



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:06 PM UTC

PDB ID : 8FJZ / pdb_00008fjz
Title : Crystal structure of HPK1 kinase domain T165E,S171E phosphomimetic mutant in complex with 3-{4-[(3R,5S)-3-Amino-5-methylpiperidin-1-yl]-6-chloro-7H-pyrrolo[2,3-d]pyrimidin-5-yl}benzonitrile
Authors : McTigue, M.; Johnson, E.; Cronin, C.
Deposited on : 2022-12-20
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

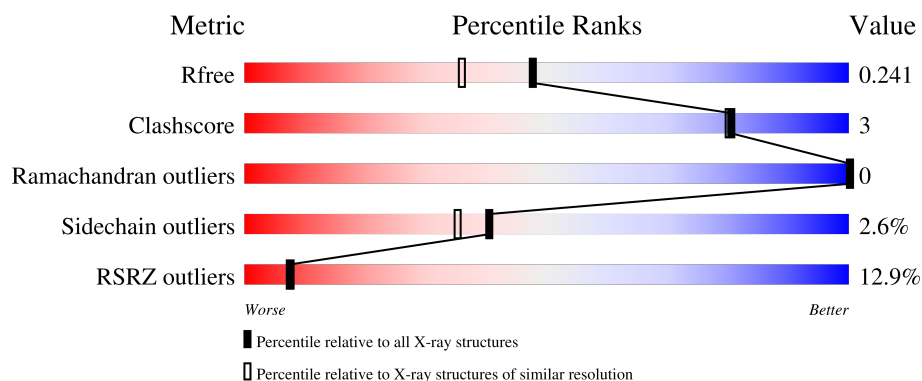
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	331	5% 78% 9% 13%
1	B	331	8% 78% 8% 14%
1	C	331	8% 78% 9% 13%
1	D	331	10% 79% 5% 16%

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Mol	Chain	Length	Quality of chain
1	E	331	11% 80% 5% 15%
1	F	331	24% 73% 10% 17%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14170 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 Mitogen-activated protein kinase kinase kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2246	1447	384	404	11			
1	B	284	Total	C	N	O	S	0	0	0
			2220	1427	384	398	11			
1	C	288	Total	C	N	O	S	0	0	0
			2246	1441	388	406	11			
1	D	279	Total	C	N	O	S	0	0	0
			2181	1403	377	390	11			
1	E	283	Total	C	N	O	S	0	0	0
			2209	1418	385	396	10			
1	F	276	Total	C	N	O	S	0	0	0
			2072	1326	360	376	10			

There are 156 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q92918
A	-22	ALA	-	expression tag	UNP Q92918
A	-21	SER	-	expression tag	UNP Q92918
A	-20	HIS	-	expression tag	UNP Q92918
A	-19	HIS	-	expression tag	UNP Q92918
A	-18	HIS	-	expression tag	UNP Q92918
A	-17	HIS	-	expression tag	UNP Q92918
A	-16	HIS	-	expression tag	UNP Q92918
A	-15	HIS	-	expression tag	UNP Q92918
A	-14	ASP	-	expression tag	UNP Q92918
A	-13	TYR	-	expression tag	UNP Q92918
A	-12	ASP	-	expression tag	UNP Q92918
A	-11	GLY	-	expression tag	UNP Q92918
A	-10	ALA	-	expression tag	UNP Q92918
A	-9	THR	-	expression tag	UNP Q92918
A	-8	THR	-	expression tag	UNP Q92918
A	-7	GLU	-	expression tag	UNP Q92918

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASN	-	expression tag	UNP Q92918
A	-5	LEU	-	expression tag	UNP Q92918
A	-4	TYR	-	expression tag	UNP Q92918
A	-3	PHE	-	expression tag	UNP Q92918
A	-2	GLN	-	expression tag	UNP Q92918
A	-1	GLY	-	expression tag	UNP Q92918
A	0	SER	-	expression tag	UNP Q92918
A	165	GLU	THR	engineered mutation	UNP Q92918
A	171	GLU	SER	engineered mutation	UNP Q92918
B	-23	MET	-	expression tag	UNP Q92918
B	-22	ALA	-	expression tag	UNP Q92918
B	-21	SER	-	expression tag	UNP Q92918
B	-20	HIS	-	expression tag	UNP Q92918
B	-19	HIS	-	expression tag	UNP Q92918
B	-18	HIS	-	expression tag	UNP Q92918
B	-17	HIS	-	expression tag	UNP Q92918
B	-16	HIS	-	expression tag	UNP Q92918
B	-15	HIS	-	expression tag	UNP Q92918
B	-14	ASP	-	expression tag	UNP Q92918
B	-13	TYR	-	expression tag	UNP Q92918
B	-12	ASP	-	expression tag	UNP Q92918
B	-11	GLY	-	expression tag	UNP Q92918
B	-10	ALA	-	expression tag	UNP Q92918
B	-9	THR	-	expression tag	UNP Q92918
B	-8	THR	-	expression tag	UNP Q92918
B	-7	GLU	-	expression tag	UNP Q92918
B	-6	ASN	-	expression tag	UNP Q92918
B	-5	LEU	-	expression tag	UNP Q92918
B	-4	TYR	-	expression tag	UNP Q92918
B	-3	PHE	-	expression tag	UNP Q92918
B	-2	GLN	-	expression tag	UNP Q92918
B	-1	GLY	-	expression tag	UNP Q92918
B	0	SER	-	expression tag	UNP Q92918
B	165	GLU	THR	engineered mutation	UNP Q92918
B	171	GLU	SER	engineered mutation	UNP Q92918
C	-23	MET	-	expression tag	UNP Q92918
C	-22	ALA	-	expression tag	UNP Q92918
C	-21	SER	-	expression tag	UNP Q92918
C	-20	HIS	-	expression tag	UNP Q92918
C	-19	HIS	-	expression tag	UNP Q92918
C	-18	HIS	-	expression tag	UNP Q92918
C	-17	HIS	-	expression tag	UNP Q92918

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	HIS	-	expression tag	UNP Q92918
C	-15	HIS	-	expression tag	UNP Q92918
C	-14	ASP	-	expression tag	UNP Q92918
C	-13	TYR	-	expression tag	UNP Q92918
C	-12	ASP	-	expression tag	UNP Q92918
C	-11	GLY	-	expression tag	UNP Q92918
C	-10	ALA	-	expression tag	UNP Q92918
C	-9	THR	-	expression tag	UNP Q92918
C	-8	THR	-	expression tag	UNP Q92918
C	-7	GLU	-	expression tag	UNP Q92918
C	-6	ASN	-	expression tag	UNP Q92918
C	-5	LEU	-	expression tag	UNP Q92918
C	-4	TYR	-	expression tag	UNP Q92918
C	-3	PHE	-	expression tag	UNP Q92918
C	-2	GLN	-	expression tag	UNP Q92918
C	-1	GLY	-	expression tag	UNP Q92918
C	0	SER	-	expression tag	UNP Q92918
C	165	GLU	THR	engineered mutation	UNP Q92918
C	171	GLU	SER	engineered mutation	UNP Q92918
D	-23	MET	-	expression tag	UNP Q92918
D	-22	ALA	-	expression tag	UNP Q92918
D	-21	SER	-	expression tag	UNP Q92918
D	-20	HIS	-	expression tag	UNP Q92918
D	-19	HIS	-	expression tag	UNP Q92918
D	-18	HIS	-	expression tag	UNP Q92918
D	-17	HIS	-	expression tag	UNP Q92918
D	-16	HIS	-	expression tag	UNP Q92918
D	-15	HIS	-	expression tag	UNP Q92918
D	-14	ASP	-	expression tag	UNP Q92918
D	-13	TYR	-	expression tag	UNP Q92918
D	-12	ASP	-	expression tag	UNP Q92918
D	-11	GLY	-	expression tag	UNP Q92918
D	-10	ALA	-	expression tag	UNP Q92918
D	-9	THR	-	expression tag	UNP Q92918
D	-8	THR	-	expression tag	UNP Q92918
D	-7	GLU	-	expression tag	UNP Q92918
D	-6	ASN	-	expression tag	UNP Q92918
D	-5	LEU	-	expression tag	UNP Q92918
D	-4	TYR	-	expression tag	UNP Q92918
D	-3	PHE	-	expression tag	UNP Q92918
D	-2	GLN	-	expression tag	UNP Q92918
D	-1	GLY	-	expression tag	UNP Q92918

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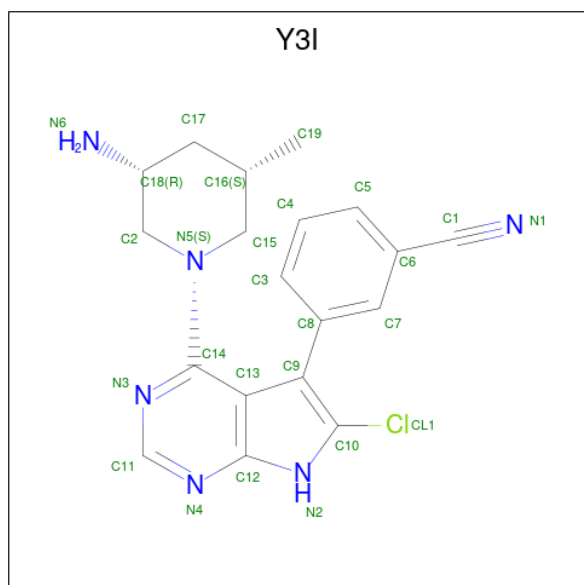
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP Q92918
D	165	GLU	THR	engineered mutation	UNP Q92918
D	171	GLU	SER	engineered mutation	UNP Q92918
E	-23	MET	-	expression tag	UNP Q92918
E	-22	ALA	-	expression tag	UNP Q92918
E	-21	SER	-	expression tag	UNP Q92918
E	-20	HIS	-	expression tag	UNP Q92918
E	-19	HIS	-	expression tag	UNP Q92918
E	-18	HIS	-	expression tag	UNP Q92918
E	-17	HIS	-	expression tag	UNP Q92918
E	-16	HIS	-	expression tag	UNP Q92918
E	-15	HIS	-	expression tag	UNP Q92918
E	-14	ASP	-	expression tag	UNP Q92918
E	-13	TYR	-	expression tag	UNP Q92918
E	-12	ASP	-	expression tag	UNP Q92918
E	-11	GLY	-	expression tag	UNP Q92918
E	-10	ALA	-	expression tag	UNP Q92918
E	-9	THR	-	expression tag	UNP Q92918
E	-8	THR	-	expression tag	UNP Q92918
E	-7	GLU	-	expression tag	UNP Q92918
E	-6	ASN	-	expression tag	UNP Q92918
E	-5	LEU	-	expression tag	UNP Q92918
E	-4	TYR	-	expression tag	UNP Q92918
E	-3	PHE	-	expression tag	UNP Q92918
E	-2	GLN	-	expression tag	UNP Q92918
E	-1	GLY	-	expression tag	UNP Q92918
E	0	SER	-	expression tag	UNP Q92918
E	165	GLU	THR	engineered mutation	UNP Q92918
E	171	GLU	SER	engineered mutation	UNP Q92918
F	-23	MET	-	expression tag	UNP Q92918
F	-22	ALA	-	expression tag	UNP Q92918
F	-21	SER	-	expression tag	UNP Q92918
F	-20	HIS	-	expression tag	UNP Q92918
F	-19	HIS	-	expression tag	UNP Q92918
F	-18	HIS	-	expression tag	UNP Q92918
F	-17	HIS	-	expression tag	UNP Q92918
F	-16	HIS	-	expression tag	UNP Q92918
F	-15	HIS	-	expression tag	UNP Q92918
F	-14	ASP	-	expression tag	UNP Q92918
F	-13	TYR	-	expression tag	UNP Q92918
F	-12	ASP	-	expression tag	UNP Q92918
F	-11	GLY	-	expression tag	UNP Q92918

