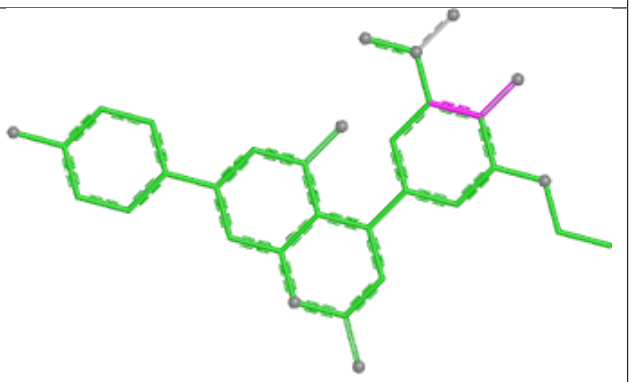
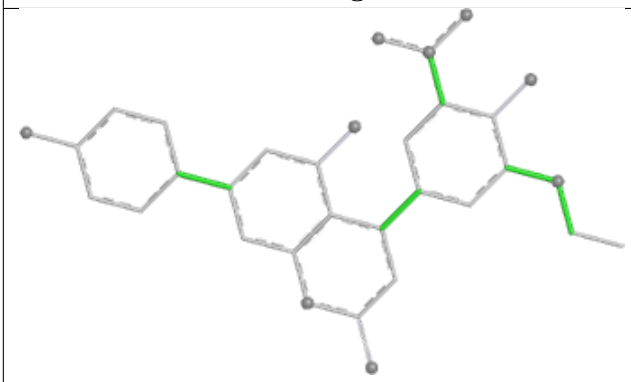


Bond angles



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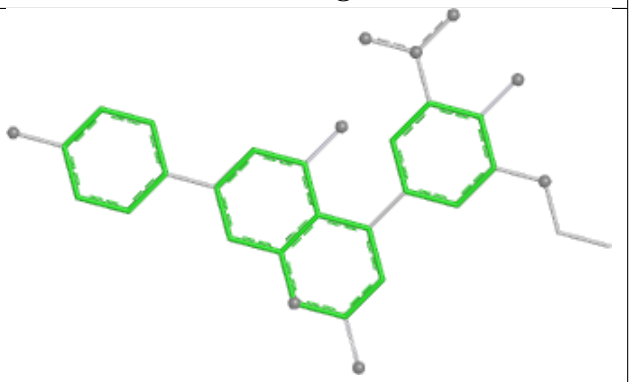
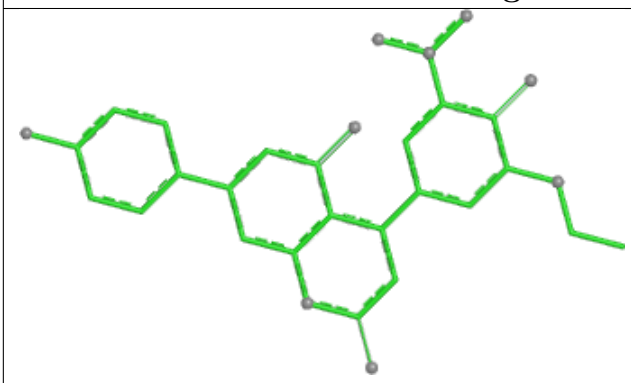


