



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:02 AM UTC

PDB ID : 8FKO / pdb_00008fko
Title : Crystal structure of HPK1 kinase domain T165E,S171E phosphomimetic mutant in complex with 3-{4-[(2S,5R)-5-Amino-2-methylpiperidin-1-yl]-6-chloro-7H-pyrrolo[2,3-d]pyrimidin-5-yl}benzonitrile
Authors : McTigue, M.; Johnson, E.; Cronin, C.
Deposited on : 2022-12-21
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

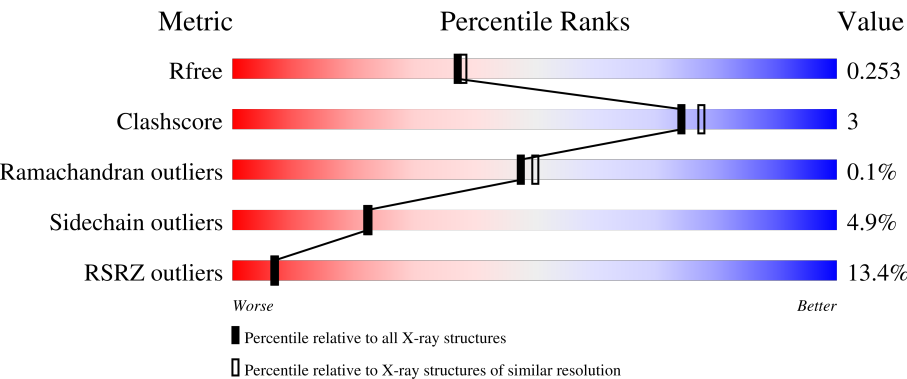
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



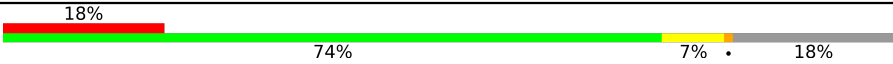
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	7% 77% 7% • 15%
1	C	331	7% 76% 9% • 13%
1	D	331	10% 75% 9% 16%

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Mol	Chain	Length	Quality of chain
1	E	331	
1	F	331	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13546 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	289	Total	C	N	O	S	0	0	0
			2273	1461	392	409	11			
1	B	281	Total	C	N	O	S	0	0	0
			2182	1402	372	397	11			
1	C	288	Total	C	N	O	S	0	0	0
			2249	1446	384	408	11			
1	D	279	Total	C	N	O	S	0	0	0
			2189	1410	380	388	11			
1	E	271	Total	C	N	O	S	0	0	0
			2108	1354	369	375	10			
1	F	224	Total	C	N	O	S	0	0	0
			1682	1077	287	309	9			

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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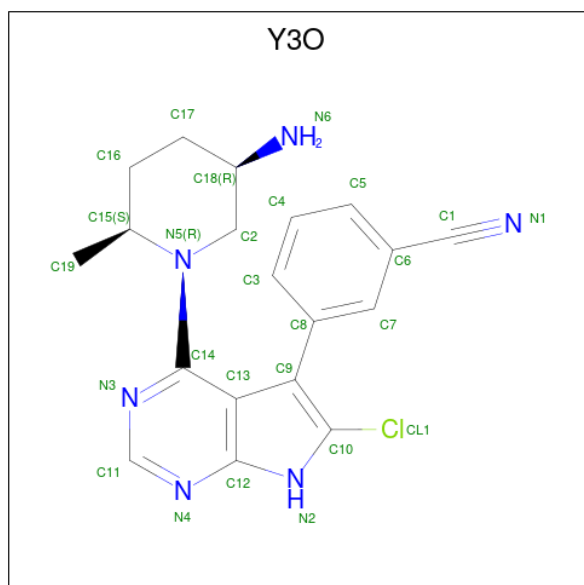
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	SER	-	expression tag	UNP Q92918
D	165	GLU	THR	engineered mutation	UNP Q92918
D	171	GLU	SER	engineered mutation	UNP Q92918
E	-23	MET	-	expression tag	UNP Q92918
E	-22	ALA	-	expression tag	UNP Q92918
E	-21	SER	-	expression tag	UNP Q92918
E	-20	HIS	-	expression 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-[(2S,5R)-5-amino-2-methylpiperidin-1-yl]-6-chloro-7H-pyrrolo[2,3-d]pyrimidin-5-yl}benzonitrile (CCD ID: Y3O) (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		

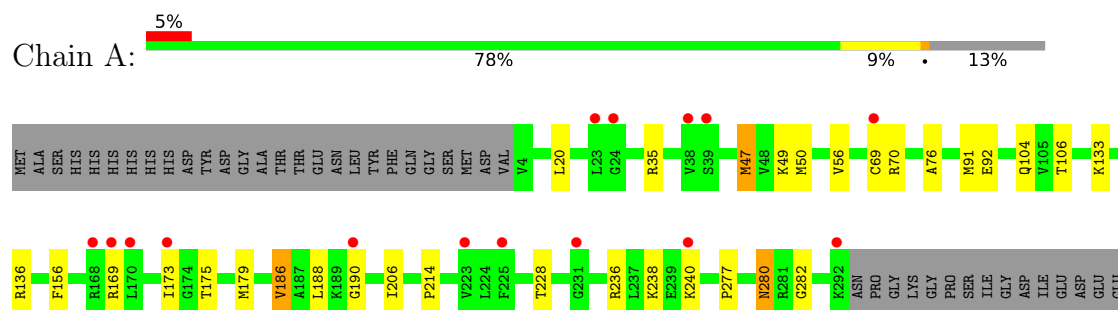
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	186	Total	O	0	0
			186	186		
3	B	176	Total	O	0	0
			176	176		
3	C	116	Total	O	0	0
			116	116		
3	D	125	Total	O	0	0
			125	125		
3	E	87	Total	O	0	0
			87	87		
3	F	43	Total	O	0	0
			43	43		

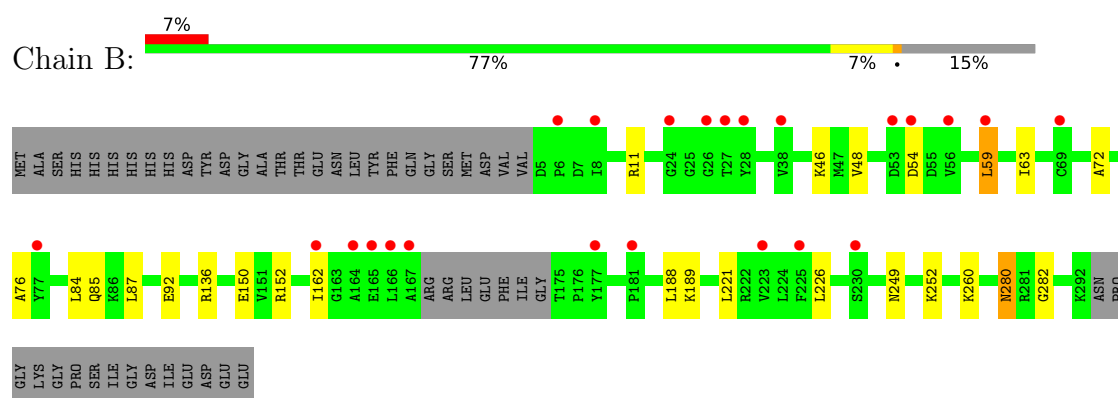
3 Residue-property plots [i](#)

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.

