Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 11:38 AM EST

PDB ID	:	4OQ5
Title	:	Crystal Structure of Human MCL-1 Bound to Inhibitor 4-(4-methylnaphthalen-1-yl)-2-{[(4-phenoxyphenyl)sulfonyl]amino}benzoic acid
Authors	:	Petros, A.M.; Swann, S.L.; Song, D.; Swinger, K.; Park, C.; Zhang, H.; Wendt, M.D.; Kunzer, A.R.; Souers, A.J.; Sun, C.
Deposited on	:	2014-02-07
Resolution	:	2.86 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

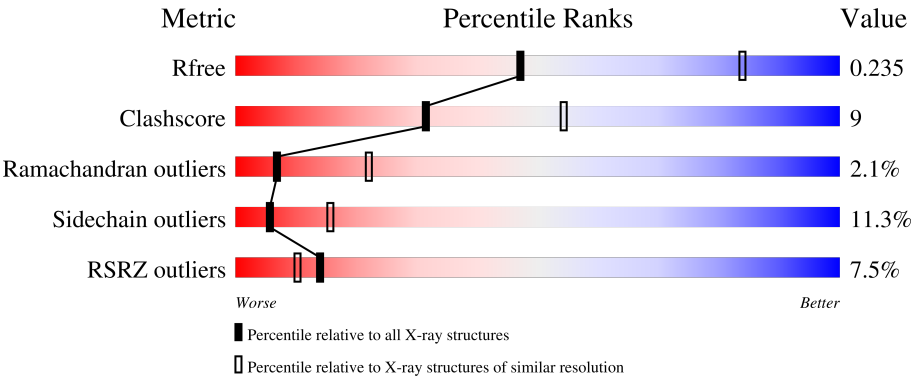
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.86 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	163	10% 69% 17% 5% • 8%
1	B	163	7% 71% 15% 6% • 7%
1	C	163	5% 71% 15% • • 9%
1	D	163	4% 66% 21% • • 9%

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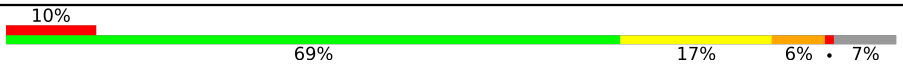
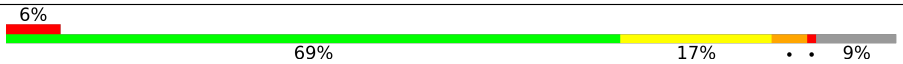
Mol	Chain	Length	Quality of chain
1	E	163	
1	F	163	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7736 atoms, of which 120 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 Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1208	758	223	222	5			
1	B	151	Total	C	N	O	S	0	0	0
			1216	764	224	223	5			
1	C	149	Total	C	N	O	S	0	0	0
			1200	754	222	219	5			
1	D	149	Total	C	N	O	S	0	0	0
			1200	754	222	219	5			
1	E	151	Total	C	N	O	S	0	0	0
			1216	764	224	223	5			
1	F	149	Total	C	N	O	S	0	0	0
			1200	754	222	219	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	expression tag	UNP Q07820
A	165	THR	-	expression tag	UNP Q07820
A	166	LEU	-	expression tag	UNP Q07820
A	167	VAL	-	expression tag	UNP Q07820
A	168	PRO	-	expression tag	UNP Q07820
A	169	ARG	-	expression tag	UNP Q07820
A	170	GLY	-	expression tag	UNP Q07820
A	171	SER	-	expression tag	UNP Q07820
A	172	MET	-	expression tag	UNP Q07820
A	173	ASP	-	expression tag	UNP Q07820
B	164	GLY	-	expression tag	UNP Q07820
B	165	THR	-	expression tag	UNP Q07820
B	166	LEU	-	expression tag	UNP Q07820
B	167	VAL	-	expression tag	UNP Q07820
B	168	PRO	-	expression tag	UNP Q07820
B	169	ARG	-	expression tag	UNP Q07820
B	170	GLY	-	expression tag	UNP Q07820

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Chain	Residue	Modelled	Actual	Comment	Reference
B	171	SER	-	expression tag	UNP Q07820
B	172	MET	-	expression tag	UNP Q07820
B	173	ASP	-	expression tag	UNP Q07820
C	164	GLY	-	expression tag	UNP Q07820
C	165	THR	-	expression tag	UNP Q07820
C	166	LEU	-	expression tag	UNP Q07820
C	167	VAL	-	expression tag	UNP Q07820
C	168	PRO	-	expression tag	UNP Q07820
C	169	ARG	-	expression tag	UNP Q07820
C	170	GLY	-	expression tag	UNP Q07820
C	171	SER	-	expression tag	UNP Q07820
C	172	MET	-	expression tag	UNP Q07820
C	173	ASP	-	expression tag	UNP Q07820
D	164	GLY	-	expression tag	UNP Q07820
D	165	THR	-	expression tag	UNP Q07820
D	166	LEU	-	expression tag	UNP Q07820
D	167	VAL	-	expression tag	UNP Q07820
D	168	PRO	-	expression tag	UNP Q07820
D	169	ARG	-	expression tag	UNP Q07820
D	170	GLY	-	expression tag	UNP Q07820
D	171	SER	-	expression tag	UNP Q07820
D	172	MET	-	expression tag	UNP Q07820
D	173	ASP	-	expression tag	UNP Q07820
E	164	GLY	-	expression tag	UNP Q07820
E	165	THR	-	expression tag	UNP Q07820
E	166	LEU	-	expression tag	UNP Q07820
E	167	VAL	-	expression tag	UNP Q07820
E	168	PRO	-	expression tag	UNP Q07820
E	169	ARG	-	expression tag	UNP Q07820
E	170	GLY	-	expression tag	UNP Q07820
E	171	SER	-	expression tag	UNP Q07820
E	172	MET	-	expression tag	UNP Q07820
E	173	ASP	-	expression tag	UNP Q07820
F	164	GLY	-	expression tag	UNP Q07820
F	165	THR	-	expression tag	UNP Q07820
F	166	LEU	-	expression tag	UNP Q07820
F	167	VAL	-	expression tag	UNP Q07820
F	168	PRO	-	expression tag	UNP Q07820
F	169	ARG	-	expression tag	UNP Q07820
F	170	GLY	-	expression tag	UNP Q07820
F	171	SER	-	expression tag	UNP Q07820
F	172	MET	-	expression tag	UNP Q07820

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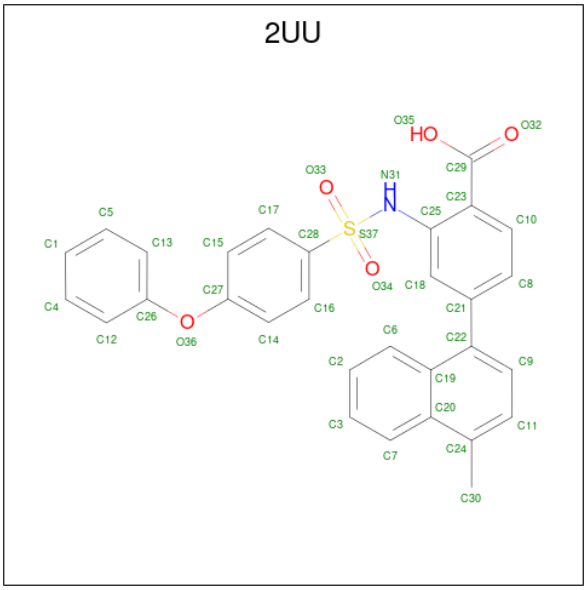
Chain	Residue	Modelled	Actual	Comment	Reference
F	173	ASP	-	expression tag	UNP Q07820

- Molecule 2 is 4-(4-methylnaphthalen-1-yl)-2-{[(4-phenoxyphenyl)sulfonyl]amino}benzoic acid (three-letter code: 2UU) (formula: $C_{30}H_{23}NO_5S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	B	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	C	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	D	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	E	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		
2	F	1	Total	C	H	N	O	S	0	0
			57	30	20	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	27	Total	O	0	0
			27	27		

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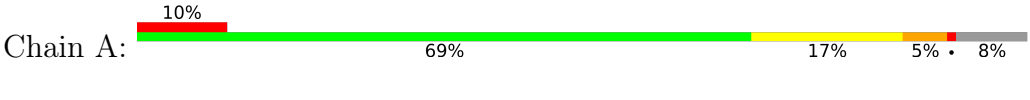
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	23	Total O 23 23	0	0
3	D	26	Total O 26 26	0	0
3	E	30	Total O 30 30	0	0
3	F	21	Total O 21 21	0	0

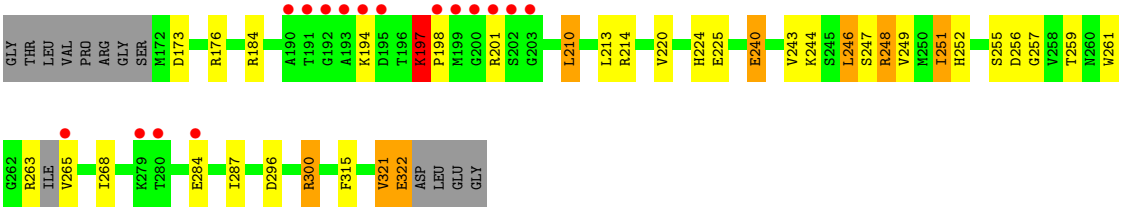
3 Residue-property plots (i)

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: Induced myeloid leukemia cell differentiation protein Mcl-1

