



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2023 – 09:44 pm GMT

PDB ID : 2JBP
Title : Protein kinase MK2 in complex with an inhibitor (crystal form-2, co-crystallization)
Authors : Hillig, R.C.; Eberspaecher, U.; Monteclaro, F.; Huber, M.; Nguyen, D.; Mengel, A.; Muller-Tiemann, B.; Egner, U.
Deposited on : 2006-12-09
Resolution : 3.31 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.8.4, 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

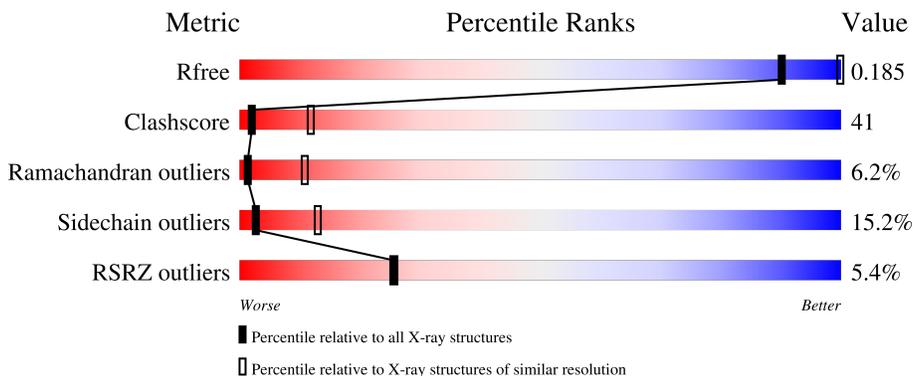
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	326	 45% 33% 8% 13%
1	B	326	 38% 40% 10% 11%
1	C	326	 35% 43% 9% 13%
1	D	326	 39% 36% 12% 12%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	326	
1	F	326	
1	G	326	
1	H	326	
1	I	326	
1	J	326	
1	K	326	
1	L	326	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P4O	I	1351	-	-	-	X
2	P4O	K	1345	-	-	-	X
2	P4O	L	1345	-	-	-	X

2 Entry composition [i](#)

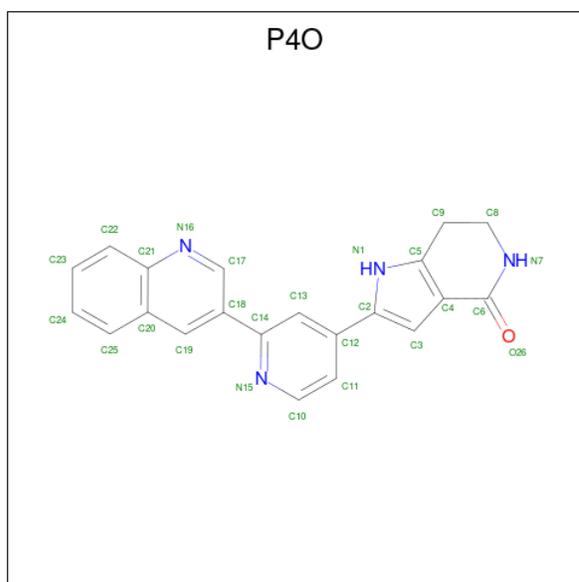
There are 3 unique types of molecules in this entry. The entry contains 27367 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MAP KINASE-ACTIVATED PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	283	2298	1467	399	415	17	0	0	0
1	B	290	2361	1510	407	427	17	0	0	0
1	C	284	2316	1485	399	415	17	0	0	0
1	D	286	2325	1486	402	420	17	0	0	0
1	E	283	2291	1467	395	412	17	0	0	1
1	F	288	2344	1499	405	423	17	0	0	1
1	G	288	2343	1498	405	423	17	0	0	1
1	H	283	2289	1464	396	412	17	0	0	1
1	I	289	2354	1503	407	427	17	0	0	0
1	J	225	1823	1167	315	326	15	0	0	1
1	K	265	2142	1367	374	384	17	0	0	1
1	L	268	2177	1390	379	391	17	0	0	1

- Molecule 2 is 2-(2-QUINOLIN-3-YLPYRIDIN-4-YL)-1,5,6,7-TETRAHYDRO-4H-PYRROLO[3,2-C]PYRIDIN-4-ONE (three-letter code: P4O) (formula: C₂₁H₁₆N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			26	21	4	1		
2	B	1	Total	C	N	O	0	0
			26	21	4	1		
2	C	1	Total	C	N	O	0	0
			26	21	4	1		
2	D	1	Total	C	N	O	0	0
			26	21	4	1		
2	E	1	Total	C	N	O	0	0
			26	21	4	1		
2	F	1	Total	C	N	O	0	0
			26	21	4	1		
2	G	1	Total	C	N	O	0	0
			26	21	4	1		
2	H	1	Total	C	N	O	0	0
			26	21	4	1		
2	I	1	Total	C	N	O	0	0
			26	21	4	1		
2	K	1	Total	C	N	O	0	0
			26	21	4	1		
2	L	1	Total	C	N	O	0	0
			26	21	4	1		

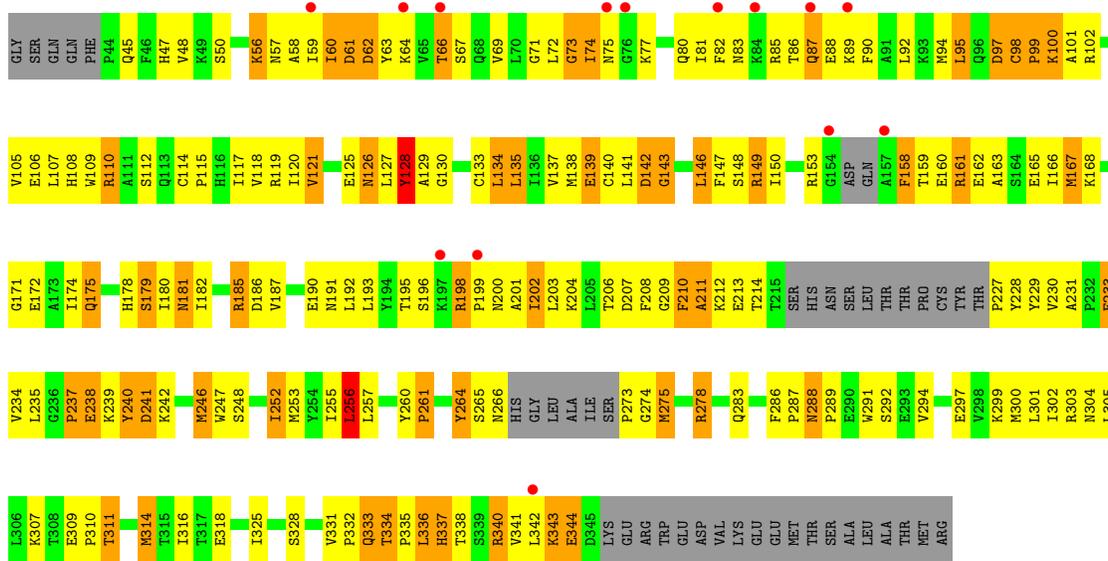
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total 4	O 4	0 0

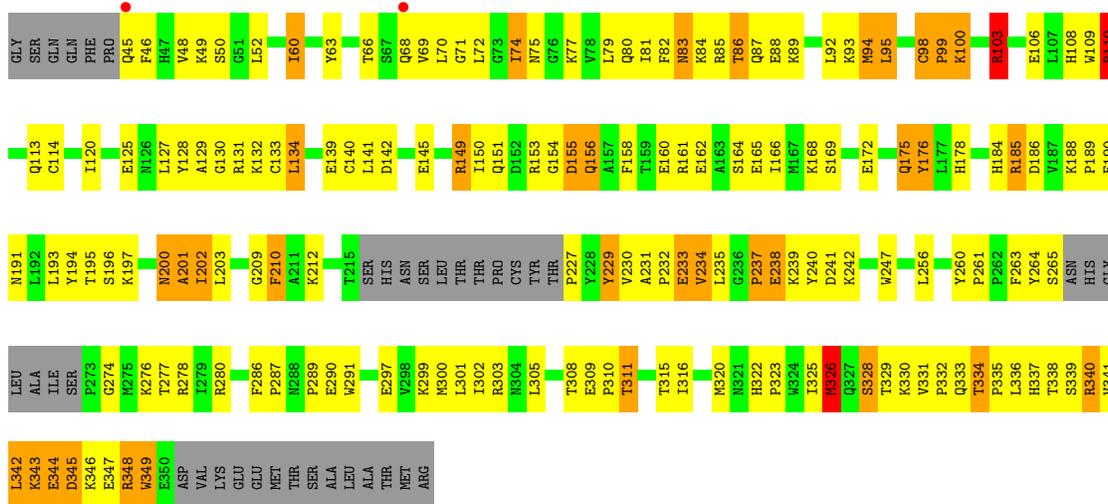
Continued on next page...

Continued from previous page...