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-10	ALA	-	expression tag	UNP Q92918
F	-9	THR	-	expression tag	UNP Q92918
F	-8	THR	-	expression tag	UNP Q92918
F	-7	GLU	-	expression tag	UNP Q92918
F	-6	ASN	-	expression tag	UNP Q92918
F	-5	LEU	-	expression tag	UNP Q92918
F	-4	TYR	-	expression tag	UNP Q92918
F	-3	PHE	-	expression tag	UNP Q92918
F	-2	GLN	-	expression tag	UNP Q92918
F	-1	GLY	-	expression tag	UNP Q92918
F	0	SER	-	expression tag	UNP Q92918
F	165	GLU	THR	engineered mutation	UNP Q92918
F	171	GLU	SER	engineered mutation	UNP Q92918

- Molecule 2 is (3P)-3-{4-[(3R,5S)-3-amino-5-methylpiperidin-1-yl]-6-chloro-7H-pyrrolo[2,3-d]pyrimidin-5-yl}benzonitrile (CCD ID: Y3I) (formula: C₁₉H₁₉ClN₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			26	19	1	6		
2	B	1	Total	C	Cl	N	0	0
			26	19	1	6		
2	C	1	Total	C	Cl	N	0	0
			26	19	1	6		
2	D	1	Total	C	Cl	N	0	0
			26	19	1	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	Cl	N	0	0
			26	19	1	6		
2	F	1	Total	C	Cl	N	0	0
			26	19	1	6		

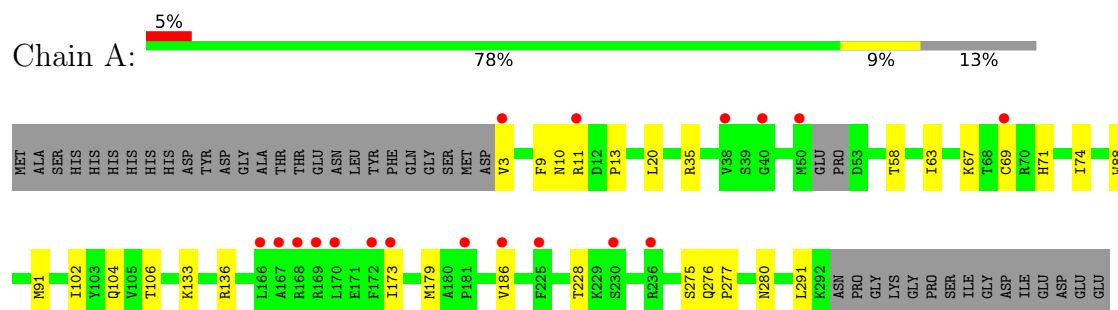
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total	O	0	0
			214	214		
3	B	190	Total	O	0	0
			190	190		
3	C	120	Total	O	0	0
			120	120		
3	D	138	Total	O	0	0
			138	138		
3	E	114	Total	O	0	0
			114	114		
3	F	64	Total	O	0	0
			64	64		

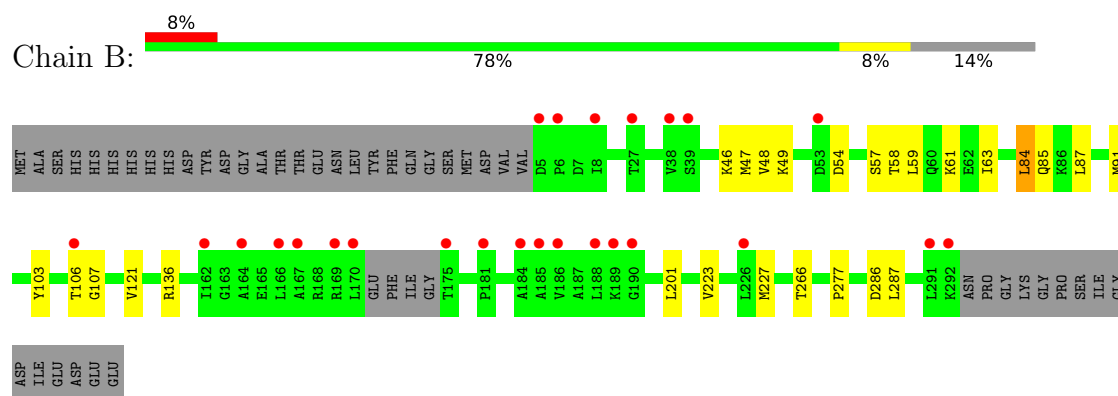
3 Residue-property plots [i](#)

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.

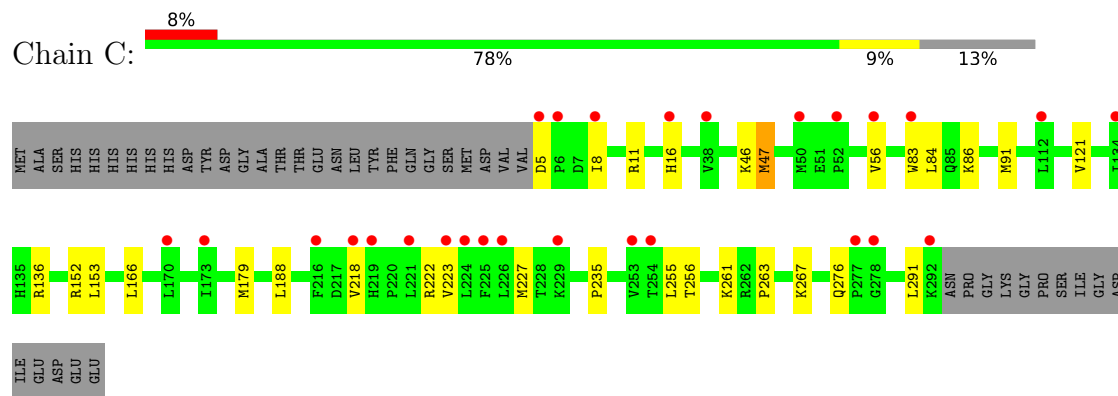
- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



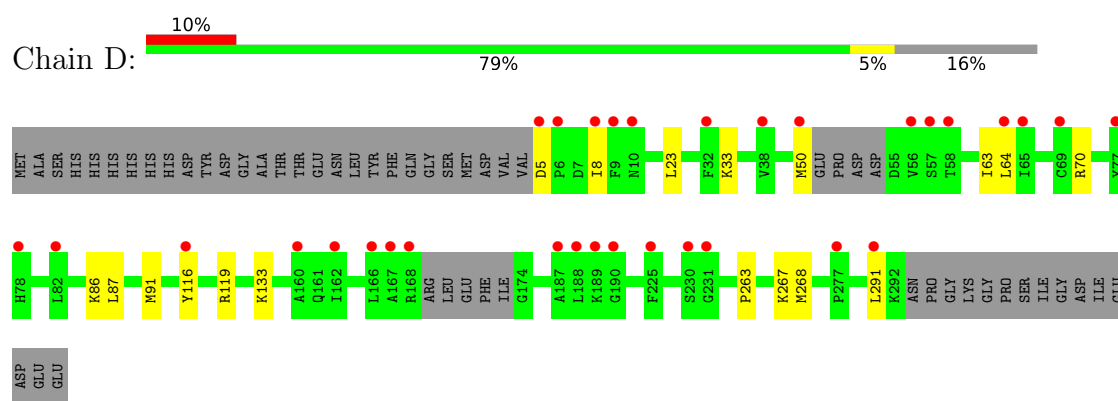
- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



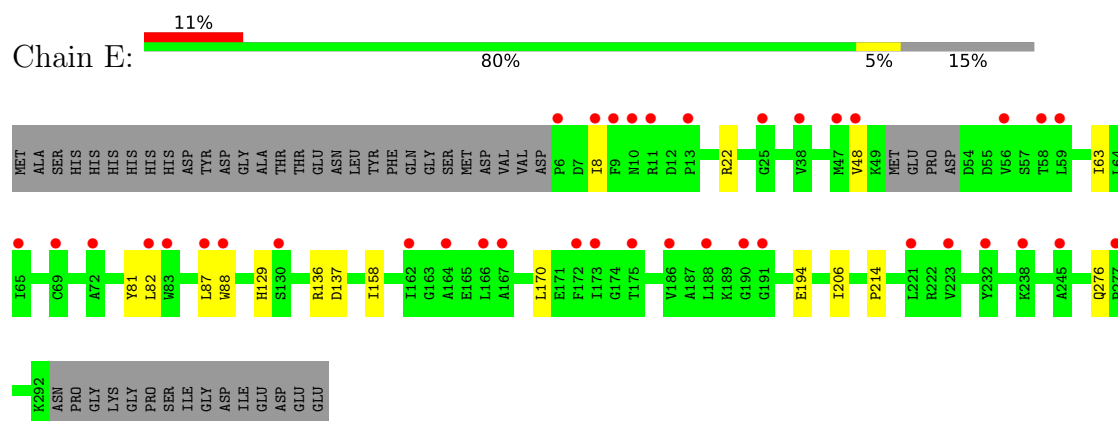
- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