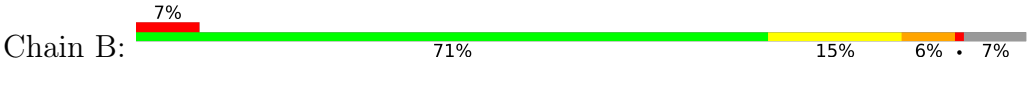
Chain A:

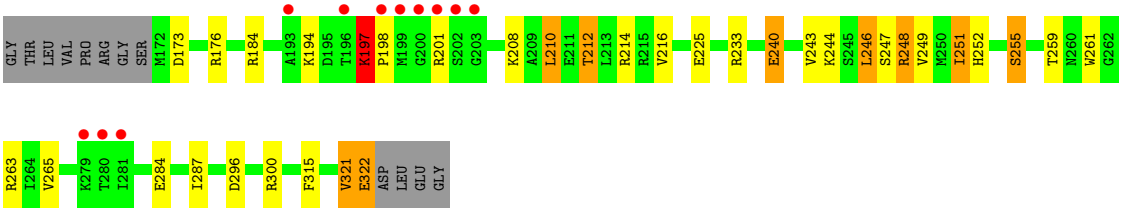




• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

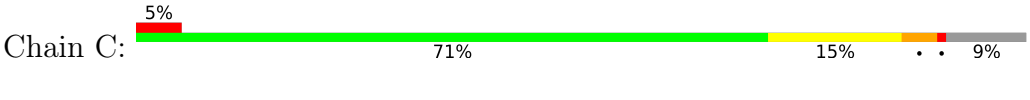
Chain B:





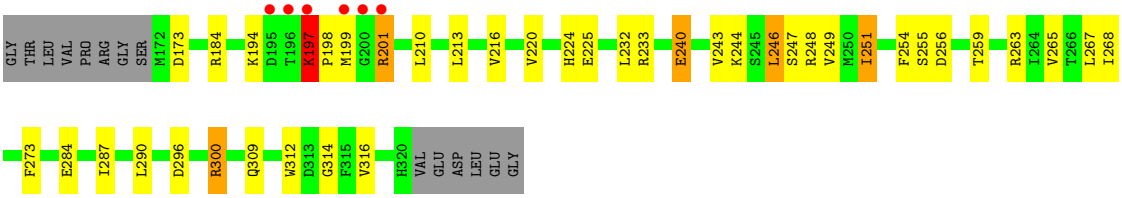
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain C:

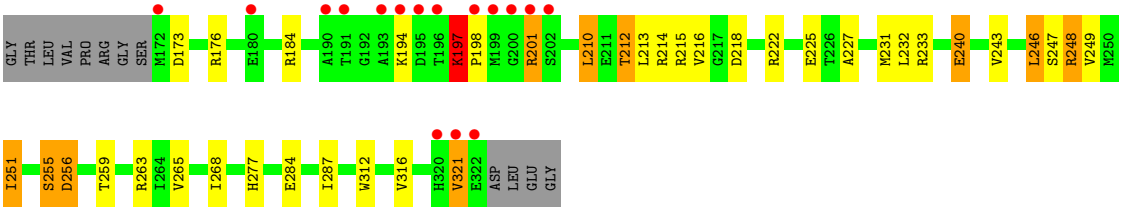


• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

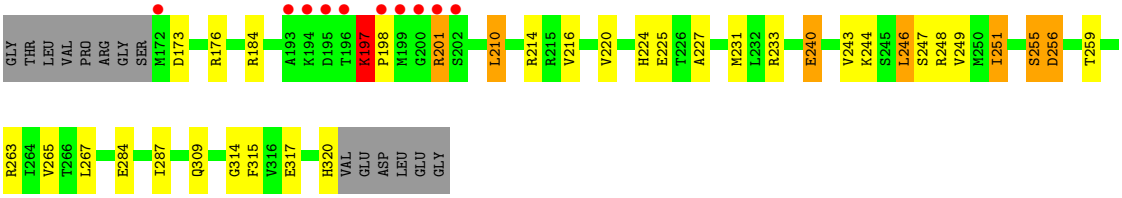
Chain D:



• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.11Å 109.75Å 76.54Å 90.00° 93.31° 90.00°	Depositor
Resolution (Å)	48.15 – 2.86 48.15 – 2.86	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.15-2.86) 97.8 (48.15-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.198 , 0.239 0.194 , 0.235	Depositor DCC
R_{free} test set	1341 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	57.6	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7736	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7063e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 2UU

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	0.52	0/1227	0.71	0/1647
1	B	0.52	0/1236	0.70	0/1661
1	C	0.52	0/1220	0.71	0/1639
1	D	0.53	0/1220	0.71	0/1639
1	E	0.51	0/1236	0.69	0/1661
1	F	0.50	0/1220	0.69	0/1639
All	All	0.52	0/7359	0.70	0/9886

There are no bond length outliers.

There are no bond angle outliers.

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	1208	0	1217	30	0
1	B	1216	0	1229	26	0
1	C	1200	0	1214	20	0
1	D	1200	0	1214	25	0
1	E	1216	0	1229	23	0
1	F	1200	0	1214	21	0
2	A	37	20	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	37	20	22	0	0
2	C	37	20	22	0	0
2	D	37	20	22	4	0
2	E	37	20	22	0	0
2	F	37	20	22	1	0
3	A	27	0	0	1	0
3	B	27	0	0	0	0
3	C	23	0	0	1	0
3	D	26	0	0	1	0
3	E	30	0	0	1	0
3	F	21	0	0	0	0
All	All	7616	120	7449	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 9.