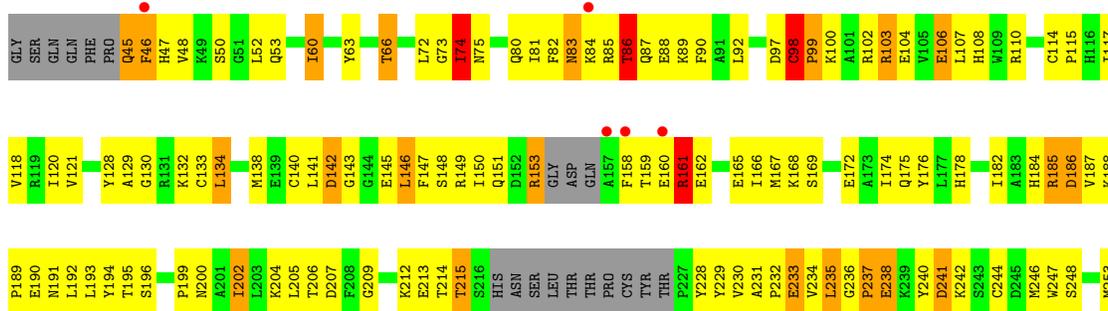
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total O 2 2	0	0
3	C	2	Total O 2 2	0	0
3	D	2	Total O 2 2	0	0
3	E	1	Total O 1 1	0	0
3	F	2	Total O 2 2	0	0
3	G	3	Total O 3 3	0	0
3	I	1	Total O 1 1	0	0
3	L	1	Total O 1 1	0	0

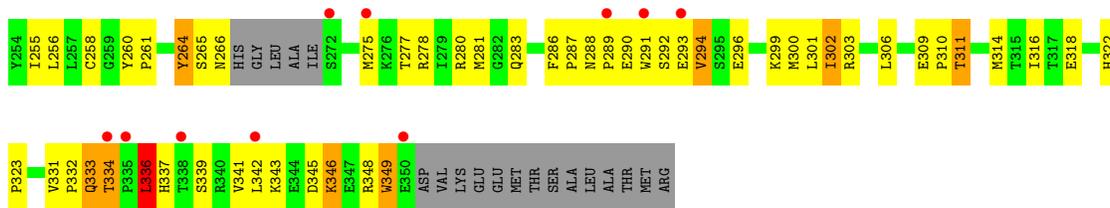


• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

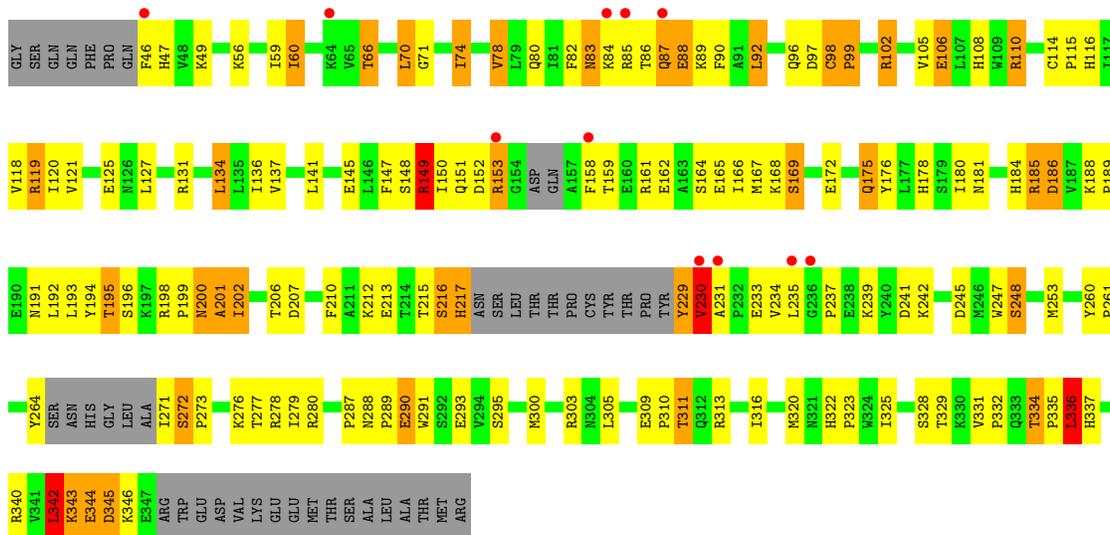


• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

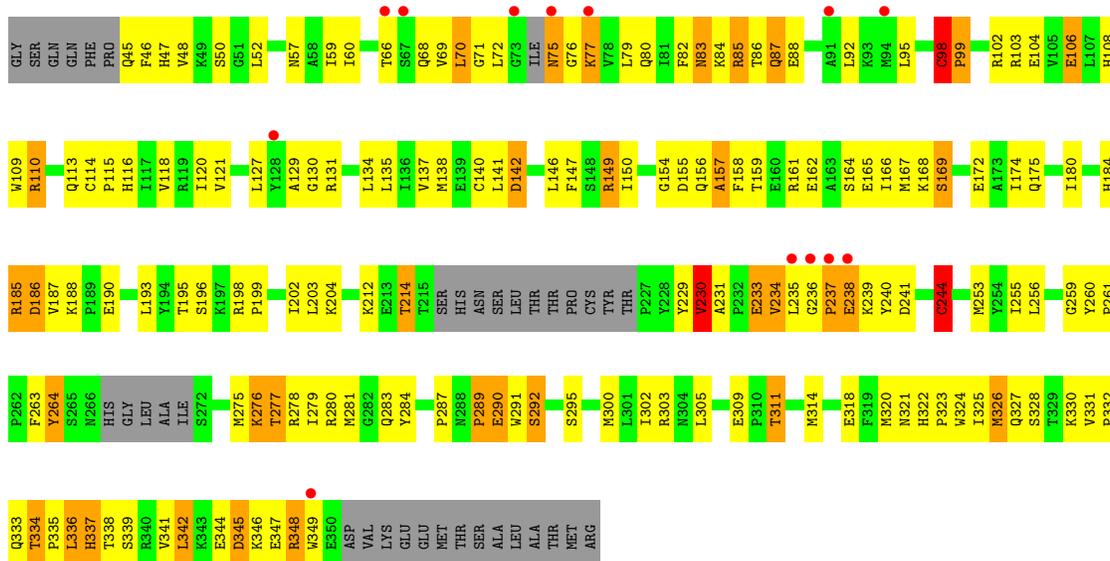




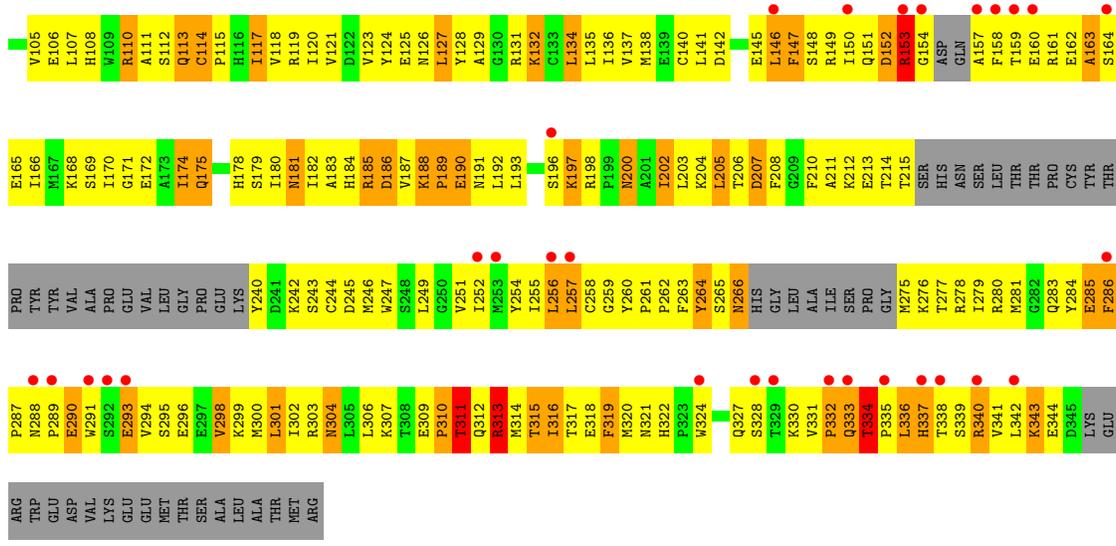
• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.98Å 215.56Å 179.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 3.31 49.08 – 3.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.08-3.31) 96.6 (49.08-3.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.33Å)	Xtrriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.215 , 0.279 0.195 , 0.185	Depositor DCC
R_{free} test set	3942 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	88.6	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 101.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27367	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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: P4O

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	0.93	3/2346 (0.1%)	0.97	8/3160 (0.3%)
1	B	0.78	1/2413 (0.0%)	0.85	2/3254 (0.1%)
1	C	0.85	1/2367 (0.0%)	0.89	2/3189 (0.1%)
1	D	0.89	5/2375 (0.2%)	0.92	2/3201 (0.1%)
1	E	0.65	0/2341	0.83	1/3155 (0.0%)
1	F	0.94	2/2396 (0.1%)	0.97	4/3230 (0.1%)
1	G	0.77	0/2394	0.91	8/3227 (0.2%)
1	H	0.65	0/2337	0.82	6/3149 (0.2%)
1	I	0.72	1/2405 (0.0%)	0.88	3/3241 (0.1%)
1	J	0.57	0/1855	0.76	0/2493
1	K	0.55	0/2184	0.74	2/2940 (0.1%)
1	L	0.59	1/2221 (0.0%)	0.78	2/2990 (0.1%)
All	All	0.76	14/27634 (0.1%)	0.87	40/37229 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
1	F	0	2
1	G	0	2
1	I	0	1
All	All	0	8

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	244	CYS	CB-SG	-7.21	1.70	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	320	MET	SD-CE	-7.17	1.37	1.77
1	A	98	CYS	CB-SG	-6.25	1.71	1.82
1	D	140	CYS	CB-SG	-6.21	1.71	1.82
1	I	244	CYS	CB-SG	-6.20	1.71	1.82

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	185	ARG	NE-CZ-NH1	-10.42	115.09	120.30
1	A	103	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	F	103	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	A	110	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	110	ARG	NE-CZ-NH2	-8.49	116.05	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	264	TYR	Sidechain
1	D	176	TYR	Sidechain
1	D	229	TYR	Sidechain
1	F	176	TYR	Sidechain
1	F	229	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2298	0	2326	135	0
1	B	2361	0	2385	185	0
1	C	2316	0	2346	174	0
1	D	2325	0	2352	171	0
1	E	2291	0	2325	238	0
1	F	2344	0	2370	172	0
1	G	2343	0	2369	186	0
1	H	2289	0	2325	157	0
1	I	2354	0	2370	176	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1823	0	1868	267	0
1	K	2142	0	2186	156	0
1	L	2177	0	2212	321	0
2	A	26	0	16	2	0
2	B	26	0	16	1	0
2	C	26	0	16	4	0
2	D	26	0	16	5	0
2	E	26	0	16	4	0
2	F	26	0	16	5	0
2	G	26	0	16	5	0
2	H	26	0	16	4	0
2	I	26	0	16	2	0
2	K	26	0	16	3	0
2	L	26	0	16	4	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
All	All	27367	0	27610	2240	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 41.