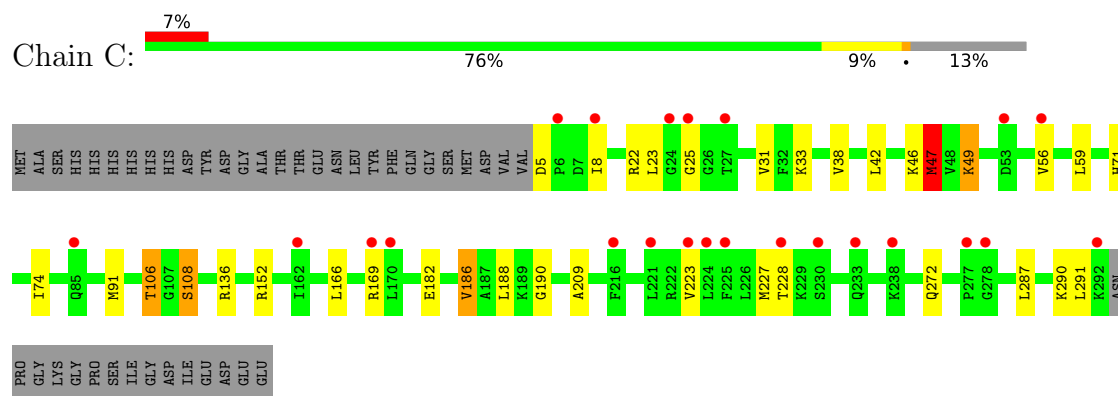
- Molecule 1: Mitogen-activated protein kinase kinase kinase 1



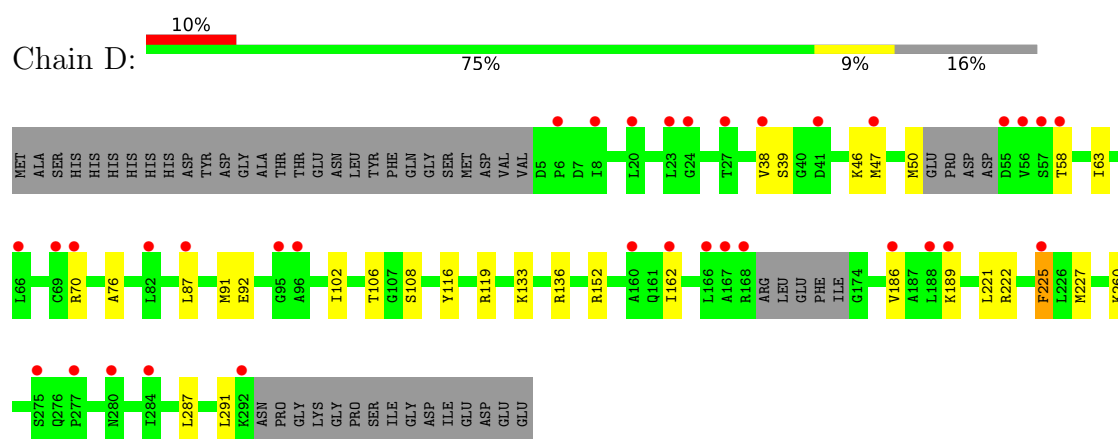
- Molecule 1: Mitogen-activated protein kinase kinase kinase 1



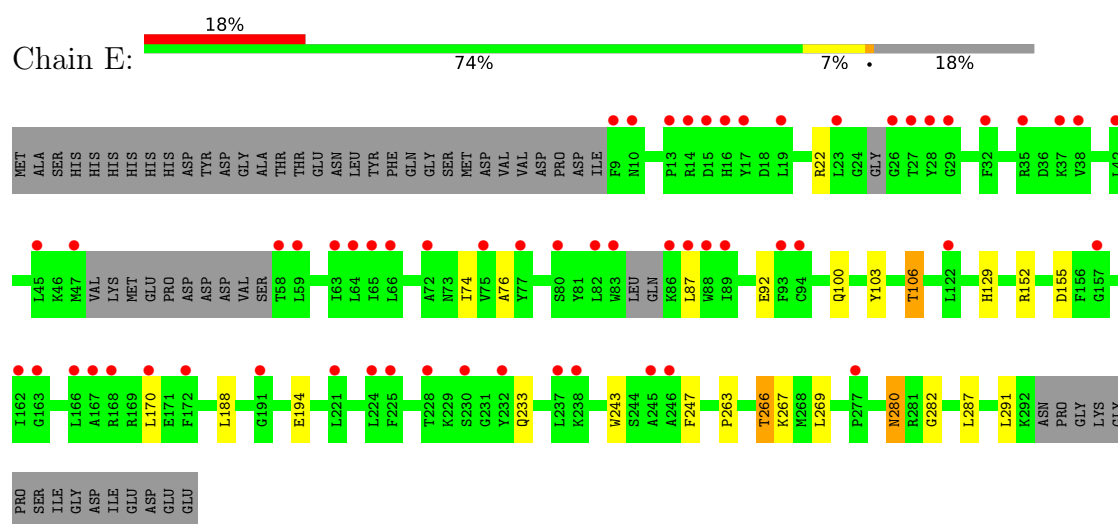
- Molecule 1: Mitogen-activated protein kinase kinase kinase 1



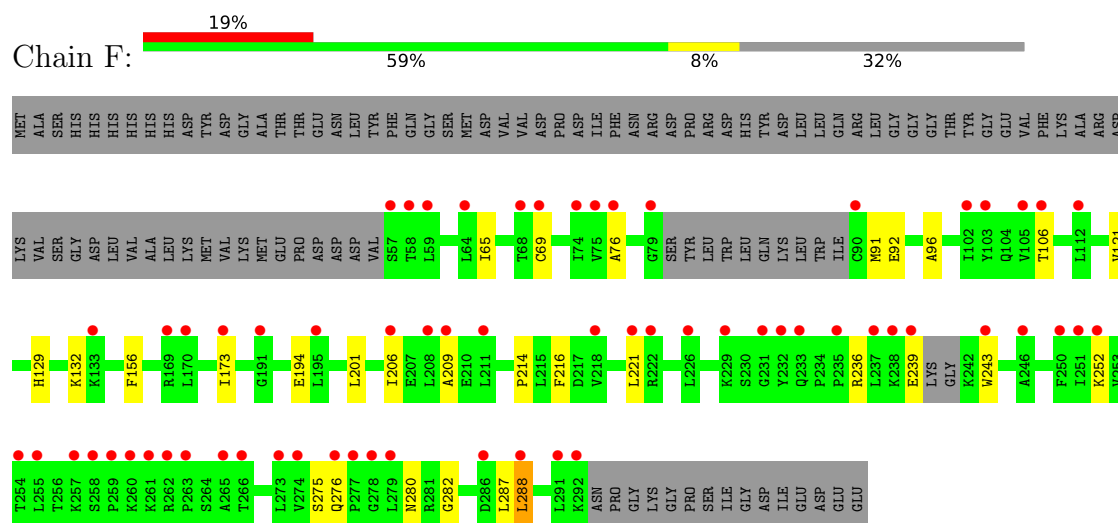
- Molecule 1: Mitogen-activated protein kinase kinase kinase 1



- 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	58.07Å 87.00Å 109.82Å 95.73° 100.64° 108.89°	Depositor
Resolution (Å)	52.91 – 2.10 52.91 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (52.91-2.10) 96.9 (52.91-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
R, R_{free}	0.220 , 0.258 0.214 , 0.253	Depositor DCC
R_{free} test set	5556 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13546	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: Y3O

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	0.77	1/2322 (0.0%)	1.07	5/3142 (0.2%)
1	B	0.74	0/2229	1.02	0/3022
1	C	0.74	1/2298 (0.0%)	1.07	3/3113 (0.1%)
1	D	0.72	0/2234	1.05	1/3017 (0.0%)
1	E	0.66	0/2151	1.02	0/2906
1	F	0.67	0/1716	1.06	2/2333 (0.1%)
All	All	0.72	2/12950 (0.0%)	1.05	11/17533 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	MET	SD-CE	-8.86	1.57	1.79
1	A	47	MET	SD-CE	-5.37	1.66	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	GLY	N-CA-C	7.27	123.54	114.37
1	A	277	PRO	N-CA-C	6.81	122.99	113.53
1	A	190	GLY	N-CA-C	5.78	122.65	114.85
1	D	225	PHE	CA-CB-CG	5.60	119.40	113.80
1	C	290	LYS	CA-C-N	5.26	127.28	120.44
1	C	290	LYS	C-N-CA	5.26	127.28	120.44
1	A	156	PHE	CA-C-N	5.08	125.57	119.94
1	A	156	PHE	C-N-CA	5.08	125.57	119.94
1	F	156	PHE	CA-C-N	5.06	125.60	119.98
1	F	156	PHE	C-N-CA	5.06	125.60	119.98
1	A	175	THR	CB-CA-C	5.04	117.98	109.67