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:A:184:ARG:HH21	1:A:198:PRO:HD2	1.50	0.76
1:B:184:ARG:HH21	1:B:198:PRO:HD2	1.51	0.75
1:A:197:LYS:HB2	1:A:198:PRO:HD3	1.69	0.74
1:B:197:LYS:HB2	1:B:198:PRO:HD3	1.70	0.74
1:E:184:ARG:HH21	1:E:198:PRO:HD2	1.52	0.73
1:E:197:LYS:HB2	1:E:198:PRO:HD3	1.69	0.73
1:D:184:ARG:HH21	1:D:198:PRO:HD2	1.53	0.72
1:F:184:ARG:HH21	1:F:198:PRO:HD2	1.53	0.72
1:C:197:LYS:HB2	1:C:198:PRO:HD3	1.70	0.71
1:F:197:LYS:HB2	1:F:198:PRO:HD3	1.71	0.71
1:D:197:LYS:HB2	1:D:198:PRO:HD3	1.71	0.71
1:C:184:ARG:HH21	1:C:198:PRO:HD2	1.52	0.71
1:D:199:MET:HA	3:D:524:HOH:O	1.92	0.69
1:A:300:ARG:HD3	1:B:255:SER:CB	2.23	0.68
1:A:300:ARG:HD3	1:B:255:SER:HB3	1.77	0.66
1:B:321:VAL:HG23	1:B:322:GLU:H	1.59	0.66
1:E:243:VAL:HA	1:E:246:LEU:HD22	1.80	0.64
1:B:216:VAL:HG12	1:B:265:VAL:HG11	1.79	0.63
1:A:256:ASP:HA	1:B:300:ARG:NH2	2.15	0.61
1:A:261:TRP:O	1:A:265:VAL:HG23	2.03	0.59
1:B:208:LYS:O	1:B:212:THR:HG23	2.01	0.59
1:F:216:VAL:HG12	1:F:265:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ALA:O	1:E:231:MET:HG3	2.03	0.58
1:C:220:VAL:O	1:C:224:HIS:HD2	1.87	0.58
1:D:243:VAL:HA	1:D:246:LEU:HD22	1.85	0.58
1:C:212:THR:HG22	1:C:215:ARG:NH2	2.19	0.58
1:E:247:SER:O	1:E:251:ILE:HG13	2.05	0.57
1:E:232:LEU:HD21	1:E:277:HIS:HB2	1.87	0.57
1:C:243:VAL:HA	1:C:246:LEU:HD22	1.86	0.56
1:D:216:VAL:HG12	1:D:265:VAL:HG11	1.86	0.56
1:D:220:VAL:O	1:D:224:HIS:HD2	1.89	0.56
1:D:247:SER:O	1:D:251:ILE:HG13	2.05	0.56
1:F:243:VAL:HA	1:F:246:LEU:HD22	1.88	0.55
1:A:247:SER:O	1:A:251:ILE:HG13	2.06	0.55
1:C:216:VAL:HG12	1:C:265:VAL:HG11	1.88	0.55
1:C:247:SER:O	1:C:251:ILE:HG13	2.06	0.55
1:E:212:THR:HG22	1:E:215:ARG:NH2	2.22	0.55
1:A:243:VAL:HA	1:A:246:LEU:HD22	1.88	0.54
1:C:184:ARG:NH2	1:C:198:PRO:HD2	2.23	0.54
1:B:243:VAL:HA	1:B:246:LEU:HD22	1.89	0.54
1:B:247:SER:O	1:B:251:ILE:HG13	2.08	0.54
1:B:261:TRP:CZ3	1:B:315:PHE:HB2	2.43	0.54
1:D:296:ASP:O	1:D:300:ARG:HB2	2.07	0.54
1:A:213:LEU:HD21	1:A:268:ILE:HG21	1.90	0.53
1:B:184:ARG:NH2	1:B:198:PRO:HD2	2.21	0.53
1:E:184:ARG:NH2	1:E:198:PRO:HD2	2.23	0.53
1:F:255:SER:O	1:F:256:ASP:C	2.46	0.53
1:F:184:ARG:NH2	1:F:198:PRO:HD2	2.23	0.53
1:F:247:SER:O	1:F:251:ILE:HG13	2.09	0.53
1:E:216:VAL:HG12	1:E:265:VAL:HG11	1.90	0.52
1:D:213:LEU:HD21	1:D:268:ILE:HG21	1.92	0.52
1:D:300:ARG:HG2	1:E:255:SER:CB	2.40	0.52
1:C:213:LEU:HD21	1:C:268:ILE:HG21	1.92	0.51
1:A:321:VAL:HG23	1:A:322:GLU:H	1.76	0.50
1:B:210:LEU:O	1:B:214:ARG:HG2	2.11	0.50
1:F:255:SER:O	1:F:256:ASP:O	2.30	0.50
1:F:227:ALA:O	1:F:231:MET:HG3	2.12	0.49
1:A:296:ASP:OD2	1:B:252:HIS:HD2	1.95	0.49
1:C:248:ARG:HD2	1:F:244:LYS:HG2	1.95	0.49
1:E:255:SER:O	1:E:256:ASP:C	2.50	0.49
1:B:243:VAL:O	1:B:246:LEU:HB2	2.13	0.48
1:E:255:SER:O	1:E:256:ASP:O	2.31	0.48
1:C:309:GLN:O	1:C:314:GLY:HA3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:NH2	1:A:198:PRO:HD2	2.23	0.48
1:A:214:ARG:HD2	3:A:523:HOH:O	2.12	0.48
1:D:312:TRP:O	1:D:316:VAL:HG23	2.14	0.48
1:C:210:LEU:HD13	1:C:214:ARG:NH2	2.28	0.47
1:A:261:TRP:O	1:A:265:VAL:CG2	2.62	0.47
1:D:184:ARG:NH2	1:D:198:PRO:HD2	2.23	0.47
1:A:210:LEU:CD1	1:A:214:ARG:NH2	2.78	0.47
1:D:197:LYS:CB	1:D:198:PRO:HD3	2.43	0.47
1:A:197:LYS:CB	1:A:198:PRO:HD3	2.42	0.47
1:A:248:ARG:HD2	1:B:244:LYS:HG2	1.95	0.47
1:F:197:LYS:CB	1:F:198:PRO:HD3	2.44	0.47
1:C:243:VAL:O	1:C:246:LEU:HB2	2.14	0.47
1:A:252:HIS:HD2	1:B:296:ASP:OD2	1.98	0.46
1:A:257:GLY:HA3	1:F:233:ARG:NH2	2.30	0.46
1:D:309:GLN:O	1:D:314:GLY:HA3	2.15	0.46
1:C:255:SER:O	1:C:256:ASP:HB3	2.16	0.46
1:B:197:LYS:CB	1:B:198:PRO:HD3	2.43	0.46
1:C:249:VAL:HG22	3:C:520:HOH:O	2.15	0.46
1:D:220:VAL:O	1:D:224:HIS:CD2	2.68	0.46
1:D:290:LEU:HD11	2:D:401:2UU:H21	1.97	0.46
1:C:220:VAL:O	1:C:224:HIS:CD2	2.67	0.46
1:A:251:ILE:HD11	1:B:251:ILE:HD11	1.98	0.45
1:B:265:VAL:HG22	1:B:315:PHE:HE1	1.81	0.45
1:D:254:PHE:HA	2:D:401:2UU:O32	2.17	0.45
1:F:243:VAL:O	1:F:246:LEU:HB2	2.17	0.45
1:A:265:VAL:HG22	1:A:315:PHE:HE1	1.82	0.45
1:E:197:LYS:CB	1:E:198:PRO:HD3	2.42	0.45
1:E:210:LEU:HD12	1:E:214:ARG:NH2	2.32	0.45
1:D:246:LEU:HG	2:D:401:2UU:H7	1.98	0.44
1:F:210:LEU:O	1:F:214:ARG:HG2	2.17	0.44
1:A:284:GLU:HA	1:A:287:ILE:HD12	2.00	0.44
1:E:210:LEU:O	1:E:214:ARG:HG2	2.17	0.44
1:E:312:TRP:O	1:E:316:VAL:HG23	2.18	0.43
1:A:243:VAL:O	1:A:246:LEU:HB2	2.18	0.43
1:A:220:VAL:O	1:A:224:HIS:HD2	2.00	0.43
1:C:197:LYS:CB	1:C:198:PRO:HD3	2.43	0.43
1:D:240:GLU:CD	1:D:240:GLU:H	2.22	0.43
1:E:284:GLU:HA	1:E:287:ILE:HD12	2.00	0.43
1:B:240:GLU:CD	1:B:240:GLU:H	2.22	0.43
1:F:240:GLU:CD	1:F:240:GLU:H	2.23	0.42
1:F:220:VAL:O	1:F:224:HIS:CD2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:VAL:O	1:F:224:HIS:HD2	2.02	0.42
1:F:309:GLN:O	1:F:314:GLY:HA3	2.20	0.42
2:F:401:2UU:H19	2:F:401:2UU:H7	1.80	0.42
1:A:240:GLU:CD	1:A:240:GLU:H	2.23	0.42
1:A:244:LYS:HG2	1:B:248:ARG:HD2	2.01	0.42
1:C:197:LYS:HB2	1:C:198:PRO:CD	2.46	0.42
1:C:240:GLU:H	1:C:240:GLU:CD	2.23	0.42
1:D:267:LEU:HD12	2:D:401:2UU:C8	2.50	0.42
1:D:244:LYS:HG2	1:E:248:ARG:HD2	2.02	0.42
1:E:240:GLU:CD	1:E:240:GLU:H	2.22	0.42
1:F:284:GLU:HA	1:F:287:ILE:HD12	2.01	0.42
1:E:218:ASP:OD1	1:E:222:ARG:HD2	2.20	0.41
1:E:176:ARG:HH11	1:E:201:ARG:HE	1.69	0.41
1:D:197:LYS:HB2	1:D:198:PRO:CD	2.47	0.41
1:D:243:VAL:O	1:D:246:LEU:HB2	2.19	0.41
2:A:401:2UU:H19	2:A:401:2UU:H7	1.81	0.41
1:B:284:GLU:HA	1:B:287:ILE:HD12	2.03	0.41
1:A:246:LEU:HG	2:A:401:2UU:H7	2.02	0.41
1:A:300:ARG:HD3	1:B:255:SER:OG	2.20	0.41
1:B:197:LYS:HB2	1:B:198:PRO:CD	2.46	0.41
1:D:232:LEU:HD22	1:D:273:PHE:CE2	2.56	0.41
1:E:213:LEU:HD21	1:E:268:ILE:HG21	2.02	0.41
1:F:176:ARG:HH11	1:F:201:ARG:HE	1.69	0.41
1:C:284:GLU:HA	1:C:287:ILE:HD12	2.03	0.40
1:F:265:VAL:CG2	1:F:315:PHE:HE1	2.35	0.40
1:E:247:SER:HB2	3:E:507:HOH:O	2.20	0.40
1:D:284:GLU:HA	1:D:287:ILE:HD12	2.02	0.40
1:A:176:ARG:HH11	1:A:201:ARG:HE	1.69	0.40
1:A:261:TRP:CZ3	1:A:315:PHE:HB2	2.56	0.40
1:B:176:ARG:HH11	1:B:201:ARG:HE	1.70	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	146/163 (90%)	136 (93%)	7 (5%)	3 (2%)	7 22
1	B	149/163 (91%)	139 (93%)	7 (5%)	3 (2%)	7 23
1	C	147/163 (90%)	140 (95%)	5 (3%)	2 (1%)	11 31
1	D	147/163 (90%)	139 (95%)	4 (3%)	4 (3%)	5 16
1	E	149/163 (91%)	138 (93%)	7 (5%)	4 (3%)	5 16
1	F	147/163 (90%)	138 (94%)	6 (4%)	3 (2%)	7 23
All	All	885/978 (90%)	830 (94%)	36 (4%)	19 (2%)	7 22

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	197	LYS
1	B	197	LYS
1	C	197	LYS
1	D	197	LYS
1	E	197	LYS
1	E	256	ASP
1	F	197	LYS
1	F	256	ASP
1	C	200	GLY
1	E	321	VAL
1	D	201	ARG
1	A	255	SER
1	B	255	SER
1	D	255	SER
1	E	255	SER
1	F	255	SER
1	D	256	ASP
1	A	321	VAL
1	B	321	VAL

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	131/141 (93%)	117 (89%)	14 (11%)	6	18
1	B	132/141 (94%)	117 (89%)	15 (11%)	5	15
1	C	130/141 (92%)	116 (89%)	14 (11%)	6	17
1	D	130/141 (92%)	115 (88%)	15 (12%)	5	15
1	E	132/141 (94%)	116 (88%)	16 (12%)	5	13
1	F	130/141 (92%)	115 (88%)	15 (12%)	5	15
All	All	785/846 (93%)	696 (89%)	89 (11%)	6	16

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	A	194	LYS
1	A	197	LYS
1	A	210	LEU
1	A	225	GLU
1	A	240	GLU
1	A	246	LEU
1	A	248	ARG
1	A	249	VAL
1	A	251	ILE
1	A	259	THR
1	A	263	ARG
1	A	300	ARG
1	A	322	GLU
1	B	173	ASP
1	B	194	LYS
1	B	197	LYS
1	B	210	LEU
1	B	212	THR
1	B	225	GLU
1	B	233	ARG
1	B	240	GLU
1	B	246	LEU
1	B	248	ARG
1	B	249	VAL
1	B	251	ILE
1	B	259	THR
1	B	263	ARG