The worst 5 of 2240 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:G:45:GLN:HG3	1:G:46:PHE:H	1.03	1.17
1:L:275:MET:HA	1:L:278:ARG:NH1	1.60	1.16
1:L:275:MET:HG3	1:L:278:ARG:HH22	1.12	1.15
1:D:264:TYR:O	1:D:275:MET:HG3	1.43	1.14
1:F:151:GLN:HE22	1:F:346:LYS:HD3	1.01	1.13

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	275/326 (84%)	244 (89%)	23 (8%)	8 (3%)	4	26
1	B	284/326 (87%)	238 (84%)	32 (11%)	14 (5%)	2	15
1	C	276/326 (85%)	245 (89%)	19 (7%)	12 (4%)	2	18
1	D	278/326 (85%)	236 (85%)	26 (9%)	16 (6%)	1	11
1	E	275/326 (84%)	210 (76%)	47 (17%)	18 (6%)	1	10
1	F	282/326 (86%)	248 (88%)	21 (7%)	13 (5%)	2	16
1	G	280/326 (86%)	238 (85%)	26 (9%)	16 (6%)	1	12
1	H	275/326 (84%)	239 (87%)	23 (8%)	13 (5%)	2	15
1	I	281/326 (86%)	245 (87%)	22 (8%)	14 (5%)	2	14
1	J	217/326 (67%)	142 (65%)	40 (18%)	35 (16%)	0	1
1	K	257/326 (79%)	221 (86%)	22 (9%)	14 (5%)	2	13
1	L	260/326 (80%)	187 (72%)	44 (17%)	29 (11%)	0	3
All	All	3240/3912 (83%)	2693 (83%)	345 (11%)	202 (6%)	1	11

5 of 202 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	237	PRO
1	B	98	CYS
1	B	156	GLN
1	B	235	LEU

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	255/294 (87%)	218 (86%)	37 (14%)	3	15
1	B	262/294 (89%)	218 (83%)	44 (17%)	2	9
1	C	256/294 (87%)	224 (88%)	32 (12%)	4	19
1	D	258/294 (88%)	228 (88%)	30 (12%)	5	22
1	E	255/294 (87%)	198 (78%)	57 (22%)	1	3
1	F	260/294 (88%)	218 (84%)	42 (16%)	2	11
1	G	261/294 (89%)	229 (88%)	32 (12%)	4	20
1	H	255/294 (87%)	221 (87%)	34 (13%)	4	17
1	I	261/294 (89%)	222 (85%)	39 (15%)	3	13
1	J	202/294 (69%)	175 (87%)	27 (13%)	4	17
1	K	239/294 (81%)	199 (83%)	40 (17%)	2	10
1	L	243/294 (83%)	201 (83%)	42 (17%)	2	9
All	All	3007/3528 (85%)	2551 (85%)	456 (15%)	3	13

5 of 456 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	311	THR
1	L	293	GLU
1	H	149	ARG
1	L	257	LEU
1	K	276	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	191	ASN
1	I	96	GLN
1	L	283	GLN
1	H	80	GLN
1	H	217	HIS

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](#)

11 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	P4O	D	1351	-	25,30,30	1.53	3 (12%)	25,43,43	1.87	8 (32%)
2	P4O	I	1351	-	25,30,30	1.53	3 (12%)	25,43,43	1.87	7 (28%)
2	P4O	K	1345	-	25,30,30	1.53	3 (12%)	25,43,43	1.91	7 (28%)
2	P4O	F	1350	-	25,30,30	1.53	3 (12%)	25,43,43	1.87	7 (28%)
2	P4O	B	1351	-	25,30,30	1.53	3 (12%)	25,43,43	1.89	8 (32%)
2	P4O	H	1347	-	25,30,30	1.53	3 (12%)	25,43,43	1.82	7 (28%)
2	P4O	C	1351	-	25,30,30	1.53	4 (16%)	25,43,43	1.83	8 (32%)
2	P4O	L	1345	-	25,30,30	1.52	3 (12%)	25,43,43	1.90	7 (28%)
2	P4O	A	1351	-	25,30,30	1.53	3 (12%)	25,43,43	1.86	7 (28%)
2	P4O	G	1350	-	25,30,30	1.52	3 (12%)	25,43,43	1.88	7 (28%)
2	P4O	E	1345	-	25,30,30	1.52	3 (12%)	25,43,43	1.97	7 (28%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P4O	D	1351	-	-	0/0/18/18	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P4O	I	1351	-	-	0/0/18/18	0/5/5/5
2	P4O	K	1345	-	-	0/0/18/18	0/5/5/5
2	P4O	F	1350	-	-	0/0/18/18	0/5/5/5
2	P4O	B	1351	-	-	0/0/18/18	0/5/5/5
2	P4O	H	1347	-	-	0/0/18/18	0/5/5/5
2	P4O	C	1351	-	-	0/0/18/18	0/5/5/5
2	P4O	L	1345	-	-	0/0/18/18	0/5/5/5
2	P4O	A	1351	-	-	0/0/18/18	0/5/5/5
2	P4O	G	1350	-	-	0/0/18/18	0/5/5/5
2	P4O	E	1345	-	-	0/0/18/18	0/5/5/5

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1351	P4O	C4-C6	-4.68	1.39	1.47
2	L	1345	P4O	C4-C6	-4.67	1.39	1.47
2	B	1351	P4O	C4-C6	-4.66	1.39	1.47
2	K	1345	P4O	C4-C6	-4.65	1.39	1.47
2	D	1351	P4O	C4-C6	-4.64	1.39	1.47

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1345	P4O	C11-C10-N15	-4.64	120.00	125.10
2	L	1345	P4O	C11-C10-N15	-4.55	120.10	125.10
2	G	1350	P4O	C11-C10-N15	-4.50	120.15	125.10
2	K	1345	P4O	C11-C10-N15	-4.42	120.25	125.10
2	I	1351	P4O	C11-C10-N15	-4.23	120.45	125.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 39 short contacts:

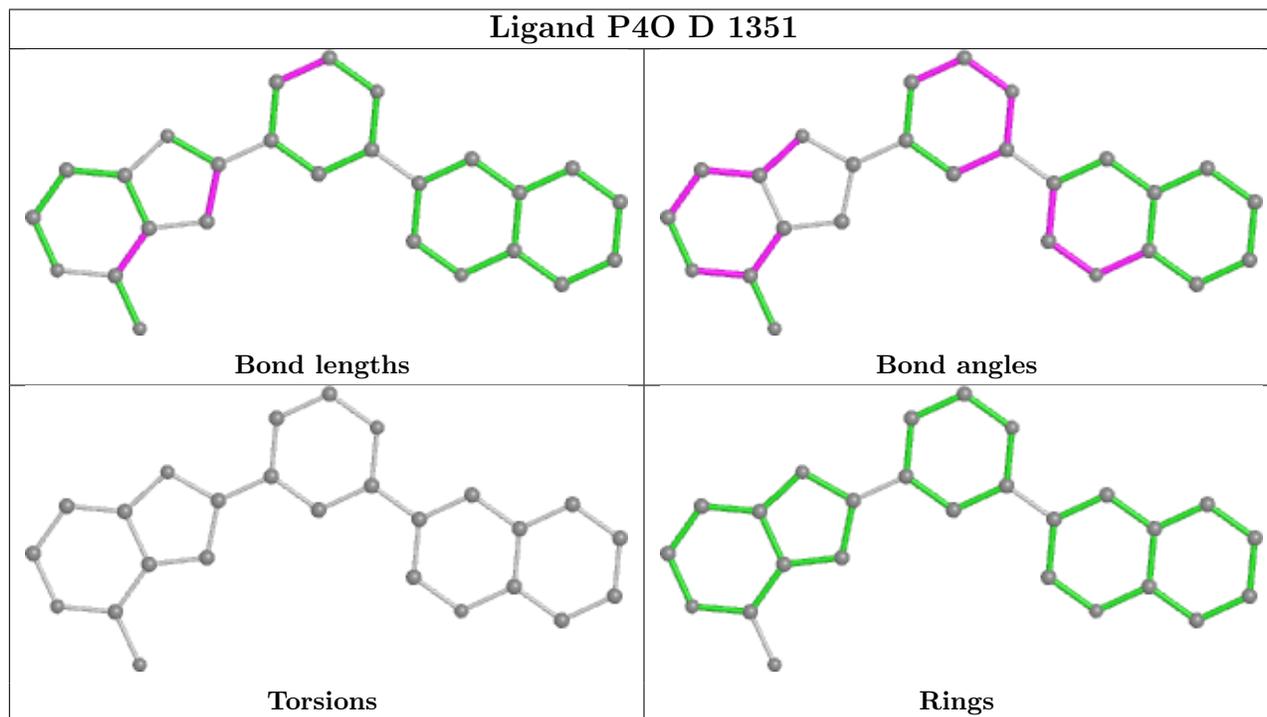
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1351	P4O	5	0
2	I	1351	P4O	2	0
2	K	1345	P4O	3	0
2	F	1350	P4O	5	0
2	B	1351	P4O	1	0
2	H	1347	P4O	4	0