Rings

Ligand A1BLX E 401



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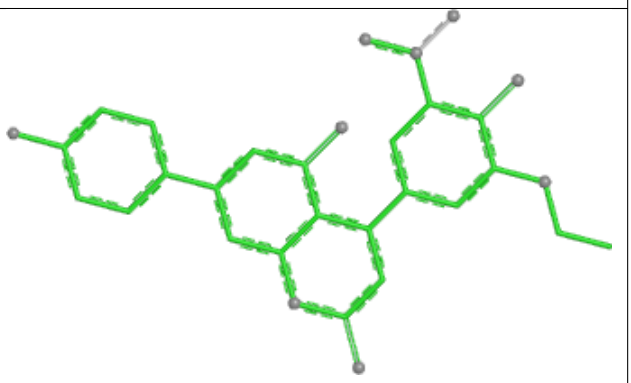
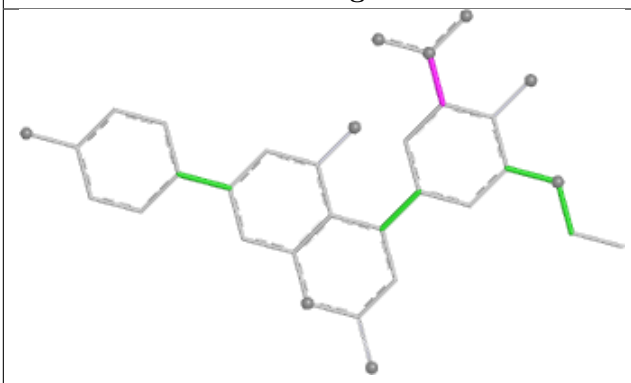
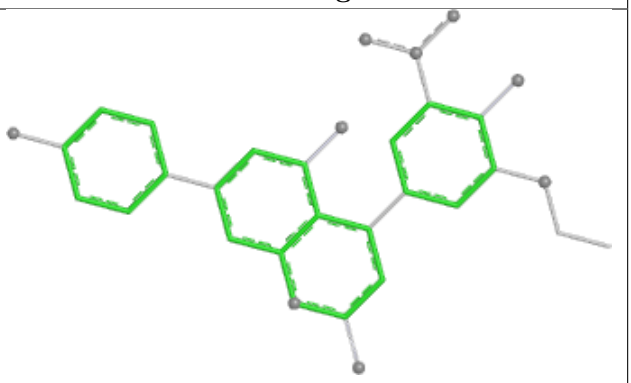