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Mol	Chain	Res	Type
1	B	322	GLU
1	C	173	ASP
1	C	194	LYS
1	C	197	LYS
1	C	210	LEU
1	C	212	THR
1	C	225	GLU
1	C	233	ARG
1	C	240	GLU
1	C	246	LEU
1	C	248	ARG
1	C	249	VAL
1	C	251	ILE
1	C	259	THR
1	C	263	ARG
1	D	173	ASP
1	D	194	LYS
1	D	197	LYS
1	D	201	ARG
1	D	210	LEU
1	D	225	GLU
1	D	233	ARG
1	D	240	GLU
1	D	246	LEU
1	D	248	ARG
1	D	249	VAL
1	D	251	ILE
1	D	259	THR
1	D	263	ARG
1	D	300	ARG
1	E	173	ASP
1	E	194	LYS
1	E	197	LYS
1	E	201	ARG
1	E	210	LEU
1	E	212	THR
1	E	225	GLU
1	E	233	ARG
1	E	240	GLU
1	E	246	LEU
1	E	248	ARG
1	E	249	VAL

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Mol	Chain	Res	Type
1	E	251	ILE
1	E	259	THR
1	E	263	ARG
1	E	321	VAL
1	F	173	ASP
1	F	197	LYS
1	F	201	ARG
1	F	210	LEU
1	F	225	GLU
1	F	240	GLU
1	F	246	LEU
1	F	248	ARG
1	F	249	VAL
1	F	251	ILE
1	F	259	THR
1	F	263	ARG
1	F	267	LEU
1	F	317	GLU
1	F	320	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	224	HIS
1	A	239	ASN
1	A	252	HIS
1	B	177	GLN
1	B	239	ASN
1	B	252	HIS
1	C	177	GLN
1	C	224	HIS
1	C	239	ASN
1	D	224	HIS
1	D	239	ASN
1	D	252	HIS
1	E	177	GLN
1	E	224	HIS
1	E	239	ASN
1	E	252	HIS
1	F	224	HIS
1	F	239	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	2UU	F	401	-	41,41,41	1.35	4 (9%)	59,59,59	0.97	1 (1%)
2	2UU	C	401	-	41,41,41	1.38	3 (7%)	59,59,59	0.90	1 (1%)
2	2UU	B	401	-	41,41,41	1.16	2 (4%)	59,59,59	1.04	2 (3%)
2	2UU	D	401	-	41,41,41	1.32	3 (7%)	59,59,59	1.11	3 (5%)
2	2UU	A	401	-	41,41,41	1.37	3 (7%)	59,59,59	1.02	2 (3%)
2	2UU	E	401	-	41,41,41	1.36	3 (7%)	59,59,59	0.90	2 (3%)

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	2UU	F	401	-	-	3/23/23/23	0/5/5/5
2	2UU	C	401	-	-	3/23/23/23	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2UU	B	401	-	-	3/23/23/23	0/5/5/5
2	2UU	D	401	-	-	3/23/23/23	0/5/5/5
2	2UU	A	401	-	-	3/23/23/23	0/5/5/5
2	2UU	E	401	-	-	3/23/23/23	0/5/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	2UU	S37-N31	5.47	1.72	1.63
2	E	401	2UU	S37-N31	5.38	1.72	1.63
2	A	401	2UU	S37-N31	5.19	1.72	1.63
2	D	401	2UU	S37-N31	4.70	1.71	1.63
2	F	401	2UU	S37-N31	4.58	1.71	1.63
2	B	401	2UU	S37-N31	4.05	1.70	1.63
2	F	401	2UU	C22-C21	-3.76	1.43	1.49
2	D	401	2UU	C22-C21	-3.76	1.43	1.49
2	E	401	2UU	C22-C21	-3.72	1.43	1.49
2	C	401	2UU	C22-C21	-3.41	1.43	1.49
2	A	401	2UU	C22-C21	-2.83	1.44	1.49
2	B	401	2UU	C22-C21	-2.78	1.44	1.49
2	A	401	2UU	C20-C19	-2.57	1.38	1.43
2	C	401	2UU	C20-C19	-2.24	1.39	1.43
2	E	401	2UU	C20-C19	-2.10	1.39	1.43
2	F	401	2UU	C7-C20	-2.10	1.38	1.42
2	F	401	2UU	C24-C20	-2.06	1.38	1.42
2	D	401	2UU	C20-C19	-2.04	1.39	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	2UU	C25-C23-C29	4.07	126.53	121.72
2	A	401	2UU	O34-S37-O33	2.81	123.00	119.55
2	C	401	2UU	O35-C29-C23	-2.52	108.05	115.31
2	B	401	2UU	C25-C23-C29	2.32	124.45	121.72
2	B	401	2UU	C18-C21-C22	-2.16	117.16	120.70
2	F	401	2UU	C25-C23-C29	2.13	124.23	121.72
2	E	401	2UU	C30-C24-C20	2.09	124.31	121.08
2	D	401	2UU	C17-C28-S37	-2.08	117.51	119.77
2	A	401	2UU	C25-N31-S37	-2.04	116.76	123.41
2	D	401	2UU	C9-C11-C24	-2.01	119.65	122.19
2	E	401	2UU	O35-C29-C23	-2.00	109.55	115.31

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	2UU	C25-N31-S37-O33
2	B	401	2UU	C25-N31-S37-O33
2	C	401	2UU	C25-N31-S37-O33
2	D	401	2UU	C25-N31-S37-O33
2	E	401	2UU	C25-N31-S37-O33
2	F	401	2UU	C25-N31-S37-O33
2	A	401	2UU	C25-N31-S37-C28
2	B	401	2UU	C25-N31-S37-C28
2	C	401	2UU	C25-N31-S37-C28
2	E	401	2UU	C25-N31-S37-C28
2	F	401	2UU	C25-N31-S37-C28
2	D	401	2UU	C25-N31-S37-C28
2	A	401	2UU	C25-N31-S37-O34
2	B	401	2UU	C25-N31-S37-O34
2	F	401	2UU	C25-N31-S37-O34
2	E	401	2UU	C25-N31-S37-O34
2	C	401	2UU	C25-N31-S37-O34
2	D	401	2UU	C25-N31-S37-O34

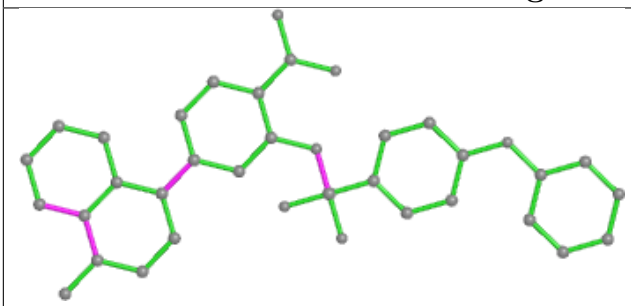
There are no ring outliers.

3 monomers are involved in 7 short contacts:

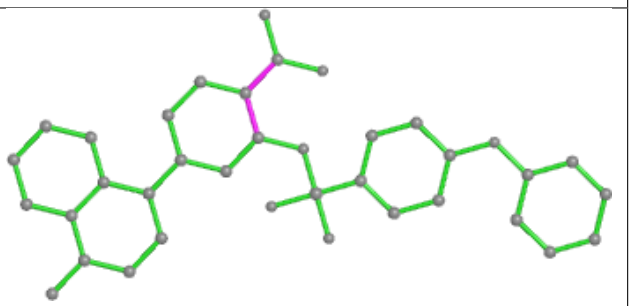
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	2UU	1	0
2	D	401	2UU	4	0
2	A	401	2UU	2	0