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	2273	0	2310	12	0
1	B	2182	0	2186	17	0
1	C	2249	0	2266	16	0
1	D	2189	0	2247	14	0
1	E	2108	0	2120	11	0
1	F	1682	0	1635	11	0
2	A	26	0	0	1	0
2	B	26	0	0	2	0
2	C	26	0	0	2	0
2	D	26	0	0	1	0
2	E	26	0	0	1	0
3	A	186	0	0	0	0
3	B	176	0	0	1	0
3	C	116	0	0	0	0
3	D	125	0	0	2	0
3	E	87	0	0	0	0
3	F	43	0	0	0	0
All	All	13546	0	12764	78	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 (78) 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:B:63:ILE:HD11	1:B:87:LEU:HD21	1.67	0.76
1:C:106:THR:HG21	1:C:287:LEU:HD11	1.67	0.76
1:B:46:LYS:HE3	2:B:401:Y3O:N1	2.02	0.73
1:F:96:ALA:HB2	1:F:288:LEU:HD21	1.76	0.66
1:C:46:LYS:HD2	2:C:401:Y3O:N1	2.12	0.65
1:B:280:ASN:HD22	1:B:282:GLY:H	1.45	0.63
1:C:23:LEU:HD11	1:C:33:LYS:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ASN:HD22	1:B:252:LYS:NZ	1.97	0.62
1:E:263:PRO:HB3	1:E:267:LYS:HD3	1.83	0.60
1:E:106:THR:HG21	1:E:287:LEU:HD11	1.85	0.58
1:E:103:TYR:HA	1:E:106:THR:HG22	1.87	0.57
1:B:48:VAL:HG11	1:B:59:LEU:HD21	1.87	0.57
1:A:69:CYS:SG	1:A:133:LYS:NZ	2.75	0.57
1:D:222:ARG:NH1	1:D:225:PHE:HE2	2.03	0.56
1:D:102:ILE:HG12	1:D:291:LEU:HD11	1.88	0.56
1:D:116:TYR:HE1	1:D:119:ARG:NH1	2.04	0.55
1:C:223:VAL:HG12	1:C:227:MET:HE2	1.88	0.55
1:F:206:ILE:HG21	1:F:214:PRO:HG3	1.90	0.54
1:C:108:SER:OG	1:C:209:ALA:O	2.26	0.53
1:E:243:TRP:HB3	1:E:247:PHE:HD2	1.75	0.52
1:F:280:ASN:HD22	1:F:282:GLY:H	1.58	0.52
1:B:72:ALA:O	1:B:152:ARG:NH1	2.43	0.51
1:A:188:LEU:HD12	1:C:228:THR:HG21	1.91	0.51
1:B:76:ALA:HB3	1:B:92:GLU:HB2	1.92	0.51
1:D:50:MET:HE2	1:D:87:LEU:HB2	1.92	0.51
1:A:20:LEU:HD11	1:A:35:ARG:HB2	1.91	0.51
1:D:222:ARG:NH1	1:D:225:PHE:CE2	2.79	0.50
1:D:76:ALA:HB3	1:D:92:GLU:HB2	1.93	0.50
1:C:166:LEU:HD12	1:C:169:ARG:HD2	1.93	0.49
1:D:260:LYS:H	1:D:260:LYS:HD2	1.78	0.49
1:C:182:GLU:O	1:C:186:VAL:HG13	2.12	0.49
1:D:63:ILE:HD11	1:D:87:LEU:HD21	1.93	0.49
1:A:91:MET:HE3	1:A:91:MET:HB2	1.84	0.48
1:A:228:THR:HG21	1:C:188:LEU:HD12	1.96	0.48
1:A:91:MET:HE3	2:A:401:Y3O:CL1	2.51	0.47
1:D:116:TYR:CE1	1:D:119:ARG:NH1	2.82	0.47
1:F:121:VAL:HG11	1:F:201:LEU:HD13	1.95	0.47
1:F:76:ALA:HB3	1:F:92:GLU:HB2	1.96	0.47
1:A:236:ARG:HB3	1:A:240:LYS:HZ1	1.80	0.47
1:B:150:GLU:OE1	1:B:152:ARG:NH2	2.48	0.46
1:C:22:ARG:NH1	1:F:216:PHE:CE1	2.83	0.46
1:D:46:LYS:HD2	2:D:401:Y3O:N1	2.30	0.46
1:C:47:MET:HE1	1:C:49:LYS:HG3	1.98	0.46
1:E:233:GLN:H	1:E:233:GLN:CD	2.23	0.46
1:E:266:THR:HA	1:E:269:LEU:HD12	1.97	0.46
1:B:249:ASN:ND2	1:B:252:LYS:NZ	2.62	0.45
1:C:25:GLY:HA2	1:C:31:VAL:HG23	1.98	0.45
1:B:46:LYS:CE	2:B:401:Y3O:N1	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ASP:HB3	1:C:8:ILE:HG13	1.98	0.45
1:E:129:HIS:CD2	1:E:194:GLU:HB2	2.51	0.45
1:B:84:LEU:O	1:B:85:GLN:HB2	2.16	0.45
1:A:76:ALA:HB3	1:A:92:GLU:HB2	1.98	0.44
1:D:189:LYS:HB2	3:D:551:HOH:O	2.18	0.44
1:E:100:GLN:HA	1:E:103:TYR:CE2	2.53	0.44
1:B:48:VAL:HG21	1:B:59:LEU:HD11	2.00	0.43
1:F:209:ALA:HB1	1:F:243:TRP:CZ2	2.54	0.43
1:B:249:ASN:HD22	1:B:252:LYS:HZ3	1.63	0.43
1:A:173:ILE:HG13	1:A:179:MET:HE1	1.99	0.43
1:D:106:THR:HG21	1:D:287:LEU:HD11	1.99	0.43
1:B:249:ASN:HD22	1:B:252:LYS:HZ1	1.64	0.43
1:D:46:LYS:NZ	3:D:505:HOH:O	2.51	0.43
1:A:280:ASN:HD22	1:A:282:GLY:H	1.67	0.43
1:C:33:LYS:HE3	1:C:42:LEU:HD13	2.01	0.43
1:F:106:THR:HG21	1:F:287:LEU:HD11	2.01	0.43
1:F:91:MET:HE3	1:F:91:MET:HB2	1.99	0.42
1:B:84:LEU:O	3:B:501:HOH:O	2.22	0.42
1:E:280:ASN:HD22	1:E:282:GLY:H	1.66	0.42
1:A:206:ILE:HG21	1:A:214:PRO:HG3	2.01	0.41
1:E:76:ALA:HB3	1:E:92:GLU:HB2	2.01	0.41
1:A:169:ARG:HH22	1:A:186:VAL:HG23	1.85	0.41
1:E:155:ASP:HB2	2:E:401:Y3O:C5	2.51	0.41
1:C:91:MET:HE3	2:C:401:Y3O:CL1	2.58	0.41
1:C:71:HIS:HB3	1:C:74:ILE:HD12	2.03	0.41
1:B:249:ASN:ND2	1:B:252:LYS:HZ3	2.18	0.40
1:B:280:ASN:HD22	1:B:282:GLY:N	2.16	0.40
1:F:129:HIS:CD2	1:F:194:GLU:HB2	2.56	0.40
1:F:65:ILE:O	1:F:69:CYS:SG	2.76	0.40
1:D:91:MET:HE3	1:D:91:MET:HB2	1.97	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	287/331 (87%)	282 (98%)	5 (2%)	0	100	100
1	B	277/331 (84%)	272 (98%)	4 (1%)	1 (0%)	30	28
1	C	286/331 (86%)	276 (96%)	10 (4%)	0	100	100
1	D	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	E	263/331 (80%)	253 (96%)	10 (4%)	0	100	100
1	F	218/331 (66%)	213 (98%)	5 (2%)	0	100	100
All	All	1604/1986 (81%)	1558 (97%)	45 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	ASP

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	243/281 (86%)	232 (96%)	11 (4%)	24	25
1	B	231/281 (82%)	221 (96%)	10 (4%)	26	27
1	C	239/281 (85%)	227 (95%)	12 (5%)	22	22
1	D	234/281 (83%)	221 (94%)	13 (6%)	19	18
1	E	219/281 (78%)	209 (95%)	10 (5%)	24	25
1	F	171/281 (61%)	162 (95%)	9 (5%)	20	19
All	All	1337/1686 (79%)	1272 (95%)	65 (5%)	22	22

