



Full wwPDB X-ray Structure Validation Report ⓘ

May 9, 2023 – 01:45 pm BST

PDB ID : 7ZSL
Title : human purine nucleoside phosphorylase in complex with JS-196
Authors : Djukic, S.; Pachl, P.; Rezacova, P.
Deposited on : 2022-05-07
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.32.2
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) : 2.32.2

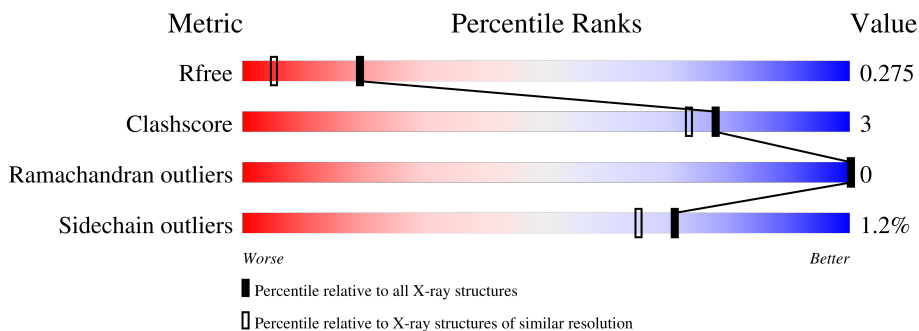
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	289	
1	B	289	
1	C	289	
1	D	289	
1	E	289	
1	F	289	

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
5	PEG	F	302	-	-	X	-

2 Entry composition [i](#)

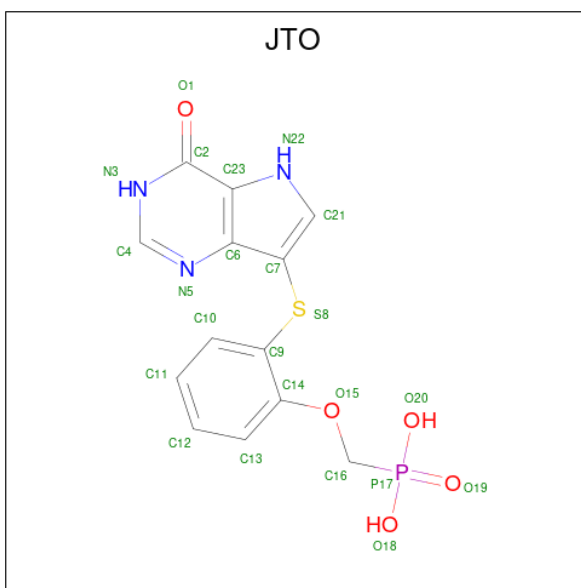
There are 6 unique types of molecules in this entry. The entry contains 13921 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Purine nucleoside phosphorylase.

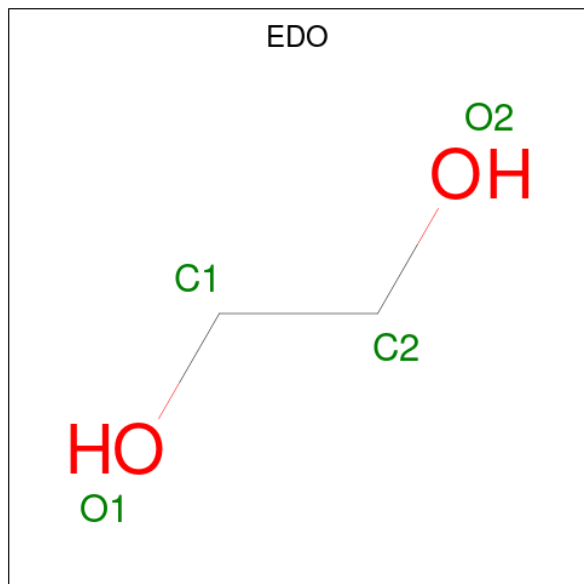
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	Total 2163	C 1379	N 376	O 391	S 17	0	3	0
1	B	274	Total 2134	C 1361	N 368	O 386	S 19	0	4	0
1	C	272	Total 2106	C 1344	N 366	O 380	S 16	0	2	0
1	D	271	Total 2119	C 1354	N 366	O 381	S 18	0	3	0
1	E	274	Total 2125	C 1359	N 367	O 382	S 17	0	2	0
1	F	270	Total 2094	C 1338	N 363	O 377	S 16	0	2	0

- Molecule 2 is [2-[(4-oxidanylidene-3,5-dihydropyrrolo[3,2-d]pyrimidin-7-yl)sulfanyl]phenoxy]methylphosphonic acid (three-letter code: JTO) (formula: C₁₃H₁₂N₃O₅PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	S	0	0
			23	13	3	5	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			23	13	3	5	1	1		
2	C	1	Total	C	N	O	P	S	0	0
			23	13	3	5	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			23	13	3	5	1	1		
2	E	1	Total	C	N	O	P	S	0	0
			23	13	3	5	1	1		
2	F	1	Total	C	N	O	P	S	0	0
			23	13	3	5	1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			4	2 2		
3	B	1	Total	C O	0	1
			8	4 4		
3	F	1	Total	C O	0	0
			4	2 2		

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0

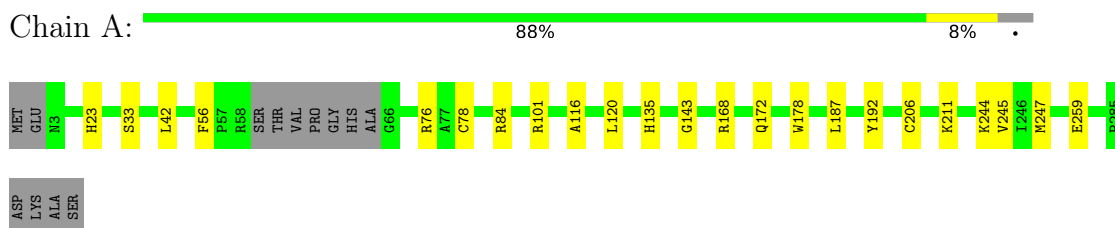
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	158	Total O 160 160	0	2
6	B	187	Total O 189 189	0	2
6	C	152	Total O 152 152	0	0
6	D	165	Total O 167 167	0	2
6	E	156	Total O 157 157	0	1
6	F	128	Total O 130 130	0	2