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

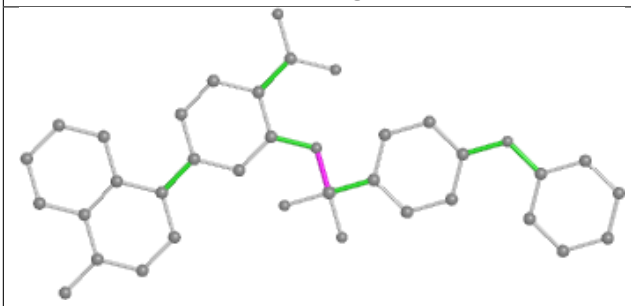
Ligand 2UU F 401



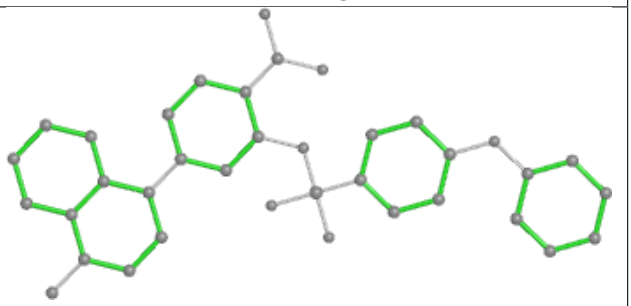
Bond lengths



Bond angles

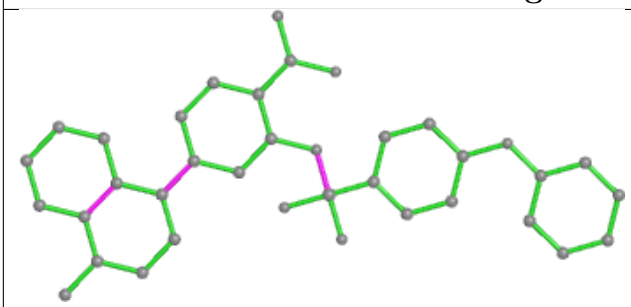


Torsions

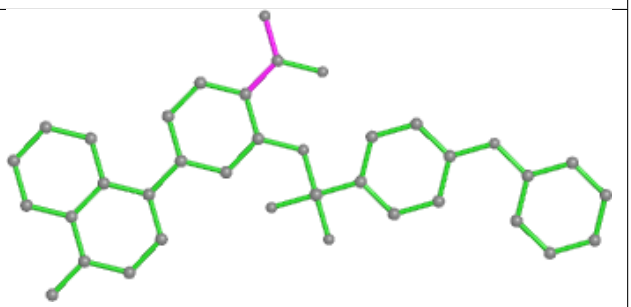


Rings

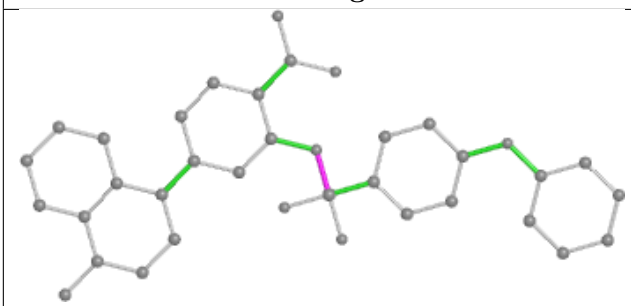
Ligand 2UU C 401



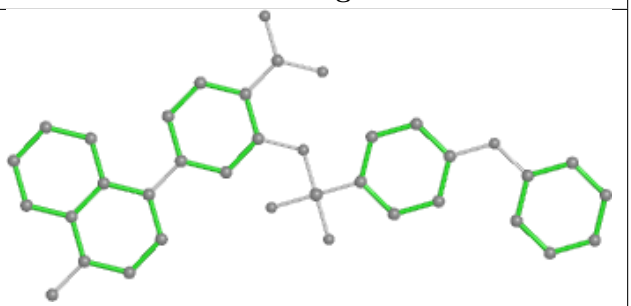
Bond lengths



Bond angles

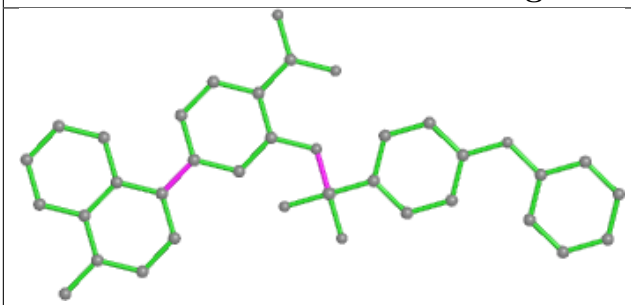


Torsions

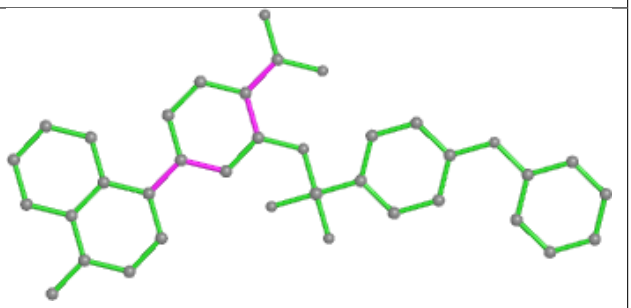


Rings

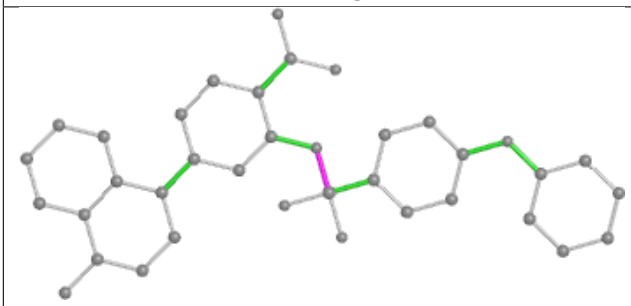
Ligand 2UU B 401



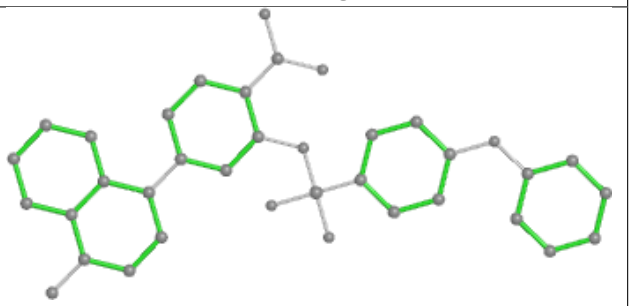
Bond lengths



Bond angles

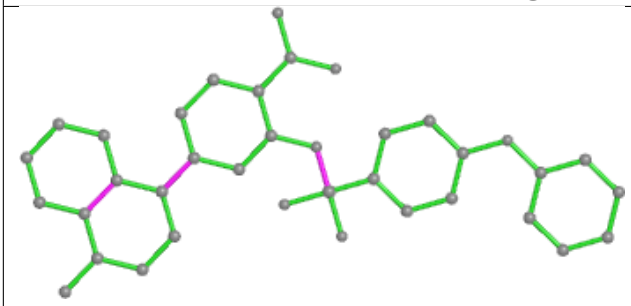


Torsions

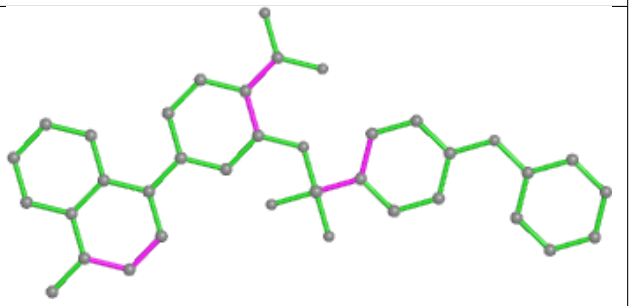


Rings

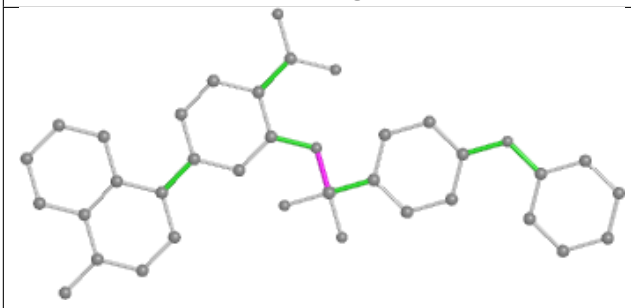
Ligand 2UU D 401



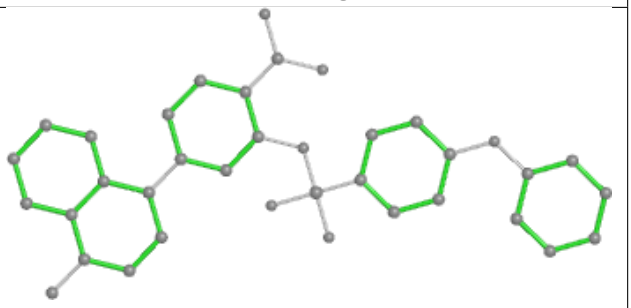
Bond lengths



Bond angles

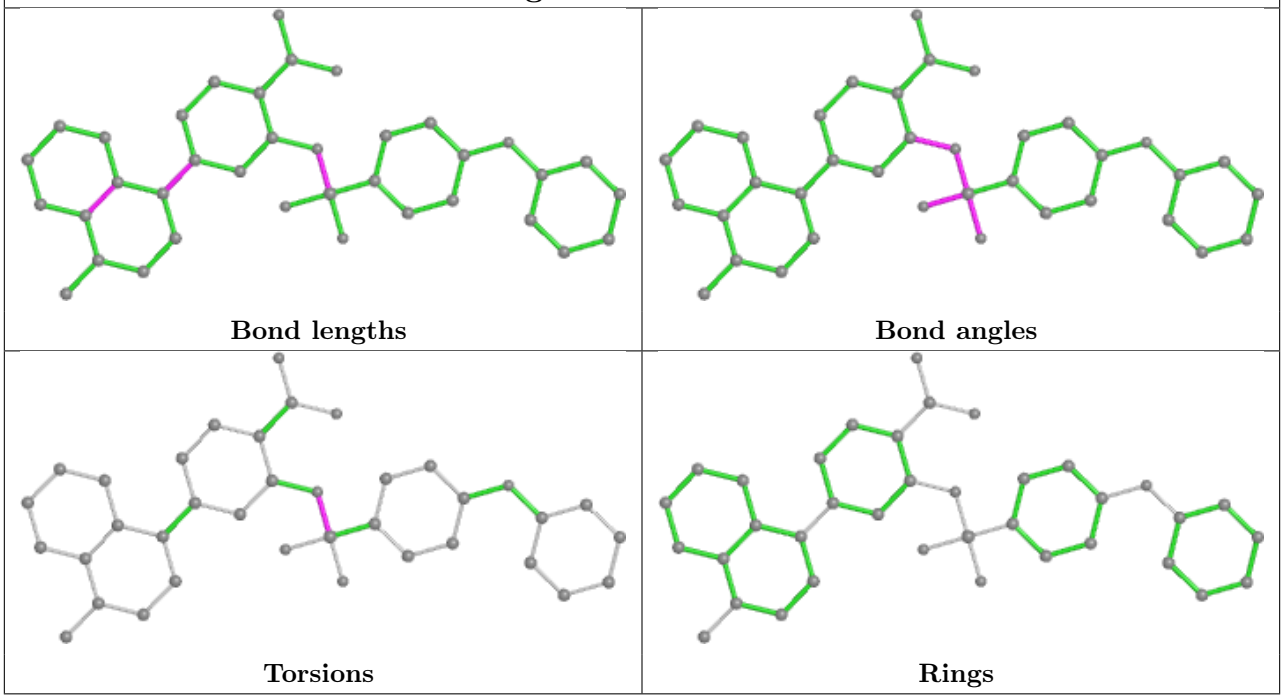


Torsions

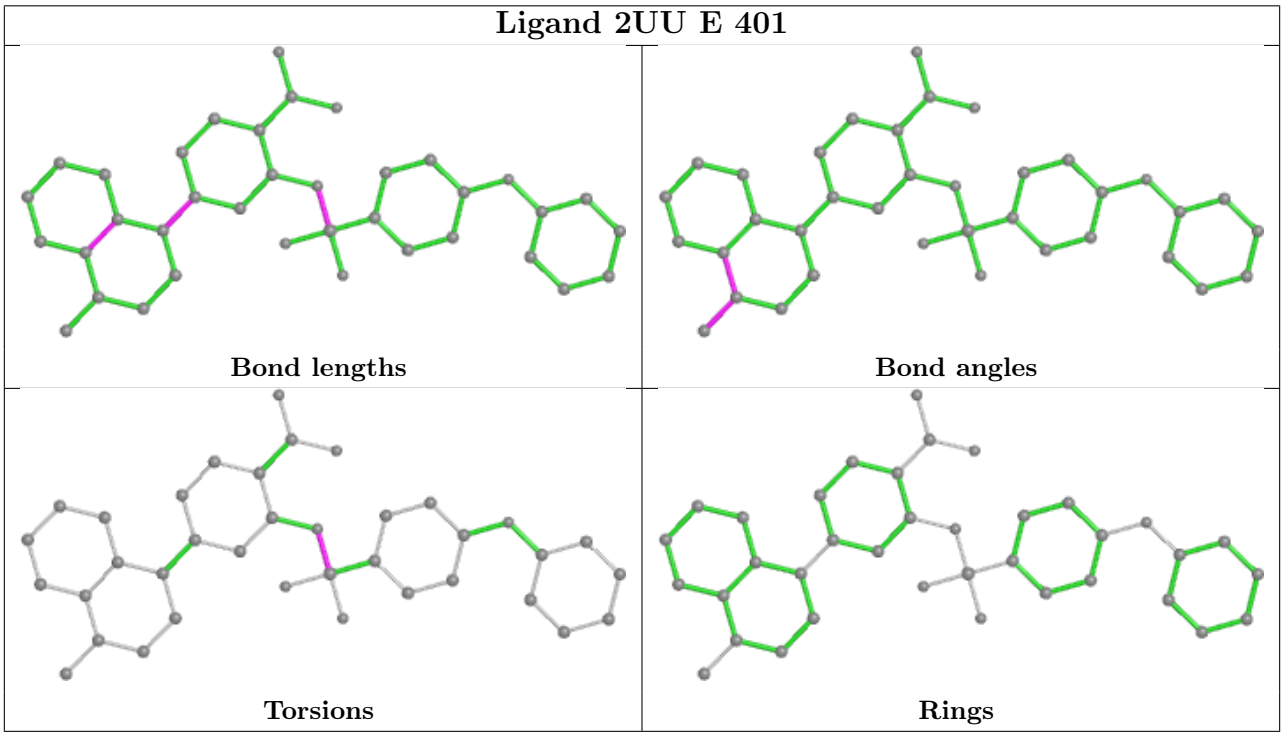


Rings

Ligand 2UU A 401



Ligand 2UU E 401



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, 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	150/163 (92%)	0.44	16 (10%) 6 4	36, 53, 110, 141	0
1	B	151/163 (92%)	0.39	11 (7%) 15 11	35, 51, 110, 137	0
1	C	149/163 (91%)	0.09	8 (5%) 25 21	37, 56, 101, 126	0
1	D	149/163 (91%)	0.06	6 (4%) 38 32	37, 52, 101, 132	0
1	E	151/163 (92%)	0.42	16 (10%) 6 4	38, 59, 110, 134	0
1	F	149/163 (91%)	0.43	10 (6%) 17 13	39, 60, 114, 136	0
All	All	899/978 (91%)	0.30	67 (7%) 14 10	35, 55, 110, 141	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	201	ARG	8.9