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	MET

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Mol	Chain	Res	Type
1	A	49	LYS
1	A	50	MET
1	A	56	VAL
1	A	70	ARG
1	A	104	GLN
1	A	106	THR
1	A	136	ARG
1	A	186	VAL
1	A	238	LYS
1	A	280	ASN
1	B	11	ARG
1	B	59	LEU
1	B	136	ARG
1	B	162	ILE
1	B	188	LEU
1	B	189	LYS
1	B	221	LEU
1	B	226	LEU
1	B	260	LYS
1	B	280	ASN
1	C	38	VAL
1	C	47	MET
1	C	49	LYS
1	C	56	VAL
1	C	59	LEU
1	C	106	THR
1	C	108	SER
1	C	136	ARG
1	C	152	ARG
1	C	186	VAL
1	C	272	GLN
1	C	291	LEU
1	D	38	VAL
1	D	39	SER
1	D	47	MET
1	D	58	THR
1	D	70	ARG
1	D	108	SER
1	D	133	LYS
1	D	136	ARG
1	D	152	ARG
1	D	162	ILE

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Mol	Chain	Res	Type
1	D	186	VAL
1	D	221	LEU
1	D	227	MET
1	E	22	ARG
1	E	74	ILE
1	E	87	LEU
1	E	106	THR
1	E	152	ARG
1	E	170	LEU
1	E	188	LEU
1	E	266	THR
1	E	280	ASN
1	E	291	LEU
1	F	132	LYS
1	F	173	ILE
1	F	221	LEU
1	F	236	ARG
1	F	239	GLU
1	F	252	LYS
1	F	275	SER
1	F	276	GLN
1	F	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	60	GLN
1	A	73	ASN
1	A	104	GLN
1	A	123	GLN
1	A	131	GLN
1	A	142	ASN
1	A	272	GLN
1	A	280	ASN
1	B	104	GLN
1	B	123	GLN
1	B	142	ASN
1	B	249	ASN
1	B	272	GLN
1	B	276	GLN
1	B	280	ASN

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Mol	Chain	Res	Type
1	C	104	GLN
1	C	142	ASN
1	D	123	GLN
1	D	142	ASN
1	D	233	GLN
1	D	276	GLN
1	E	100	GLN
1	E	104	GLN
1	E	142	ASN
1	E	233	GLN
1	E	276	GLN
1	E	280	ASN
1	F	78	HIS
1	F	100	GLN
1	F	104	GLN
1	F	142	ASN
1	F	212	GLN
1	F	280	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](#)

5 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	Y3O	D	401	-	28,29,29	0.57	0	32,42,42	0.74	0
2	Y3O	C	401	-	28,29,29	0.57	0	32,42,42	0.82	2 (6%)
2	Y3O	E	401	-	28,29,29	0.63	0	32,42,42	0.85	1 (3%)
2	Y3O	A	401	-	28,29,29	0.68	0	32,42,42	0.81	2 (6%)
2	Y3O	B	401	-	28,29,29	0.71	0	32,42,42	0.88	1 (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	Y3O	D	401	-	-	1/9/23/23	0/4/4/4
2	Y3O	C	401	-	-	1/9/23/23	0/4/4/4
2	Y3O	E	401	-	-	1/9/23/23	0/4/4/4
2	Y3O	A	401	-	-	1/9/23/23	0/4/4/4
2	Y3O	B	401	-	-	1/9/23/23	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	Y3O	CL1-C10-N2	-2.79	117.41	121.74
2	B	401	Y3O	CL1-C10-N2	-2.67	117.60	121.74
2	E	401	Y3O	CL1-C10-N2	-2.41	118.00	121.74
2	A	401	Y3O	CL1-C10-N2	-2.35	118.09	121.74
2	C	401	Y3O	C11-N3-C14	2.16	117.11	111.83
2	A	401	Y3O	C11-N3-C14	2.11	116.98	111.83

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	Y3O	N3-C14-N5-C15
2	B	401	Y3O	N3-C14-N5-C15
2	C	401	Y3O	N3-C14-N5-C15
2	D	401	Y3O	N3-C14-N5-C15

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Mol	Chain	Res	Type	Atoms
2	E	401	Y3O	N3-C14-N5-C15

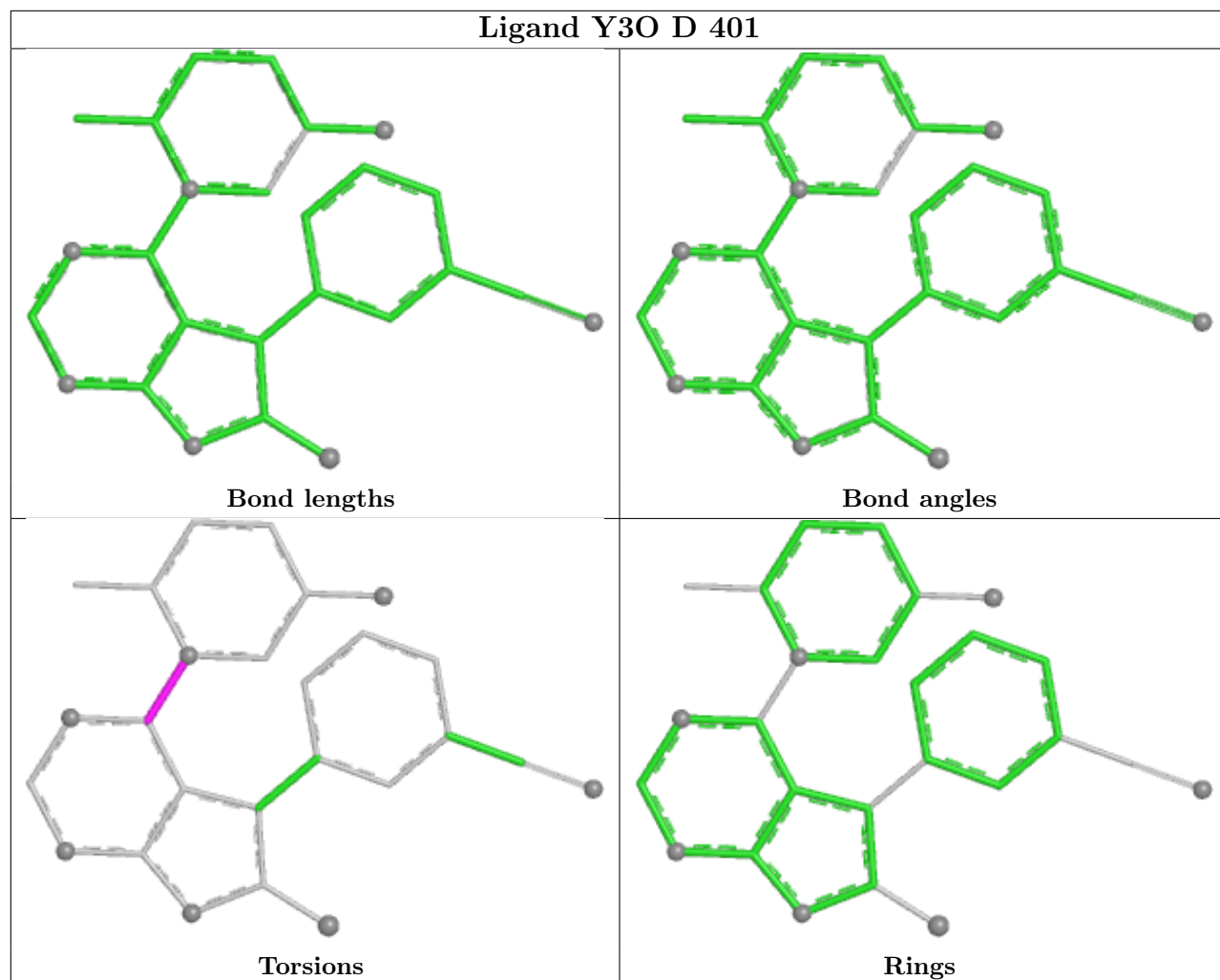
There are no ring outliers.