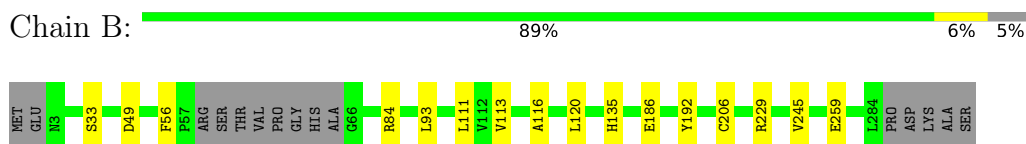
3 Residue-property plots [i](#)

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. 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. 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.

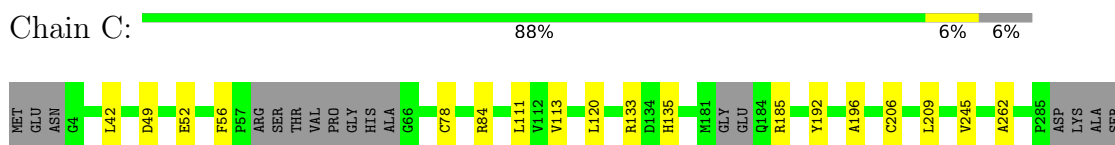
- Molecule 1: Purine nucleoside phosphorylase



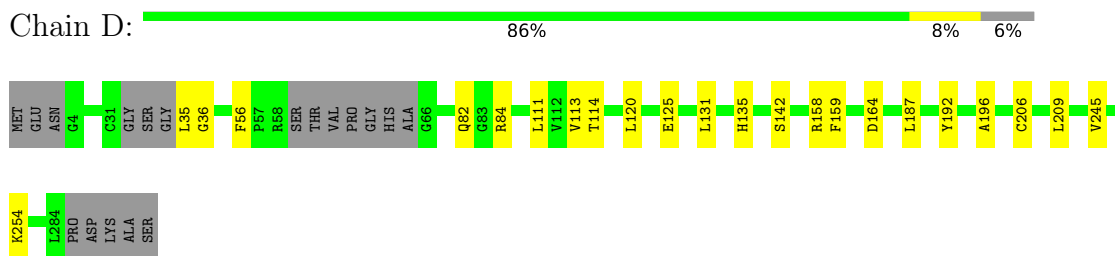
- Molecule 1: Purine nucleoside phosphorylase



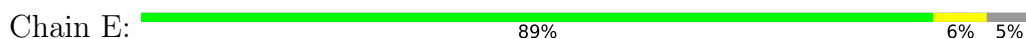
- Molecule 1: Purine nucleoside phosphorylase



- Molecule 1: Purine nucleoside phosphorylase



- Molecule 1: Purine nucleoside phosphorylase





- Molecule 1: Purine nucleoside phosphorylase

Chain F: 88% 6% 7%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.12Å 185.10Å 79.18Å 90.00° 119.94° 90.00°	Depositor
Resolution (Å)	38.76 – 1.80 38.73 – 1.80	Depositor EDS
% Data completeness (in resolution range)	86.1 (38.76-1.80) 85.8 (38.73-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.225 , 0.268 0.231 , 0.275	Depositor DCC
R_{free} test set	1565 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.218 for -h-l,k,h 0.218 for l,k,-h-l 0.278 for h,-k,-h-l 0.278 for -h-l,-k,l 0.217 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13921	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: SO4, EDO, PEG, JTO

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	0.73	0/2219	0.80	0/3003
1	B	0.75	0/2191	0.82	0/2967
1	C	0.72	0/2160	0.82	0/2925
1	D	0.74	0/2175	0.82	0/2943
1	E	0.75	0/2180	0.81	0/2950
1	F	0.72	0/2147	0.81	0/2906
All	All	0.74	0/13072	0.81	0/17694