1	B	200	GLY	8.6
1	F	201	ARG	7.9
1	A	201	ARG	7.5
1	C	201	ARG	7.3
1	B	201	ARG	7.1
1	D	201	ARG	6.4
1	B	198	PRO	6.3
1	F	200	GLY	6.2
1	D	200	GLY	5.8
1	F	193	ALA	4.8
1	F	198	PRO	4.5
1	A	200	GLY	4.4
1	E	321	VAL	4.3
1	C	200	GLY	4.3
1	A	198	PRO	4.3
1	B	202	SER	4.2
1	F	195	ASP	4.1
1	F	196	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	202	SER	4.0
1	A	193	ALA	3.9
1	E	200	GLY	3.9
1	E	198	PRO	3.9
1	F	199	MET	3.8
1	E	199	MET	3.7
1	E	196	THR	3.7
1	D	196	THR	3.6
1	A	280	THR	3.5
1	F	172	MET	3.4
1	C	196	THR	3.4
1	B	203	GLY	3.3
1	B	199	MET	3.3
1	E	322	GLU	3.2
1	A	202	SER	3.2
1	C	193	ALA	3.2
1	A	199	MET	3.2
1	C	199	MET	3.1
1	B	196	THR	3.1
1	B	280	THR	2.9
1	F	202	SER	2.9
1	D	199	MET	2.8
1	E	194	LYS	2.8
1	A	192	GLY	2.7
1	F	194	LYS	2.7
1	E	172	MET	2.7
1	C	195	ASP	2.7
1	A	191	THR	2.6
1	E	195	ASP	2.6
1	E	193	ALA	2.6
1	E	180	GLU	2.6
1	D	195	ASP	2.5
1	B	281	ILE	2.5
1	E	320	HIS	2.4
1	A	195	ASP	2.3
1	C	191	THR	2.3
1	B	193	ALA	2.3
1	A	284	GLU	2.3
1	B	279	LYS	2.3
1	A	279	LYS	2.2
1	C	198	PRO	2.1
1	E	191	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	190	ALA	2.1
1	E	190	ALA	2.0
1	A	265	VAL	2.0
1	A	194	LYS	2.0
1	D	197	LYS	2.0
1	A	203	GLY	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)

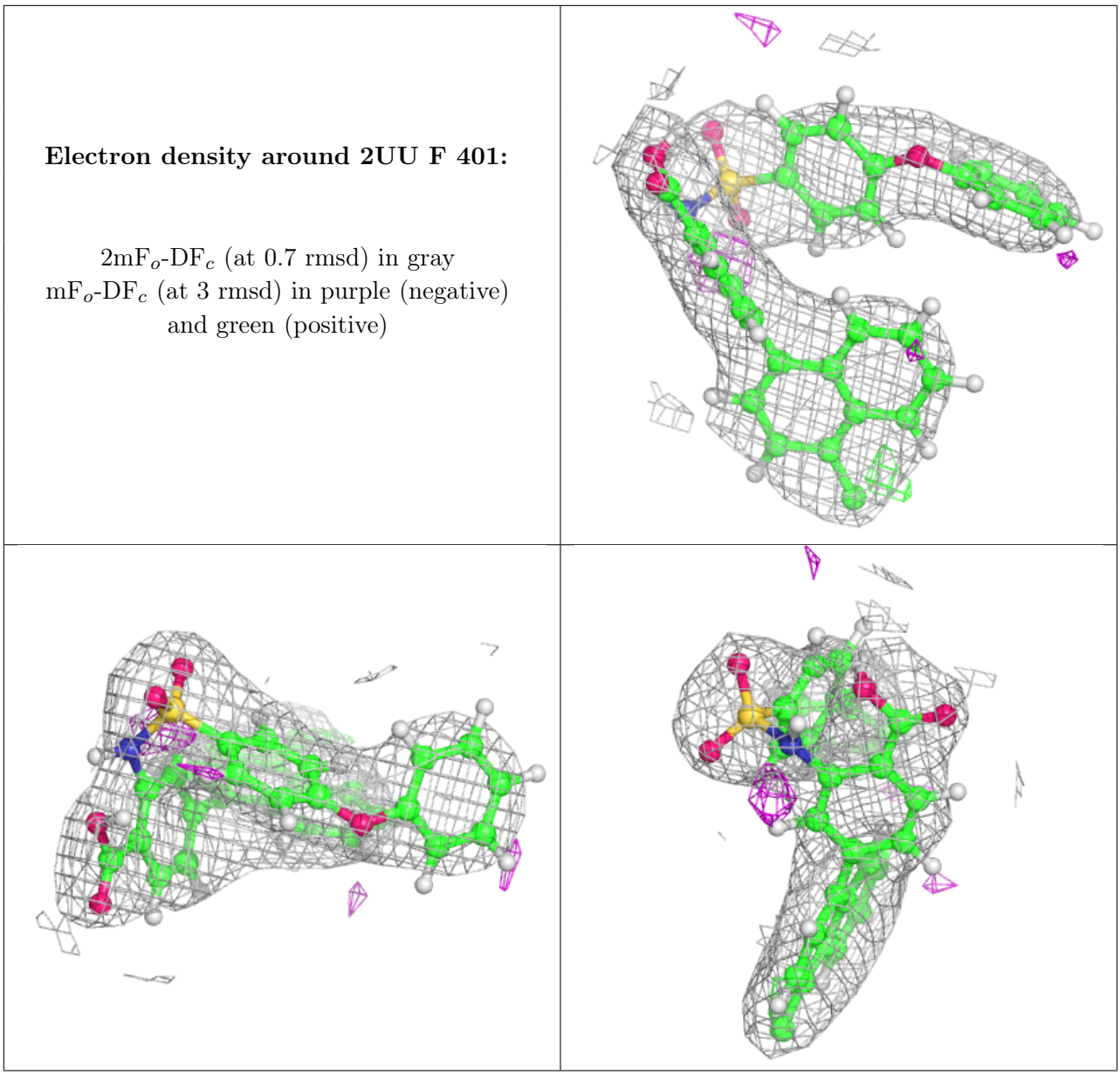
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	2UU	F	401	37/37	0.97	0.17	38,44,49,50	0
2	2UU	B	401	37/37	0.98	0.16	35,40,45,46	0
2	2UU	C	401	37/37	0.98	0.20	38,45,56,57	0
2	2UU	D	401	37/37	0.98	0.19	35,44,64,64	0
2	2UU	E	401	37/37	0.98	0.15	35,46,51,53	0
2	2UU	A	401	37/37	0.98	0.18	35,42,50,50	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.