5 monomers are involved in 7 short contacts:

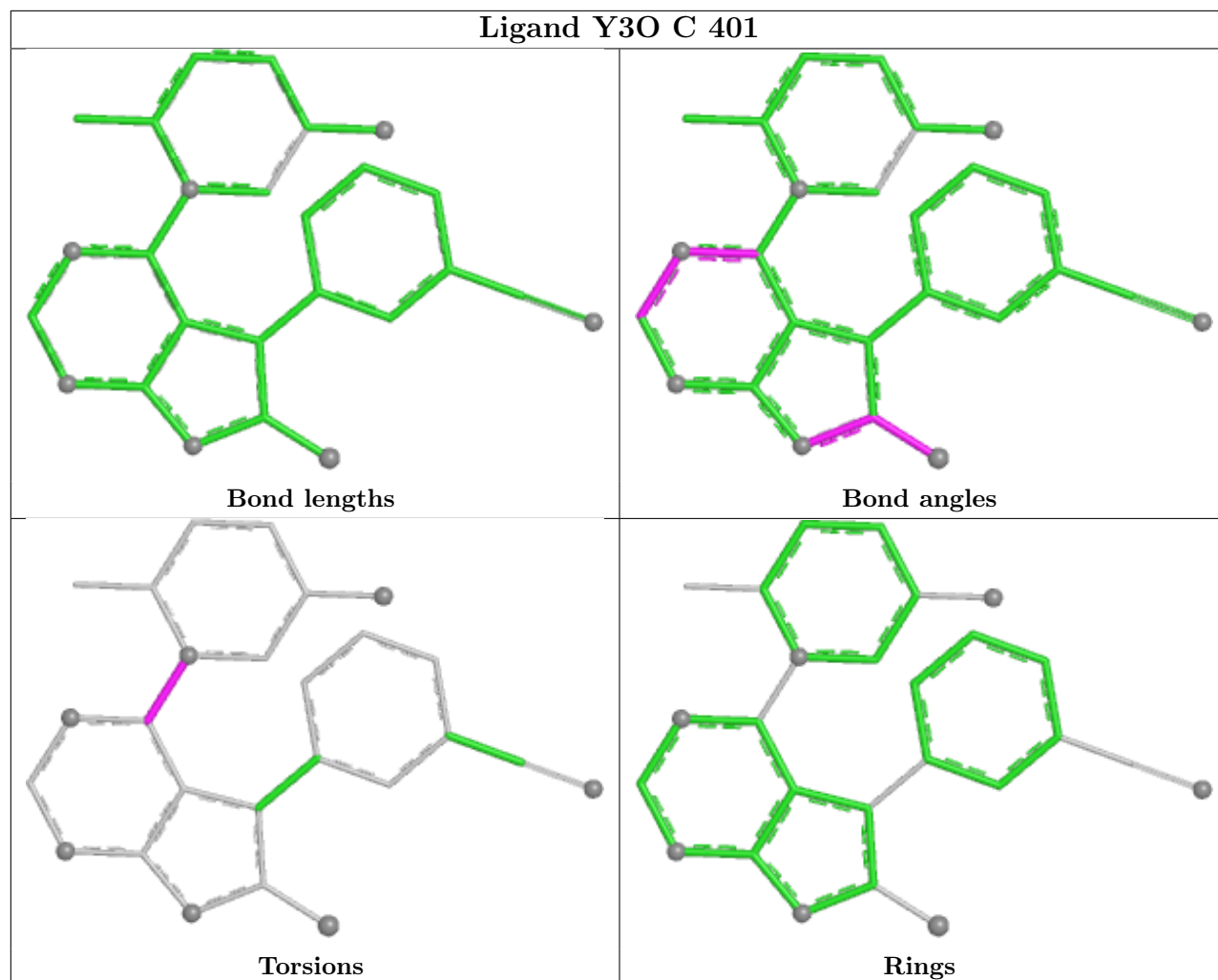
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	Y3O	1	0
2	C	401	Y3O	2	0
2	E	401	Y3O	1	0
2	A	401	Y3O	1	0
2	B	401	Y3O	2	0

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 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.