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2163	0	2128	18	0
1	B	2134	0	2089	12	0
1	C	2106	0	2056	10	0
1	D	2119	0	2085	15	0
1	E	2125	0	2093	12	0
1	F	2094	0	2052	14	0
2	A	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	23	0	0	0	0
2	C	23	0	0	0	0
2	D	23	0	0	0	0
2	E	23	0	0	0	0
2	F	23	0	0	0	0
3	A	4	0	6	3	0
3	B	8	0	12	0	0
3	F	4	0	6	0	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	15	0	0	0	0
4	E	5	0	0	0	0
4	F	10	0	0	0	0
5	A	7	0	10	0	0
5	C	7	0	10	1	0
5	F	7	0	10	4	0
6	A	160	0	0	2	0
6	B	189	0	0	2	0
6	C	152	0	0	1	0
6	D	167	0	0	0	0
6	E	157	0	0	2	0
6	F	130	0	0	0	0
All	All	13921	0	12557	74	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 (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD23	1:A:245:VAL:HG21	1.58	0.84
1:B:120:LEU:HD23	1:B:245:VAL:HG21	1.64	0.80
1:E:120:LEU:HD23	1:E:245:VAL:HG21	1.67	0.76
1:F:35:LEU:HD13	1:F:114:THR:HG21	1.73	0.70
1:B:206[B]:CYS:SG	1:B:245:VAL:HG23	2.33	0.67
1:A:206[A]:CYS:SG	1:A:245:VAL:HG23	2.37	0.65
1:D:206[A]:CYS:SG	1:D:245:VAL:HG23	2.38	0.63
1:C:206[A]:CYS:SG	1:C:245:VAL:HG23	2.38	0.62
1:B:186:GLU:OE1	1:E:207:ARG:CZ	2.49	0.61
1:E:206[A]:CYS:SG	1:E:245:VAL:HG23	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:ARG:O	1:E:211:LYS:HG2	2.05	0.57
1:A:168:ARG:NH1	1:A:172:GLN:OE1	2.39	0.56
1:B:206[B]:CYS:SG	1:B:245:VAL:CG2	2.95	0.55
1:B:111:LEU:HG	1:B:113:VAL:HG13	1.89	0.54
1:C:111:LEU:HG	1:C:113:VAL:HG13	1.91	0.53
1:B:120:LEU:HD23	1:B:245:VAL:CG2	2.38	0.51
1:D:111:LEU:HG	1:D:113:VAL:HG13	1.92	0.51
1:A:42:LEU:HD21	1:A:78[B]:CYS:SG	2.51	0.51
1:D:35:LEU:HD11	1:D:114:THR:HG21	1.93	0.51
1:F:36:GLY:O	1:F:82:GLN:NE2	2.44	0.50
1:B:120:LEU:CD2	1:B:245:VAL:HG21	2.38	0.50
1:E:207:ARG:NH1	6:E:403:HOH:O	2.44	0.50
1:F:35:LEU:CD1	1:F:114:THR:HG21	2.40	0.50
1:A:206[A]:CYS:SG	1:A:245:VAL:CG2	3.00	0.49
1:A:120:LEU:HD23	1:A:245:VAL:CG2	2.36	0.48
1:E:206[A]:CYS:SG	1:E:245:VAL:CG2	3.02	0.48
1:F:37:GLY:C	1:F:272:GLU:OE2	2.52	0.48
1:D:135:HIS:HA	1:D:192:TYR:O	2.15	0.47
1:A:33:SER:HB2	1:A:116:ALA:HB2	1.95	0.47
1:A:244:LYS:HB3	3:A:302:EDO:H11	1.95	0.47
1:E:4:GLY:N	6:E:405:HOH:O	2.47	0.47
1:D:206[A]:CYS:SG	1:D:245:VAL:CG2	3.03	0.47
1:F:159:PHE:H	5:F:302:PEG:H32	1.80	0.46
1:C:206[A]:CYS:SG	1:C:245:VAL:CG2	3.04	0.46
1:F:135:HIS:HA	1:F:192:TYR:O	2.16	0.46
1:D:142:SER:OG	1:F:142:SER:HB2	2.16	0.46
1:A:178:TRP:CG	1:A:187:LEU:HG	2.51	0.45
1:C:49:ASP:O	1:C:52:GLU:HG2	2.17	0.45
1:E:135:HIS:HA	1:E:192:TYR:O	2.16	0.45
1:A:135:HIS:HA	1:A:192:TYR:O	2.16	0.45
1:F:33:SER:HB2	1:F:116:ALA:HB2	1.97	0.45
1:C:133:ARG:NH2	6:C:408:HOH:O	2.48	0.45
1:A:244:LYS:CB	3:A:302:EDO:H11	2.46	0.45
1:F:157:ASP:HB3	5:F:302:PEG:H41	1.98	0.45
1:C:262:ALA:CB	5:C:302:PEG:H32	2.47	0.45
1:C:135:HIS:HA	1:C:192:TYR:O	2.16	0.45
1:A:211:LYS:NZ	1:D:125:GLU:OE2	2.49	0.44
1:D:164:ASP:OD2	1:E:254:LYS:HD2	2.17	0.44
1:C:42:LEU:HD21	1:C:78[B]:CYS:SG	2.57	0.44
1:A:33:SER:CB	1:A:116:ALA:HB2	2.48	0.44
1:E:87:MET:CE	1:E:93:LEU:HD21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:TRP:CG	1:E:187:LEU:HG	2.52	0.44
1:B:135:HIS:HA	1:B:192:TYR:O	2.18	0.44
1:A:120:LEU:CD2	1:A:245:VAL:HG21	2.38	0.43
1:A:76:ARG:HB2	6:A:427:HOH:O	2.17	0.43
1:A:247:MET:CE	3:A:302:EDO:O2	2.66	0.43
1:C:120:LEU:HD21	1:C:209:LEU:CB	2.49	0.42
1:D:35:LEU:HD12	1:D:114:THR:OG1	2.19	0.42
1:B:33:SER:HB2	1:B:116:ALA:HB2	2.01	0.42
1:D:254:LYS:HD3	1:F:164:ASP:CG	2.39	0.42
1:D:131:LEU:HG	1:D:187:LEU:HG	2.01	0.42
1:B:49:ASP:HB3	6:B:492:HOH:O	2.19	0.41
1:D:196:ALA:CB	1:F:143:GLY:HA2	2.50	0.41
1:B:229:ARG:HD2	1:B:229:ARG:HA	1.90	0.41
1:A:23:HIS:HB3	6:A:500:HOH:O	2.20	0.41
1:D:120:LEU:HD21	1:D:209:LEU:CB	2.50	0.41
1:D:158:ARG:HG2	1:D:159:PHE:CE2	2.56	0.41
1:F:157:ASP:HB3	5:F:302:PEG:H32	2.02	0.41
1:F:33:SER:CB	1:F:116:ALA:HB2	2.51	0.41
1:B:93:LEU:HB2	6:B:512:HOH:O	2.20	0.40
1:F:157:ASP:HB3	5:F:302:PEG:C4	2.50	0.40
1:A:143:GLY:HA2	1:C:196:ALA:CB	2.51	0.40
1:E:158:ARG:HG2	1:E:159:PHE:CE2	2.56	0.40
1:D:36:GLY:O	1:D:82:GLN:NE2	2.55	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	275/289 (95%)	272 (99%)	3 (1%)	0	100 100
1	B	274/289 (95%)	270 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	268/289 (93%)	264 (98%)	4 (2%)	0	100	100
1	D	268/289 (93%)	265 (99%)	3 (1%)	0	100	100
1	E	272/289 (94%)	268 (98%)	4 (2%)	0	100	100
1	F	266/289 (92%)	262 (98%)	4 (2%)	0	100	100
All	All	1623/1734 (94%)	1601 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	228/239 (95%)	224 (98%)	4 (2%)	59	48
1	B	224/239 (94%)	221 (99%)	3 (1%)	69	62
1	C	219/239 (92%)	216 (99%)	3 (1%)	67	59
1	D	223/239 (93%)	221 (99%)	2 (1%)	78	75
1	E	222/239 (93%)	220 (99%)	2 (1%)	78	75
1	F	218/239 (91%)	216 (99%)	2 (1%)	78	75
All	All	1334/1434 (93%)	1318 (99%)	16 (1%)	71	65

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	PHE
1	A	84	ARG
1	A	101	ARG
1	A	259	GLU
1	B	56	PHE
1	B	84	ARG
1	B	259	GLU
1	C	56	PHE
1	C	84	ARG

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Mol	Chain	Res	Type
1	C	185	ARG
1	D	56	PHE
1	D	84	ARG
1	E	56	PHE
1	E	84	ARG
1	F	56	PHE
1	F	84	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.