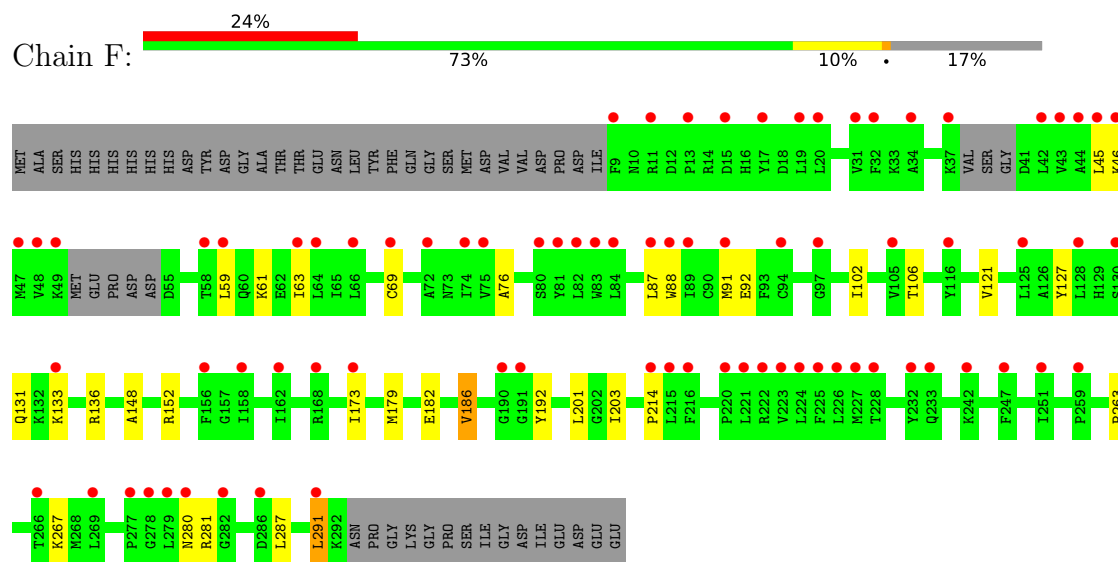
- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



- Molecule 1: Mitogen-activated protein kinase kinase kinase kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.71Å 87.40Å 109.07Å 96.43° 99.99° 108.89°	Depositor
Resolution (Å)	81.34 – 1.90 81.34 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (81.34-1.90) 96.5 (81.34-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
R, R_{free}	0.214 , 0.249 0.206 , 0.241	Depositor DCC
R_{free} test set	7448 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14170	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.59% 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: Y3I

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	0.78	0/2293	1.04	3/3105 (0.1%)
1	B	0.79	0/2267	1.00	3/3068 (0.1%)
1	C	0.77	2/2294 (0.1%)	1.03	0/3108
1	D	0.74	0/2226	1.01	0/3010
1	E	0.68	0/2254	0.98	0/3048
1	F	0.65	0/2112	0.96	0/2865
All	All	0.74	2/13446 (0.0%)	1.01	6/18204 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	MET	SD-CE	-9.29	1.56	1.79
1	C	179	MET	SD-CE	-7.38	1.61	1.79

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	PRO	N-CA-C	8.02	124.68	113.53
1	A	275	SER	CA-C-N	7.09	130.79	120.51
1	A	275	SER	C-N-CA	7.09	130.79	120.51
1	B	277	PRO	N-CA-C	6.60	122.22	113.57
1	B	84	LEU	N-CA-C	5.65	119.04	111.24
1	B	54	ASP	N-CA-C	5.24	118.03	110.28

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	2246	0	2275	11	0
1	B	2220	0	2252	14	0
1	C	2246	0	2261	15	0
1	D	2181	0	2218	8	0
1	E	2209	0	2249	6	0
1	F	2072	0	2027	19	0
2	A	26	0	0	0	0
2	B	26	0	0	1	0
2	C	26	0	0	1	0
2	D	26	0	0	0	0
2	E	26	0	0	0	0
2	F	26	0	0	3	0
3	A	214	0	0	0	0
3	B	190	0	0	0	0
3	C	120	0	0	0	0
3	D	138	0	0	0	0
3	E	114	0	0	0	0
3	F	64	0	0	0	0
All	All	14170	0	13282	70	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 3.

All (70) 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:F:173:ILE:HG13	1:F:179:MET:HE1	1.55	0.87
1:F:91:MET:HE3	2:F:401:Y3I:CL1	2.25	0.73
1:F:76:ALA:HB3	1:F:92:GLU:HB2	1.75	0.69
1:A:173:ILE:HG13	1:A:179:MET:HE1	1.80	0.63
1:C:223:VAL:HG12	1:C:227:MET:HE2	1.79	0.63
1:E:8:ILE:HD11	1:E:82:LEU:HB2	1.80	0.63
1:B:103:TYR:HA	1:B:106:THR:HG22	1.81	0.61
1:D:116:TYR:HE1	1:D:119:ARG:NH1	1.99	0.61
1:A:69:CYS:SG	1:A:133:LYS:NZ	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:ILE:HG23	1:F:291:LEU:HD11	1.86	0.57
1:C:5:ASP:HB3	1:C:8:ILE:HG13	1.87	0.57
1:F:91:MET:CE	2:F:401:Y3I:CL1	2.89	0.57
1:B:63:ILE:HD11	1:B:87:LEU:HD21	1.87	0.56
1:F:45:LEU:HD22	1:F:88:TRP:HB3	1.88	0.55
1:F:63:ILE:HD11	1:F:87:LEU:HD21	1.89	0.54
1:E:63:ILE:HD11	1:E:87:LEU:HD21	1.89	0.54
1:C:47:MET:HE3	1:C:86:LYS:HD3	1.91	0.53
1:B:84:LEU:O	1:B:85:GLN:HB2	2.08	0.53
1:D:263:PRO:HB3	1:D:267:LYS:HD3	1.90	0.53
1:D:116:TYR:CE1	1:D:119:ARG:NH1	2.77	0.52
1:F:136:ARG:NH2	1:F:192:TYR:OH	2.39	0.51
1:F:121:VAL:HG11	1:F:201:LEU:HD13	1.94	0.50
1:C:47:MET:HE3	1:C:86:LYS:CG	2.40	0.50
1:F:148:ALA:HB1	1:F:281:ARG:HH21	1.76	0.49
1:D:5:ASP:HB3	1:D:8:ILE:HB	1.94	0.49
1:E:129:HIS:CD2	1:E:194:GLU:HB2	2.48	0.49
1:C:121:VAL:HG13	1:C:153:LEU:HD21	1.94	0.48
1:F:182:GLU:O	1:F:186:VAL:HG13	2.13	0.48
1:F:203:ILE:HG23	1:F:214:PRO:HD2	1.95	0.48
1:B:47:MET:HE3	1:B:49:LYS:HG3	1.95	0.48
1:E:81:TYR:HB2	1:E:88:TRP:HB2	1.95	0.48
1:B:286:ASP:OD1	1:F:281:ARG:NH1	2.47	0.48
1:F:106:THR:HG21	1:F:287:LEU:HD11	1.96	0.47
1:B:106:THR:HG21	1:B:287:LEU:HD11	1.96	0.47
1:F:69:CYS:SG	1:F:133:LYS:NZ	2.88	0.47
1:A:9:PHE:HB3	1:A:11:ARG:HG2	1.96	0.47
1:A:71:HIS:HB3	1:A:74:ILE:HD12	1.96	0.47
1:C:83:TRP:CD1	1:C:84:LEU:HG	2.49	0.46
1:C:11:ARG:HD2	1:C:16:HIS:NE2	2.31	0.46
1:D:63:ILE:HD11	1:D:87:LEU:HD21	1.97	0.46
1:B:121:VAL:HG11	1:B:201:LEU:HD13	1.97	0.46
1:C:235:PRO:HD2	1:C:255:LEU:HD13	1.98	0.45
1:C:263:PRO:HB3	1:C:267:LYS:HD3	1.99	0.44
1:B:46:LYS:HD2	2:B:401:Y3I:N1	2.32	0.44
1:C:91:MET:HE3	1:C:91:MET:HB2	1.93	0.44
1:F:127:TYR:O	1:F:131:GLN:HG2	2.18	0.44
1:A:228:THR:HG21	1:C:188:LEU:HD12	2.00	0.43
1:D:263:PRO:HG2	1:D:268:MET:SD	2.59	0.43
1:A:102:ILE:HG12	1:A:291:LEU:HD11	2.01	0.43
1:F:263:PRO:HB3	1:F:267:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:O	1:B:85:GLN:CB	2.68	0.42
1:F:46:LYS:HD2	2:F:401:Y3I:N1	2.35	0.42
1:A:91:MET:HE3	1:A:91:MET:HB2	1.85	0.42
1:A:10:ASN:ND2	1:B:266:THR:OG1	2.53	0.41
1:A:20:LEU:HD11	1:A:35:ARG:HB2	2.02	0.41
1:B:223:VAL:CG1	1:B:227:MET:HE3	2.51	0.41
1:E:206:ILE:HG21	1:E:214:PRO:HG3	2.02	0.41
1:B:48:VAL:HG11	1:B:59:LEU:HD11	2.01	0.41
1:B:91:MET:HE3	1:B:91:MET:HB2	1.85	0.41
1:C:47:MET:HE3	1:C:86:LYS:HG2	2.02	0.41
1:D:23:LEU:HD21	1:D:33:LYS:HB2	2.02	0.41
1:E:137:ASP:CG	1:E:158:ILE:HD12	2.45	0.41
1:B:106:THR:HG23	1:B:107:GLY:O	2.21	0.41
1:D:91:MET:HE3	1:D:91:MET:HB2	1.89	0.41
1:A:13:PRO:HG3	1:A:88:TRP:CG	2.55	0.41
1:C:46:LYS:HD2	2:C:401:Y3I:N1	2.36	0.40
1:C:256:THR:HG21	1:C:261:LYS:HB2	2.03	0.40
1:F:59:LEU:HD12	1:F:87:LEU:HD23	2.02	0.40
1:A:63:ILE:O	1:A:67:LYS:HB2	2.22	0.40
1:C:47:MET:HE3	1:C:86:LYS:CD	2.52	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	284/331 (86%)	279 (98%)	5 (2%)	0	100	100
1	B	280/331 (85%)	274 (98%)	6 (2%)	0	100	100
1	C	286/331 (86%)	280 (98%)	6 (2%)	0	100	100
1	D	273/331 (82%)	265 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	279/331 (84%)	269 (96%)	10 (4%)	0	100	100
1	F	270/331 (82%)	263 (97%)	7 (3%)	0	100	100
All	All	1672/1986 (84%)	1630 (98%)	42 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/281 (85%)	231 (97%)	8 (3%)	33	26
1	B	236/281 (84%)	232 (98%)	4 (2%)	53	52
1	C	237/281 (84%)	229 (97%)	8 (3%)	32	25
1	D	232/281 (83%)	226 (97%)	6 (3%)	40	35
1	E	234/281 (83%)	229 (98%)	5 (2%)	47	44
1	F	208/281 (74%)	203 (98%)	5 (2%)	43	38
All	All	1386/1686 (82%)	1350 (97%)	36 (3%)	40	35