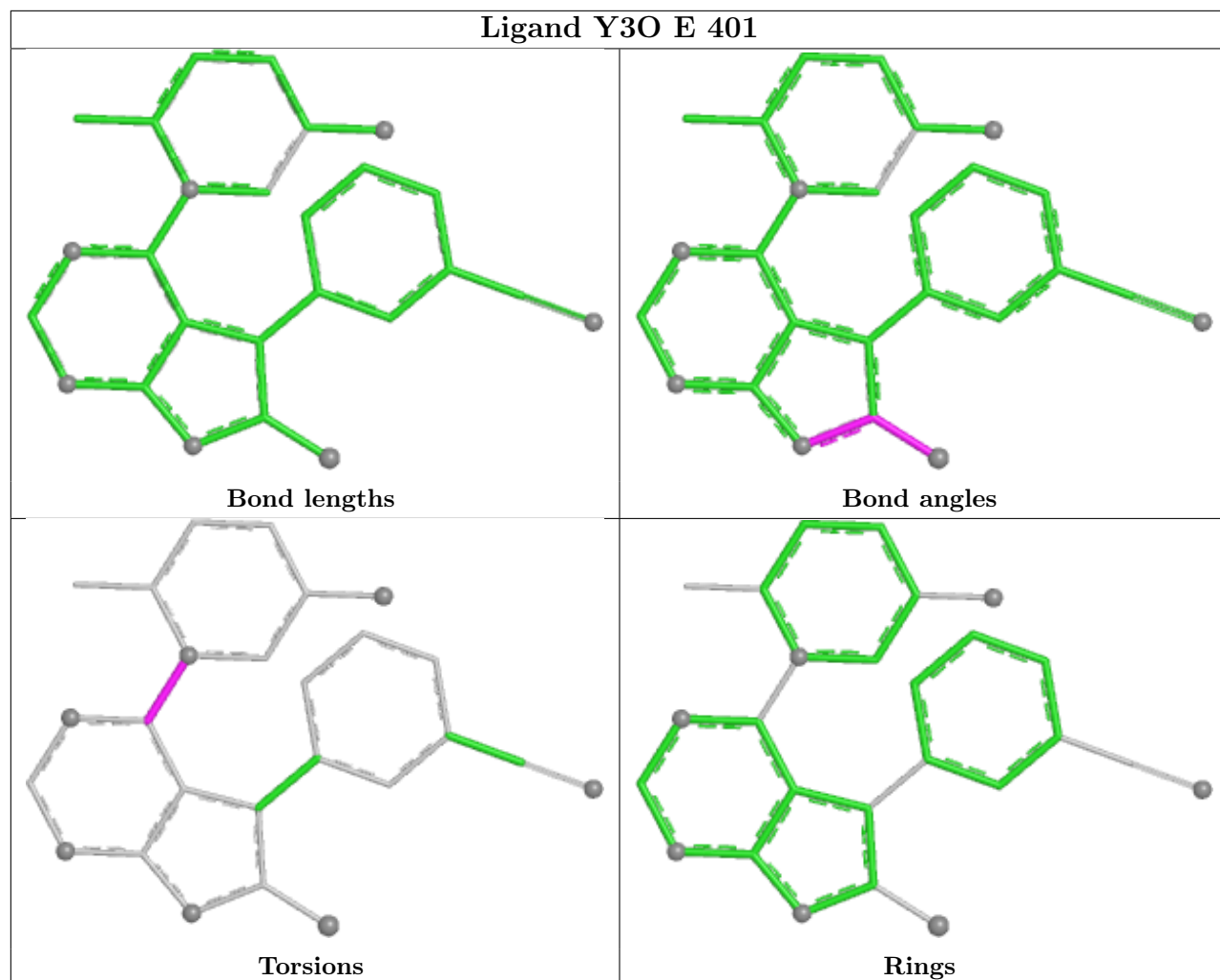
Ligand Y3O D 401



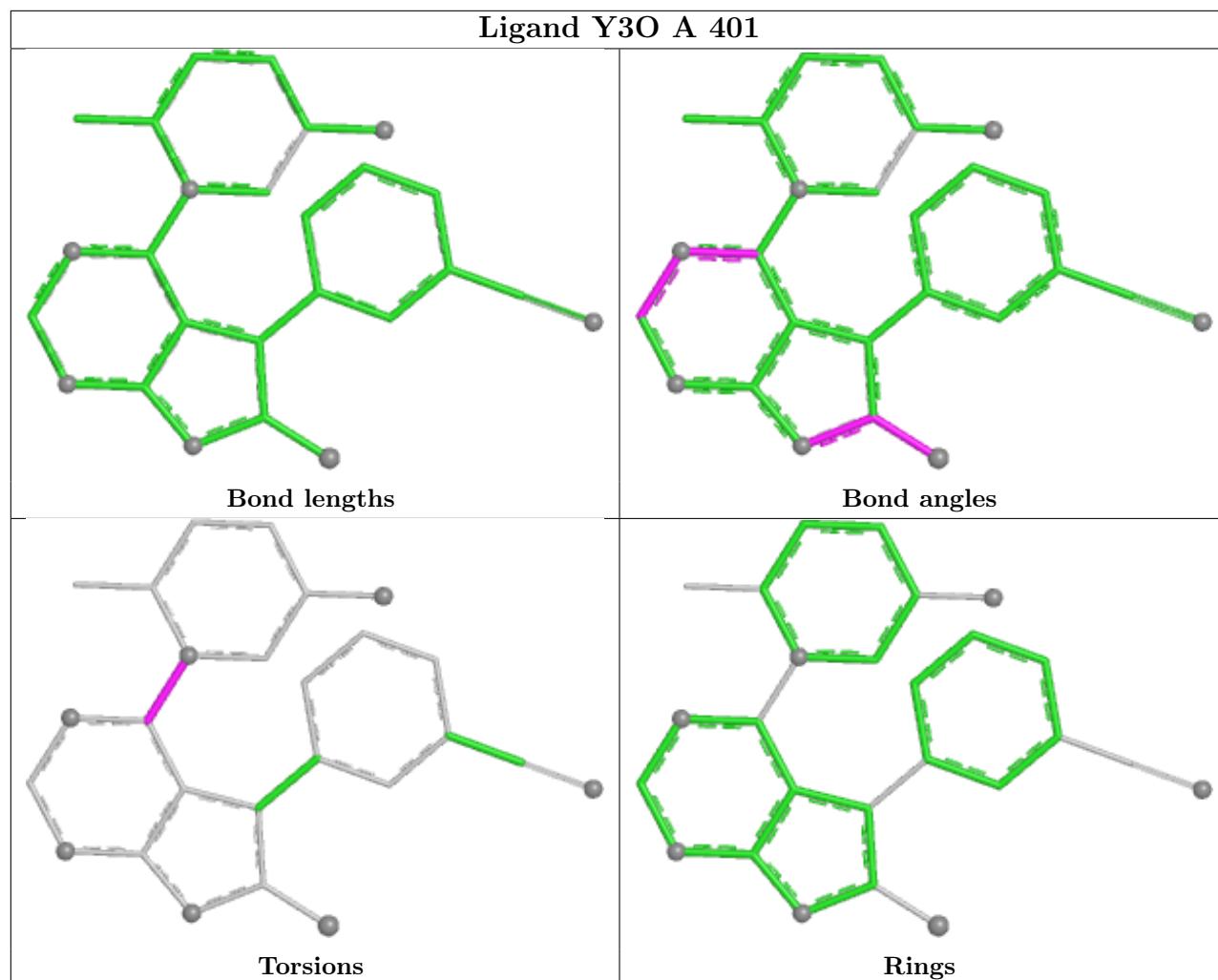
Ligand Y3O C 401

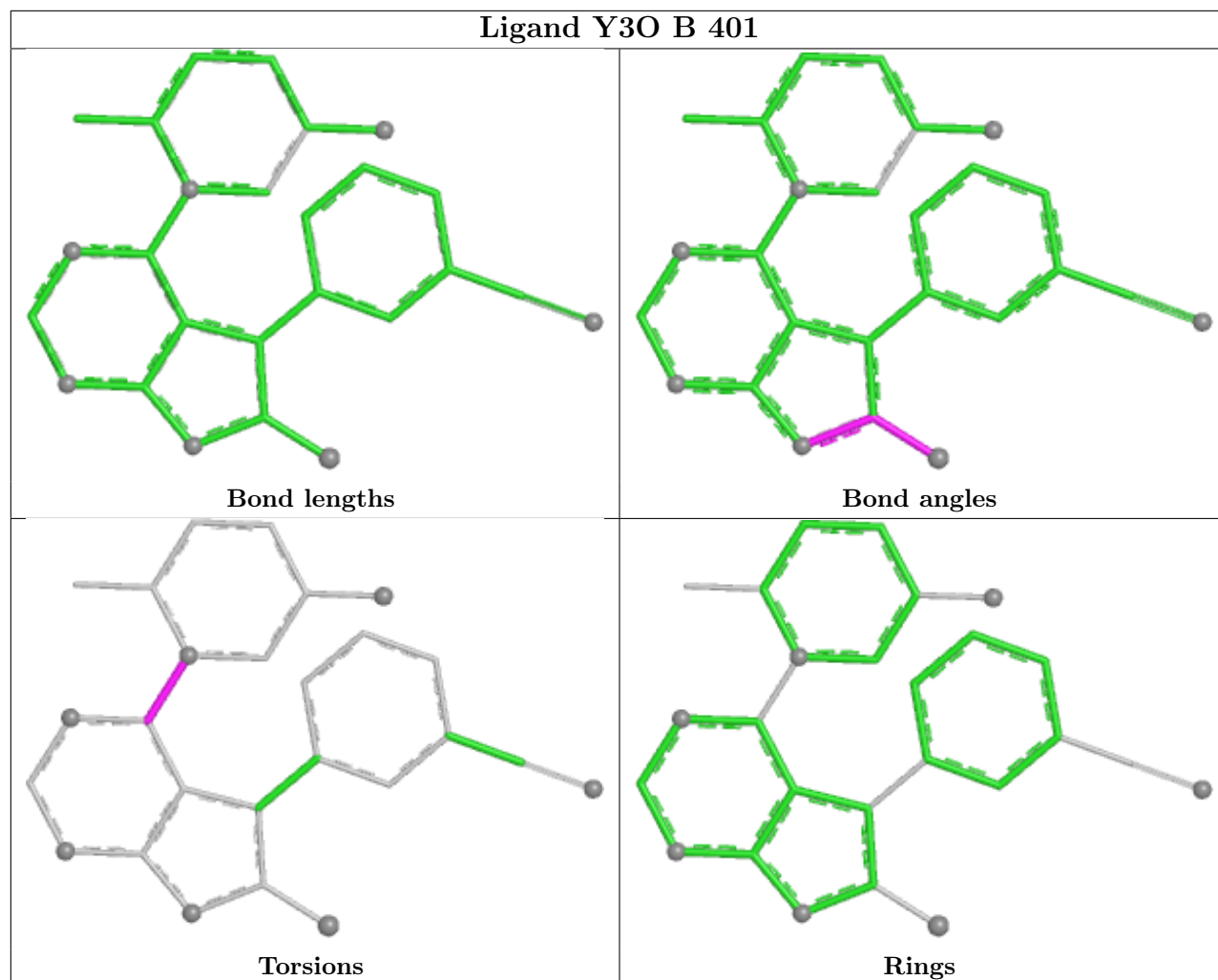


Ligand Y3O E 401



Ligand Y3O A 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, 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	289/331 (87%)	0.26	15 (5%) 33 35	19, 35, 59, 74	0
1	B	281/331 (84%)	0.43	23 (8%) 17 18	21, 38, 61, 82	0
1	C	288/331 (87%)	0.55	23 (7%) 18 19	24, 41, 65, 74	0
1	D	279/331 (84%)	0.76	34 (12%) 8 8	22, 46, 68, 80	0
1	E	271/331 (81%)	1.26	59 (21%) 2 2	24, 56, 77, 88	0
1	F	224/331 (67%)	1.48	64 (28%) 1 1	25, 61, 80, 85	0
All	All	1632/1986 (82%)	0.76	218 (13%) 7 7	19, 44, 73, 88	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	CYS	5.1
1	E	15	ASP	4.9
1	E	38	VAL	4.7
1	F	273	LEU	4.5
1	D	188	LEU	4.5
1	F	279	LEU	4.4
1	C	25	GLY	4.1
1	F	232	TYR	4.1
1	E	224	LEU	3.8
1	B	167	ALA	3.8
1	E	87	LEU	3.8
1	B	28	TYR	3.7
1	C	216	PHE	3.7
1	E	13	PRO	3.7
1	E	17	TYR	3.7
1	F	288	LEU	3.6
1	A	170	LEU	3.5
1	B	166	LEU	3.4
1	F	237	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	10	ASN	3.4
1	E	27	THR	3.4
1	E	166	LEU	3.4
1	D	69	CYS	3.4
1	B	56	VAL	3.4
1	E	32	PHE	3.4
1	F	255	LEU	3.4
1	F	265	ALA	3.3
1	F	291	LEU	3.3
1	C	230	SER	3.3
1	F	209	ALA	3.3
1	F	59	LEU	3.3
1	A	169	ARG	3.3
1	E	9	PHE	3.3
1	E	47	MET	3.3
1	F	261	LYS	3.3
1	C	225	PHE	3.3
1	B	69	CYS	3.2
1	E	246	ALA	3.2
1	F	257	LYS	3.2
1	C	53	ASP	3.2
1	D	58	THR	3.2
1	A	39	SER	3.2
1	D	82	LEU	3.1
1	D	277	PRO	3.1
1	F	263	PRO	3.1
1	E	83	TRP	3.0
1	B	38	VAL	3.0
1	D	166	LEU	3.0
1	E	89	ILE	3.0
1	F	251	ILE	3.0
1	C	24	GLY	3.0
1	A	225	PHE	3.0
1	B	225	PHE	3.0
1	F	276	GLN	3.0
1	D	8	ILE	3.0
1	D	225	PHE	3.0
1	F	57	SER	3.0
1	E	82	LEU	3.0
1	F	105	VAL	2.9
1	F	173	ILE	2.9
1	F	246	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	28	TYR	2.9
1	E	77	TYR	2.9
1	F	250	PHE	2.9
1	E	163	GLY	2.9
1	E	221	LEU	2.9
1	D	38	VAL	2.9
1	D	70	ARG	2.9
1	D	57	SER	2.9
1	E	86	LYS	2.9
1	E	88	TRP	2.9
1	F	231	GLY	2.9
1	E	35	ARG	2.8
1	F	90	CYS	2.8
1	F	238	LYS	2.8
1	F	76	ALA	2.8
1	A	23	LEU	2.8
1	A	38	VAL	2.8
1	D	186	VAL	2.8
1	F	277	PRO	2.8
1	B	8	ILE	2.8
1	C	224	LEU	2.8
1	F	208	LEU	2.8
1	E	162	ILE	2.8
1	F	278	GLY	2.7
1	E	45	LEU	2.7
1	C	228	THR	2.7
1	B	6	PRO	2.7
1	D	6	PRO	2.7
1	F	274	VAL	2.7
1	A	173	ILE	2.7
1	D	41	ASP	2.7
1	E	168	ARG	2.7
1	F	195	LEU	2.7
1	D	95	GLY	2.7
1	F	58	THR	2.6
1	F	266	THR	2.6
1	D	284	ILE	2.6
1	F	222	ARG	2.6
1	F	254	THR	2.6
1	C	6	PRO	2.6
1	F	226	LEU	2.6