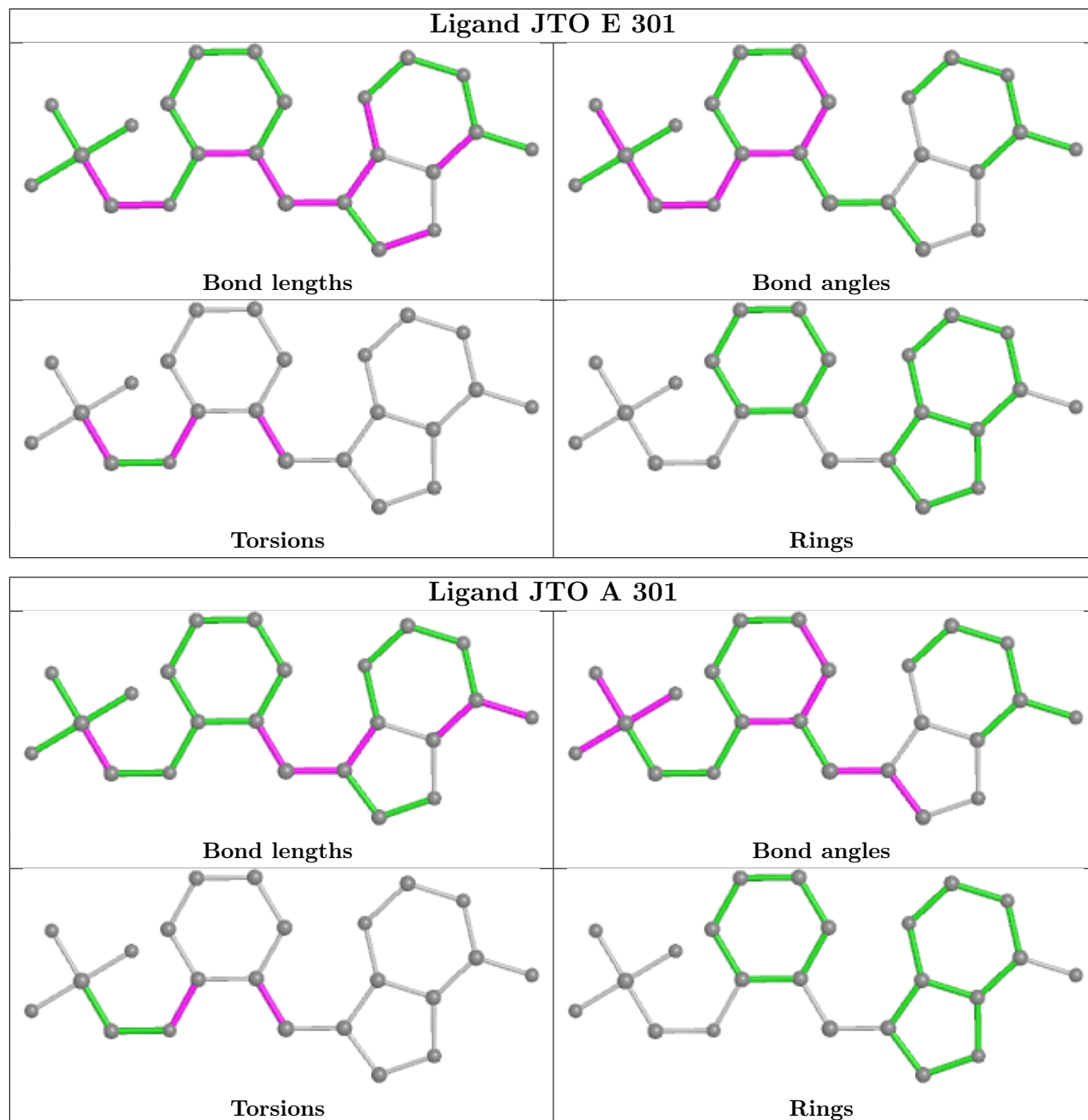
5.6 Ligand geometry [i](#)