Bond angles

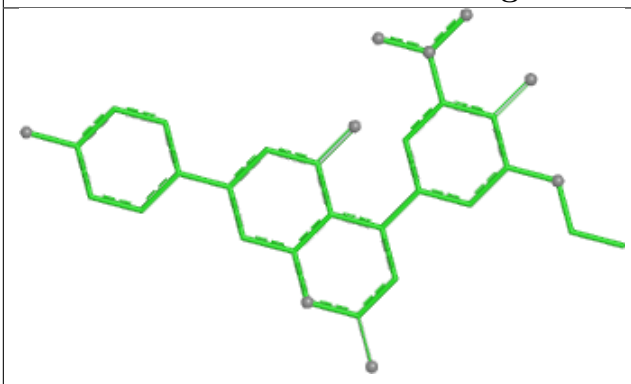


Torsions

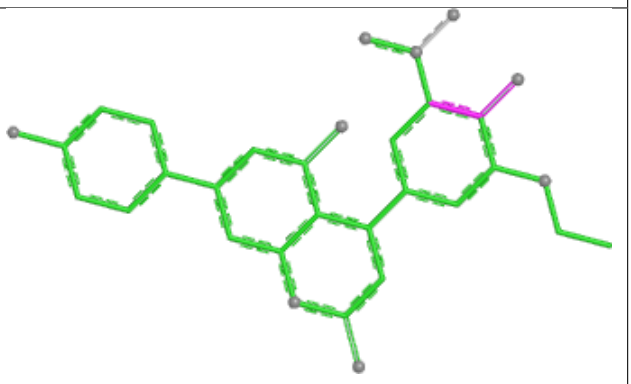


Rings

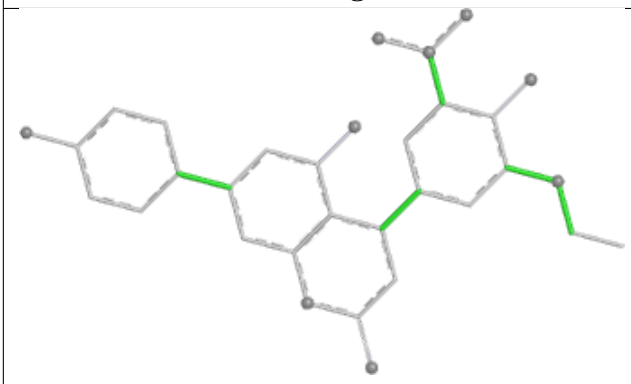
Ligand A1BLX D 401



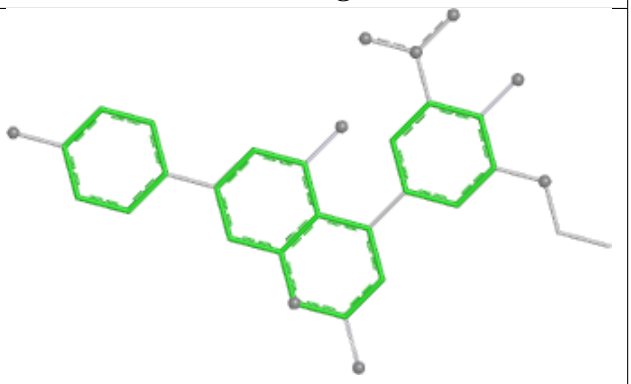
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	314/322 (97%)	0.09	2 (0%)	85	83	26, 40, 66, 77	0
1	B	315/322 (97%)	0.24	12 (3%)	44	40	25, 43, 70, 101	0
1	C	313/322 (97%)	0.36	11 (3%)	47	43	31, 48, 76, 93	0
1	D	318/322 (98%)	0.43	11 (3%)	47	43	32, 49, 72, 79	0
1	E	311/322 (96%)	0.16	7 (2%)	61	56	25, 44, 68, 102	1 (0%)
1	F	314/322 (97%)	0.27	9 (2%)	54	49	21, 45, 72, 88	2 (0%)
1	G	314/322 (97%)	0.43	16 (5%)	34	30	22, 52, 82, 100	2 (0%)
1	H	313/322 (97%)	0.40	8 (2%)	57	53	22, 49, 81, 94	2 (0%)
All	All	2512/2576 (97%)	0.30	76 (3%)	52	48	21, 46, 75, 102	7 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	101	CYS	6.1
1	H	101	CYS	6.0
1	F	101	CYS	5.1
1	G	22	LEU	5.0
1	D	22	LEU	3.9
1	E	151	PRO	3.9
1	B	101	CYS	3.8
1	A	22	LEU	3.8
1	F	22	LEU	3.7
1	C	23	ALA	3.4
1	E	23	ALA	3.3
1	E	153	GLY	3.2
1	F	312	ASP	3.1
1	H	95	VAL	3.1
1	B	240	GLN	3.1
1	B	150	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	168[A]	CYS	2.8
1	D	339	VAL	2.8
1	G	226	ASN	2.8
1	B	149	LEU	2.8
1	D	154	GLY	2.8
1	E	150	SER	2.7
1	G	101	CYS	2.7
1	H	340	THR	2.7
1	H	303	GLU	2.7
1	E	240	GLN	2.7
1	G	339	VAL	2.6
1	E	307	GLN	2.6
1	B	151	PRO	2.6
1	C	310	ASN	2.6
1	B	95	VAL	2.6
1	F	231	PRO	2.5
1	D	98	ASN	2.5
1	G	151	PRO	2.5
1	C	307	GLN	2.5
1	D	310	ASN	2.5
1	H	24	GLU	2.5
1	B	152	THR	2.5
1	D	274	THR	2.5
1	H	319[A]	GLN	2.5
1	B	300	PHE	2.5
1	C	312	ASP	2.5
1	G	302	ARG	2.4
1	F	310	ASN	2.4
1	C	95	VAL	2.4
1	D	151	PRO	2.4
1	G	168[A]	CYS	2.4
1	G	269	THR	2.4
1	E	149	LEU	2.3
1	G	23	ALA	2.3
1	C	339	VAL	2.3
1	G	310	ASN	2.3
1	C	303	GLU	2.3
1	B	22	LEU	2.2
1	B	134	VAL	2.2
1	D	23	ALA	2.2
1	F	23	ALA	2.2
1	B	153	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	268	PRO	2.2
1	G	338	LEU	2.2
1	F	93	SER	2.2
1	C	232	ASP	2.2
1	A	339	VAL	2.2
1	C	340	THR	2.1
1	D	155	GLU	2.1
1	G	312	ASP	2.1
1	G	153	GLY	2.1
1	H	25	TYR	2.1
1	F	339	VAL	2.0
1	G	235	ARG	2.0
1	B	228	TYR	2.0
1	C	311	GLU	2.0
1	G	232	ASP	2.0
1	H	304	LYS	2.0
1	D	276	GLU	2.0
1	G	303	GLU	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 monosaccharides 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, 95^{th} 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
2	A1BLX	D	401	32/32	0.91	0.09	36,43,46,47	0
2	A1BLX	E	401	32/32	0.92	0.09	28,34,40,44	0
2	A1BLX	A	401	32/32	0.93	0.08	31,39,45,46	0
2	A1BLX	B	401	32/32	0.93	0.08	28,33,36,40	0
2	A1BLX	G	401	32/32	0.93	0.08	32,37,44,46	0