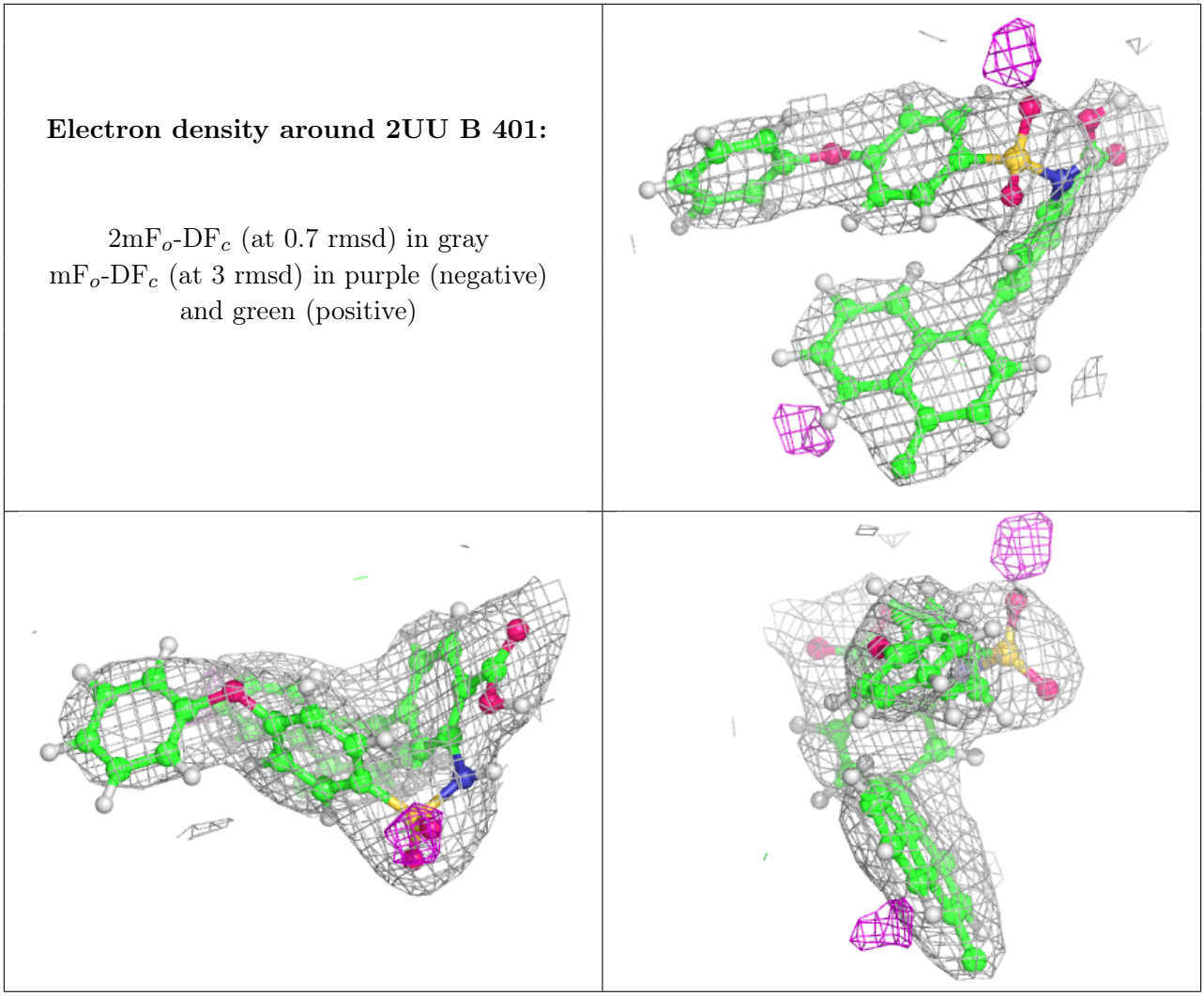
Electron density around 2UU F 401:

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



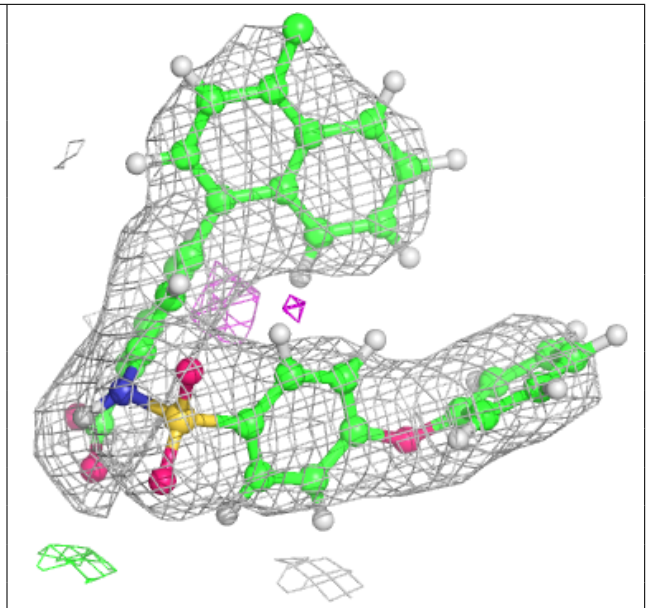
Electron density around 2UU B 401:

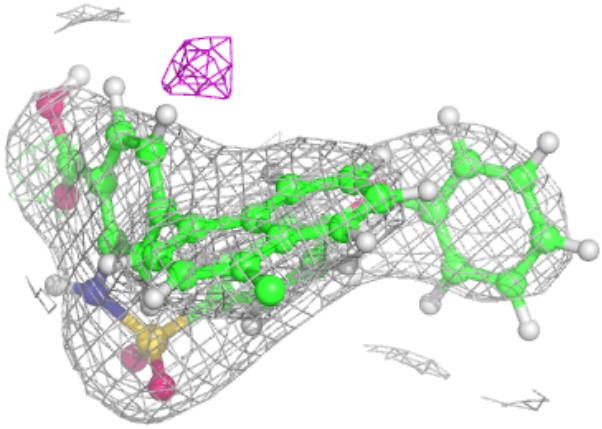
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

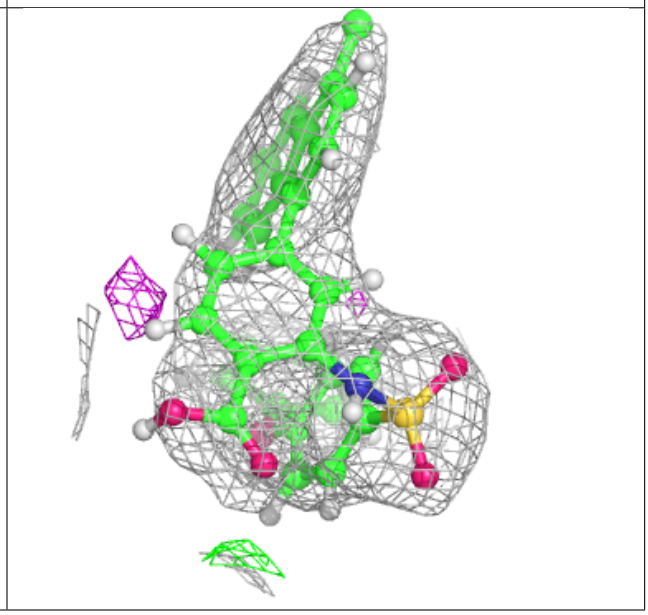


Electron density around 2UU C 401:

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

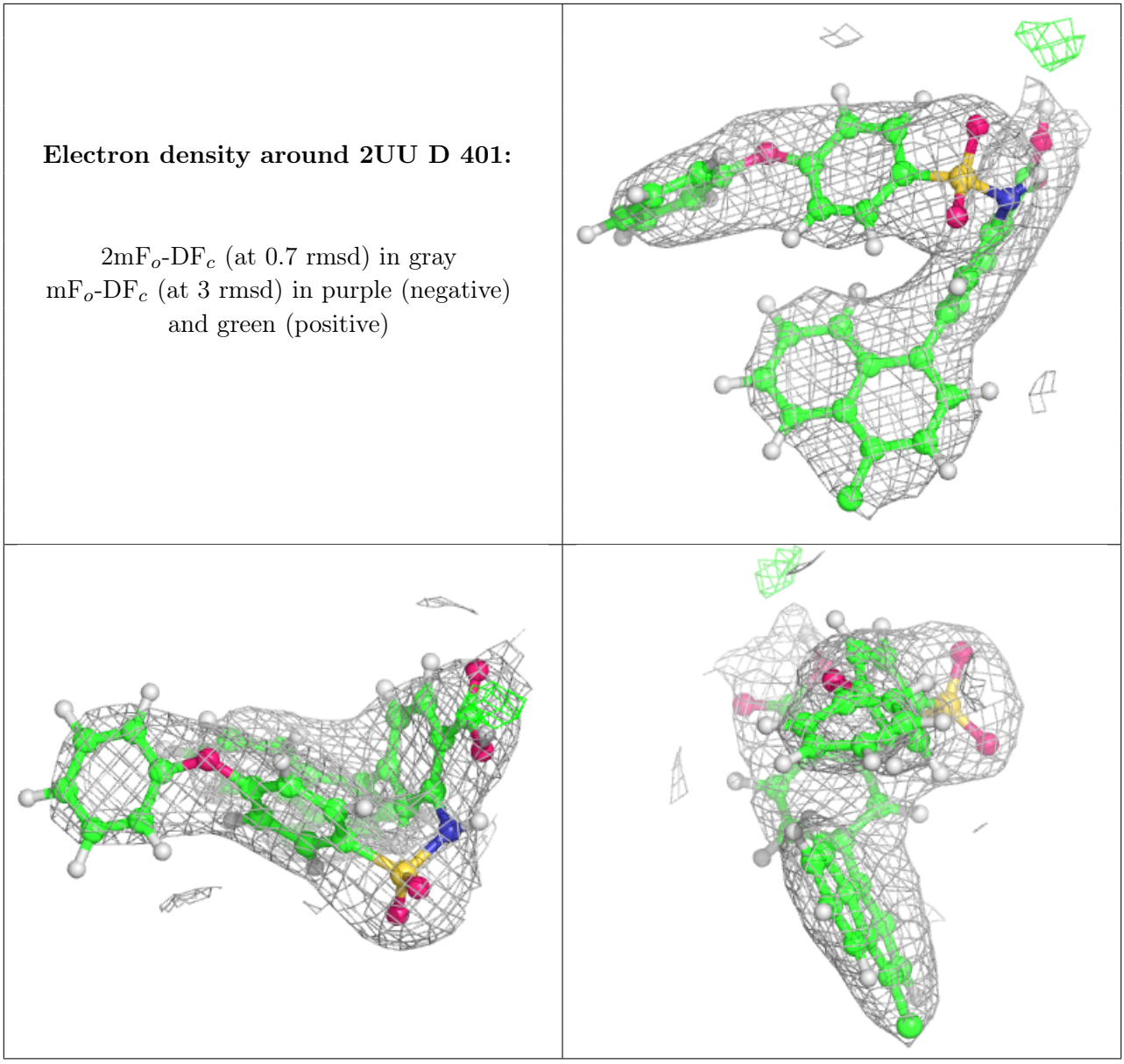






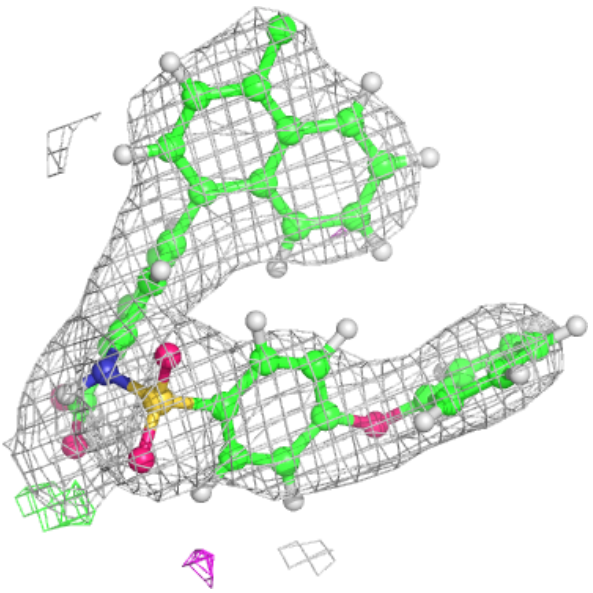
Electron density around 2UU D 401:

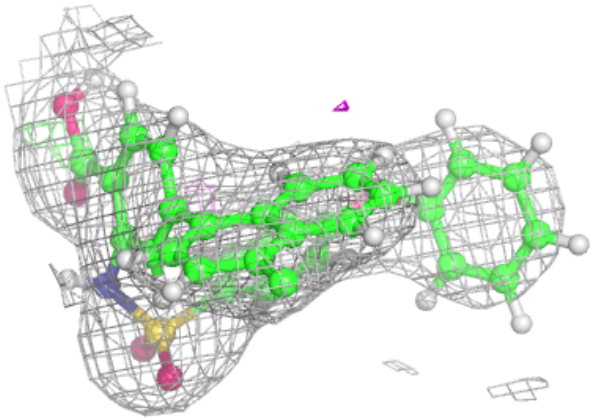
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

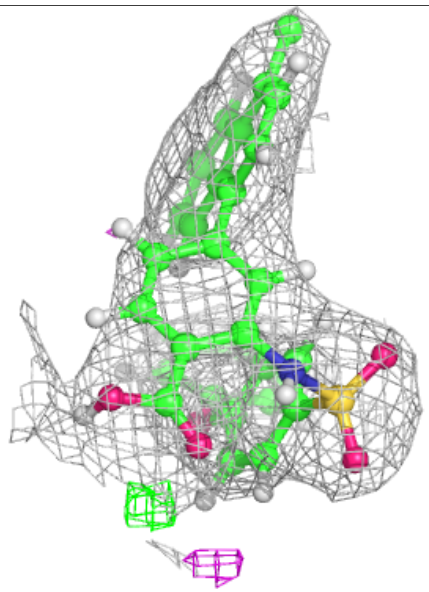


Electron density around 2UU E 401:

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

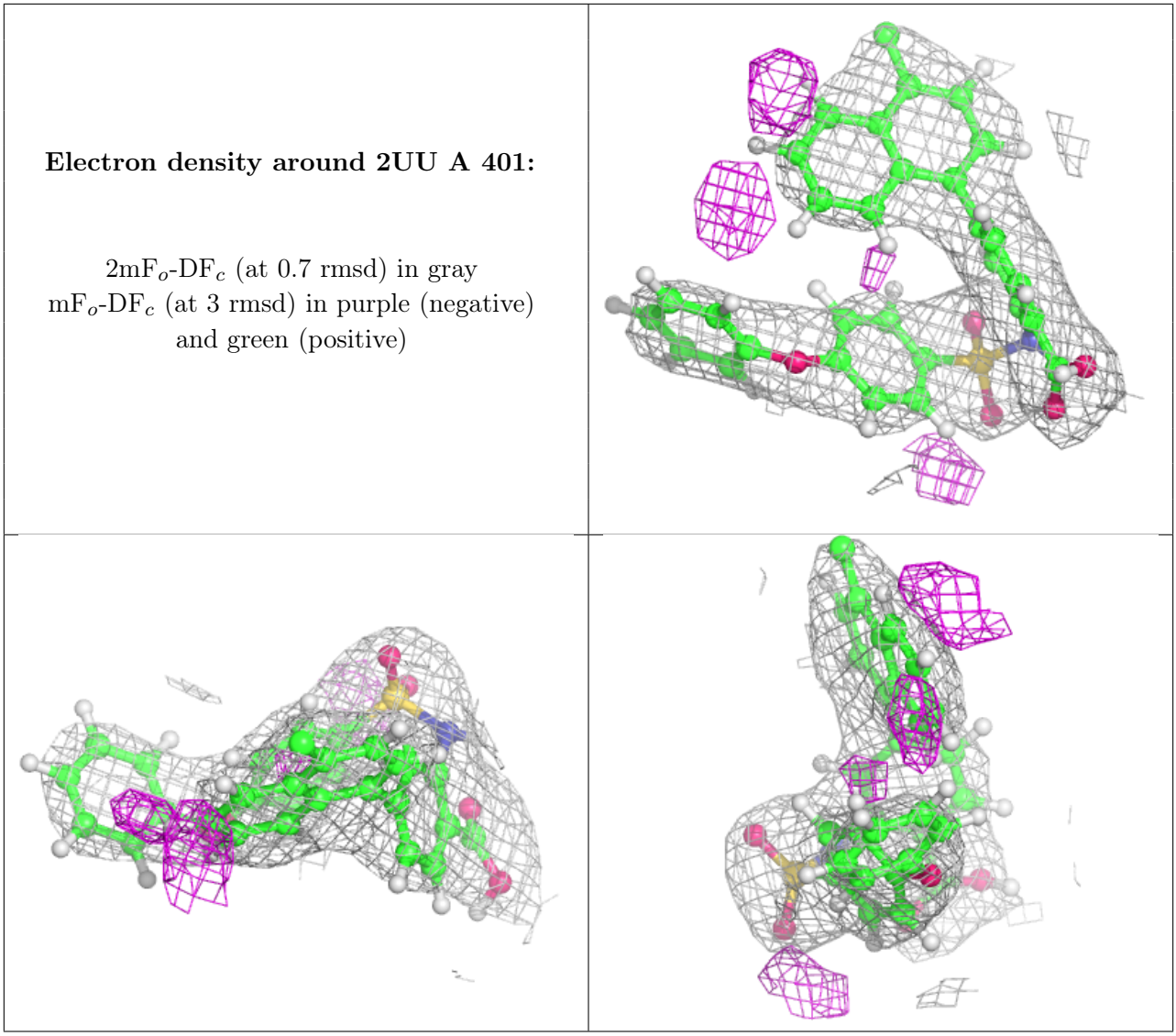






Electron density around 2UU A 401:

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



6.5 Other polymers

There are no such residues in this entry.