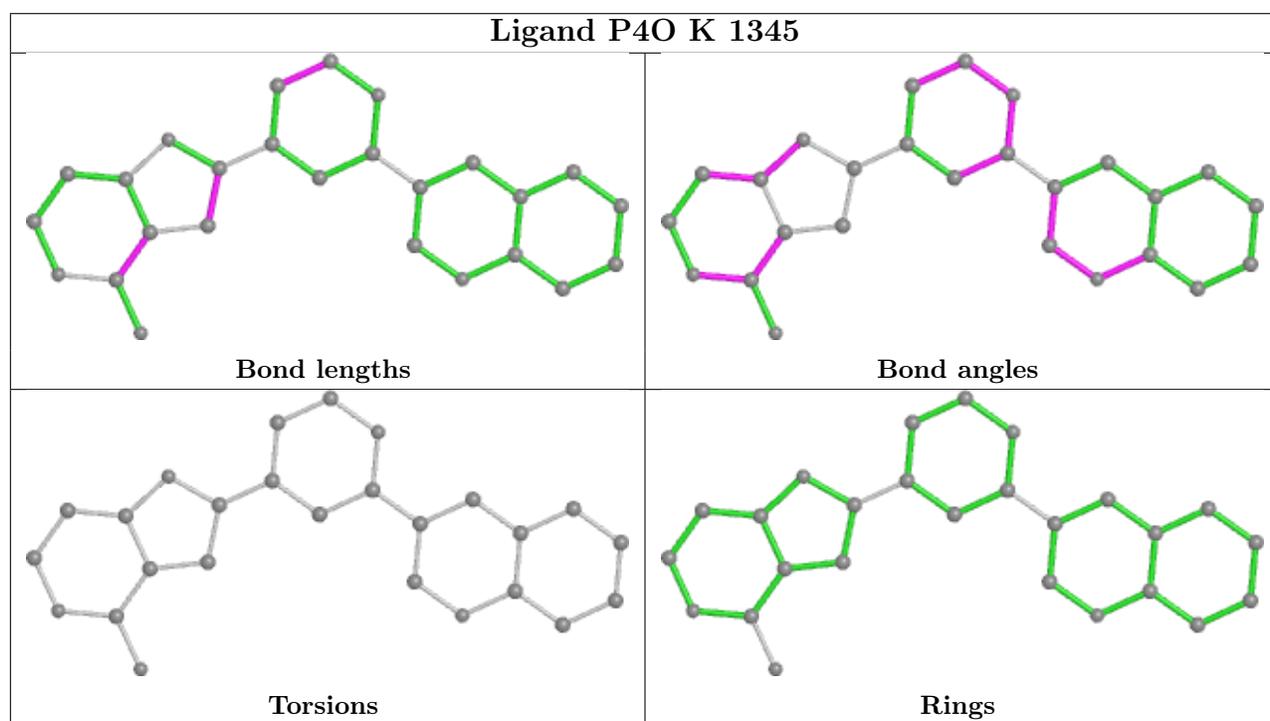
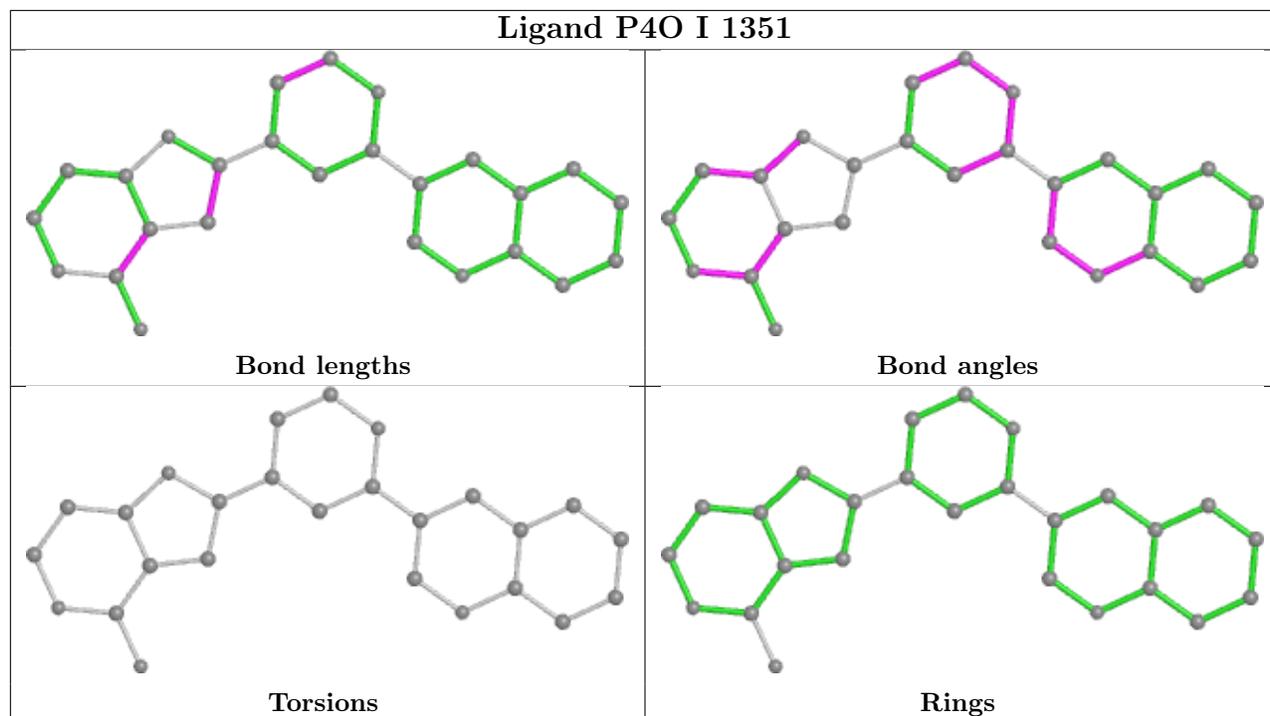
Continued on next page...

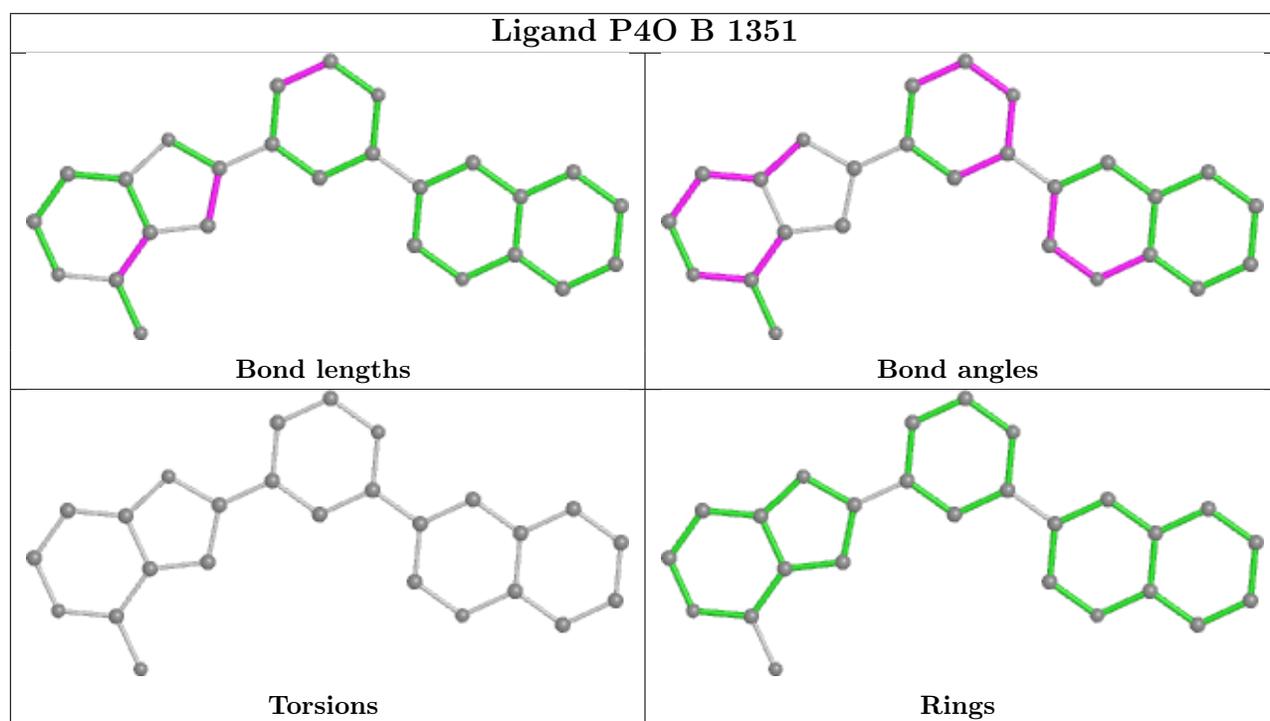
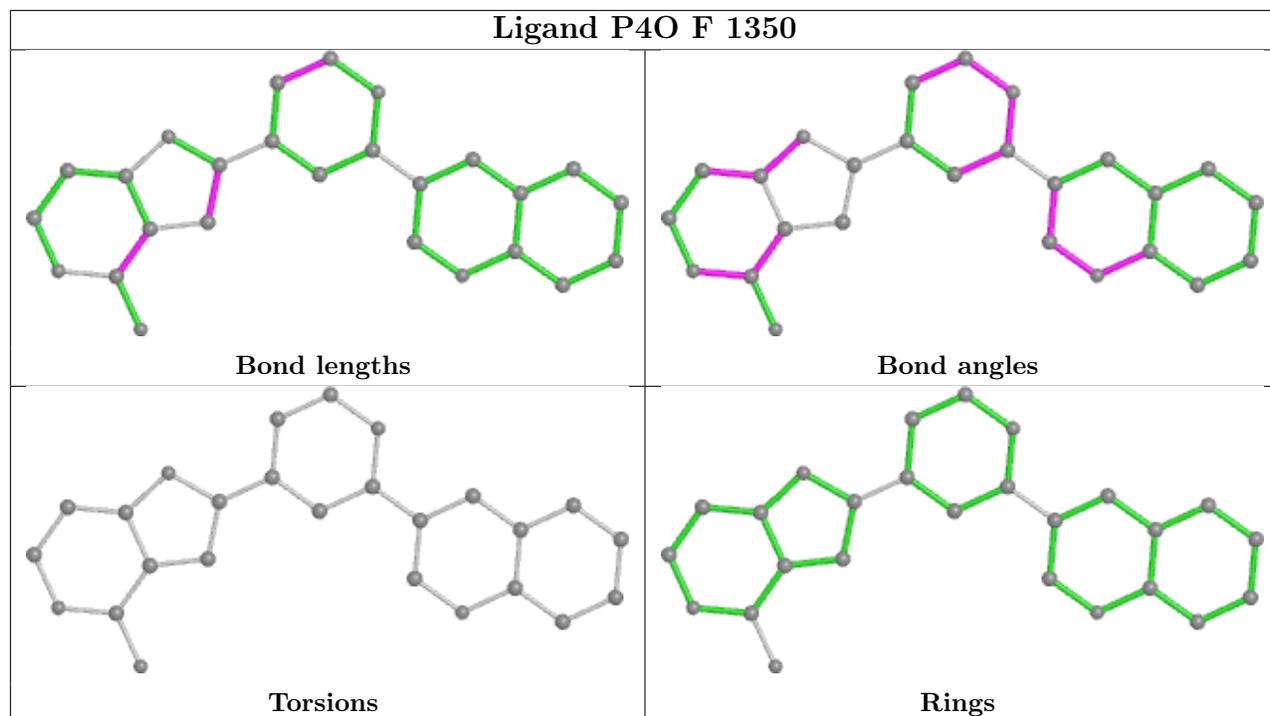
Continued from previous page...