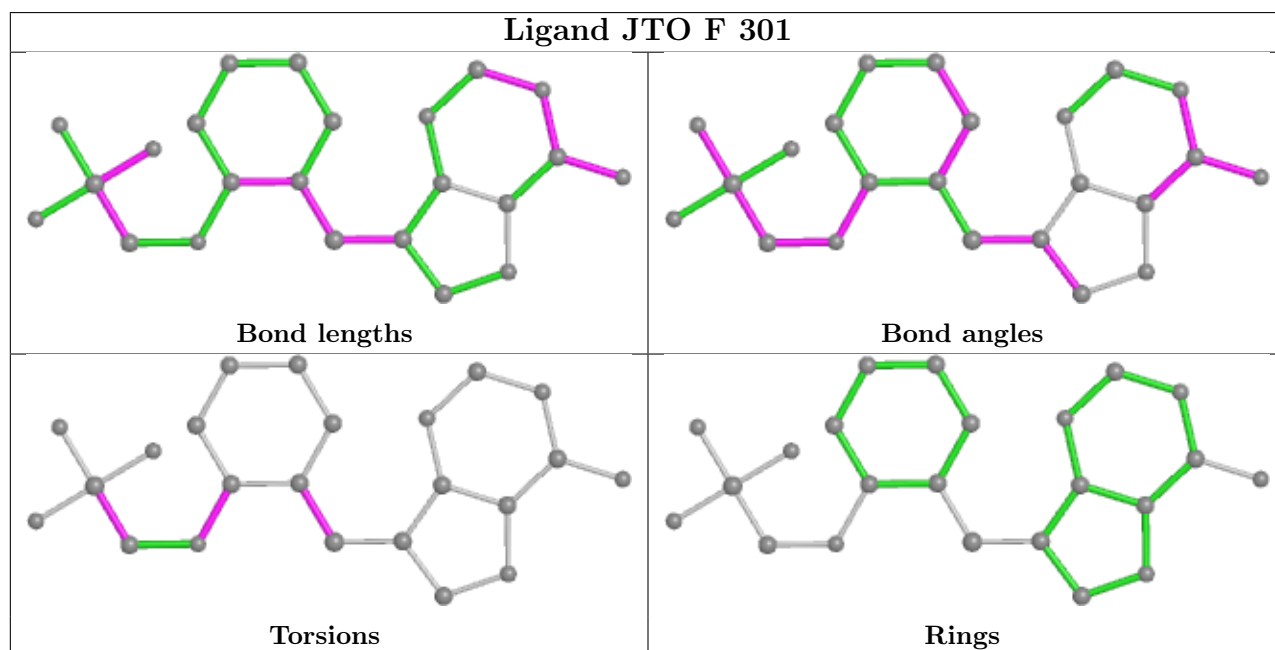
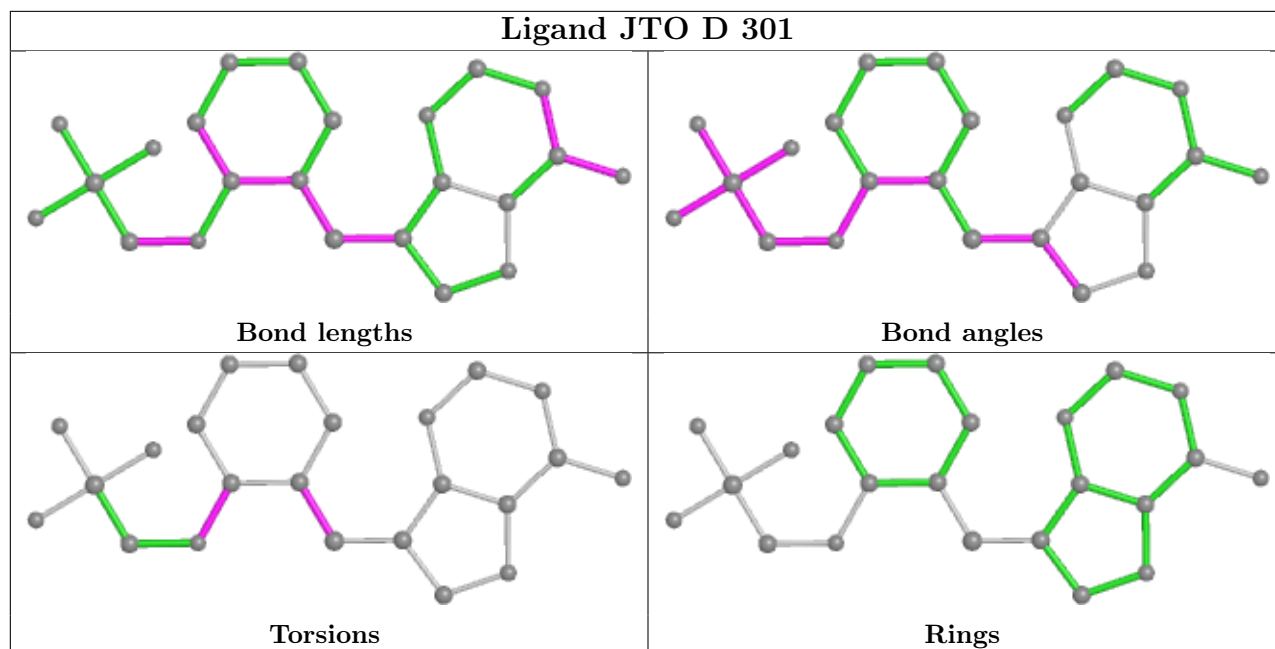
23 ligands are modelled in this entry.