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

Mol	Chain	Res	Type
1	A	3	VAL
1	A	58	THR
1	A	104	GLN
1	A	106	THR
1	A	136	ARG
1	A	186	VAL
1	A	276	GLN
1	A	280	ASN
1	B	57	SER
1	B	58	THR
1	B	61	LYS
1	B	136	ARG

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Mol	Chain	Res	Type
1	C	56	VAL
1	C	136	ARG
1	C	152	ARG
1	C	166	LEU
1	C	218	VAL
1	C	222	ARG
1	C	276	GLN
1	C	291	LEU
1	D	50	MET
1	D	64	LEU
1	D	70	ARG
1	D	86	LYS
1	D	133	LYS
1	D	291	LEU
1	E	22	ARG
1	E	48	VAL
1	E	136	ARG
1	E	170	LEU
1	E	276	GLN
1	F	61	LYS
1	F	152	ARG
1	F	186	VAL
1	F	280	ASN
1	F	291	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	104	GLN
1	B	60	GLN
1	B	78	HIS
1	B	104	GLN
1	B	131	GLN
1	C	123	GLN
1	C	276	GLN
1	D	10	ASN
1	D	100	GLN
1	D	104	GLN
1	E	100	GLN
1	E	104	GLN
1	F	21	GLN

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Mol	Chain	Res	Type
1	F	78	HIS
1	F	100	GLN
1	F	104	GLN
1	F	123	GLN
1	F	142	ASN
1	F	272	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	Y3I	A	401	-	28,29,29	0.77	0	34,42,42	0.64	0
2	Y3I	D	401	-	28,29,29	0.63	0	34,42,42	0.73	0
2	Y3I	F	401	-	28,29,29	0.66	0	34,42,42	0.71	0
2	Y3I	B	401	-	28,29,29	0.61	0	34,42,42	0.75	2 (5%)
2	Y3I	C	401	-	28,29,29	0.97	1 (3%)	34,42,42	0.81	2 (5%)
2	Y3I	E	401	-	28,29,29	0.78	1 (3%)	34,42,42	0.93	3 (8%)

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	Y3I	A	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	D	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	F	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	B	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	C	401	-	-	0/10/22/22	0/4/4/4
2	Y3I	E	401	-	-	0/10/22/22	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	Y3I	C17-C18	3.41	1.60	1.53
2	E	401	Y3I	C17-C18	2.35	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	Y3I	CL1-C10-N2	-2.52	117.83	121.74
2	E	401	Y3I	C16-C15-N5	2.36	115.50	111.82
2	C	401	Y3I	CL1-C10-N2	-2.33	118.12	121.74
2	E	401	Y3I	C11-N3-C14	2.21	117.24	111.83
2	E	401	Y3I	CL1-C10-N2	-2.11	118.46	121.74
2	B	401	Y3I	C11-N3-C14	2.07	116.89	111.83
2	C	401	Y3I	C11-N3-C14	2.04	116.81	111.83

There are no chirality outliers.

There are no torsion outliers.

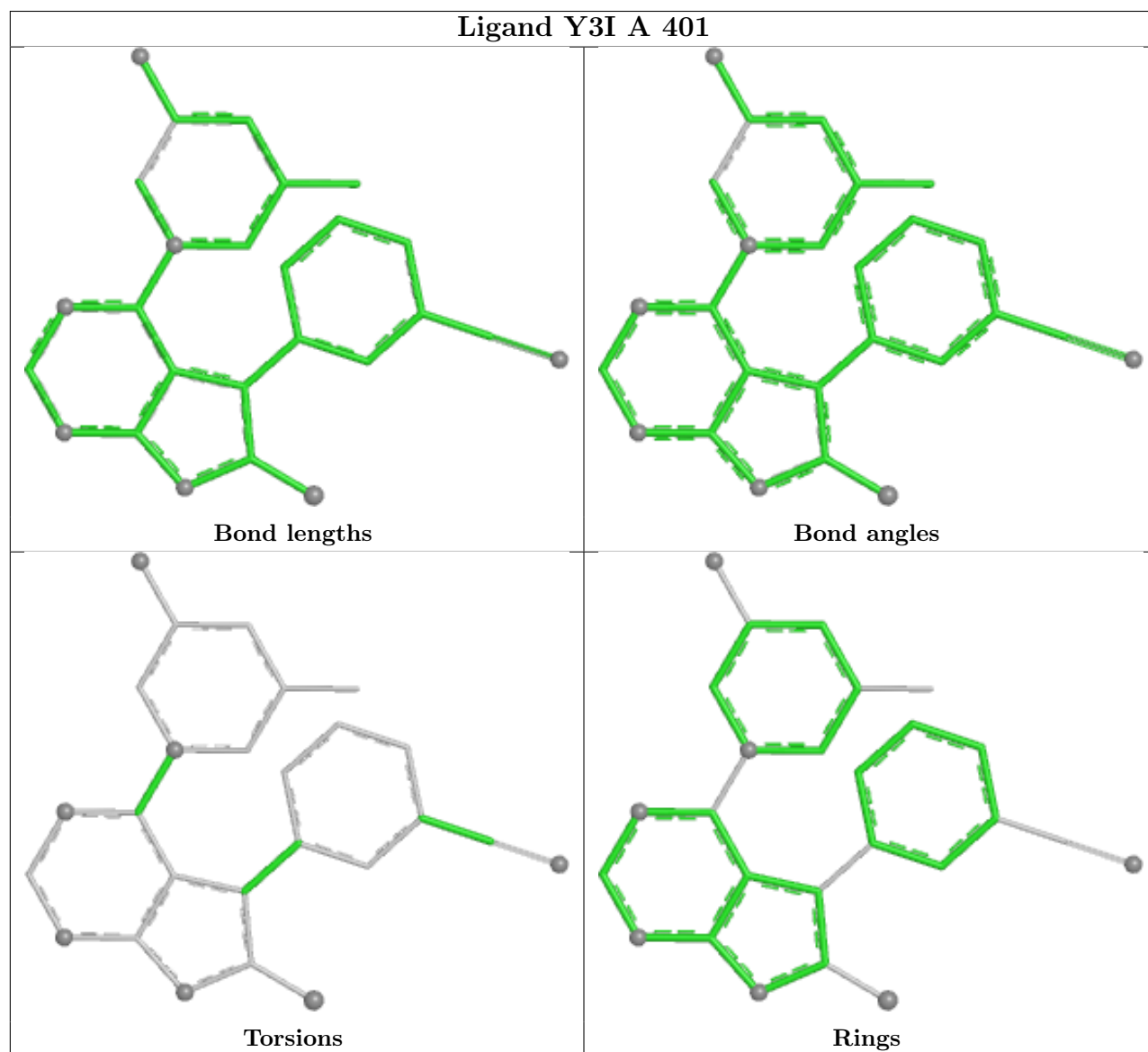
There are no ring outliers.

3 monomers are involved in 5 short contacts:

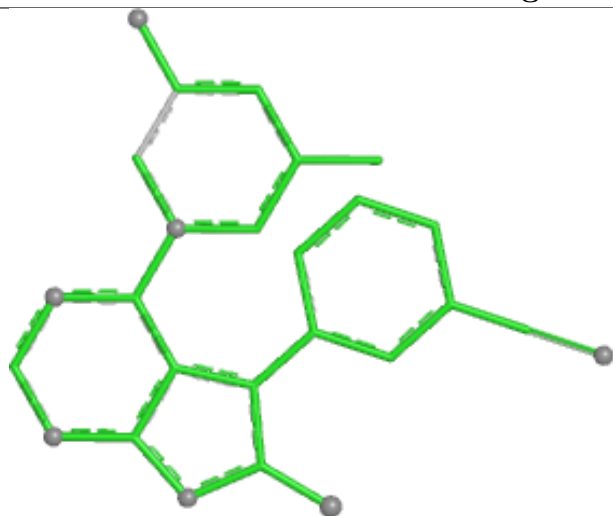
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	Y3I	3	0
2	B	401	Y3I	1	0
2	C	401	Y3I	1	0

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

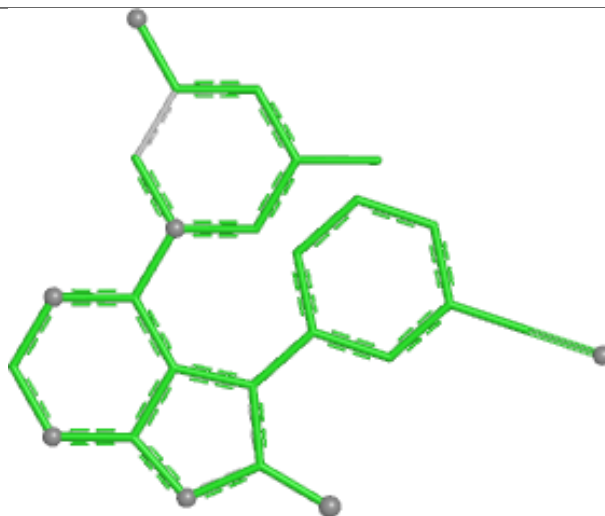
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