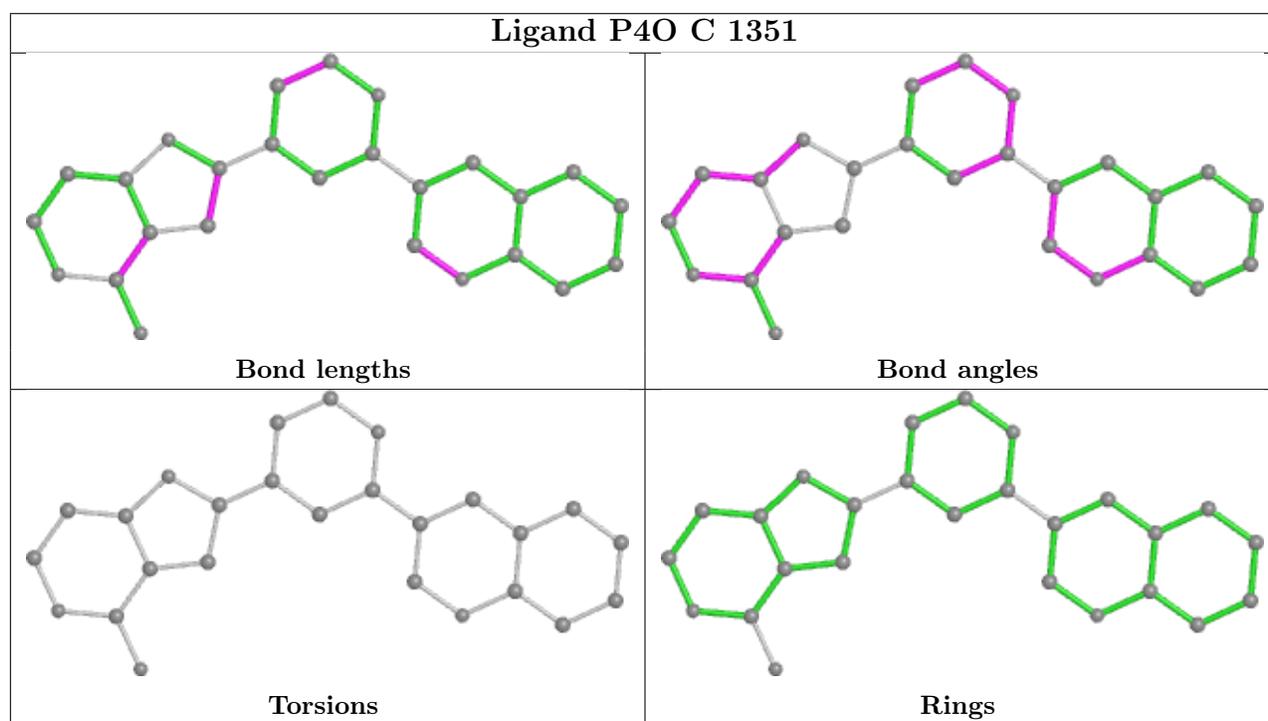
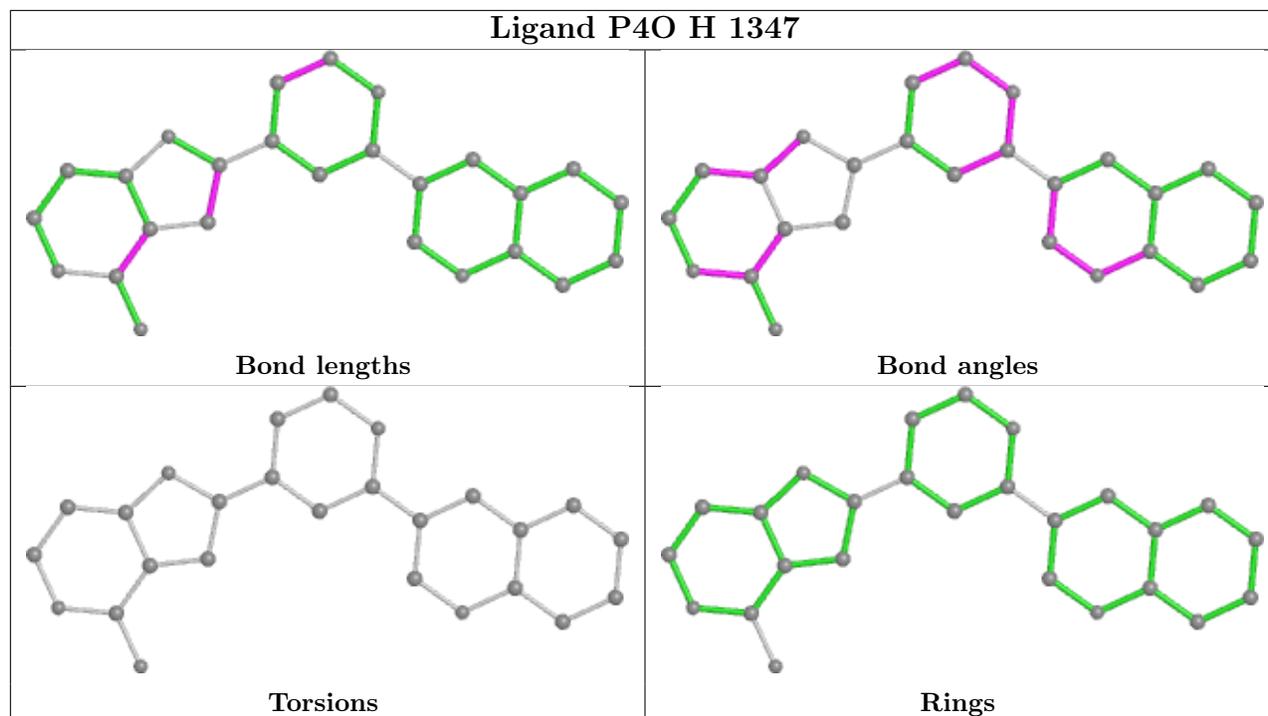
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1351	P4O	4	0
2	L	1345	P4O	4	0
2	A	1351	P4O	2	0
2	G	1350	P4O	5	0
2	E	1345	P4O	4	0