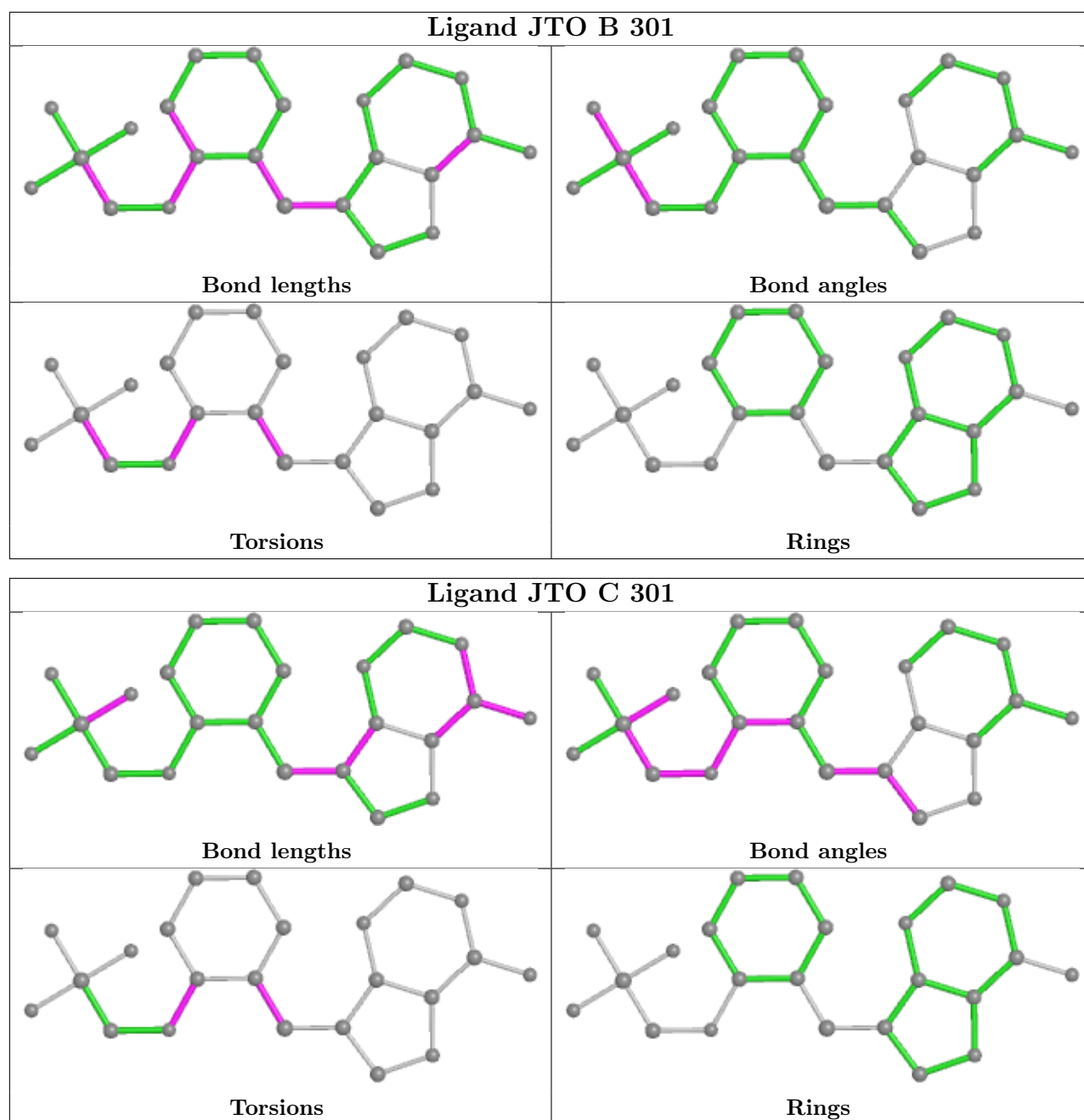
In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists 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
5	PEG	F	302	-	6,6,6	0.48	0	5,5,5	0.35	0
2	JTO	E	301	-	23,25,25	2.31	9 (39%)	23,36,36	1.99	5 (21%)
3	EDO	B	302[A]	-	3,3,3	0.66	0	2,2,2	0.61	0

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 [i](#)

There are no chain breaks in this entry.

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

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

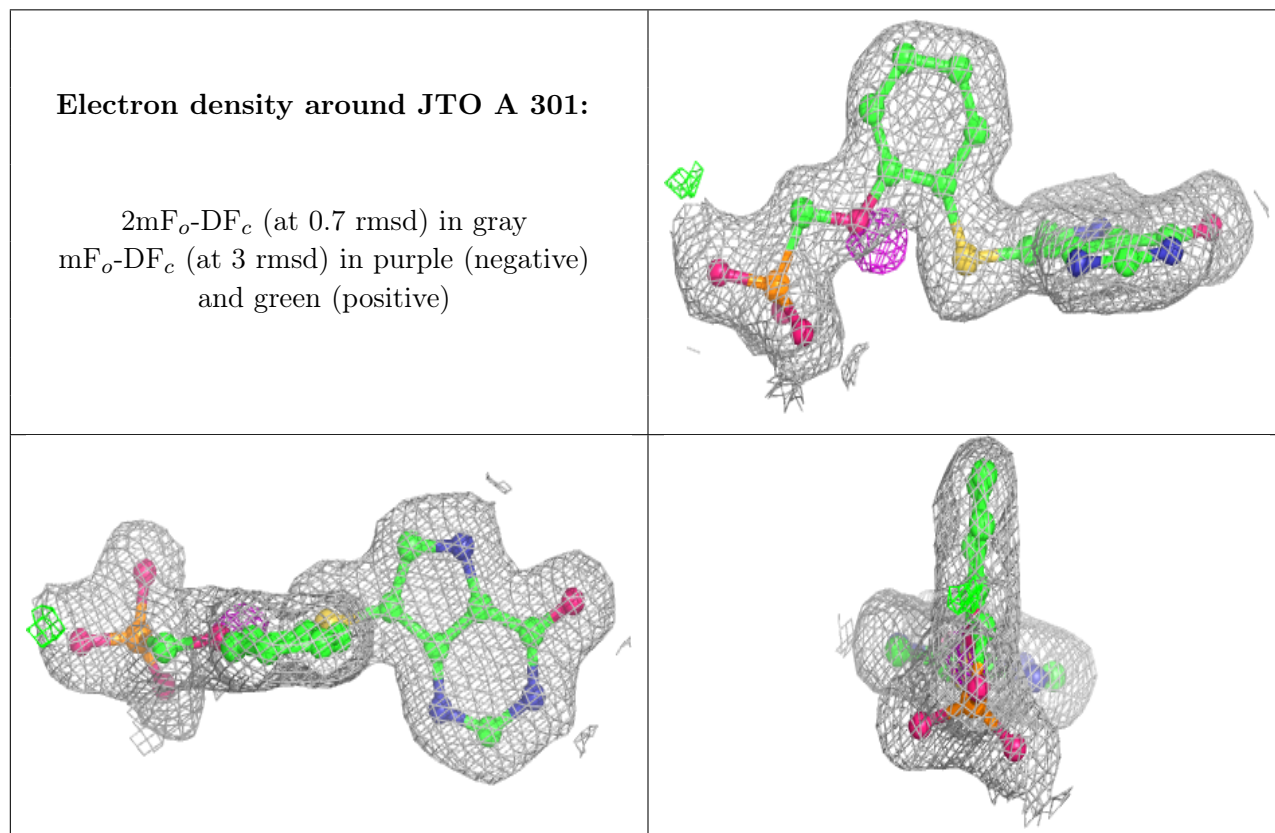
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