1	D	162	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	63	ILE	2.6
1	F	74	ILE	2.6
1	E	16	HIS	2.6
1	E	23	LEU	2.6
1	F	170	LEU	2.6
1	E	172	PHE	2.6
1	D	24	GLY	2.6
1	B	59	LEU	2.6
1	C	170	LEU	2.6
1	D	275	SER	2.6
1	E	42	LEU	2.6
1	E	230	SER	2.6
1	F	239	GLU	2.5
1	B	26	GLY	2.5
1	B	53	ASP	2.5
1	E	66	LEU	2.5
1	F	243	TRP	2.5
1	A	231	GLY	2.5
1	D	292	LYS	2.5
1	B	164	ALA	2.5
1	B	181	PRO	2.5
1	C	233	GLN	2.5
1	E	228	THR	2.5
1	E	19	LEU	2.5
1	F	211	LEU	2.5
1	C	278	GLY	2.5
1	F	102	ILE	2.5
1	E	277	PRO	2.5
1	F	260	LYS	2.5
1	D	56	VAL	2.4
1	F	218	VAL	2.4
1	B	54	ASP	2.4
1	B	165	GLU	2.4
1	E	232	TYR	2.4
1	C	221	LEU	2.4
1	F	221	LEU	2.4
1	D	168	ARG	2.4
1	B	162	ILE	2.4
1	E	14	ARG	2.4
1	E	167	ALA	2.4
1	C	56	VAL	2.4
1	E	37	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	64	LEU	2.4
1	F	191	GLY	2.4
1	F	75	VAL	2.4
1	C	292	LYS	2.4
1	C	85	GLN	2.3
1	A	168	ARG	2.3
1	A	292	LYS	2.3
1	C	8	ILE	2.3
1	D	87	LEU	2.3
1	B	230	SER	2.3
1	F	258	SER	2.3
1	E	75	VAL	2.3
1	F	68	THR	2.3
1	E	245	ALA	2.3
1	F	286	ASP	2.3
1	F	292	LYS	2.3
1	E	58	THR	2.3
1	F	106	THR	2.3
1	D	189	LYS	2.3
1	E	72	ALA	2.3
1	E	29	GLY	2.3
1	E	122	LEU	2.3
1	E	170	LEU	2.3
1	E	225	PHE	2.2
1	A	223	VAL	2.2
1	F	206	ILE	2.2
1	F	252	LYS	2.2
1	D	55	ASP	2.2
1	E	94	CYS	2.2
1	E	64	LEU	2.2
1	E	237	LEU	2.2
1	E	80	SER	2.2
1	B	27	THR	2.2
1	C	27	THR	2.2
1	D	47	MET	2.2
1	F	235	PRO	2.2
1	D	66	LEU	2.2
1	F	259	PRO	2.1
1	C	162	ILE	2.1
1	E	65	ILE	2.1
1	E	93	PHE	2.1
1	E	157	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	69	CYS	2.1
1	F	233	GLN	2.1
1	A	24	GLY	2.1
1	C	223	VAL	2.1
1	C	169	ARG	2.1
1	C	277	PRO	2.1
1	A	190	GLY	2.1
1	E	191	GLY	2.1
1	D	20	LEU	2.1
1	E	59	LEU	2.1
1	D	280	ASN	2.1
1	D	27	THR	2.1
1	E	26	GLY	2.1
1	F	79	GLY	2.1
1	E	238	LYS	2.1
1	F	229	LYS	2.1
1	B	223	VAL	2.1
1	D	96	ALA	2.1
1	F	112	LEU	2.0
1	F	262	ARG	2.0
1	C	238	LYS	2.0
1	F	133	LYS	2.0
1	D	160	ALA	2.0
1	D	167	ALA	2.0
1	D	23	LEU	2.0
1	F	169	ARG	2.0
1	A	240	LYS	2.0
1	B	24	GLY	2.0
1	B	77	TYR	2.0
1	B	177	TYR	2.0
1	F	103	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

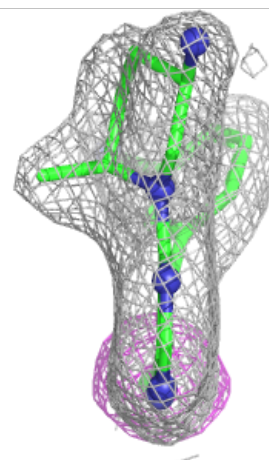
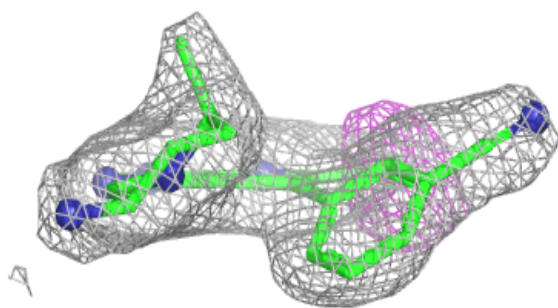
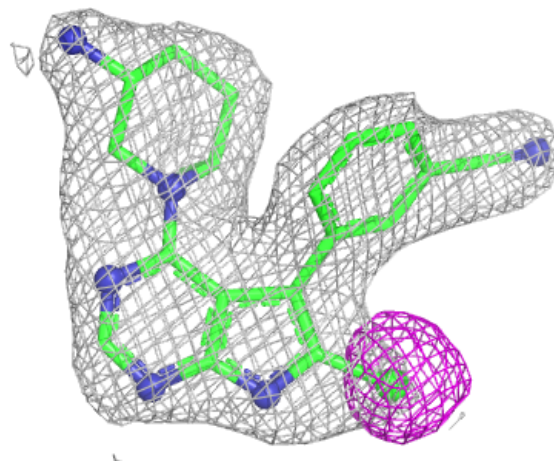
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	Y3O	E	401	26/26	0.84	0.11	45,51,52,57	0
2	Y3O	C	401	26/26	0.85	0.10	30,33,38,42	0
2	Y3O	B	401	26/26	0.86	0.09	30,32,37,42	0
2	Y3O	D	401	26/26	0.87	0.10	47,49,51,54	0
2	Y3O	A	401	26/26	0.87	0.09	28,32,36,42	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.