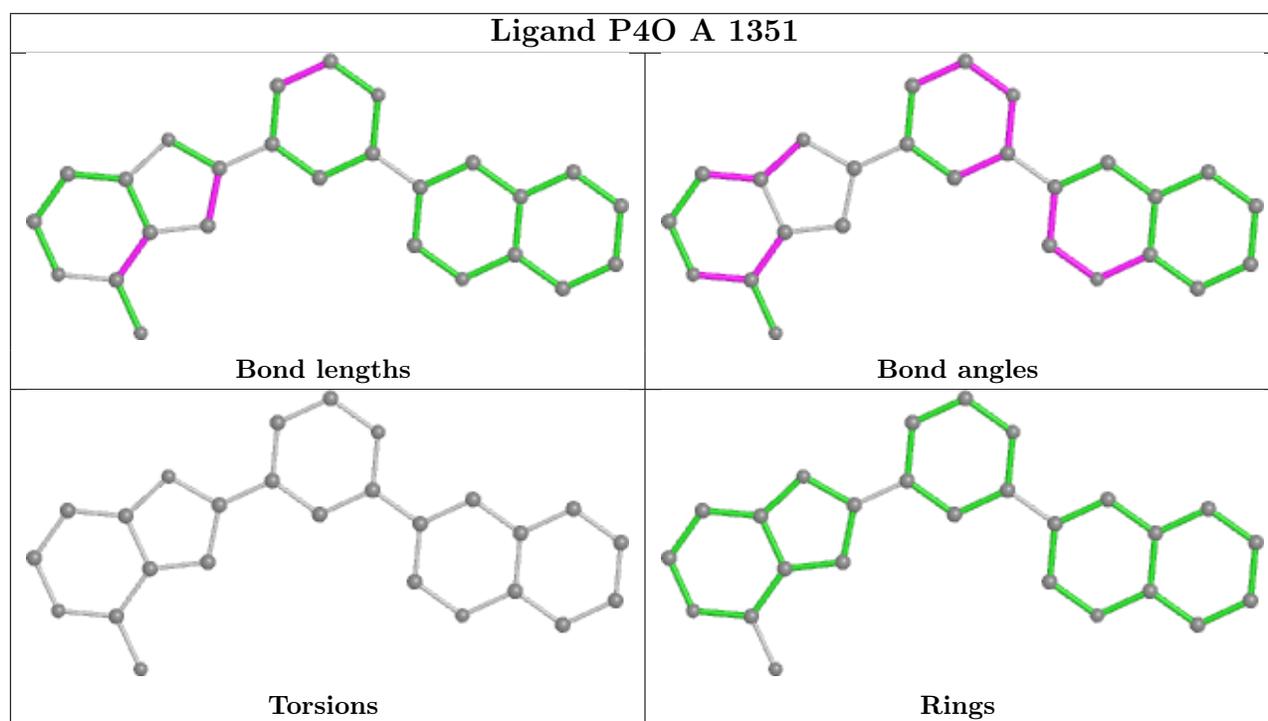
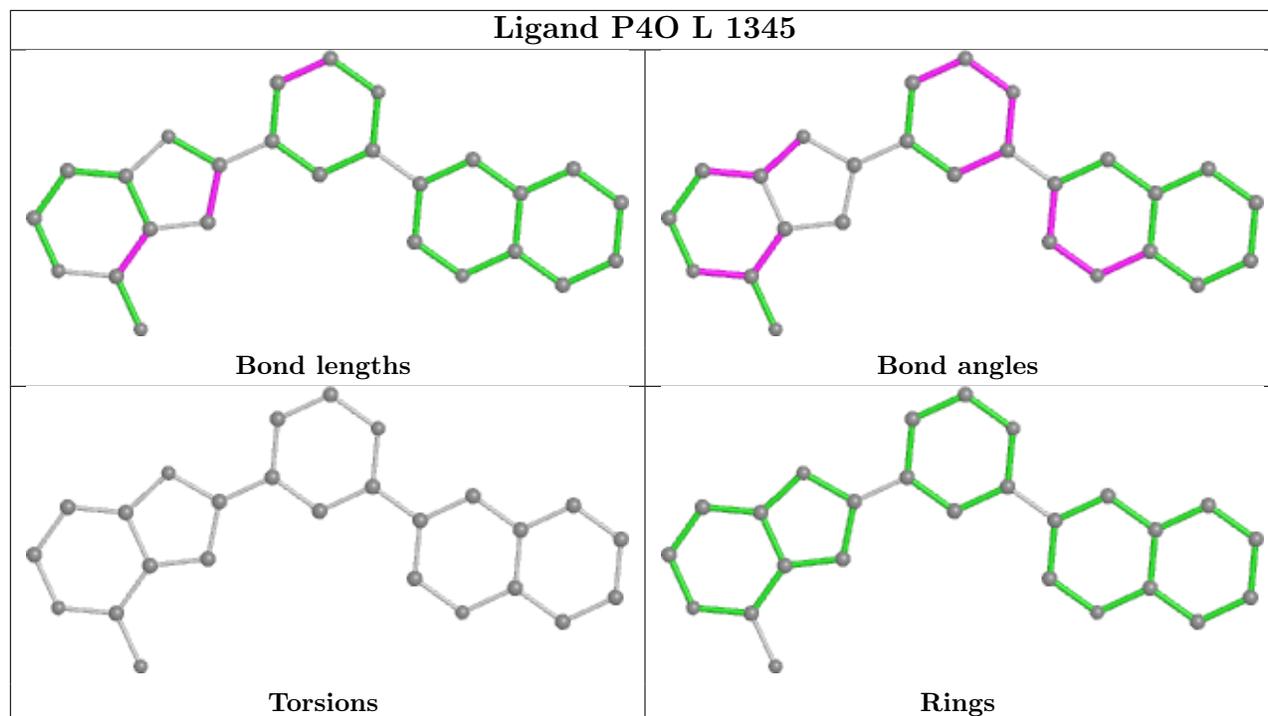
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

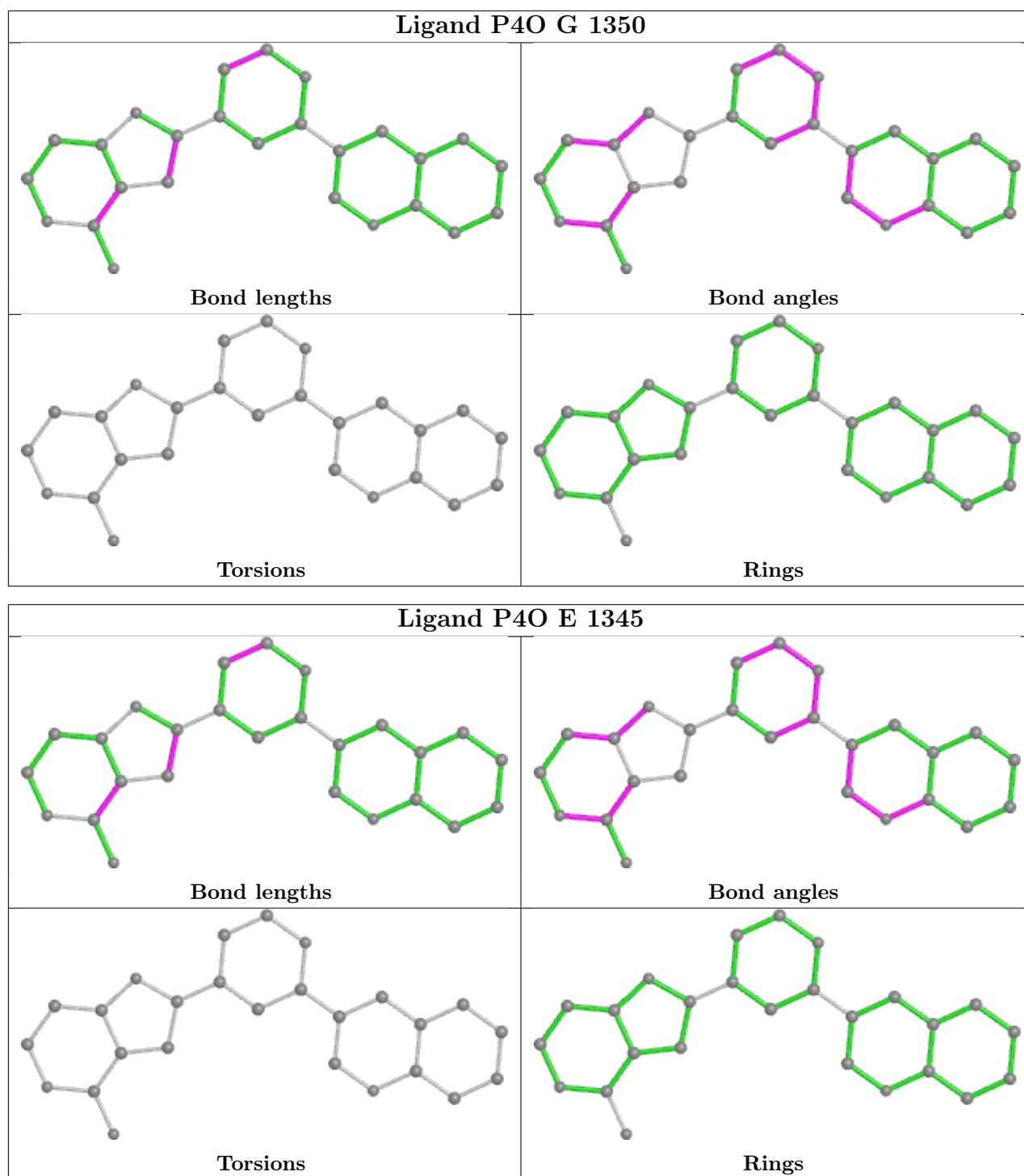












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	283/326 (86%)	-0.17	4 (1%) 75 75	13, 40, 110, 170	0
1	B	290/326 (88%)	0.03	8 (2%) 53 51	20, 63, 141, 173	0
1	C	284/326 (87%)	0.04	4 (1%) 75 75	19, 54, 127, 169	0
1	D	286/326 (87%)	0.03	9 (3%) 49 48	16, 51, 125, 171	0
1	E	283/326 (86%)	0.17	14 (4%) 29 29	33, 81, 140, 174	0
1	F	288/326 (88%)	-0.05	2 (0%) 87 89	13, 47, 116, 156	0
1	G	288/326 (88%)	0.21	15 (5%) 27 27	19, 74, 150, 194	0
1	H	283/326 (86%)	0.20	11 (3%) 39 38	36, 76, 137, 186	0
1	I	289/326 (88%)	0.17	13 (4%) 33 33	31, 72, 152, 180	0
1	J	225/326 (69%)	0.50	21 (9%) 8 9	51, 120, 170, 198	0
1	K	265/326 (81%)	0.80	47 (17%) 1 1	50, 127, 177, 198	0
1	L	268/326 (82%)	0.51	32 (11%) 4 3	35, 113, 174, 188	0
All	All	3332/3912 (85%)	0.19	180 (5%) 25 26	13, 73, 157, 198	0