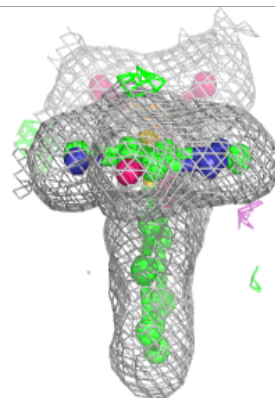
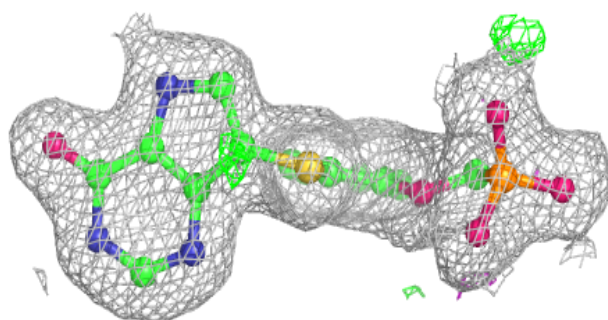
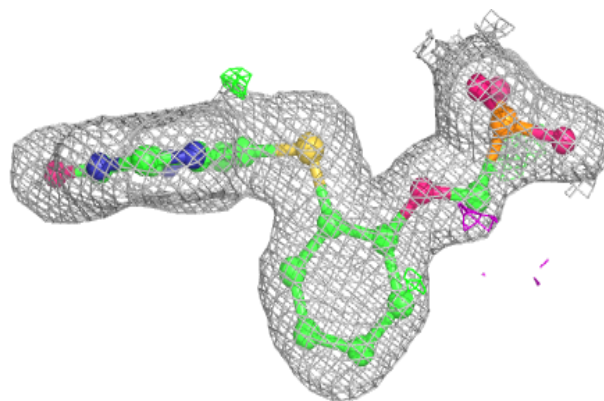
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

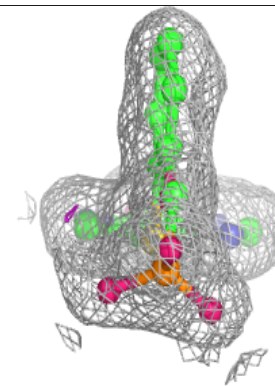
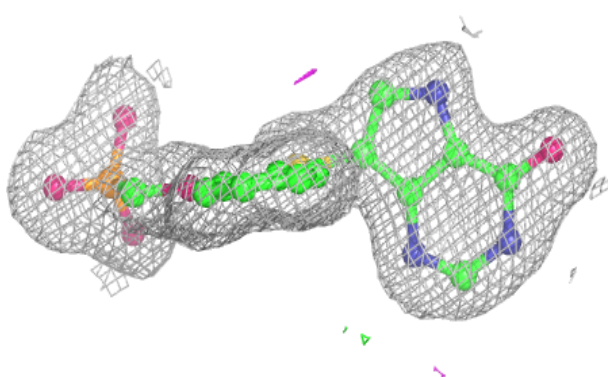
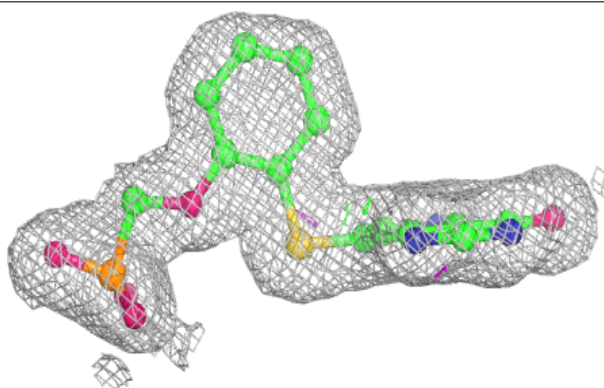


Electron density around JTO B 301:

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

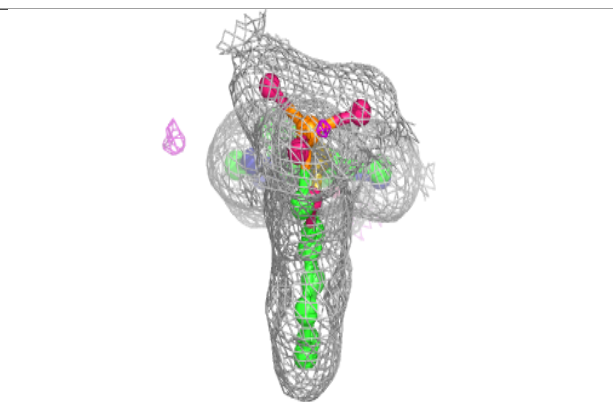
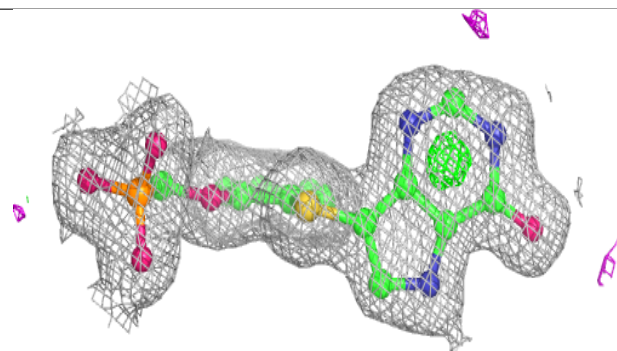
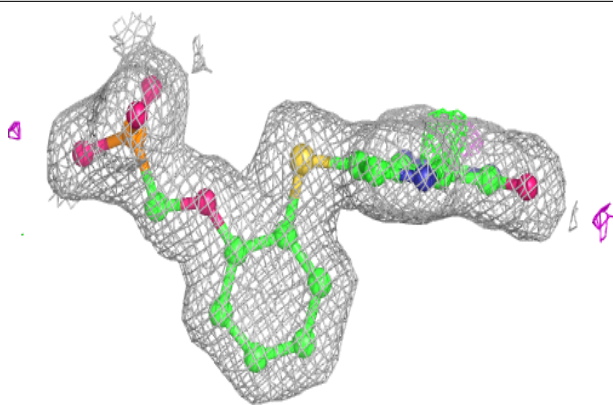
**Electron density around JTO C 301:**