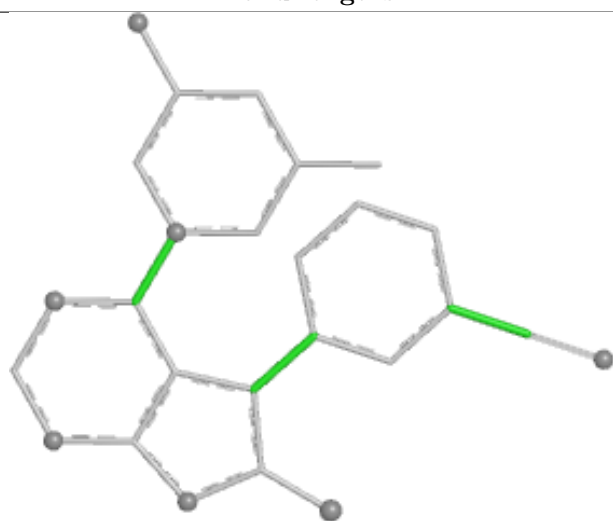
Ligand Y3I D 401



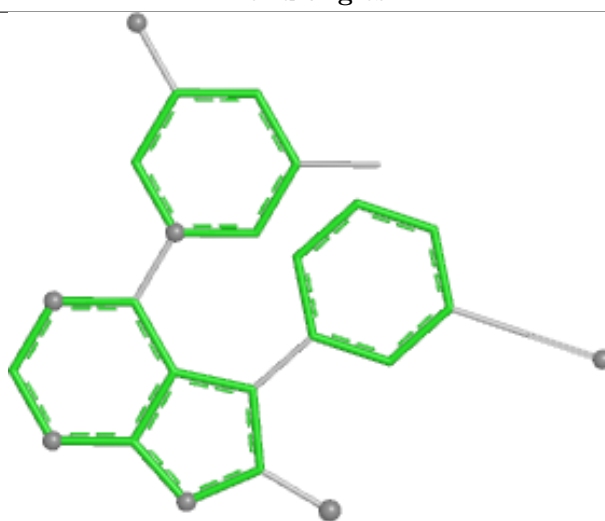
Bond lengths



Bond angles

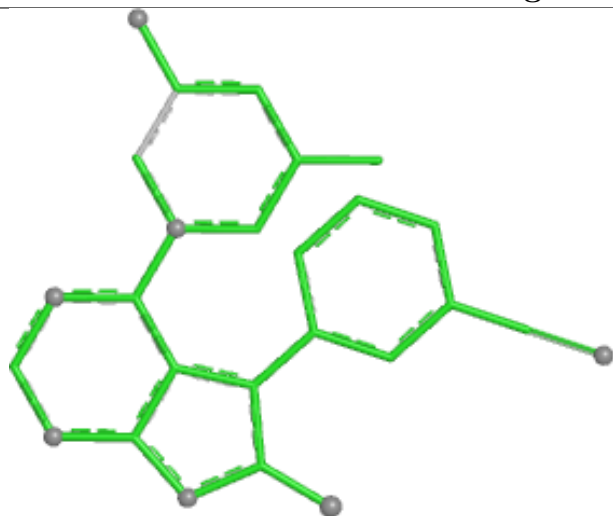


Torsions

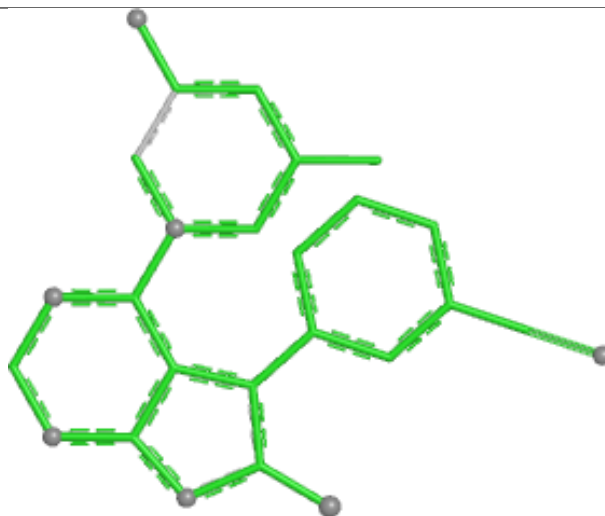


Rings

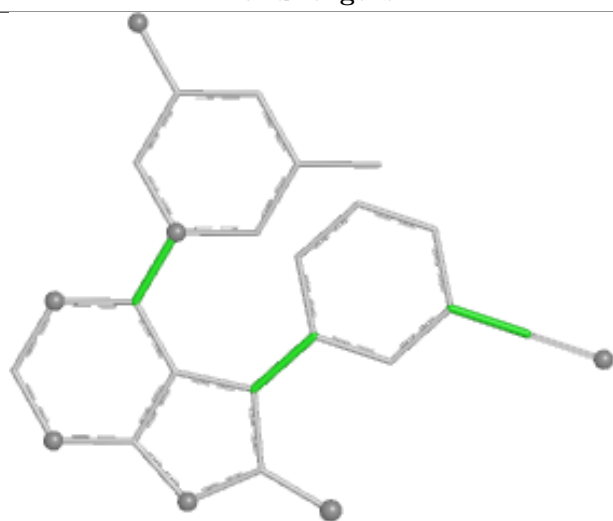
Ligand Y3I F 401



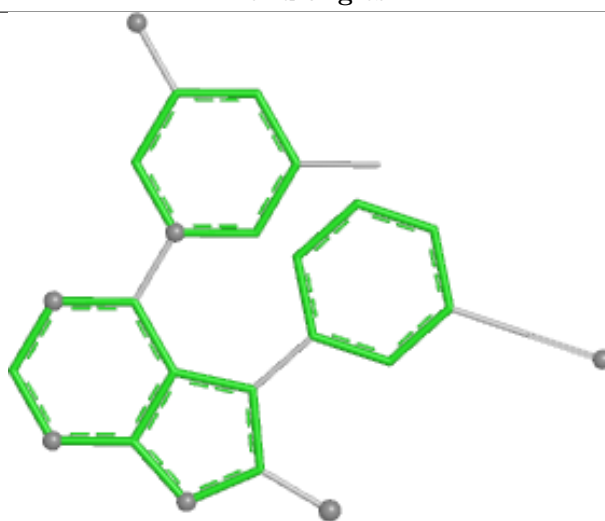
Bond lengths



Bond angles

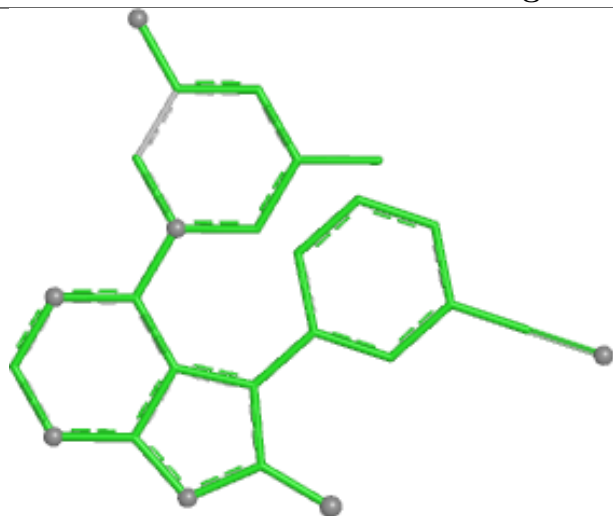


Torsions

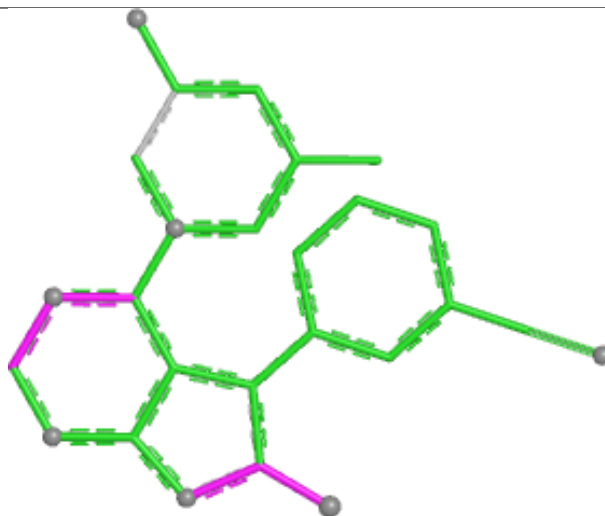


Rings

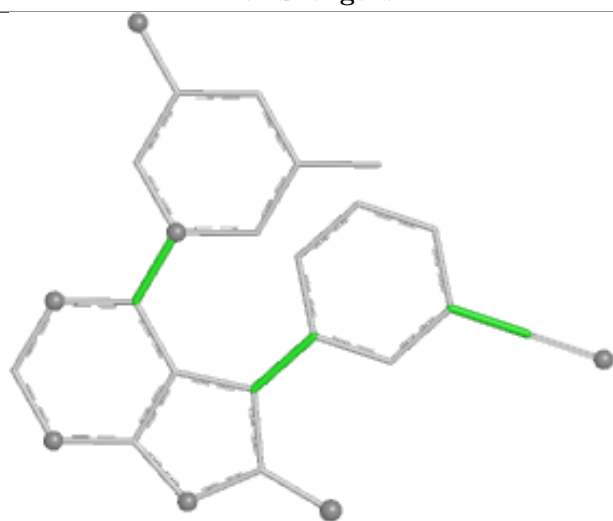
Ligand Y3I B 401



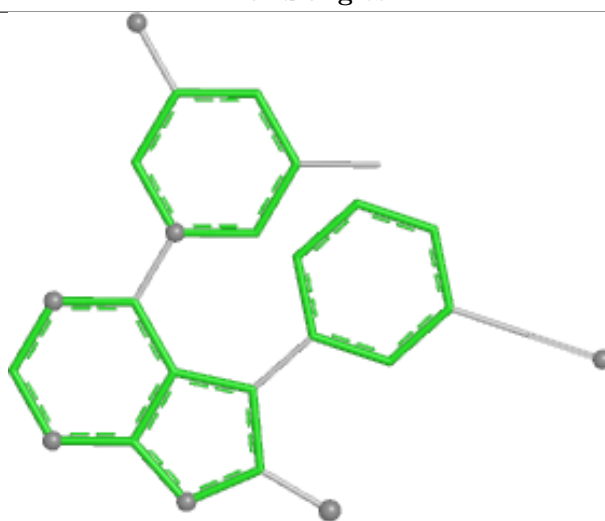
Bond lengths



Bond angles

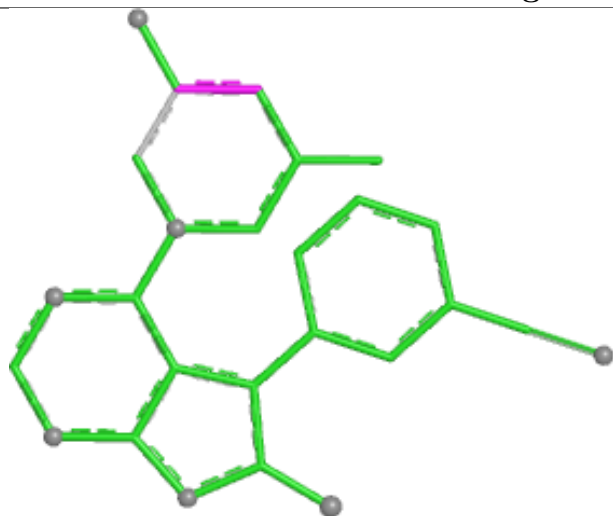


Torsions

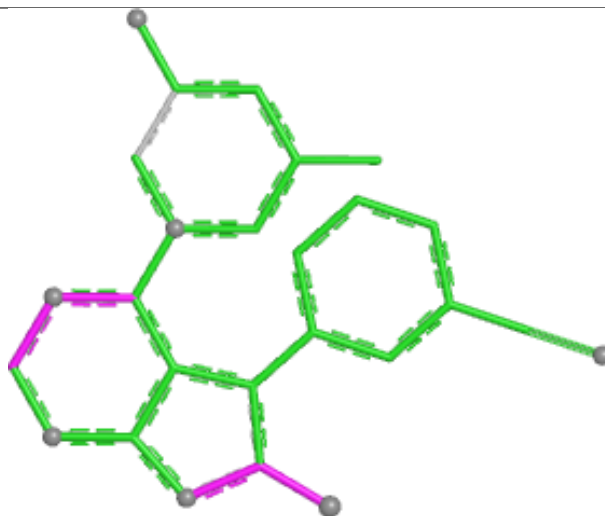


Rings

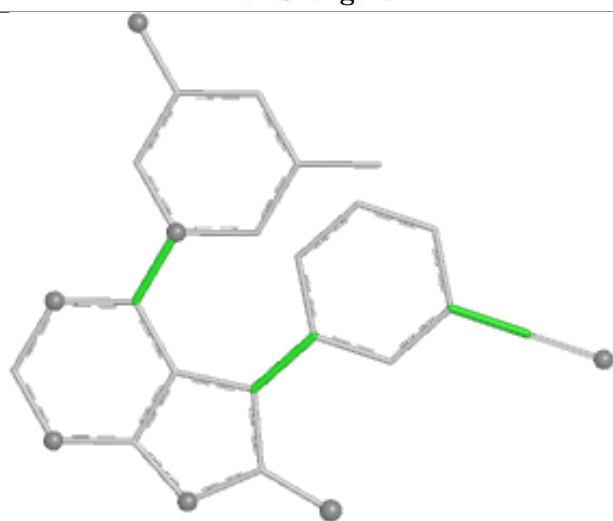
Ligand Y3I C 401



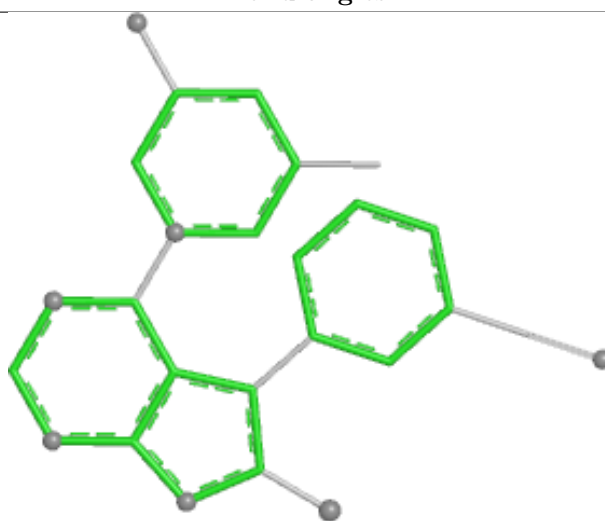
Bond lengths



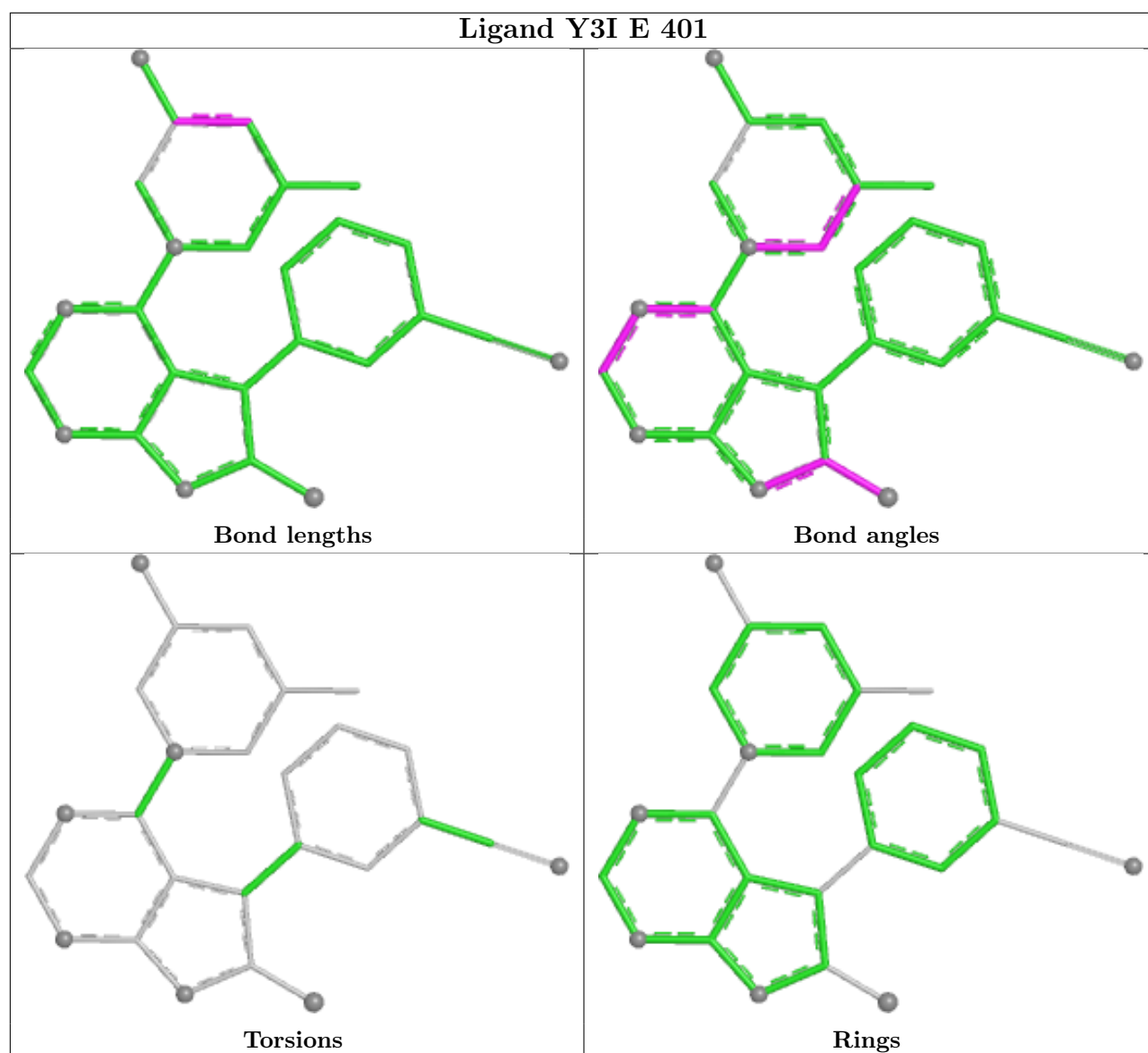
Bond angles



Torsions



Rings



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	288/331 (87%)	0.33	18 (6%) 26 27	21, 34, 56, 70	0
1	B	284/331 (85%)	0.39	25 (8%) 15 16	22, 34, 59, 83	0
1	C	288/331 (87%)	0.88	27 (9%) 14 14	24, 42, 65, 73	0
1	D	279/331 (84%)	0.77	32 (11%) 9 10	22, 43, 69, 87	0
1	E	283/331 (85%)	0.86	38 (13%) 7 7	24, 45, 69, 84	0
1	F	276/331 (83%)	1.49	79 (28%) 1 1	25, 56, 82, 88	0
All	All	1698/1986 (85%)	0.78	219 (12%) 7 7	21, 42, 71, 88	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	224	LEU	5.6
1	B	170	LEU	5.2
1	F	43	VAL	4.6
1	D	38	VAL	4.4
1	F	17	TYR	4.4
1	F	32	PHE	4.3
1	D	162	ILE	4.3
1	E	162	ILE	4.2
1	F	221	LEU	4.2
1	F	34	ALA	4.1
1	F	81	TYR	4.0
1	F	83	TRP	4.0
1	B	53	ASP	4.0
1	F	59	LEU	3.9
1	D	56	VAL	3.9
1	A	170	LEU	3.8
1	F	82	LEU	3.8
1	C	38	VAL	3.8
1	A	225	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	69	CYS	3.7
1	A	186	VAL	3.5
1	E	58	THR	3.5
1	F	9	PHE	3.5
1	F	91	MET	3.4
1	E	164	ALA	3.4
1	F	19	LEU	3.4
1	F	222	ARG	3.4
1	C	224	LEU	3.3
1	D	188	LEU	3.3
1	F	44	ALA	3.3
1	F	84	LEU	3.3
1	F	48	VAL	3.2