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	201	ALA	5.7
1	G	338	THR	5.3
1	K	289	PRO	4.9
1	H	235	LEU	4.7
1	H	231	ALA	4.7

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](#)

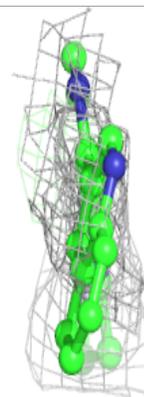
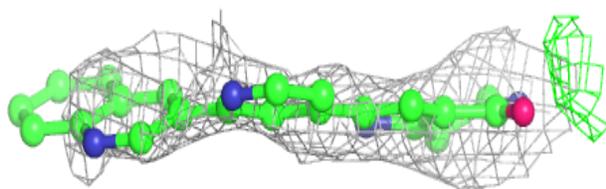
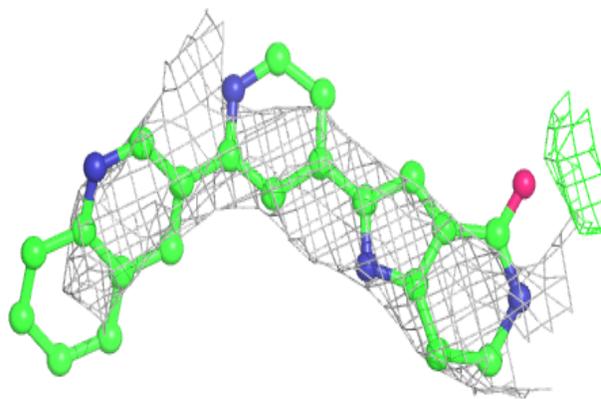
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	P4O	K	1345	26/26	0.73	0.51	133,152,162,171	0
2	P4O	I	1351	26/26	0.78	0.51	117,137,150,162	0
2	P4O	L	1345	26/26	0.80	0.41	125,139,158,161	0
2	P4O	E	1345	26/26	0.83	0.42	79,115,138,145	0
2	P4O	B	1351	26/26	0.85	0.55	54,105,135,142	0
2	P4O	H	1347	26/26	0.90	0.50	37,88,111,116	0
2	P4O	G	1350	26/26	0.91	0.28	39,98,121,130	0
2	P4O	C	1351	26/26	0.92	0.53	55,84,118,136	0
2	P4O	D	1351	26/26	0.92	0.35	42,78,99,104	0
2	P4O	F	1350	26/26	0.93	0.44	28,79,116,121	0
2	P4O	A	1351	26/26	0.96	0.22	25,57,77,89	0

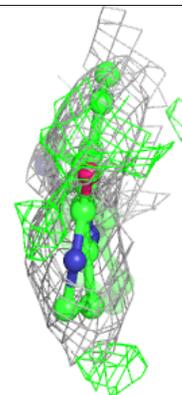
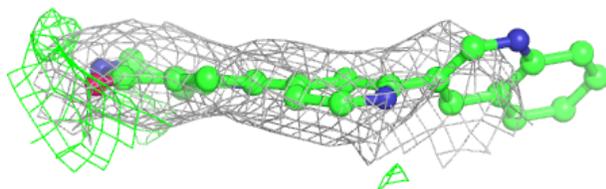
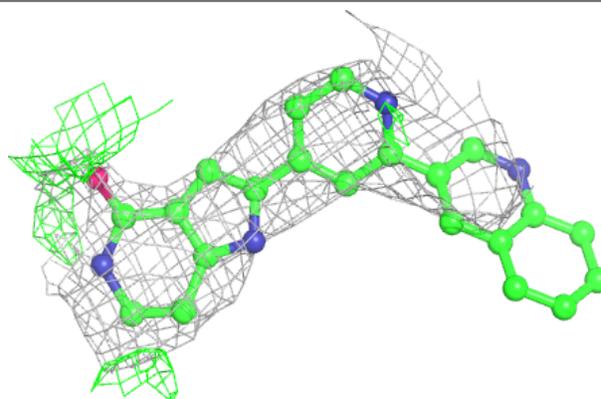
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P4O K 1345:

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

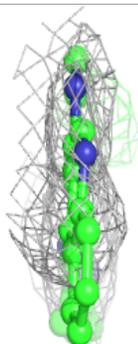
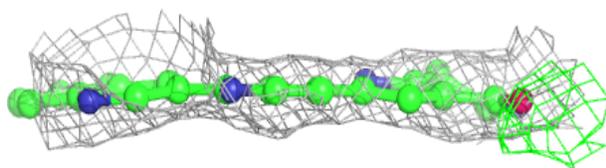
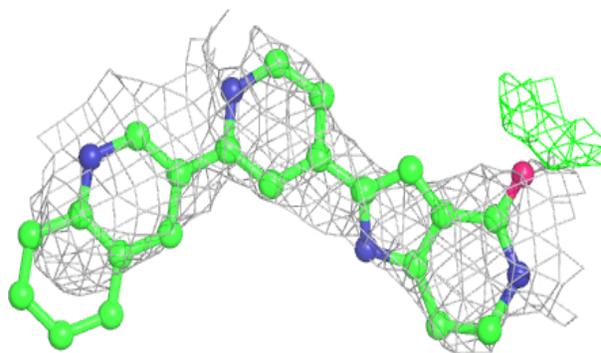
**Electron density around P4O I 1351:**

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

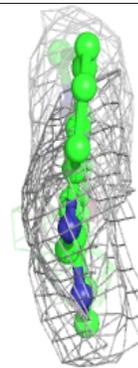
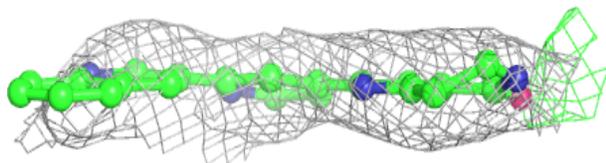
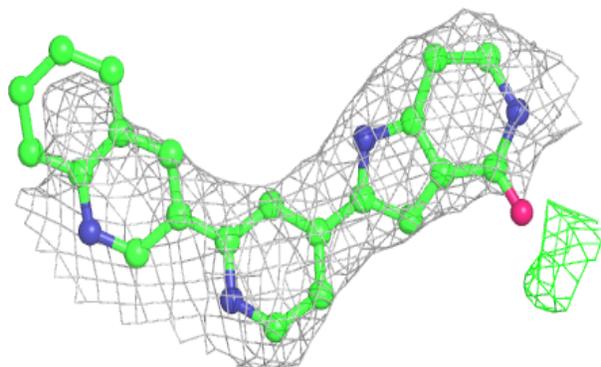


Electron density around P4O L 1345:

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

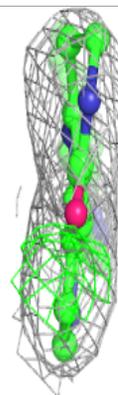
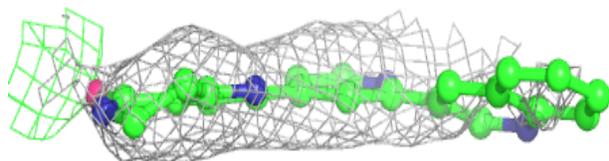
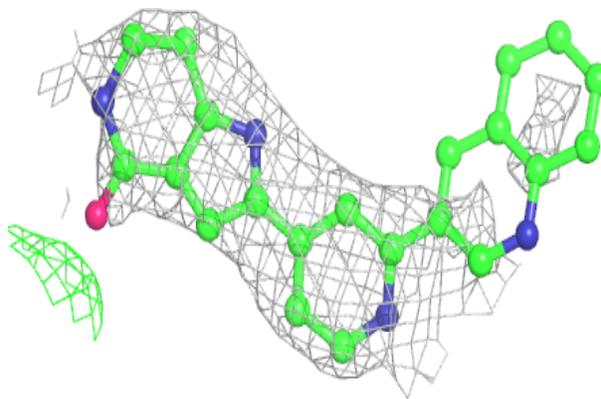
**Electron density around P4O E 1345:**

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

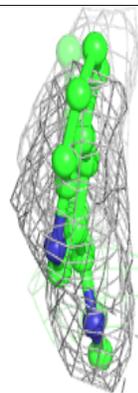
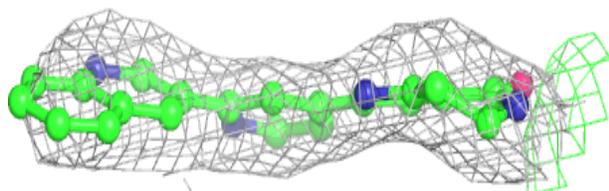
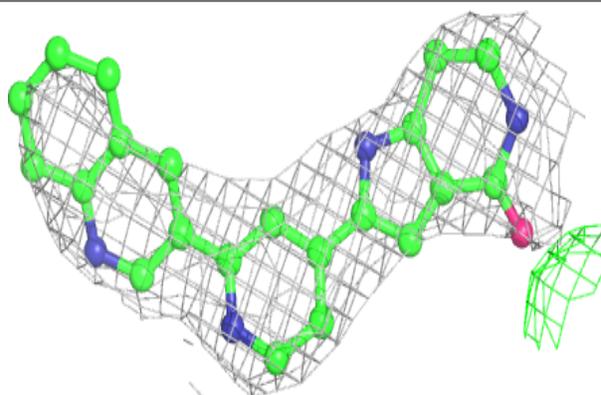