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

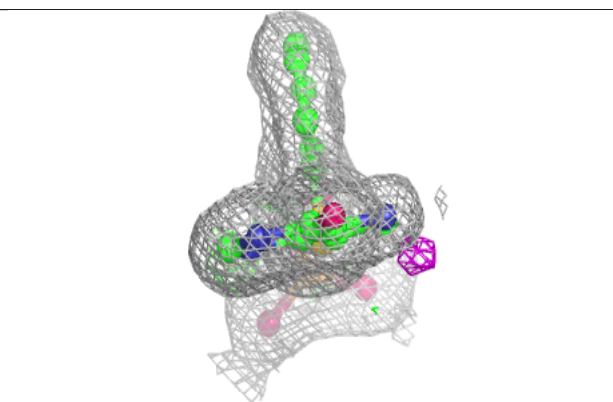
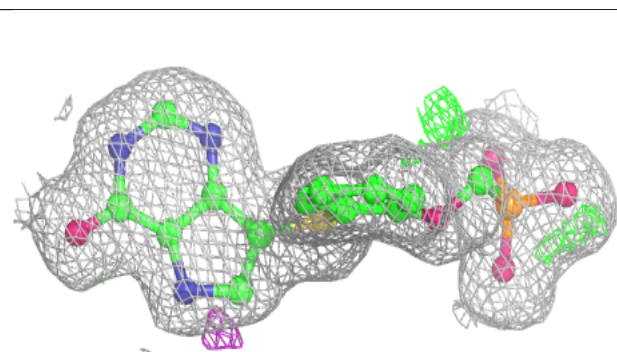
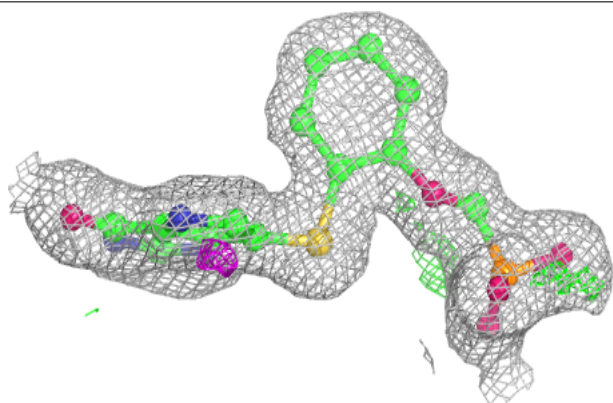


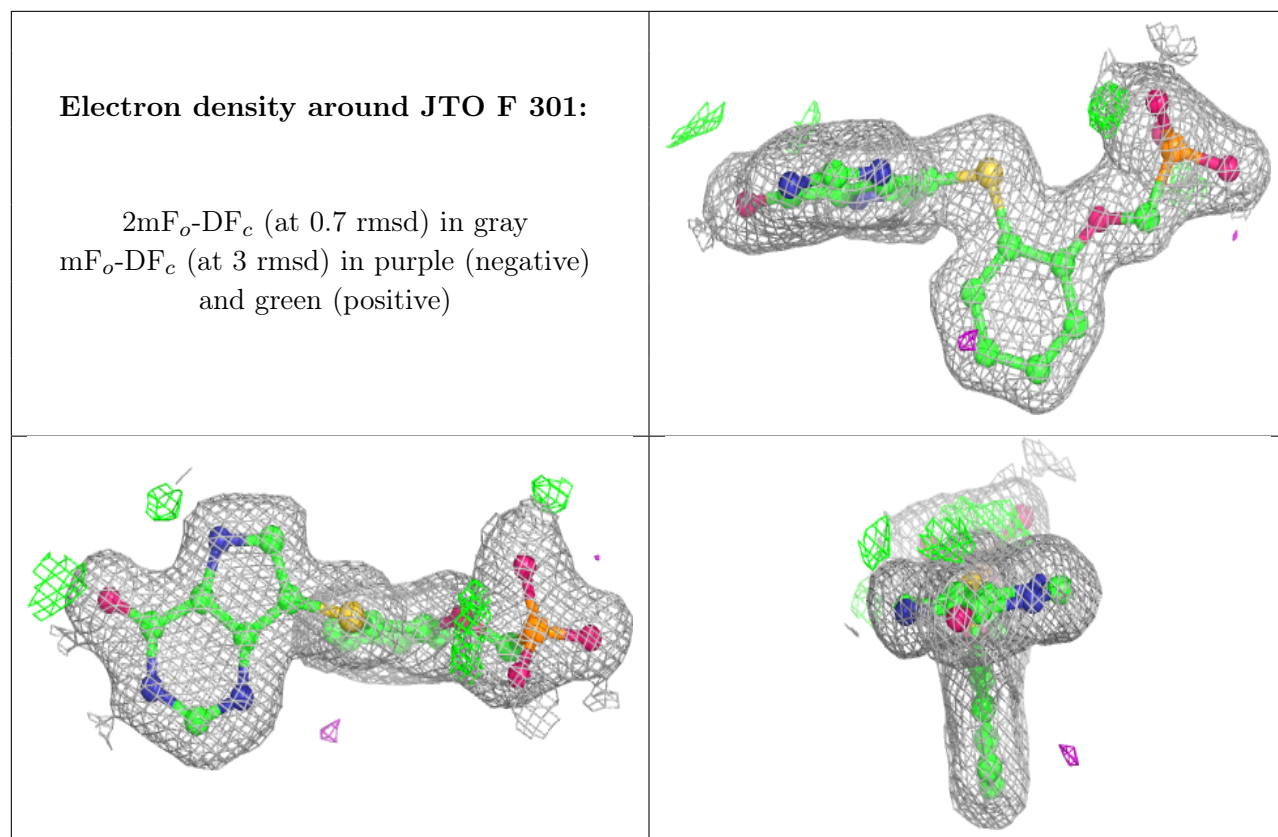
Electron density around JTO D 301:

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

**Electron density around JTO E 301:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.