1	F	220	PRO	3.2
1	C	292	LYS	3.2
1	F	69	CYS	3.2
1	F	20	LEU	3.2
1	F	215	LEU	3.2
1	D	231	GLY	3.2
1	E	56	VAL	3.2
1	F	64	LEU	3.2
1	D	9	PHE	3.1
1	F	89	ILE	3.1
1	F	232	TYR	3.1
1	E	190	GLY	3.1
1	B	226	LEU	3.1
1	D	167	ALA	3.1
1	E	8	ILE	3.0
1	F	63	ILE	3.0
1	C	225	PHE	3.0
1	D	166	LEU	3.0
1	C	223	VAL	3.0
1	E	59	LEU	3.0
1	D	189	LYS	3.0
1	F	156	PHE	3.0
1	F	277	PRO	3.0
1	D	69	CYS	3.0
1	A	173	ILE	3.0
1	E	65	ILE	3.0
1	F	279	LEU	2.9
1	B	106	THR	2.9
1	F	291	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	166	LEU	2.9
1	C	170	LEU	2.9
1	E	166	LEU	2.9
1	B	38	VAL	2.9
1	C	218	VAL	2.9
1	D	58	THR	2.9
1	E	25	GLY	2.9
1	F	190	GLY	2.9
1	C	52	PRO	2.9
1	F	225	PHE	2.9
1	F	247	PHE	2.9
1	B	164	ALA	2.9
1	F	280	ASN	2.8
1	F	233	GLN	2.8
1	C	229	LYS	2.8
1	E	10	ASN	2.8
1	F	37	LYS	2.8
1	E	87	LEU	2.8
1	F	42	LEU	2.8
1	B	186	VAL	2.8
1	F	223	VAL	2.8
1	A	169	ARG	2.8
1	F	45	LEU	2.8
1	E	172	PHE	2.7
1	E	6	PRO	2.7
1	D	160	ALA	2.7
1	F	49	LYS	2.7
1	C	216	PHE	2.7
1	E	69	CYS	2.7
1	F	266	THR	2.7
1	E	221	LEU	2.7
1	C	6	PRO	2.7
1	F	80	SER	2.7
1	F	191	GLY	2.7
1	D	6	PRO	2.7
1	B	162	ILE	2.7
1	C	134	ILE	2.7
1	C	173	ILE	2.6
1	B	39	SER	2.6
1	E	83	TRP	2.6
1	A	181	PRO	2.6
1	D	277	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	97	GLY	2.6
1	F	13	PRO	2.6
1	D	190	GLY	2.6
1	F	31	VAL	2.6
1	F	130	SER	2.6
1	D	225	PHE	2.5
1	A	167	ALA	2.5
1	C	254	THR	2.5
1	F	228	THR	2.5
1	F	11	ARG	2.5
1	D	5	ASP	2.5
1	F	216	PHE	2.5
1	F	251	ILE	2.5
1	E	167	ALA	2.5
1	B	175	THR	2.5
1	E	130	SER	2.5
1	F	286	ASP	2.5
1	C	277	PRO	2.5
1	D	77	TYR	2.4
1	D	82	LEU	2.4
1	F	87	LEU	2.4
1	D	8	ILE	2.4
1	F	227	MET	2.4
1	F	269	LEU	2.4
1	C	253	VAL	2.4
1	F	88	TRP	2.4
1	C	219	HIS	2.4
1	D	230	SER	2.4
1	E	188	LEU	2.4
1	D	65	ILE	2.4
1	F	214	PRO	2.4
1	E	48	VAL	2.4
1	B	169	ARG	2.3
1	B	188	LEU	2.3
1	D	168	ARG	2.3
1	F	125	LEU	2.3
1	D	57	SER	2.3
1	F	75	VAL	2.3
1	C	5	ASP	2.3
1	B	291	LEU	2.3
1	E	9	PHE	2.3
1	E	232	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	245	ALA	2.3