Electron density around P4O B 1351:

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

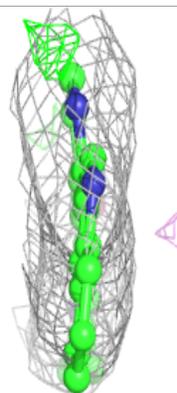
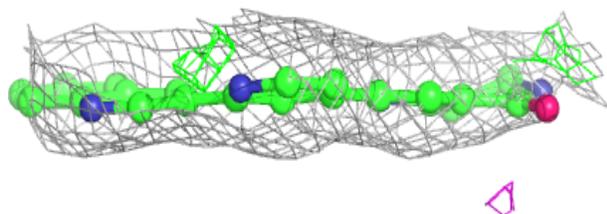
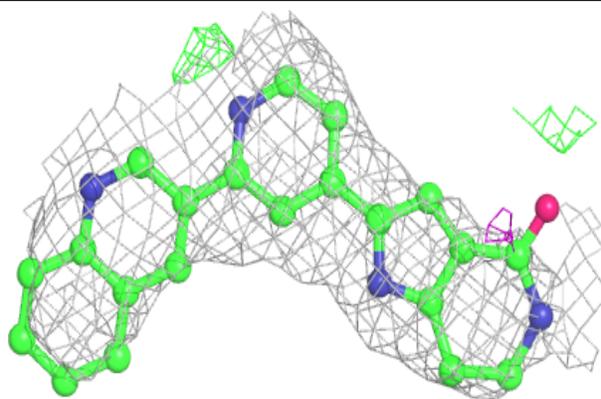
**Electron density around P4O H 1347:**

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

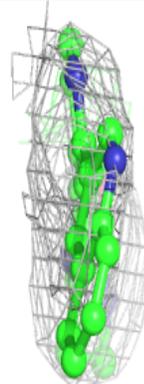
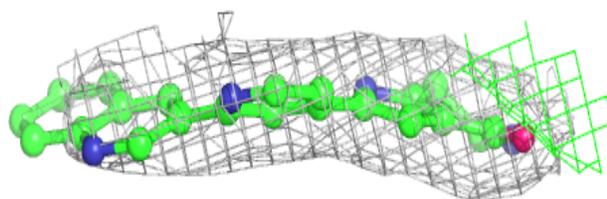
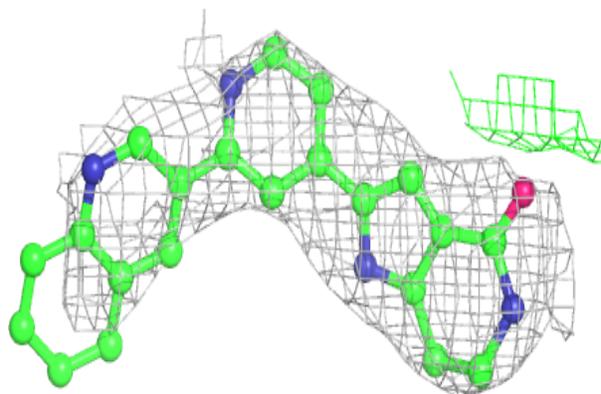


Electron density around P4O G 1350:

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

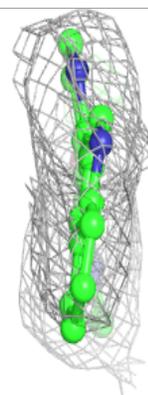
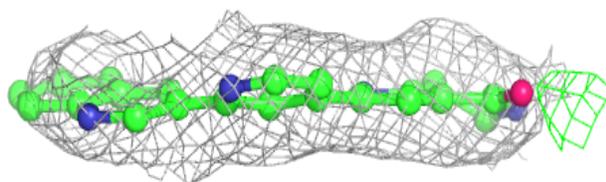
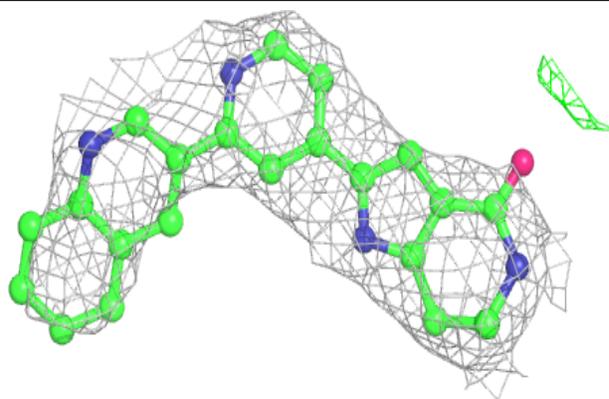
**Electron density around P4O C 1351:**

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

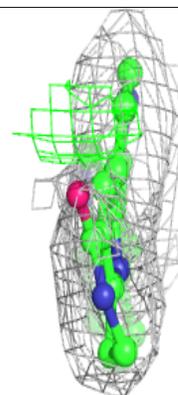
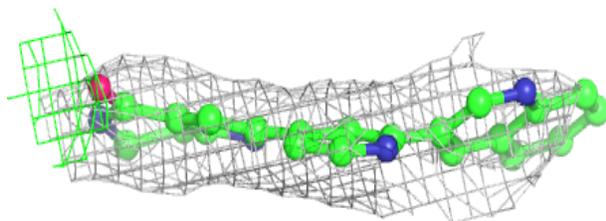
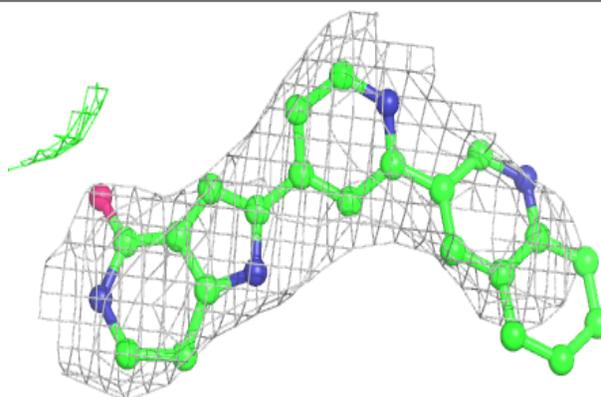


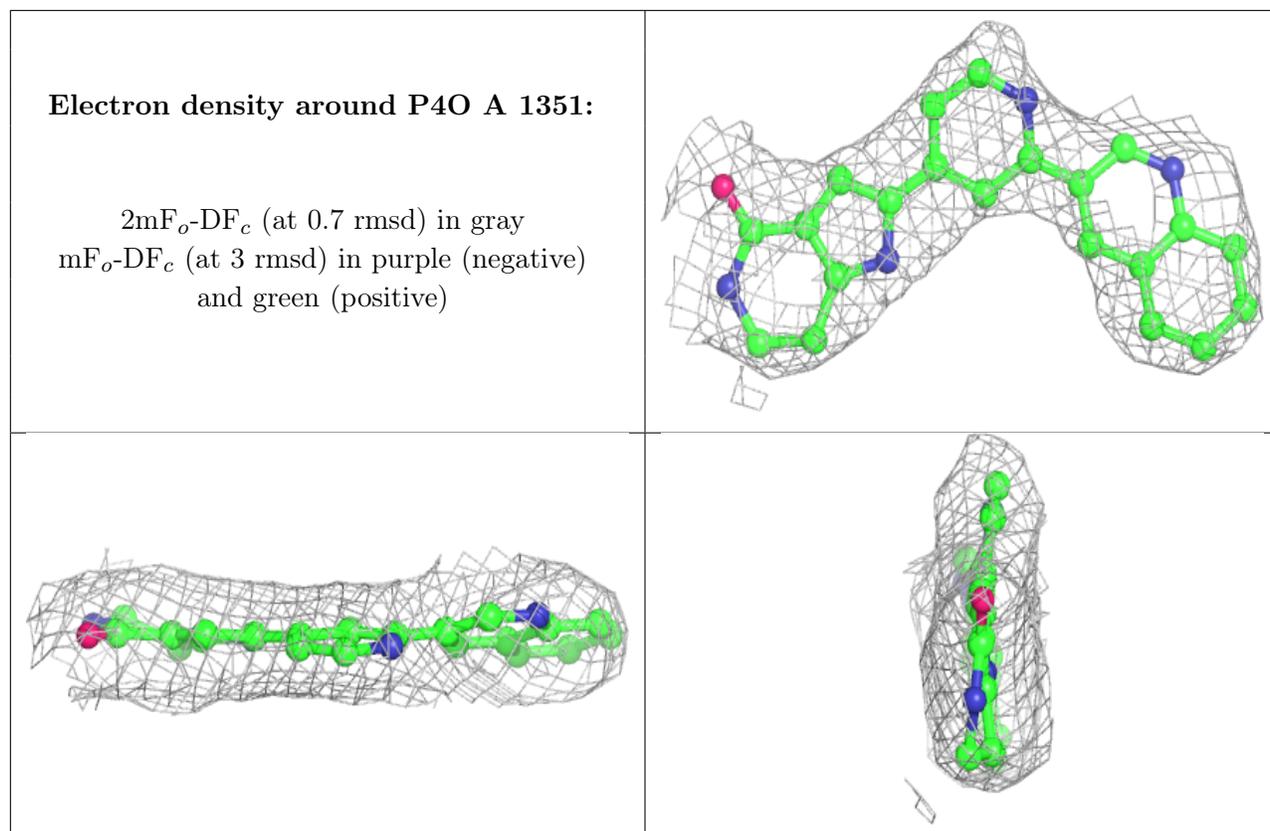
Electron density around P4O D 1351:

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

**Electron density around P4O F 1350:**

$2mF_o-DF_c$ (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.