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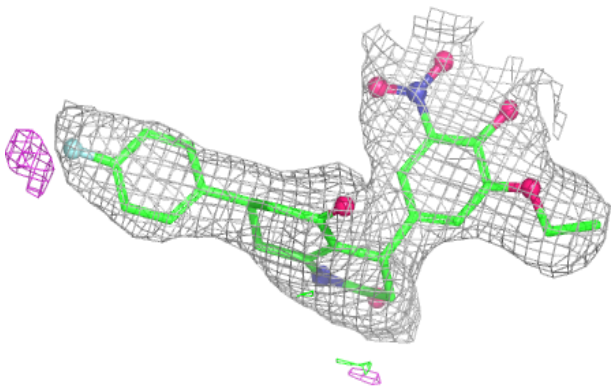
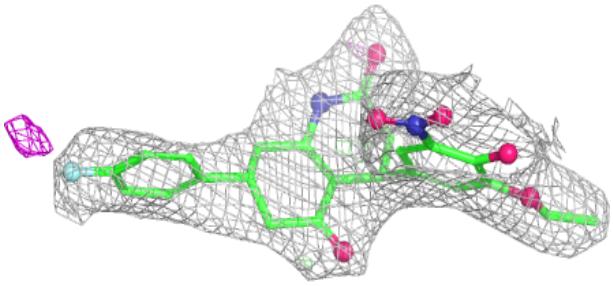
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1BLX	H	401	32/32	0.93	0.09	34,40,48,53	0
2	A1BLX	C	401	32/32	0.94	0.08	33,38,45,51	0
2	A1BLX	F	401	32/32	0.95	0.07	29,33,35,36	0

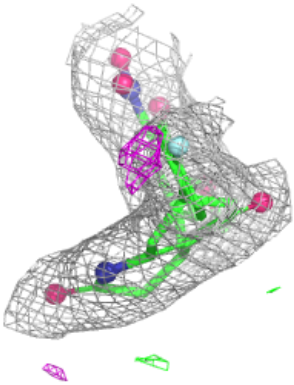
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BLX D 401:

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

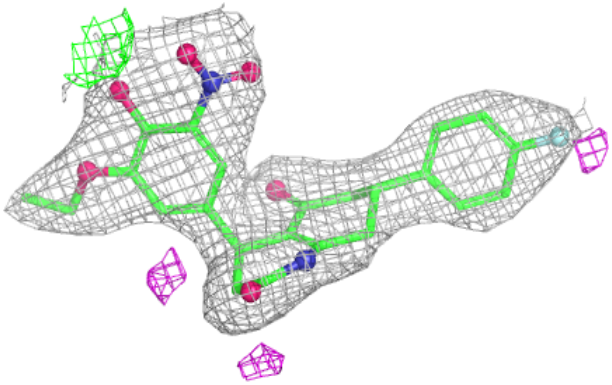


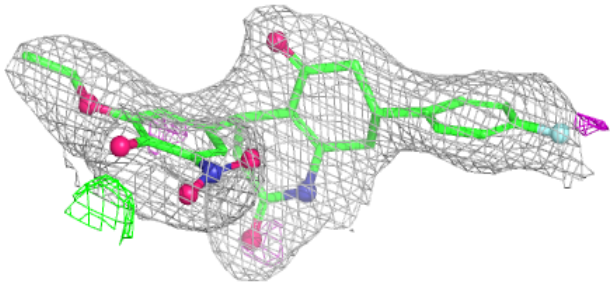


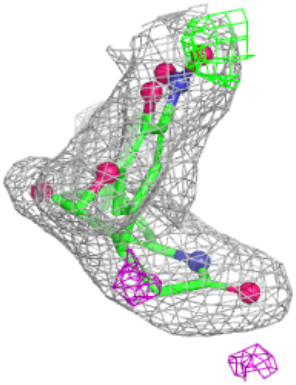


Electron density around A1BLX E 401:

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

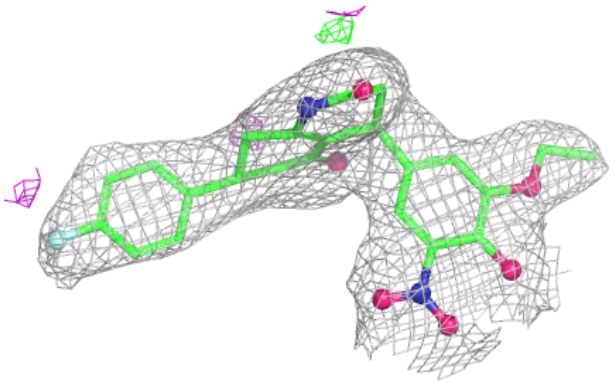


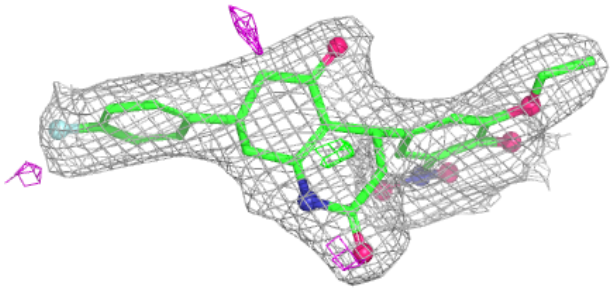


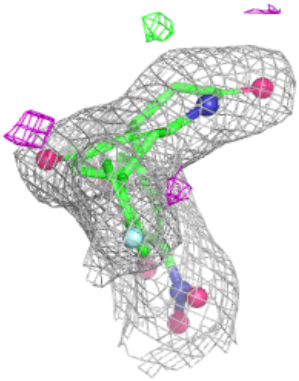


Electron density around A1BLX A 401:

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

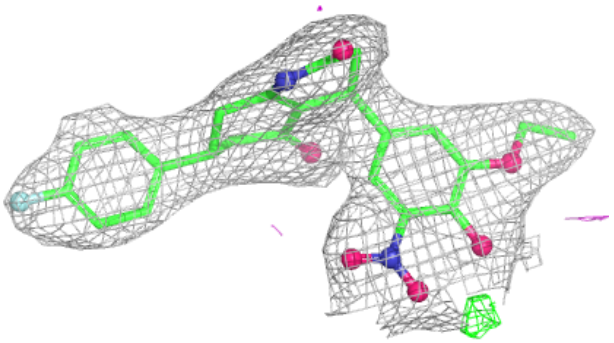


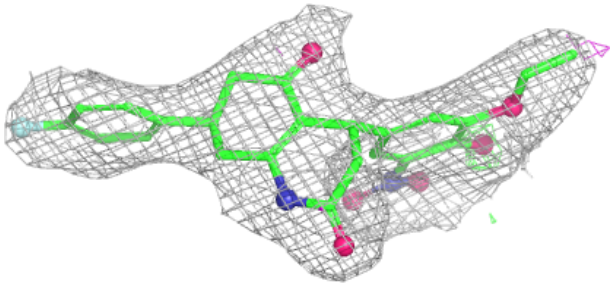


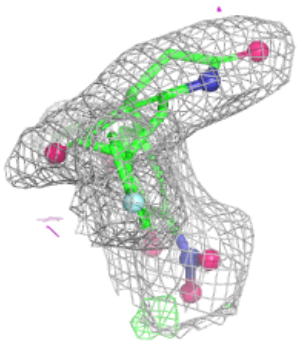


Electron density around A1BLX B 401:

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

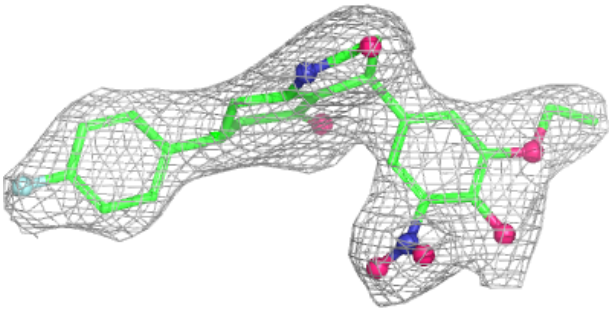


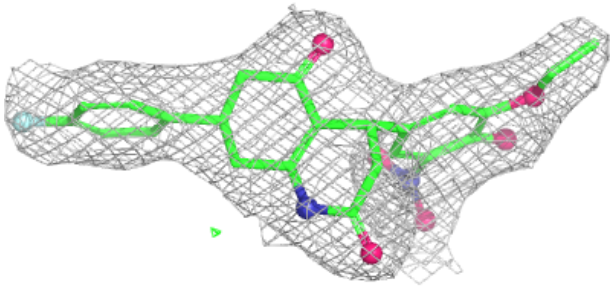


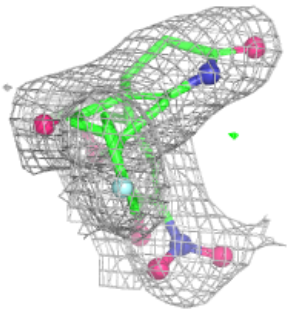


Electron density around A1BLX G 401:

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

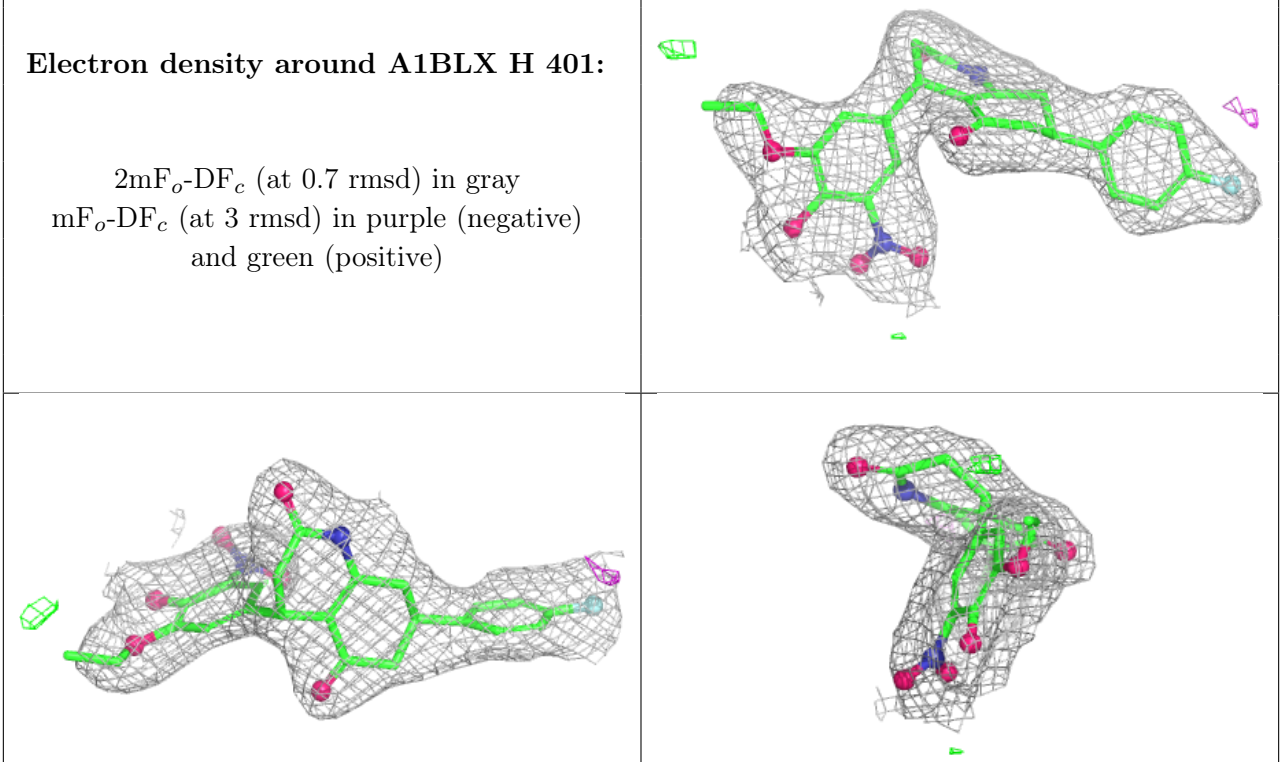






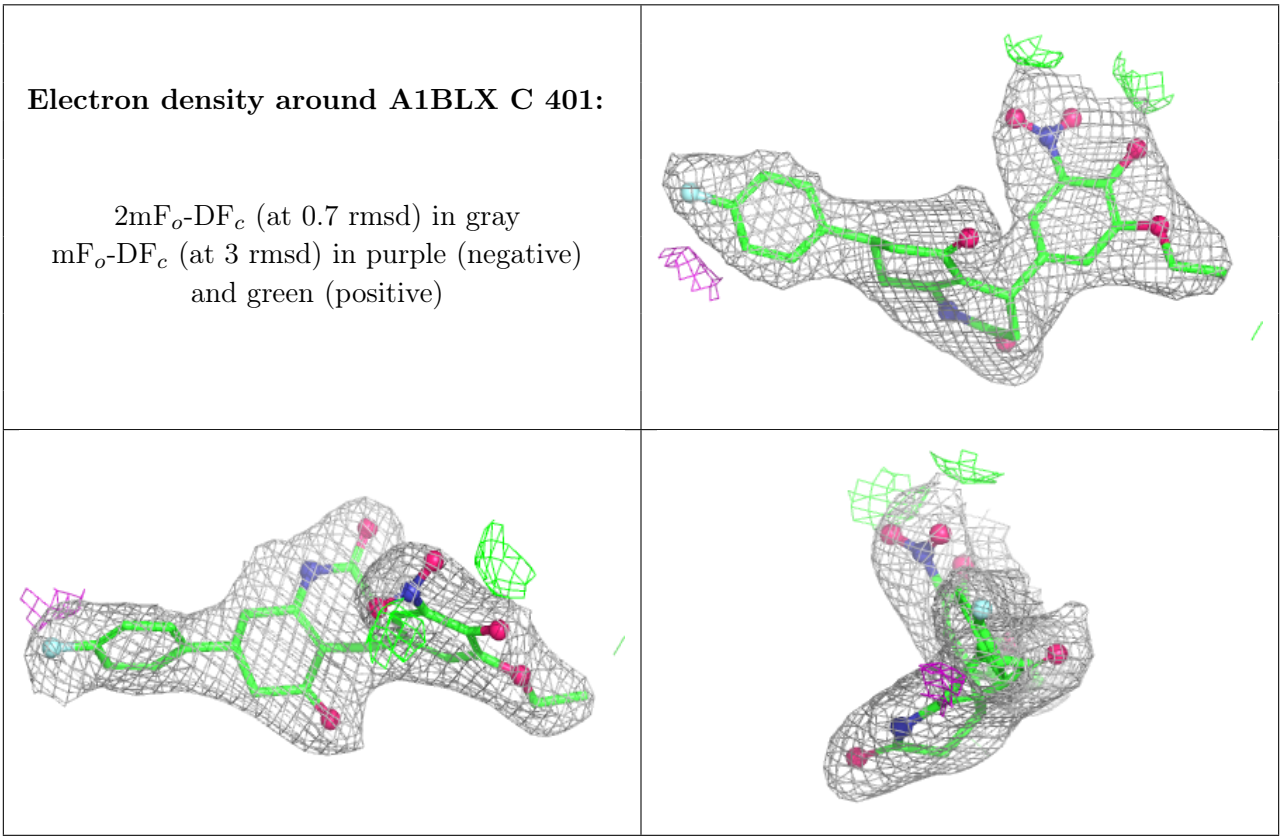
Electron density around A1BLX H 401:

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



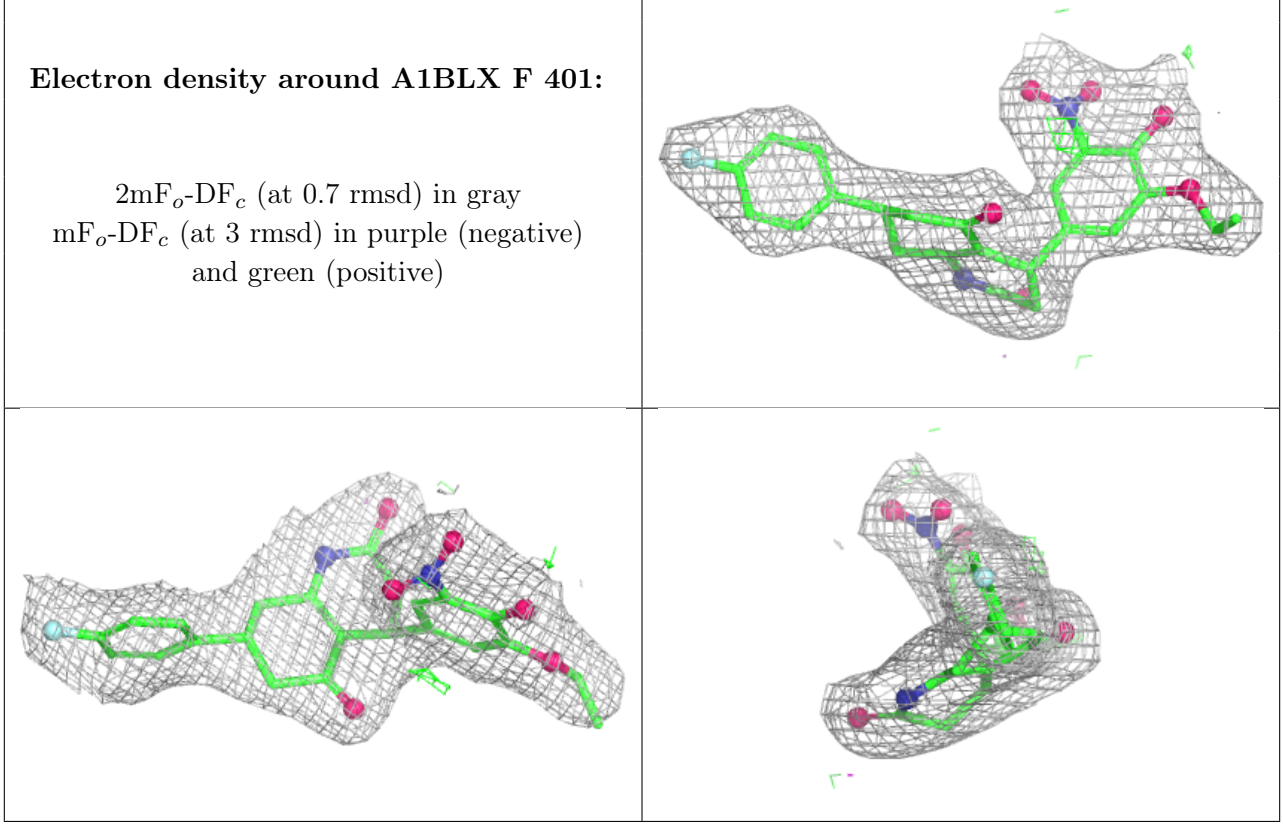
Electron density around A1BLX C 401:

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



Electron density around A1BLX F 401:

$2mF_o$-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.