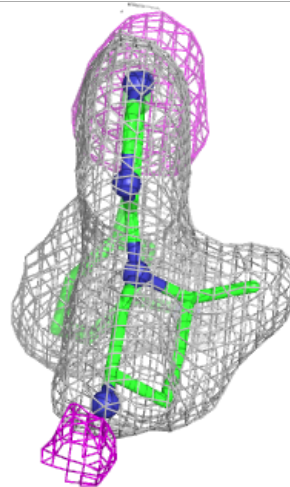
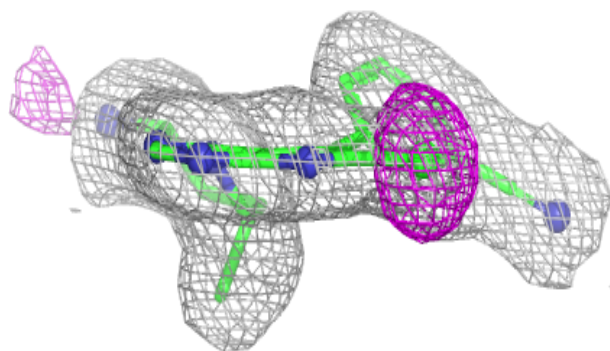
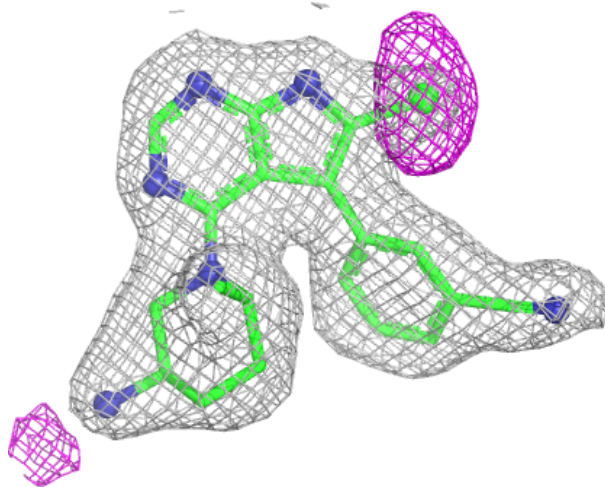
Electron density around Y3O E 401:

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



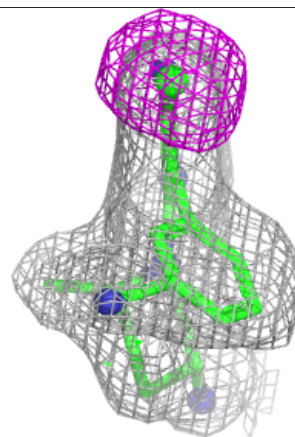
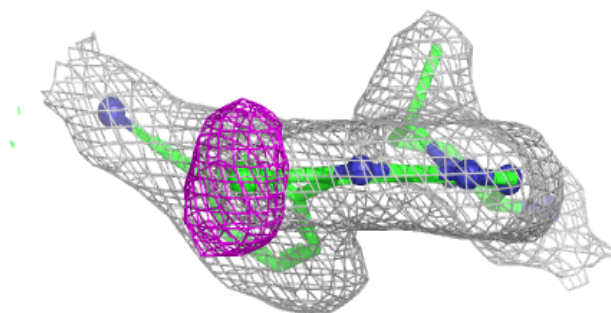
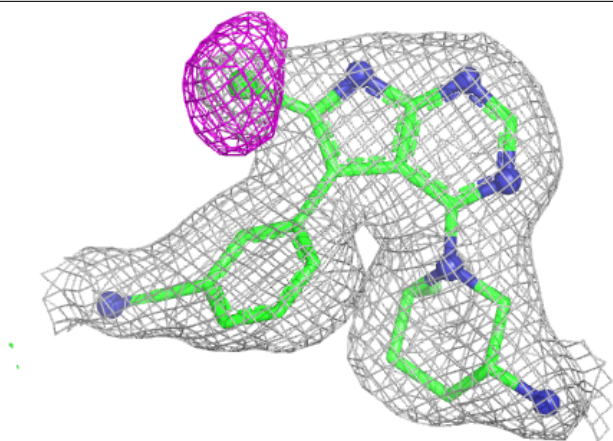
Electron density around Y3O C 401:

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



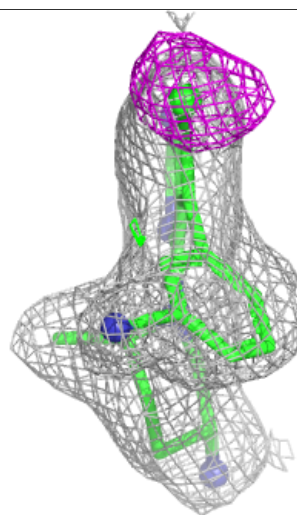
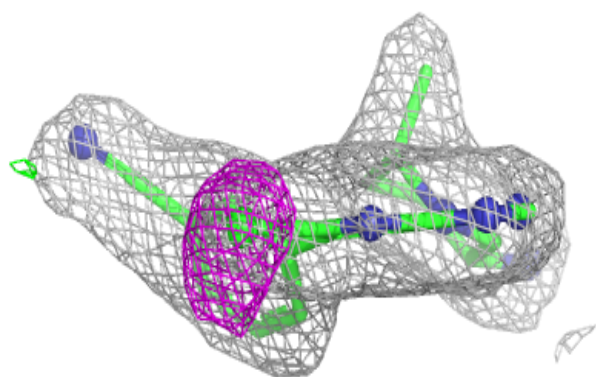
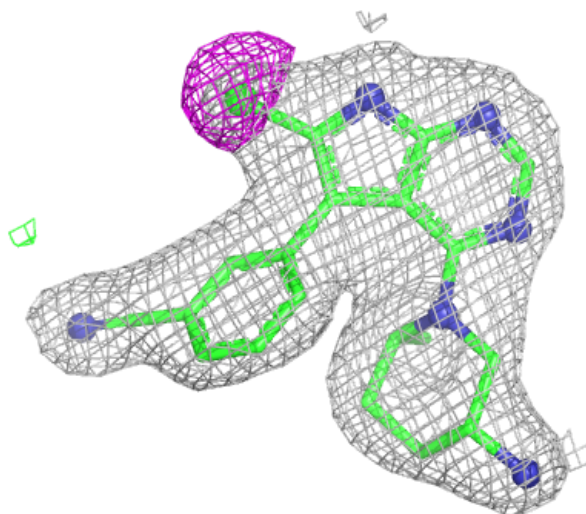
Electron density around Y3O B 401:

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



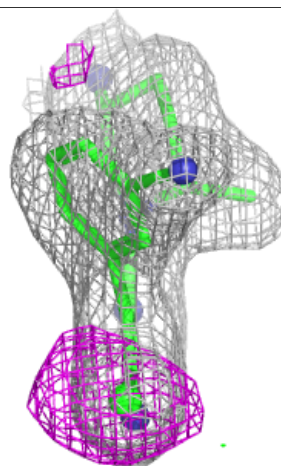
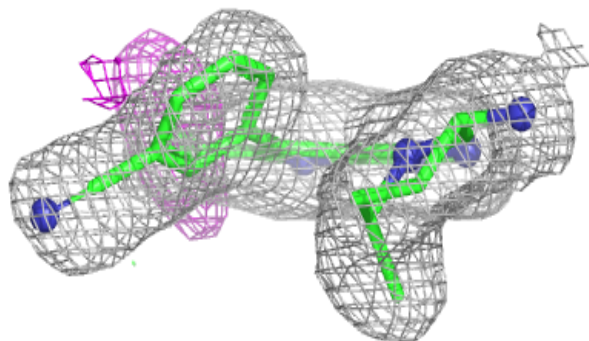
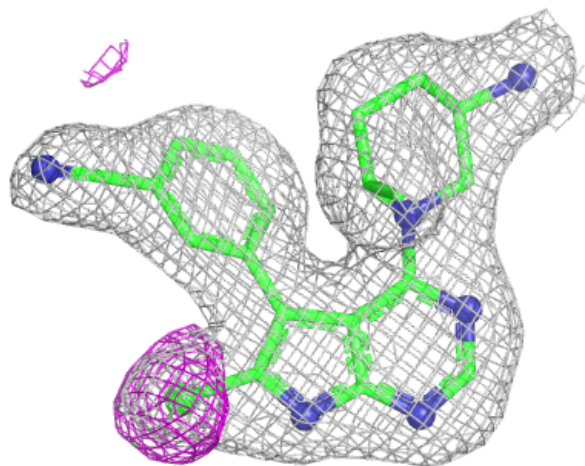
Electron density around Y3O D 401:

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



Electron density around Y3O 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.