1	B	181	PRO	2.3
1	A	168	ARG	2.3
1	E	38	VAL	2.3
1	B	6	PRO	2.3
1	B	184	ALA	2.3
1	D	187	ALA	2.3
1	E	277	PRO	2.3
1	C	278	GLY	2.3
1	A	3	VAL	2.3
1	C	226	LEU	2.3
1	D	291	LEU	2.3
1	E	82	LEU	2.3
1	E	11	ARG	2.2
1	E	88	TRP	2.2
1	A	38	VAL	2.2
1	E	47	MET	2.2
1	E	238	LYS	2.2
1	F	58	THR	2.2
1	F	226	LEU	2.2
1	A	230	SER	2.2
1	C	8	ILE	2.2
1	B	189	LYS	2.2
1	D	50	MET	2.2
1	F	133	LYS	2.2
1	F	242	LYS	2.2
1	C	56	VAL	2.2
1	E	186	VAL	2.2
1	E	223	VAL	2.2
1	B	5	ASP	2.2
1	F	278	GLY	2.2
1	E	13	PRO	2.2
1	F	72	ALA	2.2
1	A	172	PHE	2.2
1	D	116	TYR	2.2
1	F	116	TYR	2.2
1	C	50	MET	2.2
1	D	10	ASN	2.2
1	E	191	GLY	2.2
1	F	66	LEU	2.2
1	F	282	GLY	2.2
1	B	167	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	236	ARG	2.2
1	F	74	ILE	2.1
1	F	162	ILE	2.1
1	B	27	THR	2.1
1	F	105	VAL	2.1
1	F	128	LEU	2.1
1	B	292	LYS	2.1
1	B	185	ALA	2.1
1	D	32	PHE	2.1
1	F	158	ILE	2.1
1	F	173	ILE	2.1
1	C	83	TRP	2.1
1	A	11	ARG	2.1
1	B	190	GLY	2.1
1	C	16	HIS	2.1
1	F	47	MET	2.1
1	F	46	LYS	2.1
1	C	112	LEU	2.1
1	D	64	LEU	2.1
1	E	72	ALA	2.1
1	F	15	ASP	2.1
1	B	8	ILE	2.0
1	E	173	ILE	2.0
1	E	175	THR	2.0
1	D	78	HIS	2.0
1	F	259	PRO	2.0
1	A	166	LEU	2.0
1	C	221	LEU	2.0
1	F	94	CYS	2.0
1	F	168	ARG	2.0
1	A	50	MET	2.0
1	A	40	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 oligosaccharides in this entry.

6.4 Ligands

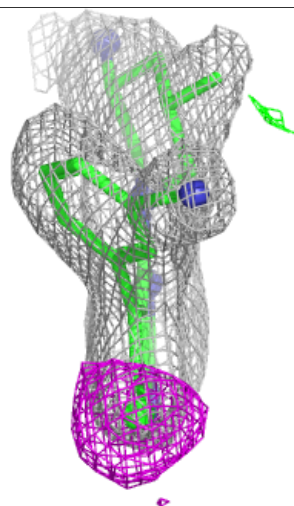
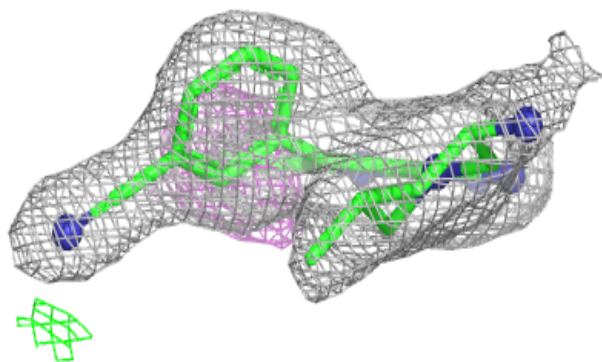
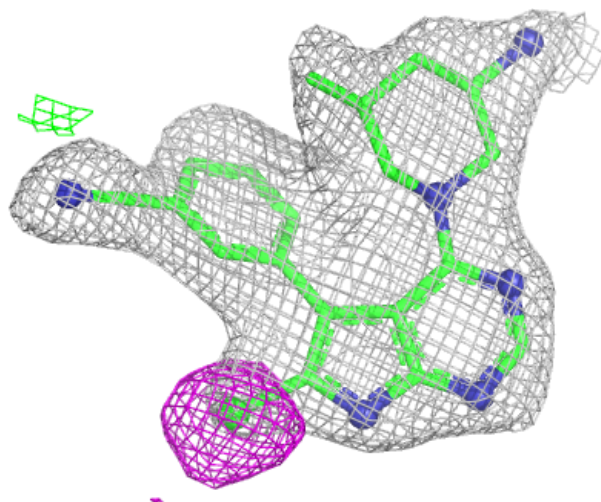
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	Y3I	F	401	26/26	0.83	0.13	56,57,59,62	0
2	Y3I	A	401	26/26	0.87	0.09	25,27,31,41	0
2	Y3I	E	401	26/26	0.88	0.10	29,34,38,44	0
2	Y3I	C	401	26/26	0.89	0.10	28,30,36,41	0
2	Y3I	D	401	26/26	0.89	0.10	35,38,41,46	0
2	Y3I	B	401	26/26	0.90	0.09	24,28,34,42	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.

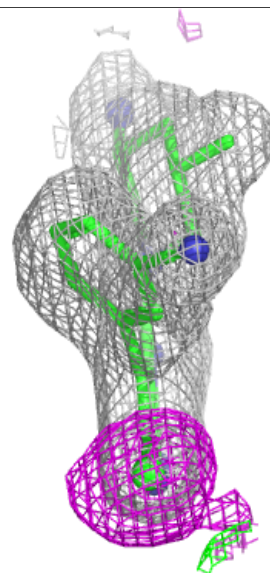
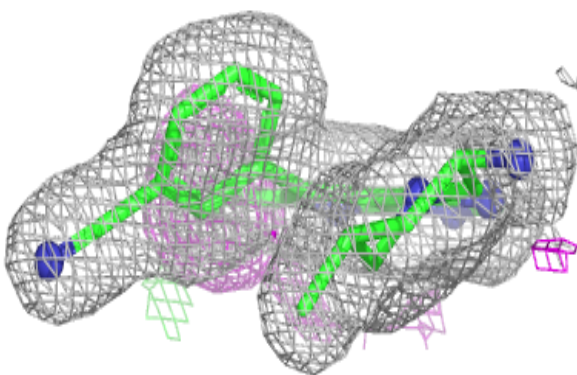
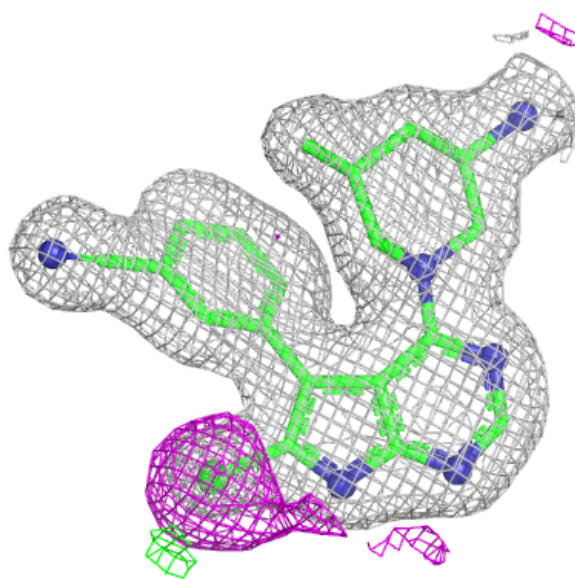
Electron density around Y3I F 401:

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



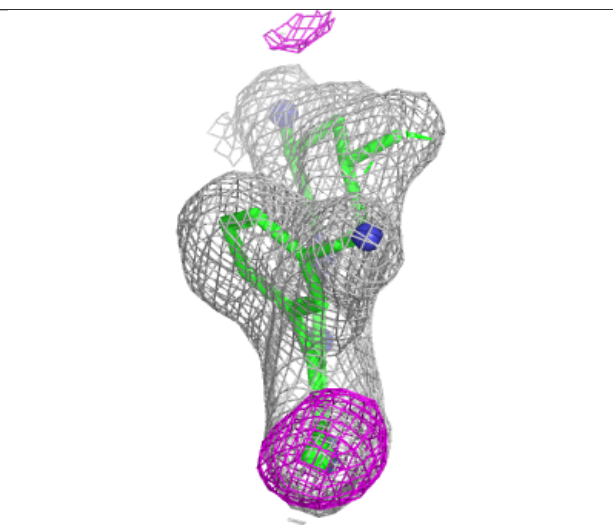
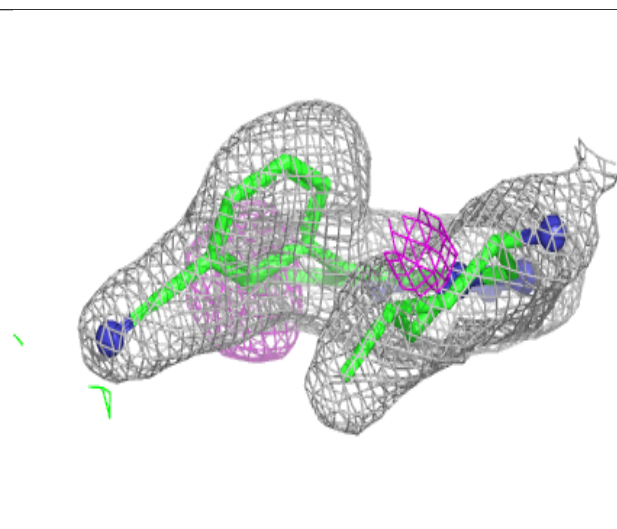
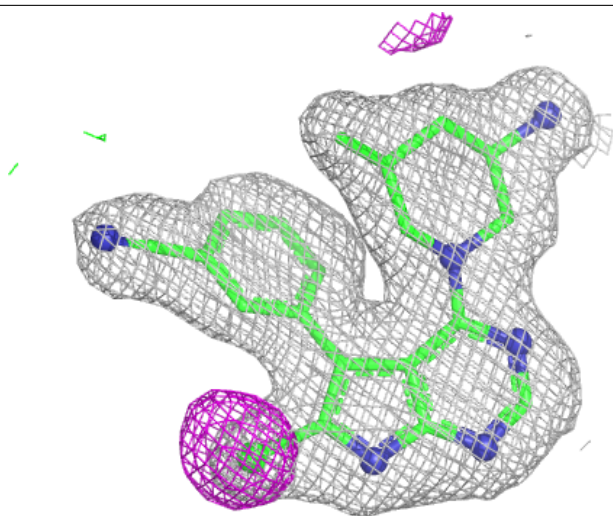
Electron density around Y3I A 401:

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



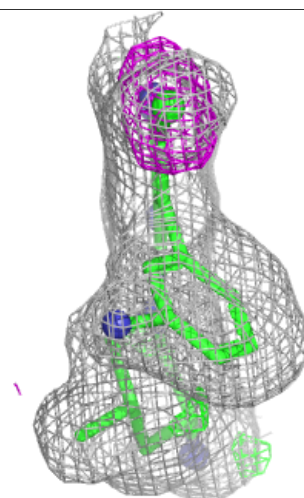
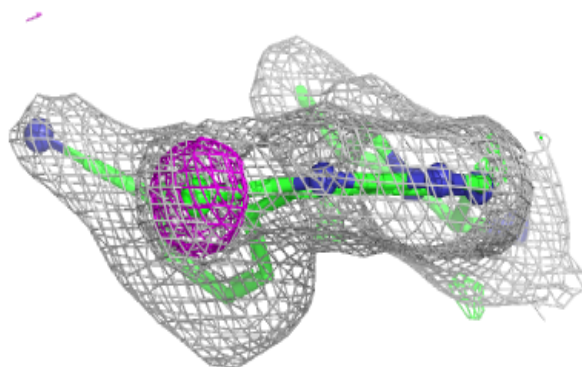
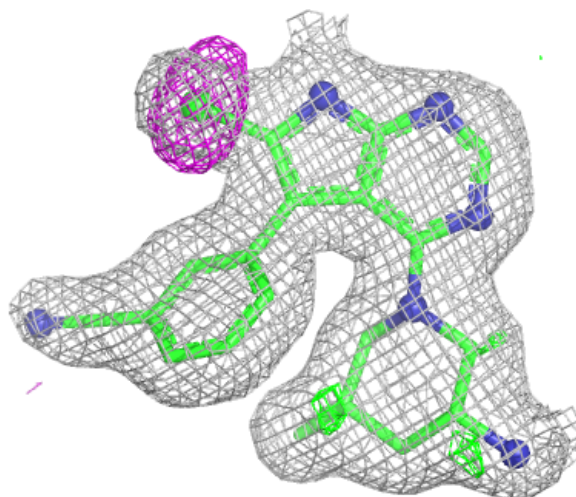
Electron density around Y3I E 401:

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



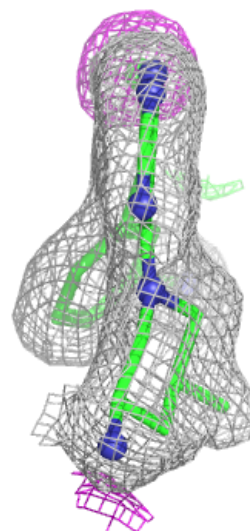
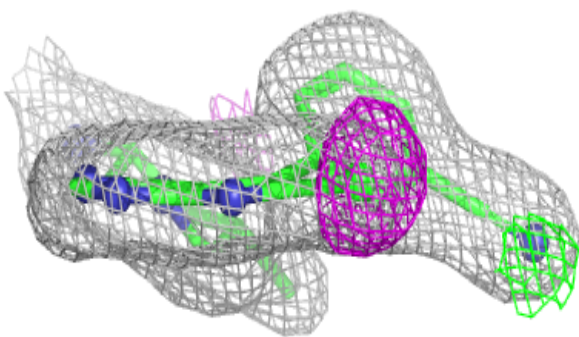
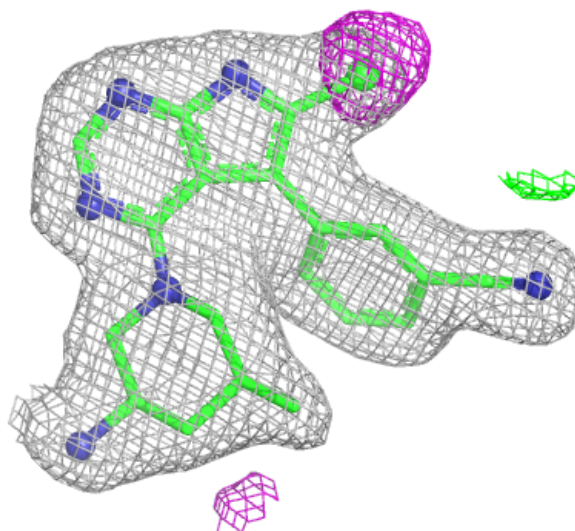
Electron density around Y3I C 401:

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



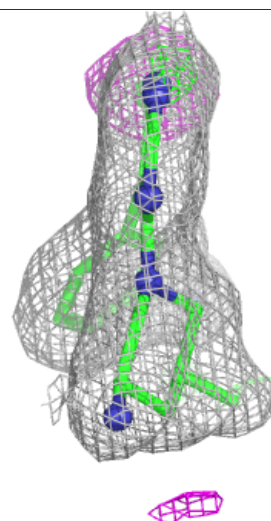
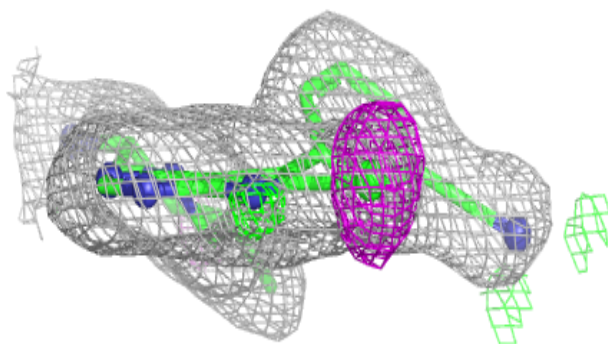
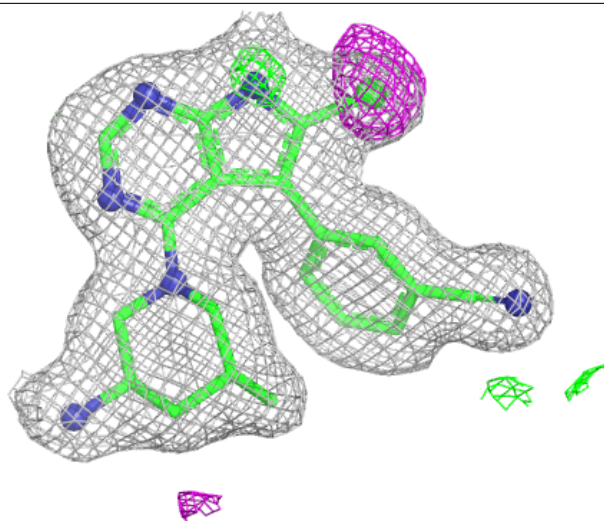
Electron density around Y3I D 401:

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



Electron density around Y3I 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.